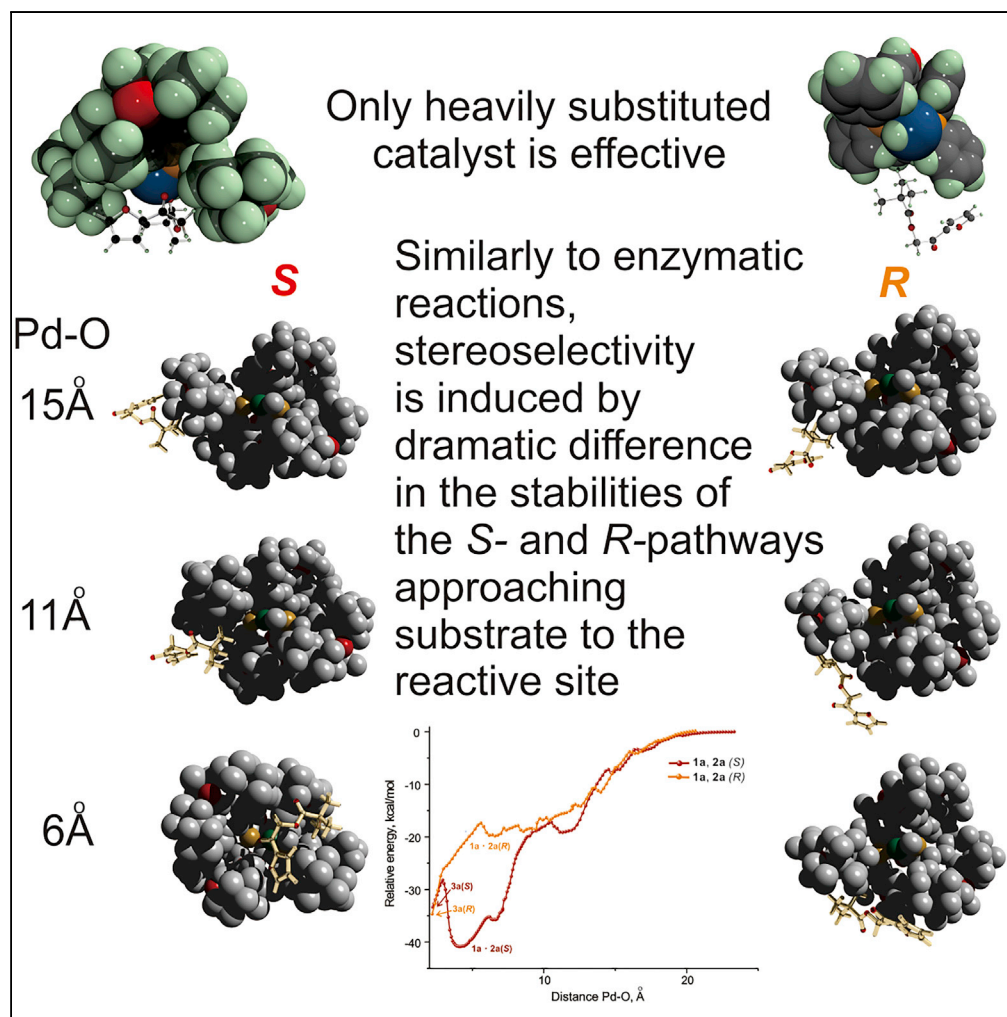


Article

Size is Important: Artificial Catalyst Mimics Behavior of Natural Enzymes



Jianzhong Chen,
Ilya D. Gridnev

gridnev.ilya.a6@tohoku.ac.jp

HIGHLIGHTS

Non-covalent interactions substrate-DTBM-SegPHOS Pd are essential for reactivity

Stereoselectivity is induced during approach of a substrate to the reactive site

This mechanism of enantioselection mimics enzymatic transformations

Performance of a catalyst can be improved via increasing the size of its ligand

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Article

Size is Important: Artificial Catalyst Mimics Behavior of Natural Enzymes

Jianzhong Chen¹ and Ilya D. Gridnev^{2,3,*}**SUMMARY**

Heavily substituted (*R*)-DTBM-SegPHOS is active in the asymmetric Pd(II)-catalyzed hydrogenation or C–O bond cleavage of α -pivaloyloxy-1-(2-furyl)ethanone, whereas (*R*)-SegPHOS fails to catalyze either of these transformations. An extensive network of C–H \cdots H–C interactions provided by the heavily substituted phenyl rings of (*R*)-DTBM-SegPHOS leads to increased stabilities of all intermediates and transition states in the corresponding catalytic cycles compared with the unsubstituted analogues. Moreover, formation of the encounter complex and its rearrangement into the reactive species proceeds in a fashion similar to that seen in natural enzymatic reactions. Computations demonstrate that this feature is the origin of enantioselection in asymmetric hydrogenation, since the stable precursor is formed only when the catalyst is approached by one prochiral plane of the substrate.

INTRODUCTION

Catalytic reactions constitute the most effective and environmentally friendly transformations available in the contemporary chemical industry. Synthetic studies of various catalytic cycles helped to improve the performance and selectivity levels of practically important transformations. However, the standards seen in the biochemical reactions catalyzed by natural enzymes are not achieved yet.

Although it had been noticed already quite early that the bulkiness of a catalyst usually improves its performance, it had been thought for many years that this is due to the increasing limitation of space remaining for the coordination of the substrate. Recently, it has been recognized, however, that in fact the bulkiness of the ligands increases the number of non-covalent attractive disperse interactions, thus stabilizing intermediates and transition states.

Differing from covalent interactions, which can be easily detected and analyzed in molecular structures, London forces, one of a number of noncovalent interactions, are difficult to observe within the bonding network (Johnson et al., 2010; Wagner and Schreiner, 2015). Recently, it has been recognized that the London dispersion interactions, a type of van der Waals interaction, play an important role in improving reactivity and securing the generation of chirality in the asymmetric catalytic reactions; most examples have been reported in the fields of biochemistry and organocatalysis (Johnson et al., 2010; Wagner and Schreiner, 2015; Cheong et al., 2011; Wheeler et al., 2016; Gridnev and Dub, 2016; Strauss and Wegner, 2019; Neuvonen et al., 2017; Motherwell et al., 2018; Fabrizio and Corminboeuf, 2018; Rösel et al., 2018; Reddi et al., 2019). The significant effects of London dispersion interactions between substrate and ligand in homogeneous transition-metal catalyzed enantioselective transformations have been less widely described (Wang et al., 2011; Ding et al., 2012; Lu et al., 2017; Thomas et al., 2018; Gridnev, 2016; Chen et al., 2018; Li et al., 2019; Lyngvi et al., 2015; Wolters et al., 2015; Sperger et al., 2016; Meyer et al., 2017).

In the mainstream of the theory of molecular catalysis, the selectivity of catalytic reactions is thought to be mainly determined by the difference in stabilities of diastereomeric transition states of the rate-determining stages of the catalytic cycles. The importance of the relative stabilities of the precursors is largely neglected, mostly due to established traditions, although the equilibrium constant reflecting the relative abundance of the precursors is clearly seen in the equation for calculating selectivity (e.g., Equation 1).

In some of our own recent studies, we have found that the approach of the substrate to the catalyst (Liu et al., 2014) or intramolecular rearrangement of the initially formed encounter complex (Imamoto et al., 2012; Gridnev et al., 2014a, 2014b; Gridnev and Imamoto, 2015, 2016) was seemingly strongly affecting the high enantioselectivities experimentally observed in these catalytic reactions.

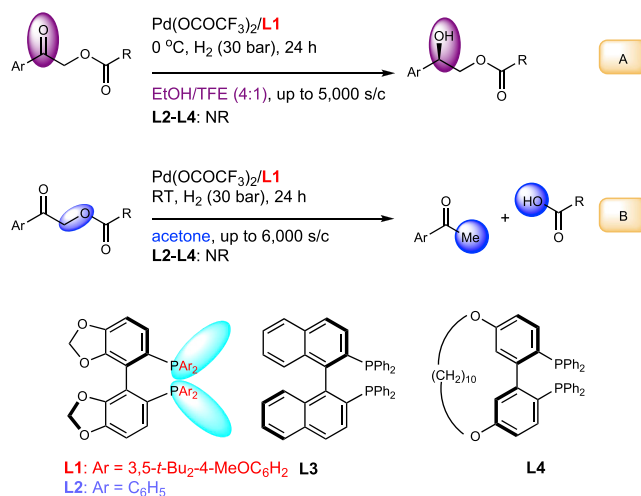
¹Shanghai Key Laboratory for Molecular Engineering of Chiral Drugs, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai 200240, P. R. China

²Department of Chemistry, Graduate School of Science, Tohoku University, Aramaki 3-6, Aoba-ku, Sendai 8578, Japan

³Lead Contact

*Correspondence: gridnev.ilya.a6@tohoku.ac.jp
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Scheme 1. Enantioselective Hydrogenation and C-O Bond Cleavage of α -Acetoxy Ketones

Herein we report for the first time a clear-cut case in which the relative stabilities of the competing transition states are irrelevant for the handedness and order of enantioselection. Instead, the initially formed weak encounter complexes are rearranging, keeping the substrate coordinated via intermolecular C–H \cdots H–C interactions, and the existence of a favorable pathway between the encounter complex and the active site discriminates between productive and unfavorable encounter complexes. This behavior mimics the experimentally supported and well-documented mechanism of perfect enantioselectivity in enzymatic transformations (Crowley and Ubbink, 2003; Tang et al., 2006; Xu et al., 2008; Andraloć et al., 2017).

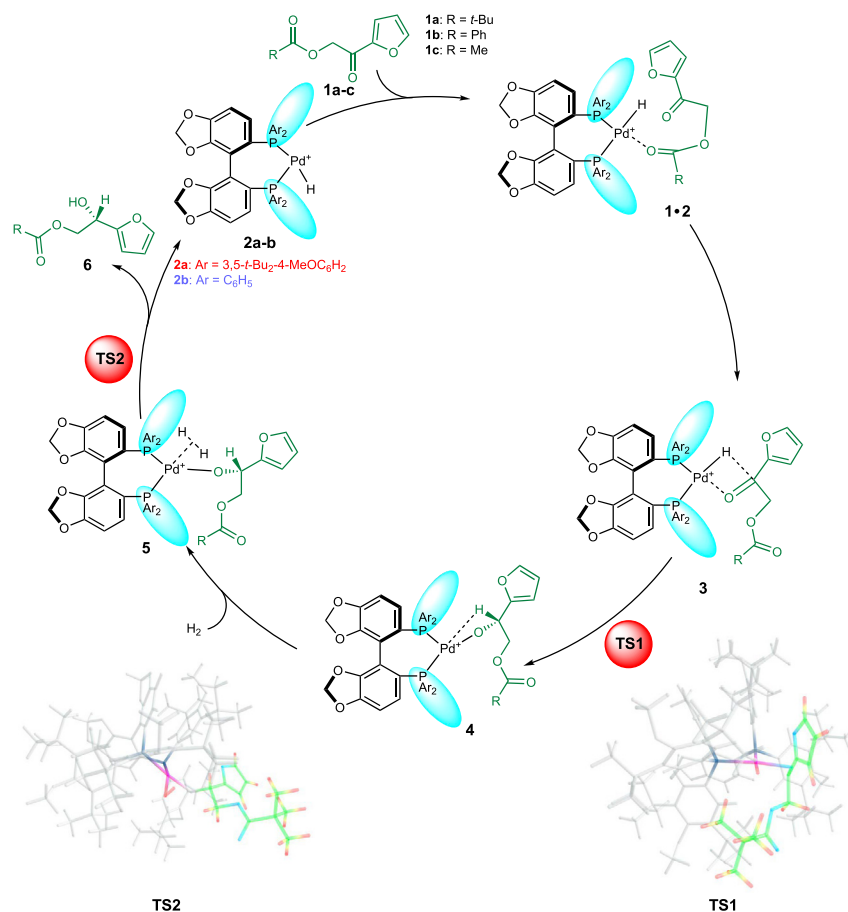
Our computational results reported in this paper demonstrate clearly that:

- (1) Numerous additional *t*-Bu (and OMe) substituents seen in the (*R*)-DTBM-SegPHOS provide an extended framework of C–H \cdots H–C interactions for coordination of a substrate. In the *S*-pathway of the asymmetric hydrogenation, an encounter complex is formed already at the long distances between the reactive centers. Furthermore, the substrate remains safely coordinated during its accommodation leading to the formation of highly reactive configuration. The same is not possible for the *R*-pathway that results in a high *S*-enantioselectivity of the reaction. This completely unrecognized mechanism of enantioselection provides important information for directed catalyst design.
- (2) The decisive factor determining the enantioselectivity is the Boltzmann distribution between *S*- and *R*- precursors that reaches approximately 2,300:1, whereas the ratio of the rates of competing reactions is much smaller.
- (3) The lack of an extended framework of C–H \cdots H–C interactions in the unsubstituted SegPHOS catalyst makes its Pd-complex ineffective.
- (4) The extended network of C–H \cdots H–C interactions is able to stabilize intermediates with significant charge separation, as is seen in the example with the catalytic C–O bond cleavage reaction. This conclusion opens the door for discovering so far unknown catalytic transformations.
- (5) The overall picture of effective and stereoselective catalytic transformations outlined in this work closely resembles the highly specific enzymatic reactions taking place in Nature.

RESULTS AND DISCUSSION

Scope of the Study

Recently, palladium-catalyzed asymmetric hydrogenations of α -acyloxy-1-arylethanones were reported by our group (Chen et al., 2013) (Scheme 1A). Interestingly, only (*R*)-DTBM-SegPHOS (**L1**) proved to be an effective catalyst (up to 5,000 S/C), whereas structurally similar ligands **L2**–**L4** with non-substituted phenyl rings were ineffective. Remarkably, application of the same catalytic system to the same substrates



Scheme 2. Computed Catalytic Cycles for the Enantioselective Hydrogenation of 1a with 2a and 2b

in acetone instead of EtOH/TFE led to a different reaction yielding the corresponding ketones even at low catalytic loadings (Chen et al., 2016; Transparent Methods 6) (Scheme 1B). In this case, the application of heavily substituted ligand L1 was also essential.

We have tried to isolate the Pd-complexes and identify palladium hydrogen species of DTBM-SegPHOS by NMR, but our attempts were unsuccessful. Nevertheless, according to the recent mechanistic studies, hydrogenation of the precatalyst in a similar system results in generation of a Pd⁺-H complex **2** that was shown to be an active species (Scheme 2) (Duan et al., 2014). Hence, we investigated the enantioselective reactions of **2a** and **2b** with **1a-c** (*t*-Bu, Ph, Me, see Supplemental Information for their enantioselectivities and yields), since **1a** afforded the highest enantioselectivity detected experimentally, whereas **1b** and **1c** provide representative examples of various substituted substrates.

Catalytic Cycle of Pd-Catalyzed Asymmetric Hydrogenation

The catalytic cycle computed for the hydrogenation of **1a** is shown in Scheme 2. Hydride transfer takes place after the proper orientation of the C=O bond is achieved in the adduct **3a** via **1a**•**2a**. The resulting alkoxide **4a** coordinates an H₂ molecule, and insertion of hydride into the Pd-O bond releases the product **6a** and regenerates the catalyst **2a**. Of interest is the strongly exothermic formation of the reactive catalyst-adduct **3a**. Moreover, when calculating the approach of the substrate to the catalyst, we observed the initial formation of an adduct **1a**•**2a**, which is approximately 12 kcal/mol more stable than **3a** in terms of electronic energy; this results in a 2.5 kcal/mol difference in free energy (Figure 1). The adduct **1a**•**2a** is formed via numerous weak intramolecular interactions between the *t*-Bu groups of the catalyst and the substrate (see Figure 2). Noteworthy, the highest point of the catalytic cycle,

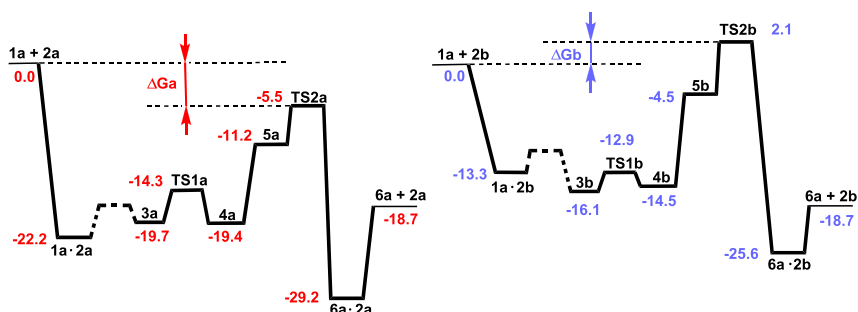


Figure 1. The Energy Profiles of the Catalytic Cycles for the Hydrogenation of 1a with 2a and 2b

TS2a, is 5.5 kcal/mol more stable than the initial mixture of the catalyst and the substrate (Scheme 2, Table 1, entry 1).

The relative stability of 1a·2a, as well as of 3a, is due to the numerous weak intramolecular interactions between the substrate and *t*-Bu groups of the catalyst 2a (Figure 2). There are ten C-H \cdots H-C interactions in the range of 2.21–2.68 Å, two C-H \cdots π interactions (2.94 and 3.10 Å), and two C-H \cdots O interactions (2.70 and 2.92 Å). To achieve a configuration that is appropriate for rapid hydrogenation (3a), half of the C-H \cdots H-C interactions must be broken, accounting for the energy difference of 2.5 kcal/mol between 1a·2a and 3a.

Comparison of Three Catalytic Systems

In the case of the computed catalytic cycle for 2b catalyzed hydrogenation of 1a, the *t*-Bu groups in the catalyst are absent (Scheme 2, Table 1, entry 7) and the encounter complex 1a·2b is less stable than the reactive catalyst-substrate complex 3b (Figure 1, –13.3 kcal/mol versus –16.1 kcal/mol). Moreover, since TS2b is 2.1 kcal/mol less stable than 1a + 2b, 3b is more likely to dissociate back to 1a + 2b, than to undergo two migratory insertions yielding the hydrogenation product. The importance of *t*-Bu groups within the catalyst for binding the substrate is further illustrated by the computational results for the catalytic cycles with the catalyst 2b and the substrates 1b, c (Table 1, entries 9–12) that lack *t*-Bu groups themselves. Graphically, this conclusion is illustrated in Figure 3, which shows that a significant difference in stabilizing energy is observed throughout the whole process for the approach of the substrate to the catalyst; this applies to all three studied examples, although the extent of this stabilization is evidently smaller in the two latter cases.

Interestingly, the observed high *S*-enantioselectivity in the hydrogenation of 1a with 2a as a catalyst 97% ee (*S*) cannot be satisfactorily accounted for by the computed parameters of the catalytic cycles using the

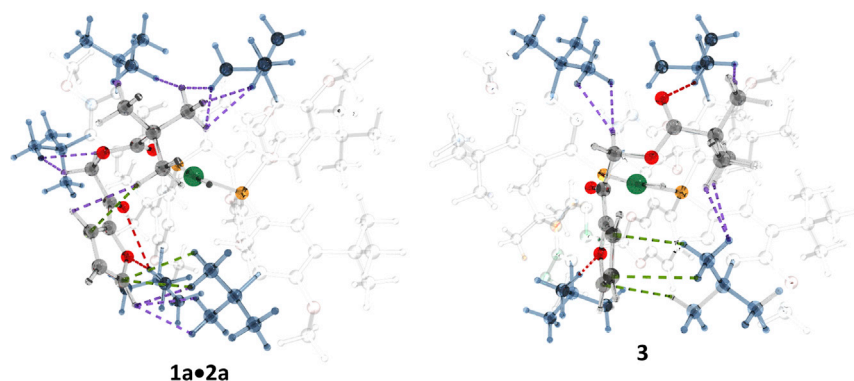


Figure 2. Optimized Structures of 1a·2a and 3a and Stabilizing Intramolecular Interactions (Shown in Dashed Lines): C-H \cdots H-C (Violet), C-H \cdots O (Red) and C-H \cdots π (Green)

See text for details

Entry	Substrate, Catalyst, Pathway	3	TS1	4	5	TS2	6·2
1	1a, 2a (S)	-19.7	-14.3	-19.4	-11.2	-5.5	-29.2
2	1a, 2a (R)	-21.2	-14.7	-15.4	-15.0	-8.0	-31.9
3	1b, 2a (S)	-8.2	-1.9	-9.1	0.2	10.1	-21.6
4	1b, 2a (R)	-7.1	-1.5	-10.2	-5.3	6.9	-23.6
5	1c, 2a (S)	-8.8	-2.4	-8.4	-2.9	7.5	-15.9
6	1c, 2a (R)	-9.8	0.2	-13.6	-0.4	0.8	-19.7
7	1a, 2b (S)	-16.1	-12.9	-14.5	-4.5	2.1	-25.6
8	1a, 2b (R)	-17.4	-6.6	-11.9	-1.7	3.4	-25.5
9	1b, 2b (S)	-8.5	-2.3	-3.5	8.1	21.8	-12.4
10	1b, 2b (R)	-5.4	3.5	-1.8	5.0	13.6	-15.3
11	1c, 2b (S)	-5.8	-0.3	-0.6	3.7	13.7	-16.8
12	1c, 2b (R)	-8.6	2.1	-1.5	5.5	13.8	-18.0

Table 1. Relative Gibbs Free Energies (kcal/mol) of Intermediates and Transition States of the Catalytic Cycles

In all cases 0.0 kcal/mol is attributed to the energy of the corresponding pair 1 + 2.

common approach based on the relative stabilities of the corresponding transition states. Indeed, the relative stabilities of either TS1 or TS2 for S- and R-pathways do not demonstrate the regularity expected in the case if the stereoselection was to take place in either or both of these states.

To gain further insight into the mechanism of enantioselection in this case, we have studied in detail the process of the formation of reactive complexes 3(S) and 3(R). Inspecting Figures 4 and 5, one can see that the association pathways differ significantly starting from the Pd-O distances of approximately 15 Å. Moreover, a deep minimum corresponding to the formation of 1a·2b is not observed in the case of the R-pathway. Therefore, almost complete dissociation must take place for the convergence of these pathways, and the enantioselectivity is largely determined by their relative abundance.

Since the R-pathway does not have really deep minima, we were unable to estimate accurately the free energy gap between two pathways. For an approximate estimation we used the coefficient 4.8 obtained above from comparing the differences in electronic energies and Gibbs free energies between 1a·2a(S) and 3a(S) (*vide supra*). Thus, the difference of 22 kcal/mol (see Figure 4) approximately corresponds to

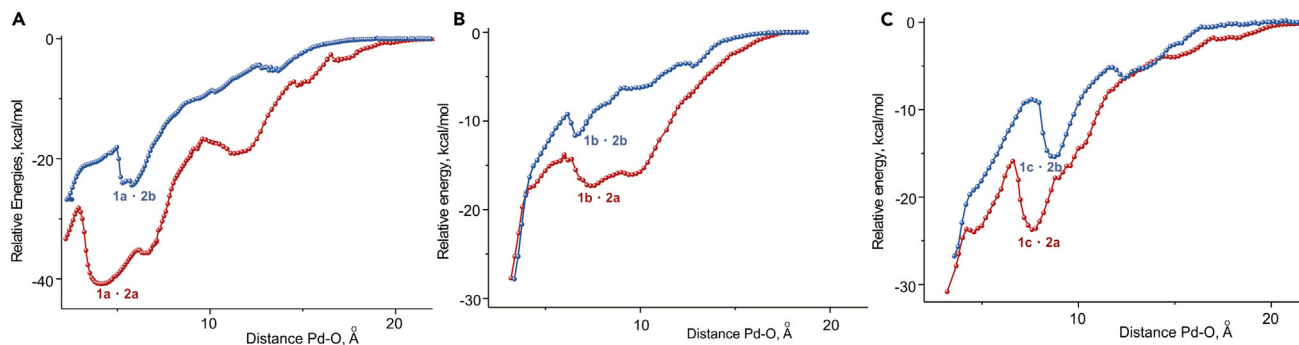


Figure 3. Scans of the Relative Energy Versus the Interatomic Distance Pd-O

(A) For 1a approaching 2a (red) and 2b (blue); (B) for 1b approaching 2a (red) and 2b (blue); (C) for 1c approaching 2a (red) and 2b (blue). In each case the energy of separated species is taken as the zero point.

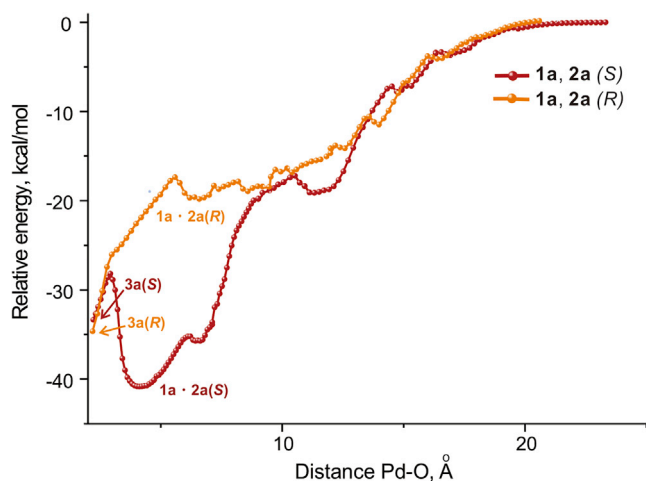


Figure 4. Scans of the Relative Energy Versus the Interatomic Distance Pd-O

1a approaching **2a** to form S-product (red) and R-product (orange). Note the similarity of the orange curve to the blue curve in the [Figure 3A](#)—both belong to reactions that do not take place.

4.6 kcal/mol difference in Gibbs free energy for **1a**·**2a(S)** and **1a**·**2a(R)** that gives a 2,343:1 ratio of precursors.

In the case of complete absence of exchange between the precursors, the optical yield is determined entirely by their relative abundance ([Halpern, 1982](#); [Landis and Halpern, 1987](#); [Drexler et al., 2005](#); [Schmidt et al., 2008](#); [Hartwig, 2010](#)) and the estimated value of the free energy difference attests for the perfect S-enantioselection, whereas the experimental ee value is 97% ee (S).

In the Curtin-Hammett conditions (all equilibria between the precursors are faster than productive transformations) the ee should be estimated by [Equation 1](#) ([Hartwig, 2010](#)).

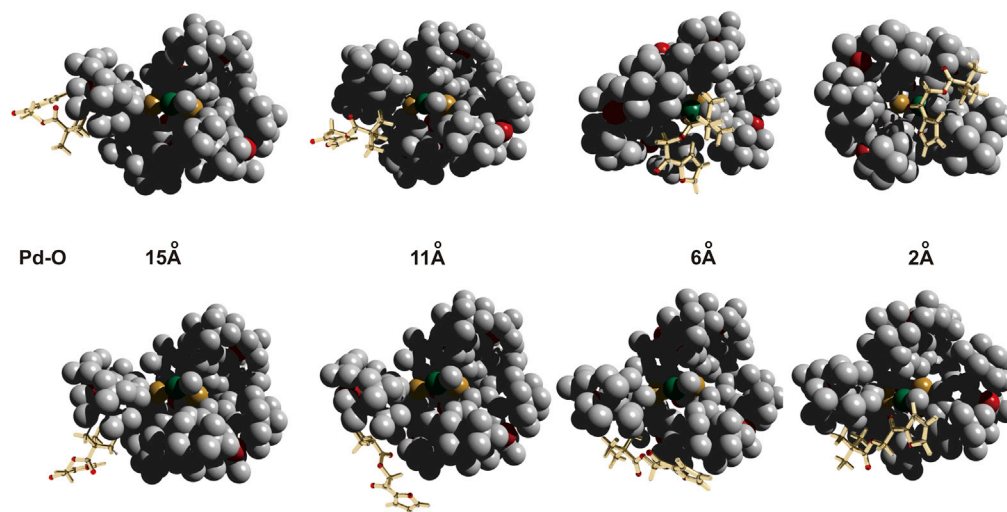
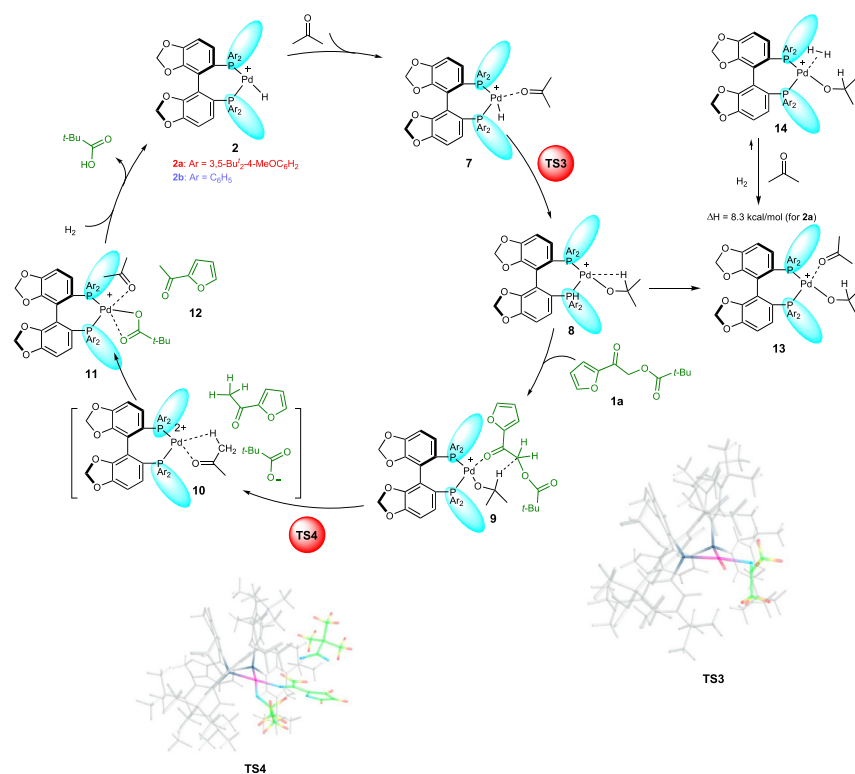


Figure 5. Structures of the Catalyst-Product Adducts at Different Distances Pd-O

Top: In the case of the S-pathway, the substrate can approach the reactive site moving in the valley between several t-Bu groups keeping numerous C-H interactions to reach the deep minimum with the oxygen atom of t-BuCO group coordinated to Pd. Bottom: The same level of stabilization cannot be achieved in the R-pathway, because the C₄H₃O group (C₄H₃O: furyl) must be kept dissociated to be able to switch the prochiral planes. Even at 15 Å the modes of coordination are different; therefore, to cross-over the pathways, the substrate must come back at least thus far.



Scheme 3. Mechanism of the C–O Bond Cleavage

$$\frac{[S]}{[R]} = K_{\text{eq}} \left(\frac{k_i}{k_f} \right) \quad (\text{Equation 1})$$

Using Equation 1, data of Table 1 for TS1 and TS2, and assuming instant achievement of equilibrium, we can obtain:

$$[S]/[R] = e^{4.6/0.593} \times (1/e^{0.4/0.593} \times 1/e^{2.5/0.593}) = 2343 \times 1/1.95 \times 1/68 = 17.7$$

That corresponds to 89% ee (S), an underestimation, but still clearly indicating the strong S-bias.

We conclude therefore that the enantioselection in the reaction under study is determined by the relative abundance of the precursors, which is a relatively rare case, although there is precedence of such a phenomenon (Liu et al., 2014; Drexler et al., 2005; Schmidt et al., 2008).

We are convinced that the presented evidence demonstrates an important feature of bulky catalysts, approaching in size to natural enzymes and able to participate in a large number of weak intramolecular interactions with the substrate. Similarly to the enzymatic catalysis (Strauss and Wegner, 2019), the initial weak encounter complexes are formed not selectively (Pd–O distances from 20 to 15 Å in the Figure 4). But the pathways for the closer association ultimately leading to the configuration appropriate for a very fast transformation are significantly different (Figure 5), thus ensuring high selectivity of the overall reaction.

It is clear that similar differences in the ability to bind the substrate and keep it in a proper conformation must be observed in the destructive C–O bond cleavage reaction that can also be catalyzed by the palladium complex of the ligand L1, whereas the palladium complex of L2 is ineffective.

Catalytic Cycle of Pd-Catalyzed C–O Bond Cleavage

We have investigated several possibilities for the hydride source in the destructive hydrogenation and have found that neither Pd–H species like 3 nor Pd–H₂ species like 5 (Scheme 2) were capable of

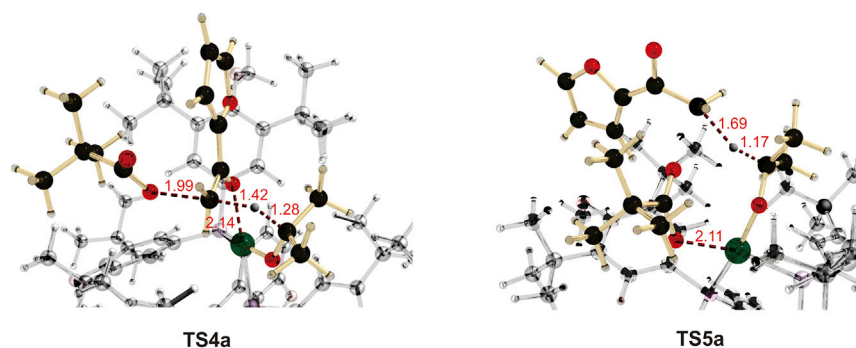


Figure 6. Partial Plots of the Transition States for the Destructive C–O Bond Cleavage

In TS4a, the hydride originating from the isopropyl alcoholate substitutes the Opiv anion in an S_N2 fashion. The alternative mode of substitution via TS5a is disfavoured by more than 30 kcal/mol (32.2 kcal/mol). Numbers indicate interatomic distances in Angström.

promoting the hydride transfer resulting in the destructive C–O bond cleavage leading to the corresponding product **12** (Scheme 3) (Transparent Methods 5). On the other hand, it was possible to locate transition states for the hydride transfer starting from the acetone alcoholate **8**, which can easily be formed from complex **7** under the reaction conditions through the transition state **TS3**. It is not further hydrogenated to 2-propanol because, in the presence of excess acetone, the formation of molecular hydrogen complex **14** is strongly endogonic (Scheme 3). On the other hand, **1a** is firmly bound via the numerous weak intramolecular interactions, similar to the previous case.

Initially, we expected that the OPiv-anion (Piv: pivaloyl) must remain attached to the Pd after the C–O bond is broken. However, the calculations showed that, in the case of this orientation of the substrate, the hydride must approach the carbon atom from the side of the broken C–O bond (Figure 6, TS5a). This makes this TS more than 30 kcal/mol less stable than another TS (Figure 6, TS4a) whereby the keto group of the substrate is coordinated to Pd and the OPiv group is replaced by the hydride similar to the usual S_N2 reaction. Despite the charges separation, the transformation from **9** to **10** was computed to proceed with an activation barrier of 28.3 kcal/mol; this is in reasonable agreement with the experimental results (Lu et al., 2017) (For the mechanism experiments see Table S1). The latter structure is not a real minimum. It spontaneously rearranges to the much more stable product **11** (Scheme 3), resulting in a strongly exogonic (41.7 kcal/mol) transformation. The transition state **TS4b** for the Pd-SEGPHOS (Pd-L2) catalysis corresponds to an activation barrier of 44.8 kcal/mol.

We have detected the production of a small amount of isopropanol in the reaction mixture by GC-MS (Transparent Methods 6, Table S1) (The substrate **1a** [R = furyl] had not been previously tried in the destructive C–O bond cleavage reaction. Hence, the corresponding experiment was carried out. Complete conversion of **1a** was achieved after 24 h reaction at 80°C and 50 atm of H_2 . See Supplemental Information for detail.). This result revealed the possibility that acetone takes part in the hydride transfer.

It is known that numerous London dispersion forces allow the Gecko a possibility to walk on walls or ceilings keeping its body upside down. The abundance of *t*-Bu groups in the molecule of the catalyst **2a** provides opportunity for a substrate to overcome Brownian motion and remain bound to the catalyst long enough to allow the reaction to proceed. Such types of catalyst can therefore be considered to be “Gecko-friendly” catalysts, as illustrated in the Figure 7. This concept suggests that an improvement in the catalytic performance of an artificial catalyst can be achieved by increasing the size of the ligand via introducing numerous *t*-Bu groups or similar substituents capable of forming catalyst-substrate adducts stabilized by non-bonding interactions.

In summary, we have discovered a catalytic reaction in which the relative stabilities of the competing transition states are irrelevant for the handedness and order of enantioselection. Similar to natural enzymatic reactions, high enantioselectivity is achieved via the stereodivergent approach of the substrate to the reactive site of the catalyst. Initially, the encounter complex is formed, which later rearranges into active species capable for extremely rapid transformation into the product. This process occurs owing

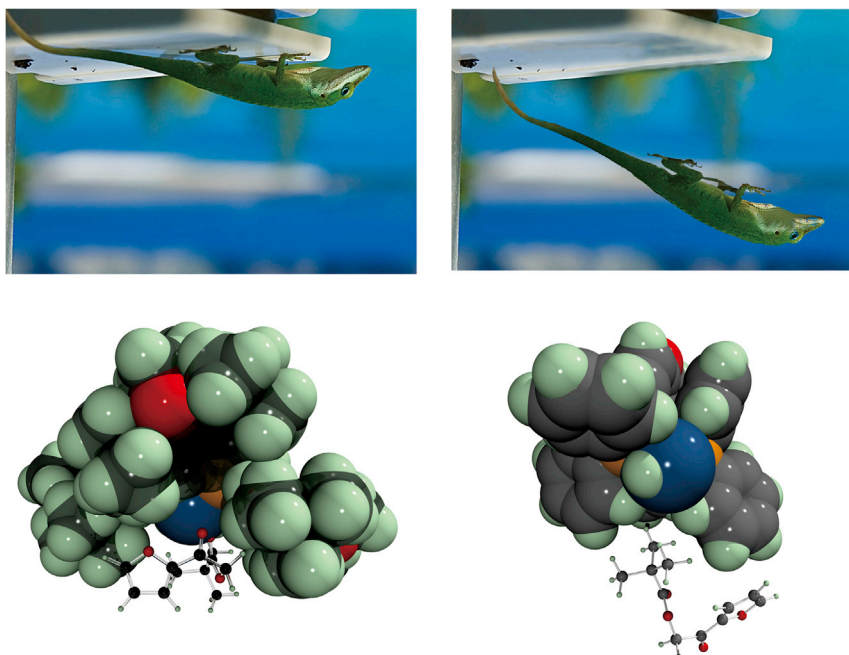


Figure 7. Gecko-Friendly Catalyst

A Gecko-friendly catalyst like **2a** (left) allows a substrate to remain bound to the catalyst through numerous London interactions long before the appropriate conformation for effectuating the reaction is achieved. Lack of Gecko-friendly structural elements in **2b** prevents the reaction that would be otherwise possible.

to the existence of an extensive network of C–H \cdots H–C interactions provided by the numerous *t*-Bu groups of the DTBM-SegPHOS ligand. Stereoselectivity is induced by dramatic difference in the stabilities of the *S*- and *R*-pathways of the approaching substrate to the reactive site. The mechanism of stereoselection mimics highly efficient enzymatic transformations taking place in Nature.

The normal SegPHOS ligand lacking the *t*-Bu groups is unable to promote the same catalytic transformations. The extended network of C–H \cdots H–C interactions is able to stabilize intermediates with significant charge separation, as is seen in the example concerning catalytic C–O bond cleavage reaction.

Limitations of the Study

The results of a purely computational study are presented here. Evidently, experimental research on the catalyst-substrate interactions for large-sized artificial catalysts must be induced by our findings.

METHODS

All methods can be found in the accompanying [Transparent Methods supplemental file](#).

SUPPLEMENTAL INFORMATION

Supplemental Information can be found online at <https://doi.org/10.1016/j.isci.2020.100960>.

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AUTHOR CONTRIBUTIONS

J.C. designed and carried out all experiments. I.D.G. made all computations. Both authors contributed equally to discussion and writing the paper.

DECLARATION OF INTERESTS

No competing interests are declared.

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Supplemental Information

Size is Important: Artificial Catalyst Mimics Behavior of Natural Enzymes

Jianzhong Chen and Ilya D. Gridnev

Supplemental Information

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Transparent Methods

1. Computational details

Computations were carried out using the range separated hybrid functional with damped atom-atom dispersion (WB97XD) (Chai, J.-D., and Head-Gordon, M., 2008) as implemented in the GAUSSIAN 09 software package. (Frisch et al. 2009). For palladium atom the SDD basis set (Bergner, A. et al. 1993) with the associated effective core potential was employed. All other atoms were described with 6-31G** basis with additional diffuse function for phosphorus (Ditchfield, R. et al., 1971; Gordon, M. S., 1980; Hariharan, P. C., and Pople, J. A., 1973; 1974; Hehre, W. J. et al., 1972). Non-specific solvation was introduced by using the SMD continuum model (Marenich, A. V. et al., 2009) (ethanol or acetone for hydrogenation and destructive cleavage respectively).

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2. Data S1. Cartesian coordinates. Related to Table 1.

2.1 Catalysts, starting compounds and products.

H₂

RwB97XD SCF energy	-1.174642 a.u.
RwB97XD SCF enthalpy	-1.161194 a.u.
RwB97XD SCF free energy	-1.175987 a.u.

2a

RwB97XD SCF energy	-4292.091722 a.u.
RwB97XD SCF enthalpy	-4290.379889 a.u.
RwB97XD SCF free energy	-4290.590561 a.u.
Three lowest frequencies (cm ⁻¹)	16.3, 18.4, 21.1

Cartesian coordinates:

1	6	0	-0.325089	-0.818663	1.922347
2	6	0	-0.114124	-1.784125	2.884063
3	6	0	-0.706020	-3.043061	2.852126
4	6	0	-1.531480	-3.422093	1.823313
5	6	0	-1.760300	-2.465603	0.825062
6	6	0	-1.195995	-1.188679	0.856769
7	1	0	-2.000885	-4.397834	1.791194
8	1	0	-2.426853	-2.740087	0.017172
9	6	0	0.320970	0.506569	2.135237
10	6	0	1.349322	1.072014	1.333727
11	6	0	-0.029347	1.227257	3.256810
12	6	0	1.909299	2.303448	1.665304
13	6	0	0.540630	2.452971	3.584025
14	6	0	1.509535	3.028866	2.799404
15	1	0	2.693867	2.721970	1.044978
16	1	0	1.959763	3.982391	3.048858
17	8	0	-0.327827	-3.749504	3.948817
18	8	0	0.675418	-1.689236	3.991731
19	8	0	-0.956332	0.895162	4.200102
20	8	0	-0.021378	2.912183	4.740805
21	6	0	0.289864	-2.791367	4.812019
22	1	0	1.169930	-3.230057	5.278576
23	1	0	-0.441757	-2.452718	5.555252
24	6	0	-0.686946	1.773919	5.291924
25	1	0	-0.018878	1.272111	6.002825
26	1	0	-1.622772	2.081926	5.755714
27	15	0	1.831546	0.193218	-0.193822
28	15	0	-1.583825	-0.040052	-0.517457
29	46	0	0.145091	0.296243	-1.880090
30	6	0	2.279877	-1.487413	0.303445
31	6	0	3.127788	-1.774347	1.363692
32	6	0	1.727189	-2.527655	-0.440388
33	6	0	3.422504	-3.093512	1.728190
34	1	0	3.573951	-0.952163	1.914279
35	6	0	1.931389	-3.859860	-0.100267
36	1	0	1.101810	-2.268017	-1.286224
37	6	0	2.722246	-4.112972	1.046917
38	6	0	3.308396	1.019275	-0.857053
39	6	0	4.563479	0.417559	-0.905243
40	6	0	3.115203	2.245201	-1.486795
41	6	0	5.648938	1.055126	-1.505599
42	1	0	4.684849	-0.565732	-0.470951
43	6	0	4.158133	2.941979	-2.104210
44	1	0	2.118353	2.674993	-1.491813
45	6	0	5.440093	2.359217	-2.020147
46	6	0	-3.049433	-0.769208	-1.305872
47	6	0	-4.335110	-0.368222	-0.964091
48	6	0	-2.870643	-1.766949	-2.254751
49	6	0	-5.456235	-0.983958	-1.516677
50	1	0	-4.461759	0.442410	-0.261635
51	6	0	-3.946457	-2.443587	-2.834504
52	1	0	-1.857357	-2.025819	-2.540304
53	6	0	-5.238239	-2.077530	-2.390262
54	6	0	-2.101125	1.525838	0.228896
55	6	0	-1.675443	2.719000	-0.333727
56	6	0	-2.936398	1.549849	1.349012
57	6	0	-2.123149	3.959170	0.133322
58	1	0	-0.967189	2.682962	-1.155840
59	6	0	-3.466292	2.746203	1.821895

60	1	0	-3.182913	0.614385	1.836474
61	6	0	-3.118873	3.932619	1.126226
62	6	0	-1.439530	5.209560	-0.466035
63	6	0	-1.823625	5.357532	-1.949526
64	1	0	-1.307850	6.219954	-2.386420
65	1	0	-1.542458	4.471361	-2.528973
66	1	0	-2.900355	5.511580	-2.073891
67	6	0	-1.724309	6.533303	0.264590
68	1	0	-1.544170	6.448680	1.339653
69	1	0	-1.041553	7.294054	-0.129516
70	1	0	-2.738764	6.902954	0.111967
71	6	0	0.089535	5.000827	-0.369764
72	1	0	0.405775	4.892817	0.673341
73	1	0	0.435225	4.121286	-0.919511
74	1	0	0.599578	5.871621	-0.793551
75	6	0	-4.322397	2.771382	3.103906
76	6	0	-3.649794	3.710624	4.125245
77	1	0	-3.695853	4.752190	3.801633
78	1	0	-4.150962	3.631915	5.096282
79	1	0	-2.595996	3.449103	4.259298
80	6	0	-5.765736	3.241452	2.841274
81	1	0	-6.227947	2.673305	2.026498
82	1	0	-6.368150	3.081685	3.742387
83	1	0	-5.815693	4.303511	2.599578
84	6	0	-4.412002	1.374051	3.739764
85	1	0	-4.948202	0.664310	3.099848
86	1	0	-3.425509	0.959821	3.968571
87	1	0	-4.966858	1.448223	4.680120
88	8	0	-3.775863	5.086969	1.471924
89	8	0	-6.349675	-2.748859	-2.838638
90	8	0	2.811485	-5.412986	1.480688
91	8	0	6.540531	3.040578	-2.481946
92	6	0	7.048771	4.001535	-1.559835
93	1	0	7.987087	4.371024	-1.977702
94	1	0	6.361445	4.842261	-1.430544
95	1	0	7.236155	3.550033	-0.580341
96	6	0	3.783940	4.260180	-2.824776
97	6	0	4.805270	4.742472	-3.871274
98	1	0	4.359505	5.573231	-4.428690
99	1	0	5.733875	5.109321	-3.434885
100	1	0	5.051725	3.953189	-4.587825
101	6	0	3.559388	5.363286	-1.773369
102	1	0	3.200221	6.278992	-2.256408
103	1	0	2.813081	5.052638	-1.036194
104	1	0	4.479148	5.607115	-1.233860
105	6	0	-4.792658	5.448533	0.540153
106	1	0	-5.271285	6.347112	0.933247
107	1	0	-4.376244	5.662245	-0.449140
108	1	0	-5.537500	4.651430	0.439389
109	6	0	-6.633317	-3.968826	-2.157337
110	1	0	-7.688088	-4.190164	-2.332534
111	1	0	-6.034191	-4.796959	-2.546025
112	1	0	-6.54212	-3.874293	-1.081885
113	6	0	-6.858418	-0.403029	-1.228492
114	6	0	-6.776521	0.818823	-0.293682
115	1	0	-6.384499	0.553677	0.694617
116	1	0	-6.157900	1.622454	-0.707077
117	1	0	-7.783185	1.223451	-0.149842
118	6	0	-7.474996	0.073416	-2.557889
119	1	0	-7.585078	-0.749403	-3.267549
120	1	0	-8.466280	0.504862	-2.378134
121	1	0	-6.850471	0.846108	-3.019545
122	6	0	-7.799969	-1.417140	-0.552217
123	1	0	-8.119146	-2.203547	-1.235201
124	1	0	-7.327661	-1.880218	0.320764
125	1	0	-8.701693	-0.899711	-0.206971
126	6	0	-3.612703	-3.519273	-3.895945
127	6	0	-3.255258	-4.841408	-3.188994
128	1	0	-2.414149	-4.698153	-2.501991
129	1	0	-4.091352	-5.242857	-2.611275
130	1	0	-2.963276	-5.95573	-3.928480
131	6	0	-4.733642	-3.749471	-4.926669
132	1	0	-4.347502	-4.389123	-5.727167
133	1	0	-5.611906	-4.242978	-4.513905
134	1	0	-5.056201	-2.806135	-5.379123
135	6	0	-2.373106	-3.083814	-4.711653
136	1	0	-2.221599	-3.790352	-5.533593

137	1	0	-2.505019	-2.085887	-5.143827
138	1	0	-1.449548	-3.087939	-4.125685
139	6	0	6.986247	0.301603	-1.683890
140	6	0	2.456745	4.056386	-3.594464
141	1	0	2.532006	3.226000	-4.305260
142	1	0	1.602682	3.872045	-2.937518
143	1	0	2.225919	4.964214	-4.161087
144	6	0	7.275499	0.167769	-3.192103
145	1	0	8.210509	-0.383169	-3.344087
146	1	0	6.472714	-0.382807	-3.695032
147	1	0	7.376234	1.144180	-3.671018
148	6	0	8.171371	1.000643	-0.991047
149	1	0	7.940043	1.237686	0.052954
150	1	0	9.038196	0.330551	-0.993916
151	1	0	8.467226	1.915904	-1.502749
152	6	0	6.906874	-1.118791	-1.100092
153	1	0	6.111041	-1.716695	-1.556310
154	1	0	7.853587	-1.634389	-1.289097
155	1	0	6.752952	-1.102043	-0.016613
156	6	0	1.974208	-5.684796	2.601906
157	1	0	2.121397	-6.737138	2.851630
158	1	0	2.240193	-5.065243	3.464059
159	1	0	0.921476	-5.509895	2.359928
160	6	0	4.522189	-3.286613	2.801641
161	6	0	4.010343	-2.802827	4.169549
162	1	0	4.817135	-2.846420	4.909784
163	1	0	3.647725	-1.771032	4.126554
164	1	0	3.194529	-3.436306	4.529704
165	6	0	5.062771	-4.719927	2.948591
166	1	0	5.943315	-4.687738	3.599756
167	1	0	4.351899	-5.407633	3.406955
168	1	0	5.375365	-5.136765	1.987234
169	6	0	5.741142	-2.428092	2.391113
170	1	0	6.132023	-2.754844	1.421789
171	1	0	5.514958	-1.360755	2.327187
172	1	0	6.538202	-2.545458	3.132938
173	6	0	1.383530	-4.978944	-1.011671
174	6	0	0.587885	-4.394717	-2.193584
175	1	0	0.240973	-5.215360	-2.829205
176	1	0	-0.295921	-3.840712	-1.856358
177	1	0	1.194888	-3.733660	-2.821247
178	6	0	0.441835	-5.951286	-0.277929
179	1	0	-0.338492	-5.412135	0.268434
180	1	0	-0.051476	-6.600267	-1.010001
181	1	0	0.979334	-6.594613	0.418966
182	6	0	2.577821	-5.762517	-1.590172
183	1	0	3.229815	-5.106164	-2.177021
184	1	0	3.173726	-6.222228	-0.797984
185	1	0	2.218707	-6.558612	-2.252361
186	1	0	-1.023651	0.442306	-2.920804

2b

RwB97XD SCF energy -2576.351388 a.u.
 RwB97XD SCF enthalpy -2575.734158a.u.
 RwB97XD SCF free energy -2575.843968 a.u.
 Three lowest frequencies (cm⁻¹) 10.9, 29.4, 38.2

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.327403	1.542941	0.169377
2	6	0	0.027959	2.855070	-0.123537
3	6	0	0.616663	3.556564	-1.170765
4	6	0	1.573500	2.985701	-1.973358
5	6	0	1.922901	1.659117	-1.682855
6	6	0	1.331614	0.940690	-0.644295
7	1	0	2.037488	3.527880	-2.788491
8	1	0	2.683734	1.193053	-2.297837
9	6	0	-0.405324	0.883613	1.287197
10	6	0	-1.422247	-0.096184	1.119820
11	6	0	-0.135777	1.258079	2.584752
12	6	0	-2.053705	-0.657759	2.225909
13	6	0	-0.756850	0.675235	3.684170
14	6	0	-1.724089	-0.288863	3.540498

15	1	0	-2.825093	-1.406935	2.084092
16	1	0	-2.211308	-0.741661	4.395977
17	8	0	0.096620	4.806962	-1.232423
18	8	0	-0.876337	3.648897	0.507780
19	8	0	0.774554	2.176059	3.003721
20	8	0	-0.238674	1.198866	4.828132
21	6	0	-0.883394	4.895475	-0.192898
22	1	0	-1.868801	5.060048	-0.636918
23	1	0	-0.611571	5.698732	0.495898
24	6	0	0.625549	2.263750	4.423187
25	1	0	0.165922	3.224167	4.679169
26	1	0	1.599240	2.142088	4.900852
27	15	0	-1.744983	-0.726942	-0.568088
28	15	0	1.784307	-0.817745	-0.425524
29	46	0	0.130678	-2.118399	-1.157258
30	6	0	-2.173415	0.747518	-1.544735
31	6	0	-3.008461	1.748486	-1.035129
32	6	0	-1.593937	0.903282	-2.807537
33	6	0	-3.269764	2.886639	-1.790448
34	1	0	-3.438575	1.649553	-0.042541
35	6	0	-1.842897	2.053046	-3.552471
36	1	0	-0.928126	0.136703	-3.196023
37	6	0	-2.679740	3.043967	-3.044123
38	6	0	-3.242819	-1.759707	-0.430662
39	6	0	-4.542382	-1.269719	-0.589970
40	6	0	-3.049194	-3.118412	-0.146223
41	6	0	-5.631006	-2.127467	-0.458307
42	6	0	-4.140371	-3.971121	-0.008060
43	1	0	-2.040806	-3.512276	-0.024535
44	6	0	-5.432567	-3.474816	-0.164655
45	6	0	3.368608	-1.022912	-1.308597
46	6	0	4.600680	-0.810580	-0.685204
47	6	0	3.329832	-1.365486	-2.665849
48	6	0	5.779923	-0.941560	-1.414864
49	1	0	4.655848	-0.557437	0.367561
50	6	0	4.509247	-1.478766	-3.393261
51	1	0	2.374450	-1.542925	-3.152806
52	6	0	5.736599	-1.269608	-2.766982
53	6	0	2.071820	-1.033454	1.356769
54	6	0	1.505644	-2.123669	2.024337
55	6	0	2.796020	-0.075470	2.076408
56	6	0	1.662577	-2.254194	3.400761
57	1	0	0.924803	-2.855611	1.469443
58	6	0	2.963582	-0.220619	3.449260
59	1	0	3.206540	0.796341	1.575787
60	6	0	2.391074	-1.303925	4.112849
61	1	0	1.384411	-3.032972	-1.323759
62	1	0	4.468769	-1.738343	-4.446403
63	1	0	6.659155	-1.369349	-3.330446
64	1	0	6.733942	-0.787315	-0.920720
65	1	0	1.208798	-3.094720	3.915936
66	1	0	2.510123	-1.405435	5.187019
67	1	0	3.527377	0.523671	4.002530
68	1	0	-3.924462	3.657216	-1.395261
69	1	0	-2.870577	3.942945	-3.622229
70	1	0	-1.376380	2.177814	-4.524655
71	1	0	-4.713498	-0.223492	-0.820568
72	1	0	-6.636878	-1.739397	-0.585144
73	1	0	-6.284653	-4.139865	-0.062836
74	1	0	-3.979741	-5.021353	0.214228

1a

RwB97XD SCF energy -728.280036 a.u.
 RwB97XD SCF enthalpy -728.025798 a.u.
 RwB97XD SCF free energy -728.085088 a.u.
 Three lowest frequencies (cm⁻¹) 30.3, 40.0, 63.3

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.327403	1.542941	0.169377
2	6	0	0.027959	2.855070	-0.123537
3	6	0	0.616663	3.556564	-1.170765
4	6	0	1.573500	2.985701	-1.973358
5	6	0	1.922901	1.659117	-1.682855
6	6	0	1.331614	0.940690	-0.644295
7	1	0	2.037488	3.527880	-2.788491
8	1	0	2.683734	1.193053	-2.297837
9	6	0	-0.405324	0.883613	1.287197
10	6	0	-1.422247	-0.096184	1.119820
11	6	0	-0.135777	1.258079	2.584752
12	6	0	-2.053705	-0.657759	2.225909
13	6	0	-0.756850	0.675235	3.684170
14	6	0	-1.724089	-0.288863	3.540498

1	6	0	2.564033	0.055597	-0.018582
2	6	0	2.781491	-1.285722	-0.176859
3	8	0	3.752479	0.699605	0.163847
4	6	0	4.187393	-1.475957	-0.086895
5	1	0	2.026228	-2.043077	-0.335986
6	6	0	4.718023	-0.237979	0.117521
7	1	0	4.731460	-2.405546	-0.164473
8	1	0	5.729520	0.117968	0.245440
9	6	0	1.359583	0.879079	-0.006912
10	8	0	1.394554	2.083460	0.178493
11	6	0	0.061629	0.122874	-0.244651
12	1	0	0.117136	-0.371597	-1.218903
13	1	0	-0.039005	-0.636813	0.533824
14	8	0	-0.988904	1.070142	-0.224956
15	6	0	-2.312347	0.811826	-0.167899
16	8	0	-3.027149	1.786088	-0.282968
17	6	0	-2.879112	-0.593320	0.087497
18	6	0	-4.400866	-0.511132	-0.102769
19	1	0	-4.841730	-1.487581	0.119081
20	1	0	-4.850402	0.228339	0.563666
21	1	0	-4.658214	-0.247794	-1.132965
22	6	0	-2.589286	-0.982035	1.550856
23	1	0	-1.522123	-1.075445	1.766314
24	1	0	-3.011303	-0.244596	2.240750
25	1	0	-3.055000	-1.950232	1.759274
26	6	0	-2.330230	-1.649866	-0.890458
27	1	0	-2.326360	-1.278320	-1.920230
28	1	0	-1.325825	-1.993389	-0.640076
29	1	0	-2.984077	-2.526467	-0.856131

1b

RwB97XD SCF energy -802.054407 a.u.
 RwB97XD SCF enthalpy -801.832638 a.u.
 RwB97XD SCF free energy -801.891375 a.u.
 Three lowest frequencies (cm⁻¹) 22.4, 26.5, 38.7

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.383081	-1.659951	0.328526
2	6	0	2.441307	-1.044543	-0.152362
3	6	0	2.360304	0.404358	-0.002172
4	6	0	3.154426	1.254939	0.717854
5	8	0	1.380019	1.114108	-0.636071
6	6	0	2.630960	2.559422	0.516282
7	1	0	4.005769	0.968287	1.318061
8	6	0	1.559799	2.408143	-0.312274
9	1	0	2.997138	3.488058	0.928213
10	1	0	0.855522	3.105007	-0.741709
11	6	0	1.410727	-1.812927	-0.968693
12	1	0	1.380552	-2.835277	-0.585960
13	1	0	1.740153	-1.827082	-2.010570
14	8	0	0.104589	-1.245211	-0.998135
15	6	0	-0.508907	-1.129707	0.188391
16	8	0	-0.004876	-1.523580	1.223549
17	6	0	-1.832385	-0.467388	0.090646
18	6	0	-2.628489	-0.411988	1.237909
19	6	0	-2.277460	0.111658	-1.101666
20	6	0	-3.868404	0.212801	1.191242
21	1	0	-2.269412	-0.860394	2.158241
22	6	0	-3.517007	0.739623	-1.141213
23	1	0	-1.655206	0.076506	-1.988605
24	6	0	-4.312501	0.788697	0.002094
25	1	0	-4.488004	0.252145	2.081284
26	1	0	-3.862704	1.192362	-2.064899
27	1	0	-5.280546	1.278934	-0.033239

1c

RwB97XD SCF energy -610.375418 a.u.
 RwB97XD SCF enthalpy -610.210715 a.u.
 RwB97XD SCF free energy -610.260952 a.u.
 Three lowest frequencies (cm⁻¹) 31.9, 55.7, 83.1

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-0.605242	2.539370	0.309794
2	6	0	-0.281262	1.455062	-0.155335
3	6	0	-1.194395	0.320493	-0.066629
4	6	0	-2.399815	0.213123	0.571197
5	8	0	-0.891406	-0.860027	-0.682819
6	6	0	-2.861897	-1.109365	0.335809
7	1	0	-2.885764	0.993783	1.138377
8	6	0	-1.906678	-1.708015	-0.429296
9	1	0	-3.778460	-1.559499	0.687221
10	1	0	-1.813859	-2.695764	-0.855614
11	6	0	1.042750	1.346049	-0.899628
12	1	0	1.709358	2.114552	-0.501643
13	1	0	0.855077	1.547057	-1.957590
14	8	0	1.674339	0.068373	-0.869814
15	6	0	1.981575	-0.408312	0.348955
16	8	0	1.716880	0.196095	1.368181
17	6	0	2.663086	-1.738872	0.261810
18	1	0	3.625526	-1.620108	-0.244410
19	1	0	2.817847	-2.140583	1.261502
20	1	0	2.053502	-2.422906	-0.331870

6a

RwB97XD SCF energy -729.506698 a.u.
 RwB97XD SCF enthalpy -729.228585 a.u.
 RwB97XD SCF free energy -729.291024 a.u.
 Three lowest frequencies (cm⁻¹) 18.2, 30.3, 35.5

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.712054	-0.039891	0.087248
2	6	0	-3.248374	1.154515	-0.276613
3	8	0	-3.700869	-0.886942	0.492694
4	6	0	-4.663561	1.039994	-0.079997
5	1	0	-2.706274	2.016205	-0.640129
6	6	0	-4.877541	-0.216229	0.382181
7	1	0	-5.414929	1.795378	-0.259491
8	1	0	-5.762724	-0.762782	0.670320
9	6	0	-1.330549	-0.615439	0.086225
10	8	0	-1.128001	-1.504241	-1.005964
11	6	0	-0.299166	0.488269	-0.027840
12	1	0	-0.369523	0.985075	-0.999918
13	1	0	-0.434714	1.227432	0.765519
14	8	0	0.984152	-0.131908	0.100453
15	6	0	2.051915	0.663528	-0.027543
16	8	0	1.954304	1.859398	-0.222084
17	6	0	3.356457	-0.114673	0.098968
18	6	0	4.533263	0.847542	-0.070363
19	1	0	5.473085	0.293461	0.015050
20	1	0	4.511624	1.334580	-1.049701
21	1	0	4.524907	1.626308	0.697898
22	6	0	3.391060	-1.195057	-0.995861
23	1	0	2.564197	-1.901729	-0.886463
24	1	0	3.332172	-0.747456	-1.993555
25	1	0	4.331102	-1.751748	-0.928025
26	6	0	3.404832	-0.772200	1.489160
27	1	0	3.340833	-0.021375	2.283772
28	1	0	2.588795	-1.487281	1.622675
29	1	0	4.352135	-1.308430	1.604308
30	1	0	-1.672406	-2.284880	-0.852041
31	1	0	-1.172660	-1.145362	1.035617

6b

RwB97XD SCF energy -803.265890 a.u.
 RwB97XD SCF enthalpy -803.018917 a.u.

RwB97XD SCF free energy -803.078129 a.u.
 Three lowest frequencies (cm⁻¹) 18.7, 35.9, 49.2
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.595638	-1.674800	-0.562402
2	6	0	2.337872	-1.027377	-0.693856
3	6	0	2.347796	0.353597	-0.121269
4	6	0	1.979635	0.886870	1.074867
5	8	0	2.895812	1.322368	-0.909337
6	6	0	2.319538	2.277580	1.020352
7	1	0	1.508921	0.360002	1.892576
8	6	0	2.871050	2.480585	-0.201596
9	1	0	2.168780	3.021489	1.789279
10	1	0	3.273268	3.349396	-0.700425
11	6	0	1.254991	-1.905852	-0.070361
12	1	0	1.385917	-1.991029	1.010043
13	1	0	1.298647	-2.899842	-0.518831
14	8	0	-0.029201	-1.352904	-0.376199
15	6	0	-0.845506	-1.012555	0.627888
16	8	0	-0.597485	-1.217575	1.801280
17	1	0	2.155090	-0.953429	-1.770299
18	1	0	3.832432	-1.667191	0.373740
19	6	0	-2.091318	-0.359823	0.144660
20	6	0	-3.043782	0.024805	1.092227
21	6	0	-2.319996	-0.119697	-1.213575
22	6	0	-4.218595	0.644446	0.684281
23	1	0	-2.856655	-0.163920	2.143974
24	6	0	-3.497264	0.500104	-1.616787
25	1	0	-1.580641	-0.415460	-1.948753
26	6	0	-4.445913	0.881940	-0.670098
27	1	0	-4.956604	0.943247	1.421535
28	1	0	-3.674480	0.686032	-2.671200
29	1	0	-5.363836	1.366273	-0.988786

6c
 RwB97XD SCF energy -611.586578 a.u.
 RwB97XD SCF enthalpy -611.397074 a.u.
 RwB97XD SCF free energy -611.448738 a.u.
 Three lowest frequencies (cm⁻¹) 31.8, 56.1, 73.5
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	-1.329003	2.496792	0.255751
2	6	0	-0.604361	1.432611	-0.345070
3	6	0	-1.212480	0.097192	-0.058438
4	6	0	-0.928969	-0.900369	0.821761
5	8	0	-2.330534	-0.219660	-0.771508
6	6	0	-1.937671	-1.901215	0.638395
7	1	0	-0.097896	-0.926005	1.512654
8	6	0	-2.757100	-1.432841	-0.334880
9	1	0	-2.033779	-2.841862	1.161213
10	1	0	-3.642450	-1.823911	-0.813050
11	6	0	0.854251	1.504701	0.100337
12	1	0	0.948177	1.320856	1.172892
13	1	0	1.253723	2.493494	-0.130430
14	8	0	1.612421	0.538362	-0.636154
15	6	0	2.371481	-0.337167	0.040806
16	8	0	2.523233	-0.308828	1.245422
17	1	0	-0.656817	1.614102	-1.423030
18	1	0	-1.371201	2.323157	1.204842
19	6	0	2.965868	-1.357071	-0.880415
20	1	0	3.341311	-0.885826	-1.790765
21	1	0	3.765044	-1.895770	-0.372130
22	1	0	2.178842	-2.062837	-1.165267

2.2. Catalytic cycle **2a – 1a(S)**.

1a2a (S)

RwB97XD SCF energy -5020.436758 a.u.
 RwB97XD SCF enthalpy -5018.468193 a.u.
 RwB97XD SCF free energy -5018.711040 a.u.
 Three lowest frequencies (cm⁻¹) 16.1, 17.4, 20.8
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.922493	-0.256276	2.606677
2	6	0	-0.822526	-0.988658	3.771887
3	6	0	-1.415213	-2.234278	3.947811
4	6	0	-2.116850	-2.847079	2.939713
5	6	0	-2.218641	-2.138534	1.735190
6	6	0	-1.658670	-0.872819	1.555734
7	1	0	-2.581797	-3.817131	3.068570
8	1	0	-2.772770	-2.599478	0.926170
9	6	0	-0.314976	1.105984	2.602700
10	6	0	0.797913	1.535690	1.827538
11	6	0	-0.804829	2.023209	3.508691
12	6	0	1.305715	2.823641	1.981467
13	6	0	-0.287795	3.305228	3.655328
14	6	0	0.766924	3.744561	2.894429
15	1	0	2.165464	3.135701	1.400939
16	1	0	1.182072	4.739381	3.005868
17	8	0	-1.170405	-2.681337	5.207839
18	8	0	-0.154633	-0.645496	4.910746
19	8	0	-1.835919	1.850386	4.384746
20	8	0	-0.987759	3.963581	4.626315
21	6	0	-0.610497	-1.563833	5.902566
22	1	0	0.228893	-1.895997	6.511924
23	1	0	-1.391502	-1.088149	6.507680
24	6	0	-1.720973	2.939073	5.300340
25	1	0	-1.159351	2.609678	6.183477
26	1	0	-2.713015	3.305746	5.560538
27	15	0	1.494410	0.361648	0.600992
28	15	0	-1.833771	-0.085819	-0.087268
29	46	0	0.045707	0.083703	-1.286482
30	6	0	1.845755	-1.111043	1.602099
31	6	0	2.596654	-1.016151	2.765052
32	6	0	1.392151	-2.354195	1.174214
33	6	0	2.913911	-2.138708	3.534789
34	1	0	2.963087	-0.041588	3.070634
35	6	0	1.618272	-3.506857	1.921308
36	1	0	0.847096	-2.403422	0.241121
37	6	0	2.328162	-3.360294	3.138726
38	6	0	3.116228	1.004463	0.079411
39	6	0	4.268645	0.230098	0.200264
40	6	0	3.171723	2.180920	-0.658521
41	6	0	5.491643	0.657821	-0.308153
42	1	0	4.200080	-0.734132	0.683264
43	6	0	4.372761	2.685230	-1.169951
44	1	0	2.248101	2.718889	-0.849908
45	6	0	5.539618	1.950018	-0.882794
46	6	0	-3.182545	-1.013687	-0.876441
47	6	0	-4.518113	-0.752303	-0.578515
48	6	0	-2.869335	-2.018710	-1.777896
49	6	0	-5.543252	-1.534153	-1.101206
50	1	0	-4.758608	0.073424	0.075897
51	6	0	-3.850518	-2.824129	-2.364749
52	1	0	-1.827189	-2.175340	-2.034325
53	6	0	-5.173747	-2.630329	-1.920952
54	6	0	-2.453077	1.595792	0.215178
55	6	0	-1.951585	2.633555	-0.555824
56	6	0	-3.386153	1.876060	1.214611
57	6	0	-2.375700	3.955490	-0.397653
58	1	0	-1.190711	2.406583	-1.294068
59	6	0	-3.921129	3.153193	1.362227
60	1	0	-3.698977	1.078453	1.877502

61	6	0	-3.452367	4.165526	0.484982	134	1	0	-5.150027	-3.663541	-4.732896
62	6	0	-1.591815	5.033745	-1.182304	135	6	0	-2.468962	-3.002787	-4.444385
63	6	0	-1.997887	5.001278	-2.666293	136	1	0	-2.142180	-3.659632	-5.257168
64	1	0	-1.381528	5.700131	-3.243040	137	1	0	-3.020475	-2.165879	-4.886498
65	1	0	-1.858220	4.001406	-3.088690	138	1	0	-1.567248	-2.604372	-3.972026
66	1	0	-3.046270	5.277826	-2.810651	139	6	0	6.699950	-0.301949	-0.322645
67	6	0	-1.747184	6.459660	-0.625743	140	6	0	3.182903	3.733419	-3.102064
68	1	0	-1.541981	6.492539	0.448904	141	1	0	3.458269	2.901218	-3.759464
69	1	0	-1.019742	7.108839	-1.125113	142	1	0	2.206607	3.518576	-2.664865
70	1	0	-2.734560	6.887795	-0.796584	143	1	0	3.074214	4.631296	-3.719673
71	6	0	-0.079585	4.709288	-1.091194	144	6	0	7.212298	-0.439913	-1.770458
72	1	0	0.251557	4.668751	-0.047633	145	1	0	8.044677	-1.151928	-1.802830
73	1	0	0.184272	3.761575	-1.568412	146	1	0	6.421037	-0.819901	-2.426795
74	1	0	0.489831	5.494033	-1.600248	147	1	0	7.564214	0.512596	-2.170885
75	6	0	-4.937056	3.442766	2.487073	148	6	0	7.843704	0.175666	0.589744
76	6	0	-4.413446	4.595999	3.365787	149	1	0	7.482191	0.378888	1.603664
77	1	0	-4.402536	5.542031	2.822514	150	1	0	8.609657	-0.605007	0.657584
78	1	0	-5.050379	4.714583	4.249259	151	1	0	8.325631	1.074355	0.201998
79	1	0	-3.392600	4.392356	3.702747	152	6	0	6.292304	-1.711558	0.140873
80	6	0	-6.325772	3.801163	1.925616	153	1	0	5.479486	-2.124026	-0.466733
81	1	0	-6.676648	3.038184	1.221474	154	1	0	7.152607	-2.381113	0.043089
82	1	0	-7.050125	3.852840	2.746366	155	1	0	5.981373	-1.733176	1.190283
83	1	0	-6.333412	4.768232	1.422656	156	6	0	1.562575	-4.493068	5.034151
84	6	0	-5.126678	2.216083	3.395394	157	1	0	1.754834	-5.417282	5.582785
85	1	0	-5.576994	1.372484	2.860354	158	1	0	1.719786	-3.639547	5.700939
86	1	0	-4.185389	1.882733	3.841959	159	1	0	0.523838	-4.480488	4.693028
87	1	0	-5.807464	2.481797	4.210099	160	6	0	3.909580	-1.915610	4.700564
88	8	0	-4.071673	5.390096	0.546193	161	6	0	3.219761	-1.130131	5.830115
89	8	0	-6.164009	-3.506443	-2.295568	162	1	0	3.945926	-0.884534	6.613153
90	8	0	2.466830	-4.473582	3.933358	163	1	0	2.787135	-0.193972	5.462735
91	8	0	6.777398	2.247347	-1.176850	164	1	0	2.418930	-1.715178	6.291239
92	6	0	7.230823	3.394772	-0.188444	165	6	0	4.539936	-3.192691	5.284602
93	1	0	8.227795	3.718120	-0.493987	166	1	0	5.345050	-2.895456	5.965642
94	1	0	6.572987	4.267613	-0.117614	167	1	0	3.841704	-3.798333	5.862168
95	1	0	7.286716	2.921331	0.797822	168	1	0	4.978668	-3.820867	4.504242
96	6	0	4.274972	3.964929	-2.033667	169	6	0	5.097097	-1.074714	4.174431
97	6	0	5.543504	4.346897	-2.815721	170	1	0	5.612951	-1.594958	3.360361
98	1	0	5.285526	5.160444	-3.502655	171	1	0	4.802511	-0.086889	3.811834
99	1	0	6.352847	4.707929	-2.180809	172	1	0	5.819587	-0.918807	4.982479
100	1	0	5.917882	3.511938	-3.414059	173	6	0	1.215400	-4.882627	1.346690
101	6	0	3.857722	5.148755	-1.142170	174	6	0	0.455763	-4.731931	0.015854
102	1	0	3.746823	6.057111	-1.745107	175	1	0	0.209465	-5.728183	-0.365203
103	1	0	2.901488	4.958918	-0.643040	176	1	0	-0.485075	-4.183883	0.144304
104	1	0	4.606838	5.347578	-0.368378	177	1	0	1.051614	-4.228213	-0.750484
105	6	0	-4.978297	5.636841	-0.525471	178	6	0	0.311551	-5.703887	2.284057
106	1	0	-5.572477	6.506806	-0.238622	179	1	0	-0.551376	-5.118713	2.617459
107	1	0	-4.454614	5.859532	-1.459874	180	1	0	-0.068108	-6.578739	1.744781
108	1	0	-5.641125	4.780749	-0.689746	181	1	0	0.847809	-6.067994	3.159937
109	6	0	-6.156522	-4.713915	-1.536601	182	6	0	2.508174	-5.672821	1.060874
110	1	0	-7.015625	-5.298503	-1.870680	183	1	0	3.144681	-5.132097	0.351827
111	1	0	-5.240992	-5.290220	-1.701332	184	1	0	3.080141	-5.842674	1.976751
112	1	0	-6.249099	-4.508098	-0.464985	185	1	0	2.266053	-6.648460	0.623967
113	6	0	-7.014041	-1.146651	-0.839329	186	8	0	2.541489	-1.909634	-1.716482
114	6	0	-7.109227	0.152285	-0.018115	187	6	0	2.676336	-1.767100	-2.923419
115	1	0	-6.687917	0.037643	0.986975	188	1	0	-1.007564	-0.041462	-2.434418
116	1	0	-6.607708	0.992031	-0.510909	189	6	0	2.031598	-2.653716	-3.877502
117	1	0	-8.163457	0.421735	0.099112	190	6	0	2.142981	-2.809802	-5.234346
118	6	0	-7.710769	-0.888164	-2.189745	191	8	0	1.183599	-3.597572	-3.374035
119	1	0	-7.696287	-1.774790	-2.827300	192	6	0	1.317899	-3.911850	-5.580528
120	1	0	-8.756681	-0.607581	-2.021826	193	1	0	2.748080	-2.206959	-5.896686
121	1	0	-7.223042	-0.067660	-2.727471	194	6	0	0.764609	-4.343631	-4.411492
122	6	0	-7.777940	-2.233168	-0.059519	195	1	0	1.157064	-4.332893	-6.561852
123	1	0	-7.970331	-3.117267	-0.667835	196	1	0	0.081124	-5.144533	-4.173988
124	1	0	-7.229625	-2.537222	0.838677	197	6	0	3.542535	-6.645792	-3.499233
125	1	0	-8.748051	-1.837744	0.261463	198	1	0	4.393259	-1.056668	-4.044069
126	6	0	-3.365771	-3.798055	-3.464534	199	1	0	3.883697	-0.002660	-2.686168
127	6	0	-2.526086	-4.918901	-2.823984	200	8	0	2.805495	0.114494	-4.475400
128	1	0	-1.643782	-4.514560	-2.315711	201	6	0	1.720896	0.721369	-4.004914
129	1	0	-3.105774	-5.488520	-2.090620	202	8	0	1.503242	0.711968	-2.799799
130	1	0	-2.183083	-5.619286	-3.593855	203	6	0	0.815149	1.317257	-5.063034
131	6	0	-4.476108	-4.422901	-4.326795	204	6	0	-0.064762	2.403029	-4.436771
132	1	0	-4.004745	-4.937007	-5.171514	205	1	0	0.531321	3.247923	-4.080524
133	1	0	-5.073836	-5.163333	-3.794681	206	1	0	-0.762129	2.776245	-5.192766

207	1	0	-0.647535	2.008726	-3.600284
208	6	0	1.629336	1.889027	-6.230208
209	1	0	2.225337	1.118093	-6.724778
210	1	0	0.941091	2.311951	-6.968202
211	1	0	2.300441	2.685828	-5.894247
212	6	0	-0.071990	0.150762	-5.554424
213	1	0	-0.779273	0.534183	-6.296260
214	1	0	0.524063	-0.637207	-6.023002
215	1	0	-0.643125	-0.286104	-4.728688

3a(5)

RwB97XD SCF energy -5020.428980 a.u.
RwB97XD SCF enthalpy -5018.461076 a.u.
RwB97XD SCF free energy -5018.707100 a.u.
Three lowest frequencies (cm⁻¹) 13.1, 15.6, 18.4

Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.228973	-1.605325	-2.280844
2	6	0	-0.844731	-2.713902	-2.818368
3	6	0	-0.554265	-4.017390	-2.427961
4	6	0	0.406216	-4.287621	-1.485854
5	6	0	1.053119	-3.179892	-0.919731
6	6	0	0.757702	-1.866983	-1.288990
7	1	0	0.647040	-5.300222	-1.185293
8	1	0	1.801793	-3.369416	-0.159606
9	6	0	-0.629759	-0.269964	-2.805295
10	6	0	-1.403661	0.689426	-2.098672
11	6	0	-0.317169	0.048659	-4.107617
12	6	0	-1.755342	1.895144	-2.700296
13	6	0	-0.672792	1.254890	-4.700645
14	6	0	-1.383070	2.211581	-4.017422
15	1	0	-2.354745	2.614553	-2.154251
16	1	0	-1.663754	3.152980	-4.474891
17	8	0	-1.323665	-4.884706	-3.139419
18	8	0	-1.794659	-2.735409	-3.794269
19	8	0	0.376200	-0.710548	-5.002477
20	8	0	-0.199820	1.281164	-5.980782
21	6	0	-2.308748	-4.066701	-3.776589
22	1	0	-3.224910	-4.086218	-3.180972
23	1	0	-2.469580	-4.412376	-4.796982
24	6	0	0.171439	-0.069739	-6.262794
25	1	0	-0.648968	-0.568542	-6.792893
26	1	0	1.098392	-0.086047	-6.834982
27	15	0	-1.860214	0.277620	-0.376986
28	15	0	1.520261	-0.507348	-0.326840
29	46	0	-0.000900	0.263014	1.119870
30	6	0	-2.853351	-1.234782	-0.506291
31	6	0	-3.900315	-1.335143	-1.417604
32	6	0	-2.649518	-2.245873	0.421795
33	6	0	-4.766210	-2.428872	-1.423609
34	1	0	-4.053654	-0.522820	-2.119386
35	6	0	-3.450642	-3.391063	0.449643
36	1	0	-1.838774	-2.133057	1.135091
37	6	0	-4.468784	-3.484508	-0.525309
38	6	0	-3.023002	1.551293	0.209214
39	6	0	-4.287996	1.209156	0.681480
40	6	0	-2.568573	2.854867	0.379062
41	6	0	-5.149431	2.163798	1.216371
42	1	0	-4.602162	0.176175	0.633493
43	6	0	-3.385592	3.867407	0.894383
44	1	0	-1.547162	3.090216	0.096811
45	6	0	-4.713693	3.509983	1.207137
46	6	0	2.990540	-1.266348	0.435125
47	6	0	4.216757	-1.305994	-0.225401
48	6	0	2.883593	-1.830960	1.697642
49	6	0	5.307805	-1.987079	0.307232
50	1	0	4.319108	-0.796545	-1.172339
51	6	0	3.945532	-2.510356	2.301884
52	1	0	1.946508	-1.723670	2.234256
53	6	0	5.111674	-2.672471	1.530453
54	6	0	2.143812	0.727662	-1.492097
55	6	0	2.034400	2.070513	-1.165729
56	6	0	2.786622	0.353242	-2.675394
57	6	0	2.631532	3.089087	-1.945839
58	1	0	1.472946	2.344416	-0.276668
59	6	0	3.453763	1.290124	-3.457714
60	1	0	2.775675	-0.688975	-2.967609
61	6	0	3.444945	2.634970	-3.007320
62	6	0	2.306331	4.532058	-1.571843
63	6	0	2.920588	4.857830	-0.199027
64	1	0	2.687660	5.890188	0.085509
65	1	0	2.525390	4.202013	0.582352
66	1	0	4.010028	4.749428	-0.216772
67	6	0	2.747601	5.596362	-2.590604

68	1	0	2.399918	5.361280	-3.600146
69	1	0	2.299234	6.551920	-2.297069
70	1	0	3.827342	5.744822	-2.623136
71	6	0	0.769783	4.659372	-1.473296
72	1	0	0.296316	4.452800	-2.439491
73	1	0	0.338294	3.980756	-0.733995
74	1	0	0.506983	5.679709	-1.176035
75	6	0	4.098766	0.879418	-4.797361
76	6	0	3.445094	1.703609	-5.924166
77	1	0	3.669976	2.767405	-5.823658
78	1	0	3.813878	1.366927	-6.899644
79	1	0	2.357217	1.587353	-5.908963
80	6	0	5.623383	1.095569	-4.816810
81	1	0	6.105086	0.627798	-3.951975
82	1	0	6.042947	0.638171	-5.719272
83	1	0	5.888456	2.153550	-4.835385
84	6	0	3.852952	-0.608132	-5.099120
85	1	0	4.349382	-1.261197	-4.372397
86	1	0	2.787958	-0.856152	-5.118797
87	1	0	4.269015	-0.842328	-6.083969
88	8	0	4.259534	3.528900	-3.657999
89	8	0	6.111536	-3.507494	1.966576
90	8	0	-5.214165	-4.633690	-0.580527
91	8	0	-5.631527	4.477643	1.542706
92	6	0	-6.187625	5.135017	0.407403
93	1	0	-6.946630	5.823655	0.783256
94	1	0	-5.430166	5.701333	-0.143544
95	1	0	-6.650493	4.418164	-0.279205
96	6	0	-2.735193	5.259277	1.085709
97	6	0	-3.526042	6.241106	1.968712
98	1	0	-2.886896	7.106946	2.174317
99	1	0	-4.433184	6.617323	1.495835
100	1	0	-3.796822	5.792000	2.928465
101	6	0	-2.497453	5.898111	-0.295157
102	1	0	-1.986517	6.861135	-0.184078
103	1	0	-1.878507	5.256373	-0.929760
104	1	0	-3.440829	6.076996	-0.820834
105	6	0	5.457458	3.808659	-2.936150
106	1	0	6.057960	4.466340	-3.567215
107	1	0	5.250609	4.309366	-1.984739
108	1	0	6.016891	2.889240	-2.731497
109	6	0	5.819625	-4.881457	1.719619
110	1	0	6.666406	-5.454799	2.100703
111	1	0	4.904512	-5.197903	2.231693
112	1	0	5.700321	-5.072274	0.647504
113	6	0	6.684677	-1.900043	-0.383058
114	6	0	6.629938	-0.969222	-1.621102
115	1	0	5.970045	-1.385753	-2.399619
116	1	0	6.299252	0.027178	-1.372056
117	1	0	7.633182	-0.908129	-2.051379
118	6	0	7.691610	-1.278877	0.605147
119	1	0	7.802546	-1.889186	1.504032
120	1	0	8.675116	-1.188377	0.130343
121	1	0	7.371309	-0.275496	0.907479
122	6	0	7.201181	-3.272659	-0.853462
123	1	0	4.738008	-3.917008	-0.016970
124	1	0	6.455650	-3.788883	-1.467623
125	1	0	8.099184	-3.132196	-1.465111
126	6	0	3.739456	-2.921901	3.778422
127	6	0	2.604406	-3.956214	3.882352
128	1	0	1.669787	-3.581766	3.451282
129	1	0	2.866948	-4.884646	3.363406
130	1	0	2.413648	-4.197229	4.934225
131	6	0	4.976786	-3.470619	4.508171
132	1	0	4.724817	-3.579135	5.568907
133	1	0	5.292379	-4.452245	4.153371
134	1	0	5.825823	-2.786113	4.436309
135	6	0	3.339716	-1.641706	4.546130
136	1	0	3.167224	-1.876594	5.601343
137	1	0	4.143564	-0.900421	4.490728
138	1	0	2.427956	-1.180112	4.157601
139	6	0	-6.480008	1.724251	1.864369
140	6	0	-1.373403	5.073434	1.794340
141	1	0	-1.514049	4.634189	2.787700
142	1	0	-0.676548	4.444819	1.236753
143	1	0	-0.890704	6.047828	1.923397
144	6	0	-6.503899	2.205149	3.329571
145	1	0	-7.432936	1.880929	3.811926
146	1	0	-5.666282	1.777069	3.891494
147	1	0	-6.446366	3.293328	3.399362
148	6	0	-7.710408	2.273519	1.119351
149	1	0	-7.651471	2.064209	0.045828
150	1	0	-8.615763	1.790950	1.503860
151	1	0	-7.829078	3.348295	1.261069
152	6	0	-6.610061	0.190844	1.890039
153	1	0	-5.775025	-0.288927	2.411809
154	1	0	-7.527957	-0.077211	2.422829
155	1	0	-6.680865	-0.240070	0.885440
156	6	0	-4.708407	-5.616041	-1.472856
157	1	0	-5.247909	-6.542408	-1.264320
158	1	0	-4.885238	-5.336797	-2.518273
159	1	0	-3.634681	-5.779648	-1.321633
160	6	0	-5.981313	-2.362444	-2.384685

161	6	0	-5.532227	-2.661872	-3.826803	21	6	0	1.732847	-4.945012	3.483722
162	1	0	-6.350279	-2.448542	-4.524224	22	1	0	2.716382	-5.401357	3.584441
163	1	0	-4.673237	-2.046727	-4.116149	23	1	0	1.129151	-5.075678	4.389733
164	1	0	-5.259455	-3.713889	-3.953981	24	6	0	0.338624	-1.273483	6.085811
165	6	0	-7.146704	-3.299224	-2.019173	25	1	0	1.157550	-1.883730	6.484520
166	1	0	-8.005699	-3.044182	-2.649753	26	1	0	-0.568448	-1.363623	6.682717
167	1	0	-6.920222	-4.351835	-2.186819	27	15	0	2.038897	0.219458	0.245335
168	1	0	-7.450625	-3.175274	-0.975204	28	15	0	-1.255858	-0.499544	0.202836
169	6	0	-6.564251	-0.929626	-2.349884	29	46	0	0.174069	0.674801	-1.107351
170	1	0	-6.810666	-0.627265	-1.326599	30	6	0	2.750042	-1.405148	-0.114073
171	1	0	-5.890725	-0.179902	-2.772497	31	6	0	3.791226	-1.942819	0.630197
172	1	0	-7.485153	-0.897798	-2.940915	32	6	0	2.212688	-2.129118	-1.175969
173	6	0	-3.128819	-4.432808	1.549434	33	6	0	4.301151	-3.217697	0.360770
174	6	0	-1.787736	-5.107982	1.204837	34	1	0	4.220623	-1.353761	1.434737
175	1	0	-1.523319	-5.840343	1.976244	35	6	0	2.624788	-3.427384	-1.456490
176	1	0	-1.848692	-5.632948	0.245404	36	1	0	1.431904	-1.666123	-1.766757
177	1	0	-0.975721	-4.376189	1.140002	37	6	0	3.623337	-3.977551	-0.616882
178	6	0	-4.182995	-5.531625	1.769674	38	6	0	3.300428	1.488357	-0.073728
179	1	0	-4.228064	-6.248381	0.949079	39	6	0	4.576300	1.180026	-0.539840
180	1	0	-3.907918	-6.090834	2.671269	40	6	0	2.904410	2.819705	-0.004499
181	1	0	-5.182193	-5.116990	1.924837	41	6	0	5.493938	2.183738	-0.850982
182	6	0	-2.986605	-3.699260	2.902688	42	1	0	4.848982	0.140995	-0.669341
183	1	0	-2.172089	-2.971949	2.912494	43	6	0	3.770065	3.874248	-0.303176
184	1	0	-3.912059	-3.173975	3.163352	44	1	0	1.880649	3.040738	0.277759
185	1	0	-2.779670	-4.428764	3.692912	45	6	0	5.096918	3.524906	-0.629681
186	8	0	-1.340842	0.614248	2.858423	46	6	0	-2.777660	-1.041631	-0.633069
187	6	0	-0.547866	0.814110	3.802302	47	6	0	-3.944121	-1.274682	0.094530
188	1	0	1.281049	0.409330	1.999095	48	6	0	-2.768549	-1.294799	-1.996683
189	6	0	-0.248520	-0.213104	4.756084	49	6	0	-0.509216	-1.867840	-0.486436
190	6	0	0.388612	-0.201791	5.974511	50	1	0	-3.976882	-0.998075	1.138143
191	8	0	-0.672606	-1.479023	4.468319	51	6	0	-3.861999	-1.881271	-2.647401
192	6	0	0.337636	-1.529923	6.460343	52	1	0	-1.887725	-1.024876	-2.571404
193	1	0	0.827150	0.661261	6.453477	53	6	0	-4.944846	-2.272867	-1.838369
194	6	0	-0.305423	-2.256376	5.497777	54	6	0	-1.801350	0.496112	1.615552
195	1	0	0.736129	-1.907574	7.389960	55	6	0	-1.683340	1.874686	1.532495
196	1	0	-0.561129	-3.302636	5.417028	56	6	0	-2.391617	-0.078380	2.743985
197	6	0	0.056185	2.191277	3.980612	57	6	0	-2.210398	2.723096	2.513084
198	1	0	-0.357924	2.669287	4.874720	58	1	0	-1.164633	2.301170	0.678232
199	1	0	-0.195975	2.783197	3.101883	59	6	0	-3.001935	0.709395	3.715059
200	8	0	1.469993	2.063492	4.120791	60	1	0	-2.385581	-1.156929	2.843762
201	6	0	2.224079	3.013300	3.536145	61	6	0	-2.978830	2.113948	3.520713
202	8	0	1.738474	3.994712	3.012035	62	6	0	-1.852185	4.221571	2.397716
203	6	0	3.709391	2.678302	3.579751	63	6	0	-2.518096	4.816809	1.145831
204	6	0	3.959988	1.605413	2.500401	64	1	0	-2.226319	5.865381	1.020079
205	1	0	3.666744	1.965122	1.507390	65	1	0	-2.219432	4.280132	0.241032
206	1	0	5.027091	1.360926	2.472885	66	1	0	-3.609735	4.778716	1.218497
207	1	0	3.406153	0.688365	2.714135	67	6	0	-2.202429	5.086824	3.619918
208	6	0	4.512780	3.941340	3.259754	68	1	0	-1.810041	4.657578	4.545792
209	1	0	4.325050	4.729064	3.996160	69	1	0	-1.737403	6.069638	3.484511
210	1	0	5.581524	3.706676	3.277411	70	1	0	-3.272930	5.253034	3.741921
211	1	0	4.266687	4.333545	2.269889	71	6	0	-0.318045	4.321285	2.237995
212	6	0	4.098758	2.139210	4.963744	72	1	0	0.194538	3.905128	3.112183
213	1	0	5.167304	1.901714	4.970599	73	1	0	0.047466	3.798409	1.350894
214	1	0	3.913221	2.884417	5.744484	74	1	0	-0.029310	5.372626	2.139629
215	1	0	3.546989	1.231088	5.217213	75	6	0	-3.597579	0.069768	4.985931
						76	6	0	-2.866026	0.652473	6.211171
						77	1	0	-3.064833	1.720471	6.324255
						78	1	0	-3.197661	0.145894	7.124477
						79	1	0	-1.784092	0.518915	6.117735
						80	6	0	-5.112151	0.316315	5.124144
						81	1	0	-5.646942	0.025643	4.213562
						82	1	0	-5.503592	-0.290962	5.947778
						83	1	0	-5.341237	1.358194	5.348538
						84	6	0	-3.389397	-1.453511	4.989792
						85	1	0	-3.932702	-1.942933	4.173287
						86	1	0	-2.333250	-1.726791	4.913592
						87	1	0	-3.773489	-1.863399	5.929211
						88	8	0	-3.728633	2.887926	4.371300
						89	8	0	-5.938408	-3.064688	-2.360331
						90	8	0	3.944677	-5.300967	-0.790646
						91	8	0	6.049435	4.502383	-0.788696
						92	6	0	6.587910	4.980571	0.441074
						93	1	0	7.392019	5.671506	0.181514
						94	1	0	5.837347	5.511893	1.033995
						95	1	0	6.990721	4.159724	1.043352
						96	6	0	3.165154	5.299345	-0.282899
						97	6	0	3.985954	6.365981	-1.029005
						98	1	0	3.388587	7.282520	-1.086715
						99	1	0	4.920020	6.622973	-0.530734
						100	1	0	4.216524	6.053402	-2.051871
						101	6	0	2.952124	5.742318	1.176055
						102	1	0	2.438684	6.709963	1.206835

TS1a(S)

RwB97XD SCF energy -5020.425887 a.u.
 RwB97XD SCF enthalpy -5018.458665 a.u.
 RwB97XD SCF free energy -5018.698397 a.u.
 Three lowest frequencies (cm⁻¹) -428.7, 14.1, 16.7
 Imaginary frequency (cm⁻¹) -428.7
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.445557	-2.045871	1.882039
2	6	0	0.910974	-3.283987	2.273357
3	6	0	0.432370	-4.481671	1.751649
4	6	0	-0.516080	-4.506254	0.759729
5	6	0	-0.996035	-3.262397	0.326537
6	6	0	-0.556136	-2.054891	0.870645
7	1	0	-0.892521	-5.433930	0.345552
8	1	0	-1.755832	-3.260270	-0.445596
9	6	0	0.956244	-0.848073	2.603778
10	6	0	1.697673	0.226675	2.040803
11	6	0	0.732801	-0.773225	3.962564
12	6	0	2.109349	1.294667	2.835924
13	6	0	1.147839	0.297429	4.746759
14	6	0	1.831464	1.360361	4.209906
15	1	0	2.679660	2.104543	2.396889
16	1	0	2.156705	2.198903	4.814308
17	8	0	1.046516	-5.523746	2.371227
18	8	0	1.869597	-3.552332	3.204628
19	8	0	0.065770	-1.670495	4.741283
20	8	0	0.749303	0.094652	6.034033

103	1	0	2.341784	5.018308	1.724773	185	1	0	2.863734	-4.848360	-4.602486
104	1	0	3.901914	5.849773	1.708753	186	8	0	1.131260	1.900740	-2.534656
105	6	0	-4.944591	3.339643	3.778556	187	6	0	-0.035206	1.993197	-3.073502
106	1	0	-5.465898	3.922894	4.539640	188	1	0	-1.062543	1.069236	-2.080768
107	1	0	-4.758238	3.969697	2.903256	189	6	0	-0.289878	1.274384	-4.330965
108	1	0	-5.570998	2.495194	3.470377	190	6	0	-0.993964	1.596951	-5.451591
109	6	0	-5.560316	-4.439011	-2.424928	191	8	0	0.341310	0.081738	-4.496889
110	1	0	-6.378949	-4.967044	-2.916984	192	6	0	-0.773781	0.531596	-6.376138
111	1	0	-4.637672	-4.575377	-2.998767	193	1	0	-1.589585	2.486385	-5.599816
112	1	0	-5.408041	-4.853847	-1.422292	194	6	0	0.031580	-0.358697	-5.739409
113	6	0	-6.369430	-2.002281	0.315900	195	1	0	-1.173328	0.437415	-7.375161
114	6	0	-6.250991	-1.318696	1.690271	196	1	0	0.456822	-1.309717	-6.022308
115	1	0	-5.518828	-1.813543	2.337900	197	6	0	-0.824720	3.269261	-2.830047
116	1	0	-5.980790	-0.260501	1.604488	198	1	0	-0.584930	3.991814	-3.617426
117	1	0	-7.220192	-1.371954	2.195994	199	1	0	-0.536396	3.680454	-1.861193
118	6	0	-7.502674	-1.295571	-0.452729	200	8	0	-2.208819	2.943261	-2.850121
119	1	0	-7.662979	-1.744365	-1.435095	201	6	0	-3.064742	3.899553	-2.451493
120	1	0	-8.439048	-1.369768	0.111466	202	8	0	-2.699252	5.032355	-2.216097
121	1	0	-7.277356	-0.232491	-0.591524	203	6	0	-4.487352	3.368247	-2.347826
122	6	0	-6.752024	-3.472288	0.569406	204	6	0	-4.483083	2.074783	-1.513182
123	1	0	-7.083489	-3.972027	-0.341427	205	1	0	-4.032163	2.237281	-0.527093
124	1	0	-5.912268	-4.032973	0.993622	206	1	0	-5.513026	1.736160	-1.362536
125	1	0	-7.578415	-3.515532	1.287431	207	1	0	-3.934387	1.274652	-2.015811
126	6	0	-3.797642	-1.917943	-4.192361	208	6	0	-5.370264	4.426948	-1.685243
127	6	0	-2.529489	-2.661718	-4.648942	209	1	0	-5.367629	5.362351	-2.251874
128	1	0	-1.615702	-2.185855	-4.282487	210	1	0	-6.400201	4.060542	-1.634682
129	1	0	-2.536438	-3.699945	-4.298446	211	1	0	-5.035510	4.643792	-0.666082
130	1	0	-2.474683	-2.673112	-5.743037	212	6	0	-4.987783	3.079094	-3.775143
131	6	0	-5.002179	-2.529852	-4.926390	213	1	0	-5.991148	2.644209	-3.726214
132	1	0	-4.864811	-2.352614	-5.998841	214	1	0	-5.042719	3.999743	-4.365252
133	1	0	-5.085783	-3.609242	-4.789172	215	1	0	-4.333169	2.373837	-4.293767
134	1	0	-5.944727	-2.066694	-4.628474	-----					
135	6	0	-3.732145	-0.441608	-4.640742	4a(S)					
136	1	0	-3.627908	-0.378786	-5.729247	RwB97XD SCF energy -5020.436903 a.u.					
137	1	0	-4.653090	0.078205	-4.356174	RwB97XD SCF enthalpy -5018.465745 a.u.					
138	1	0	-2.889170	0.091179	-4.194014	RwB97XD SCF free energy -5018.706577 a.u.					
139	6	0	6.845056	1.824575	-1.507078	Three lowest frequencies (cm ⁻¹) 4.4, 18.7, 21.9					
140	6	0	1.789088	5.260806	-0.989823	Cartesian coordinates:					
141	1	0	1.880428	4.867114	-2.007621	-----					
142	1	0	1.052627	4.657666	-0.454097	Center Atomic Atomic Coordinates (Angstroms)					
143	1	0	1.381341	6.274896	-1.052538	Number Number Type X Y Z					
144	6	0	6.923836	2.509994	-2.885662	-----					
145	1	0	7.869513	2.253879	-3.376554	1	6	0	0.524614	-2.321076	1.678155
146	1	0	6.106634	2.174863	-3.533995	2	6	0	1.015079	-3.582846	1.937840
147	1	0	6.870036	3.596961	-2.798091	3	6	0	0.557179	-4.725918	1.288065
148	6	0	8.055249	2.241570	-0.649114	4	6	0	-0.393867	-4.684620	0.299471
149	1	0	7.955112	1.880464	0.380185	5	6	0	-0.902283	-3.391592	0.001770
150	1	0	8.966722	1.801325	-1.068485	6	6	0	-0.478963	-2.245917	0.673397
151	1	0	8.196348	3.322233	-0.629551	7	1	0	-0.751462	-5.552424	-0.208261
152	6	0	6.966635	0.309718	-1.738546	8	1	0	-1.666850	-3.315303	-0.763149
153	1	0	6.158072	-0.086309	-2.361711	9	6	0	0.982620	-1.184485	2.521934
154	1	0	7.909780	0.103359	-2.254018	10	6	0	1.633693	0.001762	2.079422
155	1	0	6.982398	-0.242247	-0.794179	11	6	0	0.761135	-1.270505	3.879577
156	6	0	3.353885	-6.147370	0.192985	12	6	0	1.976345	1.002431	2.988304
157	1	0	3.739208	-7.152960	0.014013	13	6	0	1.107762	-0.266006	4.777697
158	1	0	3.616541	-5.831968	1.207914	14	6	0	1.710975	0.895183	4.361072
159	1	0	2.263830	-6.152637	0.101768	15	1	0	2.482420	1.895279	2.642562
160	6	0	5.587224	-3.623970	1.123633	16	1	0	1.984589	1.681674	5.053956
161	6	0	5.284281	-3.785751	2.622824	17	8	0	1.192892	-5.816221	1.792021
162	1	0	6.212630	-3.981388	3.171107	18	8	0	1.973557	-3.932265	2.840027
163	1	0	4.826203	-2.887209	3.047647	19	8	0	0.150440	-2.284240	4.552572
164	1	0	4.609231	-4.628010	2.799142	20	8	0	0.734387	-0.634421	6.032387
165	6	0	6.292716	-4.897363	0.624104	21	6	0	1.863567	-5.349766	2.965378
166	1	0	7.264823	-4.963843	1.124959	22	1	0	2.855888	-5.794562	3.022058
167	1	0	5.751789	-5.814429	0.859486	23	1	0	1.257670	-5.590007	3.847343
168	1	0	6.474939	-4.867510	-0.453180	24	6	0	0.403135	-2.022751	5.932815
169	6	0	6.616808	-2.485352	0.938495	25	1	0	1.258172	-2.622622	6.265717
170	1	0	6.849246	-2.350865	-0.122725	26	1	0	-0.495326	-2.229588	6.513217
171	1	0	6.273815	-1.527540	1.338383	27	15	0	1.977727	0.236064	0.305525
172	1	0	7.546224	-2.740129	1.458525	28	15	0	-1.191026	-0.633422	0.210597
173	6	0	2.069266	-4.156584	-2.698467	29	46	0	0.176559	0.759452	-0.969187
174	6	0	0.978936	-3.320956	-3.394987	30	6	0	2.729754	-1.302608	-0.271073
175	1	0	0.624112	-3.864545	-4.276195	31	6	0	3.783209	-1.886801	0.421132
176	1	0	0.115702	-3.150393	-2.740848	32	6	0	2.239856	-1.904362	-1.427748
177	1	0	1.352129	-2.351129	-3.738255	33	6	0	4.342819	-3.101040	0.010111
178	6	0	1.440917	-5.525533	-2.379518	34	1	0	4.182456	-1.384126	1.296695
179	1	0	0.701440	-5.447225	-1.576115	35	6	0	2.705268	-3.144711	-1.851660
180	1	0	0.925025	-5.900472	-3.270107	36	1	0	1.456908	-1.396883	-1.978319
181	1	0	2.188675	-6.266819	-2.098274	37	6	0	3.701068	-3.763391	-1.058237
182	6	0	3.227095	-4.348224	-3.697549	38	6	0	3.172900	1.585931	0.131777
183	1	0	3.652944	-3.382629	-3.991501	39	6	0	4.454342	1.376814	-0.373684
184	1	0	4.025893	-4.959334	-3.269193						

40	6	0	2.734548	2.883493	0.372617	122	6	0	-6.780261	-3.498035	-0.176070
41	6	0	5.340484	2.439358	-0.546735	123	1	0	-7.100854	-3.785676	-1.178255
42	1	0	4.757760	0.372601	-0.637989	124	1	0	-5.986944	-4.179453	0.149256
43	6	0	3.567972	3.991768	0.216009	125	1	0	-7.634646	-3.637311	0.495440
44	1	0	1.705623	3.038542	0.677162	126	6	0	-3.567641	-1.319862	-4.460794
45	6	0	4.904779	3.726237	-0.146783	127	6	0	-2.387121	-2.154917	-4.986317
46	6	0	-2.669455	-1.032220	-0.766620	128	1	0	-1.443224	-1.853550	-4.525234
47	6	0	-3.870422	-1.341014	-0.127389	129	1	0	-2.538017	-3.222105	-4.789843
48	6	0	-2.605425	-1.063260	-2.153397	130	1	0	-2.284468	-2.019732	-6.068635
49	6	0	-4.973653	-1.800780	-0.835497	131	6	0	-4.815463	-1.656408	-5.295163
50	1	0	-3.934660	-1.233473	0.945466	132	1	0	-4.628175	-1.325516	-6.322765
51	6	0	-3.691819	-1.494037	-2.929008	133	1	0	-5.032121	-2.724693	-5.340101
52	1	0	-1.690932	-0.739823	-2.644829	134	1	0	-5.704670	-1.135293	-4.933563
53	6	0	-4.815111	-1.975874	-2.231593	135	6	0	-3.292835	0.178402	-4.709939
54	6	0	-1.805020	0.141090	1.728126	136	1	0	-3.131914	0.357876	-5.777845
55	6	0	-1.742673	1.521991	1.829074	137	1	0	-4.152323	0.776239	-4.390180
56	6	0	-2.390351	-0.600318	2.756445	138	1	0	-2.412053	0.539500	-4.176359
57	6	0	-2.325172	2.212797	2.897907	139	6	0	6.699471	2.213593	-1.243743
58	1	0	-1.224687	2.076317	1.051522	140	6	0	1.553460	5.397157	-0.311083
59	6	0	-3.042868	0.027646	3.812704	141	1	0	1.673785	5.174793	-1.376528
60	1	0	-2.347377	-1.681772	2.707808	142	1	0	0.836284	4.686936	0.107579
61	6	0	-3.081374	1.445838	3.802202	143	1	0	1.103018	6.390968	-0.219610
62	6	0	-2.048140	3.730884	2.971507	144	6	0	6.750342	3.081718	-2.516547
63	6	0	-2.750543	4.433695	1.796889	145	1	0	7.706243	2.931187	-3.031162
64	1	0	-2.545682	5.509822	1.817035	146	1	0	5.947798	2.803463	-3.208464
65	1	0	-2.399926	4.047198	0.835222	147	1	0	6.653536	4.144399	-2.285684
66	1	0	-3.835262	4.295149	1.844176	148	6	0	7.898311	2.549245	-0.336399
67	6	0	-2.446318	4.418914	4.288517	149	1	0	7.810135	2.053916	0.636570
68	1	0	-2.037483	3.898258	5.158711	150	1	0	8.821051	2.193700	-0.807980
69	1	0	-2.030738	5.432441	4.280069	151	1	0	8.007506	3.621625	-0.175108
70	1	0	-3.524201	4.517181	4.419739	152	6	0	6.864635	0.749232	-1.681066
71	6	0	-0.522400	3.940527	2.835511	153	1	0	6.066901	0.421665	-2.356071
72	1	0	0.013078	3.462679	3.663199	154	1	0	7.812105	0.643722	-2.218570
73	1	0	-0.119811	3.544443	1.899690	155	1	0	6.896773	0.068492	-0.824995
74	1	0	-0.299283	5.012029	2.857799	156	6	0	3.482354	-6.014454	-0.486924
75	6	0	-3.625063	-0.800070	4.976659	157	1	0	3.908965	-6.981630	-0.758694
76	6	0	-2.949792	-0.344364	6.285031	158	1	0	3.715792	-5.792197	0.558764
77	1	0	-3.203498	0.690136	6.525518	159	1	0	2.395002	-6.051867	-0.601957
78	1	0	-3.273576	-0.979176	7.117352	160	6	0	5.636676	-3.550312	0.735027
79	1	0	-1.860617	-0.413607	6.204023	161	6	0	5.332238	-3.883632	2.205302
80	6	0	-5.152807	-0.650463	5.102039	162	1	0	6.263372	-4.114558	2.734730
81	1	0	-5.650313	-0.836859	4.143916	163	1	0	4.849055	-3.049697	2.723727
82	1	0	-5.531339	-1.384062	5.822558	164	1	0	4.679395	-4.757945	2.281516
83	1	0	-5.441255	0.337656	5.460699	165	6	0	6.379573	-4.741132	0.104059
84	6	0	-3.334860	-2.299062	4.794522	166	1	0	7.352999	-4.832513	0.598428
85	1	0	-3.847409	-2.712564	3.918579	167	1	0	5.865504	-5.693446	0.238300
86	1	0	-2.264835	-2.505772	4.699698	168	1	0	6.560771	-4.590164	-0.963064
87	1	0	-3.702933	-2.838620	5.672693	169	6	0	6.631214	-2.367665	0.680528
88	8	0	-3.880920	2.069182	4.728032	170	1	0	6.878081	-2.125593	-0.358410
89	8	0	-5.809042	-2.636590	-2.909311	171	1	0	6.250419	-1.463692	1.163010
90	8	0	4.055422	-5.051545	-1.369493	172	1	0	7.559580	-2.643642	1.191639
91	8	0	5.829050	4.740949	-0.161574	173	6	0	2.197035	-3.748315	-3.177186
92	6	0	6.349156	5.054647	1.128123	174	6	0	1.142053	-2.839323	-3.830267
93	1	0	7.133595	5.798380	0.976749	175	1	0	0.826899	-3.286798	-4.778084
94	1	0	5.581005	5.472762	1.785781	176	1	0	0.249310	-2.737200	-3.202568
95	1	0	6.773960	4.167630	1.609545	177	1	0	1.531511	-1.840477	-0.049321
96	6	0	2.919745	5.383117	0.414968	178	6	0	1.543619	-5.130649	-2.997429
97	6	0	3.714412	6.560411	-0.176933	179	1	0	0.790625	-5.111670	-2.202973
98	1	0	3.088107	7.457923	-0.128162	180	1	0	1.039965	-5.416667	-3.927373
99	1	0	4.634804	6.780881	0.363029	181	1	0	2.275506	-5.905828	-2.770835
100	1	0	3.964962	6.386217	-1.227567	182	6	0	3.387612	-3.862474	-4.149098
101	6	0	2.678018	5.624995	1.915858	183	1	0	3.839078	-2.881005	-4.330571
102	1	0	2.144073	6.570297	2.064440	184	1	0	4.159473	-4.529452	-3.757399
103	1	0	2.075994	4.822368	2.353528	185	1	0	3.048664	-4.263373	-5.111133
104	1	0	3.617965	5.681083	2.473255	186	8	0	1.044485	2.102630	-2.236954
105	6	0	-5.113027	2.529310	4.175352	187	6	0	-0.179427	2.201156	-2.844198
106	1	0	-5.689322	2.947668	5.002290	188	1	0	-0.940455	1.450402	-2.343567
107	1	0	-4.955261	3.303615	3.417557	189	6	0	-0.175336	1.768018	-4.275873
108	1	0	-5.671883	1.705246	3.718774	190	6	0	-0.502630	2.367210	-5.449679
109	6	0	-5.463114	-3.992685	-3.186713	191	8	0	0.243876	0.493328	-4.500932
110	1	0	-6.295684	-4.421263	-3.746989	192	6	0	-0.263223	1.393878	-6.474728
111	1	0	-4.546783	-4.060564	-3.782846	193	1	0	-0.879461	3.372345	-5.574301
112	1	0	-5.316515	-4.557214	-2.259511	194	6	0	0.183810	0.280791	-5.842060
113	6	0	-6.318232	-2.029746	-0.116366	195	1	0	-0.409598	1.514192	-7.538395
114	6	0	-6.225432	-1.640581	1.370023	196	1	0	0.497216	-0.694736	-6.181733
115	1	0	-5.531008	-2.282932	1.922963	197	6	0	-0.872489	3.541065	-2.595877
116	1	0	-5.917930	-0.598133	1.506402	198	1	0	-0.565225	4.302329	-3.318110
117	1	0	-7.212105	-1.754535	1.829690	199	1	0	-0.619679	3.874674	-1.587915
118	6	0	-7.384987	-1.125433	-0.763861	200	8	0	-2.279185	3.299554	-2.691416
119	1	0	-7.519223	-1.353338	-1.823662	201	6	0	-3.094808	4.143107	-2.041458
120	1	0	-8.348702	-1.267343	-0.261806	202	8	0	-2.695623	5.175679	-1.542184
121	1	0	-7.109828	-0.069109	-0.669687	203	6	0	-4.527324	3.625978	-2.006808

204	6	0	-4.522393	2.222305	-1.370498
205	1	0	-4.063914	2.239148	-0.374602
206	1	0	-5.551887	1.866418	-1.261554
207	1	0	-3.979586	1.503534	-1.990127
208	6	0	-5.387263	4.580581	-1.177405
209	1	0	-5.373999	5.591681	-1.594385
210	1	0	-6.422747	4.226317	-1.171973
211	1	0	-5.038819	4.635794	-0.141871
212	6	0	-5.057468	3.553935	-3.449142
213	1	0	-6.060921	3.116617	-3.447014
214	1	0	-5.121462	4.551923	-3.895076
215	1	0	-4.415307	2.936711	-4.082233

5a(S)

RwB97XD SCF energy -5021.614667 a.u.

RwB97XD SCF enthalpy -5019.625569 a.u.

RwB97XD SCF free energy -5019.869487 a.u.

Three lowest frequencies (cm⁻¹) 8.7, 16.5, 20.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.190855	-1.966821	-2.079140
2	6	0	-0.981398	-2.500789	-3.331074
3	6	0	-1.163872	-1.773579	-4.504219
4	6	0	-1.534691	-0.451345	-4.487476
5	6	0	-1.738565	0.125090	-3.225040
6	6	0	-1.586225	-0.601591	-2.045884
7	1	0	-1.683300	0.112331	-5.400675
8	1	0	-2.048874	1.162487	-3.185198
9	6	0	-1.122483	-2.848897	-0.884477
10	6	0	-0.240785	-2.711069	0.223381
11	6	0	-2.019721	-3.892297	-0.811367
12	6	0	-0.337136	-3.577947	1.311891
13	6	0	-2.110195	-4.746688	0.282368
14	6	0	-1.285590	-4.609390	1.371861
15	1	0	0.349213	-3.479271	2.143599
16	1	0	-1.347922	-5.271835	2.226975
17	8	0	-0.925928	-2.574692	-5.574018
18	8	0	-0.595844	-3.768691	-3.639436
19	8	0	-2.971164	-4.226450	-1.725863
20	8	0	-3.113129	-5.641003	0.074146
21	6	0	-0.809251	-3.898583	-5.045959
22	1	0	0.043564	-4.398668	-5.503169
23	1	0	-1.744962	-4.441224	-5.221677
24	6	0	-3.466766	-5.497951	-1.304666
25	1	0	-2.979183	-6.288601	-1.886427
26	1	0	-4.551028	-5.520288	-1.410490
27	15	0	0.984992	-1.358008	0.246794
28	15	0	-1.819516	0.214403	-0.436956
29	46	0	0.119913	0.691091	0.704166
30	6	0	1.780981	-1.369945	-1.372707
31	6	0	2.333486	-2.531367	-1.894915
32	6	0	1.827258	-0.188486	-2.107765
33	6	0	2.919161	-2.554638	-3.165410
34	1	0	2.310114	-3.439143	-1.300427
35	6	0	2.346941	-0.151517	-3.395697
36	1	0	1.427943	0.710058	-1.656661
37	6	0	2.816302	-1.375252	-3.933655
38	6	0	2.180337	-1.740064	1.551004
39	6	0	3.515067	-2.036160	1.288464
40	6	0	1.756653	-1.572943	2.864604
41	6	0	4.414375	-2.269700	2.330433
42	1	0	3.851553	-2.077969	0.260886
43	6	0	2.609999	-1.762522	3.951228
44	1	0	0.733243	-1.262427	3.046070
45	6	0	3.913565	-2.210890	3.653473
46	6	0	-2.565409	1.839240	-0.748755
47	6	0	-3.842549	2.138095	-0.288314
48	6	0	-1.764289	2.854558	-1.257271
49	6	0	-4.368939	3.423202	-0.393274
50	1	0	-4.428913	1.354353	0.168952
51	6	0	-2.220442	4.168099	-1.380137

52	1	0	-0.743681	2.617783	-1.541354
53	6	0	-3.567717	4.405269	-1.025918
54	6	0	-3.049666	-0.703212	0.506358
55	6	0	-2.938341	-0.694129	1.887156
56	6	0	-4.154072	-1.299962	-0.101803
57	6	0	-3.952054	-1.193145	2.711774
58	1	0	-2.042780	-0.270724	2.333103
59	6	0	-5.209991	-1.787701	0.661152
60	1	0	-4.187521	-1.358090	-1.183134
61	6	0	-5.128035	-1.620340	2.068275
62	6	0	-3.646631	-1.244927	4.225547
63	6	0	-3.553322	0.186081	4.787186
64	1	0	-3.312153	0.154382	5.855603
65	1	0	-2.770643	0.764995	4.284877
66	1	0	-4.499010	0.725286	4.670798
67	6	0	-4.639626	-2.058786	5.072917
68	1	0	-4.802244	-3.056693	4.656933
69	1	0	-4.214297	-2.179668	6.075148
70	1	0	-5.607965	-1.571269	5.190873
71	6	0	-2.274589	-1.933921	4.405268
72	1	0	-2.293047	-2.955503	4.009338
73	1	0	-1.461706	-1.394962	3.911547
74	1	0	-2.029864	-1.984752	5.471046
75	6	0	-6.370619	-2.550711	-0.008762
76	6	0	-6.418801	-3.972349	0.585770
77	1	0	-6.654572	-3.951413	1.652097
78	1	0	-7.186397	-4.566832	0.077703
79	1	0	-5.455349	-4.477863	0.462790
80	6	0	-7.733662	-1.860770	0.185819
81	1	0	-7.686523	-0.801539	-0.090006
82	1	0	-8.477909	-2.339076	-0.460534
83	1	0	-8.093934	-1.940135	1.211814
84	6	0	-6.146371	-2.684377	-1.524200
85	1	0	-6.182464	-1.713638	-2.031002
86	1	0	-5.192523	-3.163679	-1.762649
87	1	0	-6.944122	-3.303093	-1.946831
88	8	0	-6.249511	-1.905315	2.806785
89	8	0	-4.135719	5.633291	-1.259359
90	8	0	3.200481	-1.384190	-5.251222
91	8	0	4.766035	-2.569824	4.668315
92	6	0	4.529811	-3.881545	5.171358
93	1	0	5.321402	-4.088385	5.893812
94	1	0	3.560479	-3.957624	5.672411
95	1	0	4.564667	-4.628083	4.369347
96	6	0	2.047396	-1.412547	5.350456
97	6	0	3.114152	-1.178084	6.435402
98	1	0	2.619596	-0.766027	7.321634
99	1	0	3.626366	-2.087812	6.747854
100	1	0	3.866682	-0.455159	6.106879
101	6	0	1.078036	-2.517756	5.807117
102	1	0	0.597590	-2.233228	6.749936
103	1	0	0.293728	-2.683440	5.061884
104	1	0	1.591278	-3.470647	5.967090
105	6	0	-6.969942	-0.734143	3.188018
106	1	0	-7.854279	-1.074466	3.729562
107	1	0	-6.372820	-0.088245	3.839270
108	1	0	-7.278967	-0.158029	2.309030
109	6	0	-4.563691	5.811505	-2.607618
110	1	0	-5.069513	6.777540	-2.650976
111	1	0	-3.720295	5.816687	-3.304560
112	1	0	-5.259315	5.021765	-2.909565
113	6	0	-5.729397	3.741243	0.265027
114	6	0	-6.311353	2.504801	0.977731
115	1	0	-6.544153	1.695885	0.276087
116	1	0	-5.641485	2.111156	1.750266
117	1	0	-7.245827	2.789824	1.470787
118	6	0	-5.515625	4.830473	1.334911
119	1	0	-5.133392	5.754430	0.895691
120	1	0	-6.465462	5.055680	1.832568
121	1	0	-4.806424	4.491310	2.098170
122	6	0	-6.785924	4.214110	-0.750696
123	1	0	-6.567988	5.209739	-1.137401
124	1	0	-6.867363	3.518902	-1.593133

125	1	0	-7.764962	4.260948	-0.261293
126	6	0	-1.180811	5.214492	-1.848706
127	6	0	-0.910189	5.028167	-3.353454
128	1	0	-0.579991	4.008393	-3.575518
129	1	0	-1.803723	5.227707	-3.952923
130	1	0	-0.124340	5.717028	-3.682887
131	6	0	-1.559612	6.680292	-1.572376
132	1	0	-0.686021	7.305883	-1.786358
133	1	0	-2.375337	7.044693	-2.196507
134	1	0	-1.831177	6.835701	-0.524013
135	6	0	0.144699	4.979017	-1.084115
136	1	0	0.876840	5.723183	-1.407401
137	1	0	0.002828	5.090761	-0.003258
138	1	0	0.590910	3.999829	-1.273942
139	6	0	5.917878	-2.468261	2.038346
140	6	0	1.256951	-0.085459	5.247753
141	1	0	1.882251	0.716022	4.840120
142	1	0	0.359078	-0.166154	4.629761
143	1	0	0.925138	0.216304	6.246564
144	6	0	6.686913	-1.285991	2.661262
145	1	0	7.759545	-1.389687	2.460920
146	1	0	6.351049	-0.337575	2.227707
147	1	0	6.545660	-1.240394	3.743755
148	6	0	6.474549	-3.798674	2.582393
149	1	0	5.847908	-4.645046	2.280866
150	1	0	7.474812	-3.964934	2.167388
151	1	0	6.568461	-3.799726	3.667907
152	6	0	6.198540	-2.465117	0.528140
153	1	0	5.873844	-1.539515	0.045004
154	1	0	7.277137	-2.556747	0.366096
155	1	0	5.717828	-3.311579	0.028454
156	6	0	2.212137	-1.939577	-6.116745
157	1	0	2.628009	-1.908816	-7.125464
158	1	0	1.979135	-2.976014	-5.852101
159	1	0	1.288650	-1.355048	-6.085931
160	6	0	3.652407	-3.859761	-3.563189
161	6	0	2.628449	-4.991272	-3.760348
162	1	0	3.146532	-5.938385	-3.947614
163	1	0	1.993194	-5.123311	-2.878994
164	1	0	1.981210	-4.789674	-4.618734
165	6	0	4.545594	-3.773838	-4.813258
166	1	0	5.122513	-4.702812	-4.880948
167	1	0	3.985521	-3.679226	-5.743488
168	1	0	5.256712	-2.945622	-4.750669
169	6	0	4.602684	-4.236536	-2.403988
170	1	0	5.341099	-3.444445	-2.241205
171	1	0	4.081038	-4.416142	-1.460647
172	1	0	5.143468	-5.155350	-2.654300
173	6	0	2.485234	1.200823	-4.127824
174	6	0	1.901704	2.349581	-3.286097
175	1	0	2.029297	3.293158	-3.825528
176	1	0	0.828643	2.215663	-3.106257
177	1	0	2.408198	2.456783	-2.321769
178	6	0	1.762562	1.231913	-5.486708
179	1	0	0.727883	0.886116	-5.393592
180	1	0	1.738163	2.261133	-5.861153
181	1	0	2.270384	0.623741	-6.235182
182	6	0	3.984842	1.488504	-4.334651
183	1	0	4.503341	1.557031	-3.372247
184	1	0	4.463843	0.708973	-4.932290
185	1	0	4.114264	2.444341	-4.854782
186	8	0	1.909590	1.212015	1.535403
187	6	0	2.465224	2.332184	0.900909
188	6	0	3.896656	2.061258	0.542268
189	6	0	5.102012	2.461699	1.029834
190	8	0	4.087190	1.185945	-0.482707
191	6	0	6.100808	1.789384	0.249041
192	1	0	5.264494	3.162666	1.836487
193	6	0	5.425236	1.029715	-0.649361
194	1	0	7.173959	1.866523	0.349718
195	1	0	5.727822	0.362931	-1.442653
196	6	0	2.330708	3.536204	1.825854
197	1	0	2.865178	3.360597	2.764596

198	1	0	1.274366	3.705924	2.050305
199	8	0	2.877263	4.686663	1.165386
200	6	0	2.930568	5.817135	1.878401
201	8	0	2.447097	5.908196	2.990285
202	6	0	3.683299	6.923806	1.148480
203	6	0	3.035916	7.168743	-0.223669
204	1	0	1.981859	7.446547	-0.119636
205	1	0	3.554868	7.989522	-0.729260
206	1	0	3.101151	6.282507	-0.860230
207	6	0	3.636540	8.200487	1.989866
208	1	0	4.098726	8.050546	2.969885
209	1	0	4.180841	8.998378	1.474937
210	1	0	2.607360	8.537589	2.146642
211	6	0	5.140817	6.461672	0.964485
212	1	0	5.710724	7.249122	0.460774
213	1	0	5.617344	6.263860	1.930610
214	1	0	5.199143	5.553566	0.357557
215	1	0	-0.532398	2.518518	1.125463
216	1	0	-0.720006	2.101774	1.745530
217	1	0	1.935999	2.570383	-0.039535

TS2a(S)

RwB97XD SCF energy -5021.600098 a.u.
RwB97XD SCF enthalpy -5019.613175 a.u.
RwB97XD SCF free energy -5019.860389 a.u.
Three lowest frequencies (cm⁻¹) -1057, 6.0, 12.2
Imaginary frequency (cm⁻¹) -1057

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.409162	-0.879209	2.461758
2	6	0	1.275628	-0.850052	3.832449
3	6	0	1.403500	0.316851	4.583588
4	6	0	1.660976	1.531244	3.995022
5	6	0	1.811106	1.530630	2.600658
6	6	0	1.701852	0.365803	1.841691
7	1	0	1.762477	2.440971	4.574508
8	1	0	2.035372	2.472141	2.113072
9	6	0	1.309038	-2.180472	1.753064
10	6	0	0.346208	-2.520909	0.762801
11	6	0	2.220759	-3.163146	2.071130
12	6	0	0.382242	-3.771587	0.147231
13	6	0	2.248583	-4.407541	1.448490
14	6	0	1.343687	-4.741521	0.470351
15	1	0	-0.356734	-4.023779	-0.603990
16	1	0	1.358977	-5.706758	-0.021097
17	8	0	1.226219	0.027030	5.896897
18	8	0	0.994503	-1.889526	4.661698
19	8	0	3.235317	-3.087384	2.973839
20	8	0	3.278232	-5.138251	1.951559
21	6	0	1.277093	-1.400139	5.970369
22	1	0	0.525573	-1.760866	6.670594
23	1	0	2.287612	-1.710798	6.263948
24	6	0	3.702494	-4.427550	3.116932
25	1	0	3.244251	-4.880207	4.004843
26	1	0	4.790704	-4.431176	3.175625
27	15	0	-0.887582	-1.281694	0.230883
28	15	0	1.878732	0.473157	0.033623
29	46	0	-0.023869	0.309074	-1.200784
30	6	0	-1.596093	-0.560714	1.728781
31	6	0	-2.093085	-1.325257	2.776325
32	6	0	-1.657011	0.828028	1.800642
33	6	0	-2.640296	-0.730573	3.920539
34	1	0	-2.054543	-2.407111	2.702800
35	6	0	-2.146908	1.483895	2.920647
36	1	0	-1.316159	1.397717	0.947824
37	6	0	-2.556966	0.676246	4.008897
38	6	0	-2.140616	-2.174093	-0.726514
39	6	0	-3.384624	-2.551603	-0.229374
40	6	0	-1.820268	-2.451420	-2.051696
41	6	0	-4.282053	-3.276925	-1.015911
42	1	0	-3.649693	-2.277197	0.783105
43	6	0	-2.675970	-3.151649	-2.900124
44	1	0	-0.874340	-2.093317	-2.438625

45	6	0	-3.879699	-3.625976	-2.330044	127	6	0	0.664179	6.254570	0.170138
46	6	0	2.575559	2.115904	-0.299200	128	1	0	0.262114	5.528357	0.883819
47	6	0	3.946779	2.309215	-0.415172	129	1	0	1.481071	6.785525	0.662494
48	6	0	1.712367	3.185521	-0.502049	130	1	0	-0.125282	6.980768	-0.053710
49	6	0	4.480709	3.567573	-0.682174	131	6	0	1.601270	6.572922	-2.164556
50	1	0	4.606249	1.460345	-0.303715	132	1	0	0.762149	7.215610	-2.450502
51	6	0	2.173234	4.469650	-0.798847	133	1	0	2.401720	7.215556	-1.804220
52	1	0	0.645379	3.001609	-0.455629	134	1	0	1.958437	6.067369	-3.067837
53	6	0	3.577010	4.653174	-0.808047	135	6	0	-0.144549	4.890332	-1.740768
54	6	0	3.104874	-0.740829	-0.499996	136	1	0	-0.821743	5.671615	-2.097472
55	6	0	2.913848	-1.371924	-1.719646	137	1	0	0.111985	4.253708	-2.594993
56	6	0	4.244590	-1.024990	0.254400	138	1	0	-0.712339	4.293247	-1.021636
57	6	0	3.866658	-2.237285	-2.264694	139	6	0	-5.669399	-2.659709	-0.452632
58	1	0	1.993099	-1.188242	-2.264333	140	6	0	-1.295868	-2.171663	-4.792817
59	6	0	5.256530	-1.831908	-0.256680	141	1	0	-1.717764	-1.192858	-4.544830
60	1	0	4.337566	-0.592198	1.242772	142	1	0	-0.305501	-2.246320	-4.333770
61	6	0	5.085175	-2.343371	-1.569573	143	1	0	-1.139872	-2.219368	-5.875102
62	6	0	3.445987	-3.005424	-3.538725	144	6	0	-6.788371	-3.155044	-1.384229
63	6	0	3.249104	-2.016559	-4.702614	145	1	0	-7.764985	-3.363240	-0.933133
64	1	0	2.913690	-2.552847	-5.597058	146	1	0	-6.706668	-2.073658	-1.529293
65	1	0	2.495532	-1.257779	-4.467198	147	1	0	-6.748512	-3.635123	-2.361723
66	1	0	4.181869	-1.499640	-4.949808	148	6	0	-5.787536	-5.183453	-0.261500
67	6	0	4.398630	-4.125987	-3.989456	149	1	0	-4.956838	-5.569530	0.339123
68	1	0	4.637881	-4.811234	-3.172770	150	1	0	-6.719261	-5.415822	0.266263
69	1	0	3.898070	-4.700050	-4.776755	151	1	0	-5.807548	-5.720308	-1.208666
70	1	0	5.332722	-3.753198	-4.410621	152	6	0	-5.904731	-3.024459	0.926777
71	6	0	2.095082	-3.696640	-3.240123	153	1	0	-5.815725	-1.934166	0.898710
72	1	0	2.200503	-4.429167	-2.432746	154	1	0	-6.917344	-3.267639	1.263262
73	1	0	1.311632	-2.990517	-2.951051	155	1	0	-5.210884	-3.413927	1.676849
74	1	0	1.748052	-4.221597	-4.135986	156	6	0	-1.872034	1.287073	6.153542
75	6	0	6.471705	-2.209693	0.614072	157	1	0	-2.249768	1.835108	7.018617
76	6	0	6.556872	-3.746741	0.704810	158	1	0	-1.627157	0.263556	6.452992
77	1	0	6.781456	-4.190621	-0.266459	159	1	0	-0.960958	1.768367	5.784641
78	1	0	7.345689	-4.037780	1.407291	160	6	0	-3.315570	-1.673467	4.947177
79	1	0	5.610493	-4.169472	1.056594	161	6	0	-2.247207	-2.484798	5.698959
80	6	0	7.791782	-1.650366	0.050459	162	1	0	-2.726599	-3.222863	6.351600
81	1	0	7.713966	-0.575680	-0.148534	163	1	0	-1.582985	-3.016657	5.011236
82	1	0	8.592647	-1.796379	0.783716	164	1	0	-1.633254	-1.833927	6.327802
83	1	0	8.090744	-2.157172	-0.867316	165	6	0	-4.231612	-0.978591	5.971204
84	6	0	6.318605	-1.664721	2.043997	166	1	0	-4.786289	-1.751854	6.513940
85	1	0	6.334676	-0.569495	2.072561	167	1	0	-3.687342	-0.392740	6.711189
86	1	0	5.395109	-2.010019	2.518546	168	1	0	-4.958585	-0.323556	5.483705
87	1	0	7.159578	-2.017178	2.648952	169	6	0	-4.227102	-2.650508	4.172053
88	8	0	6.153114	-2.974558	-2.151278	170	1	0	-4.976619	-2.101425	3.593317
89	8	0	4.124540	5.892094	-1.013500	171	1	0	-3.674893	-3.301874	3.489606
90	8	0	-2.903561	1.315232	5.170809	172	1	0	-4.755172	-3.299866	4.877681
91	8	0	-4.752112	-4.388444	-3.061812	173	6	0	-2.336784	3.105072	2.888808
92	6	0	-4.436579	-5.762494	-3.254007	174	6	0	-1.818725	3.610316	1.567791
93	1	0	-5.375382	-6.320734	-3.213003	175	1	0	-2.004776	4.688711	1.564276
94	1	0	-3.987254	-5.928441	-4.237526	176	1	0	-0.739133	3.460517	1.447685
95	1	0	-3.761161	-6.133753	-2.477090	177	1	0	-2.331026	3.188504	0.698175
96	6	0	-2.235588	-3.326524	-4.372771	178	6	0	-1.605362	3.747844	4.027512
97	6	0	-3.418980	-3.276897	-5.356585	179	1	0	-0.554622	3.444721	4.083071
98	1	0	-3.032959	-3.322191	-6.380318	180	1	0	-1.631766	4.826804	3.839567
99	1	0	-4.130474	-4.090056	-5.230237	181	1	0	-2.075355	3.571550	4.994758
100	1	0	-3.966551	-2.334799	-5.245723	182	6	0	-3.848046	3.308754	2.970599
101	6	0	-1.436915	-4.635383	-4.527349	183	1	0	-4.377661	2.846994	2.130159
102	1	0	-1.035891	-4.714651	-5.544230	184	1	0	-4.274860	2.929227	3.902594
103	1	0	-0.592575	-4.649463	-3.830078	185	1	0	-4.024211	4.389548	2.928092
104	1	0	-2.037408	-5.525779	-4.334679	186	8	0	-1.603188	0.650030	-2.625525
105	6	0	6.824416	-2.158477	-3.106878	187	6	0	-2.417567	1.703669	-2.157868
106	1	0	7.654996	-2.750162	-3.495100	188	6	0	-3.689036	1.208100	-1.543423
107	1	0	6.164189	-1.874067	-3.932488	189	6	0	-4.909238	0.847168	-0.027285
108	1	0	7.213359	-1.244742	-2.644153	190	8	0	-3.684443	1.093901	-0.188861
109	6	0	4.131755	6.785686	0.095810	191	6	0	-5.705135	0.493132	-0.890487
110	1	0	5.044799	7.381525	0.025749	192	1	0	-5.214120	0.861402	-3.063305
111	1	0	3.277353	7.468371	0.062744	193	6	0	-4.905557	0.657529	0.195549
112	1	0	4.128441	6.243754	1.046410	194	1	0	-6.735847	0.169904	-0.885329
113	6	0	6.004254	3.714551	-0.884326	195	1	0	-5.047417	0.517580	1.256694
114	6	0	6.718750	2.352985	-0.786865	196	6	0	-2.691316	2.697882	-3.286573
115	1	0	6.624498	1.905289	0.208792	197	1	0	-3.366768	2.297145	-0.044988
116	1	0	6.350418	1.634567	-1.527192	198	1	0	-1.750763	2.993251	-3.756943
117	1	0	7.785890	2.501567	-0.978110	199	8	0	-3.246831	3.863817	-2.675592
118	6	0	6.286928	4.278354	-2.290219	200	6	0	-4.539244	4.165154	-2.891342
119	1	0	5.822677	5.255513	-2.430723	201	8	0	-5.202577	3.669001	-3.774284
120	1	0	7.367425	4.386617	-2.436533	202	6	0	-5.050002	5.159136	-1.852940
121	1	0	5.909611	3.599229	-3.062559	203	6	0	-4.013117	6.262398	-1.596397
122	6	0	6.632093	4.628256	0.184785	204	1	0	-3.767293	6.801642	-2.517268
123	1	0	6.354807	5.672424	0.047400	205	1	0	-4.419264	6.983734	-0.879682
124	1	0	6.339816	4.317553	1.193633	206	1	0	-3.089361	5.852165	-1.180944
125	1	0	7.724050	4.569003	0.120198	207	6	0	-6.365909	5.764804	-2.344028
126	6	0	1.112262	5.548842	-1.123633	208	1	0	-7.113933	4.989848	-2.529494

209	1	0	-6.760446	6.453609	-1.590353
210	1	0	-6.220537	6.322920	-3.274279
211	6	0	-5.283041	4.355534	-0.556385
212	1	0	-5.649882	5.026512	0.227276
213	1	0	-6.024851	3.564403	-0.705837
214	1	0	-4.355467	3.893226	-0.206388
215	1	0	0.567801	1.408498	-2.477229
216	1	0	-0.286963	1.219690	-2.748454
217	1	0	-1.902569	2.281728	-1.372890

53	6	0	4.415458	4.079212	-0.555308
54	6	0	2.967063	-1.142042	-0.439530
55	6	0	2.787342	-1.822239	-1.633209
56	6	0	4.001492	-1.519714	0.420936
57	6	0	3.665565	-2.827122	-2.053340
58	1	0	1.938210	-1.557604	-2.256301
59	6	0	4.939999	-2.473674	0.038796
60	1	0	4.078283	-1.037643	1.388069
61	6	0	4.801776	-3.041504	-1.254132
62	6	0	3.261693	-3.607067	-3.324130
63	6	0	3.328665	-2.677972	-4.550122
64	1	0	2.993607	-3.213429	-5.445469
65	1	0	2.686016	-1.800113	-4.425392
66	1	0	4.349358	-2.325343	-4.730326
67	6	0	4.075045	-4.879972	-3.615210
68	1	0	4.109414	-5.547593	-2.749798
69	1	0	3.582095	-5.418361	-4.432220
70	1	0	5.097129	-4.676718	-3.935863
71	6	0	1.800754	-4.075265	-3.140487
72	1	0	1.706034	-4.742726	-2.276833
73	1	0	1.103216	-3.244678	-3.002711
74	1	0	1.483578	-4.623785	-4.032876
75	6	0	6.026064	-2.948122	1.026489
76	6	0	5.859008	-4.465960	1.236714
77	1	0	6.054261	-5.018815	0.315482
78	1	0	6.558059	-4.820504	2.002485
79	1	0	4.841671	-4.703110	1.562293
80	6	0	7.455302	-2.650830	0.535007
81	1	0	7.570906	-1.598707	0.253195
82	1	0	8.165403	-2.856929	1.343734
83	1	0	7.738872	-3.274985	-0.312561
84	6	0	5.870699	-2.262553	2.393444
85	1	0	6.045466	-1.182363	2.331605
86	1	0	4.882389	-2.428574	2.831374
87	1	0	6.613937	-2.672712	3.084506
88	8	0	5.821794	-3.838745	-1.712108
89	8	0	5.187212	5.215945	-0.535485
90	8	0	-3.426563	1.317106	4.998658
91	8	0	-5.145887	-3.953465	-3.404112
92	6	0	-5.027079	-5.373102	-3.381348
93	1	0	-5.919715	-5.770326	-3.868308
94	1	0	-4.144910	-5.715898	-3.929025
95	1	0	-4.971743	-5.752506	-2.356011
96	6	0	-2.369468	-3.367764	-4.467303
97	6	0	-3.439809	-3.442350	-5.571769
98	1	0	-2.933646	-3.477605	-6.542367
99	1	0	-4.073406	-4.325643	-5.506730
100	1	0	-4.084998	-2.558079	-5.563625
101	6	0	-1.558299	-4.675990	-4.432786
102	1	0	-1.060232	-4.839440	-5.395145
103	1	0	-0.792998	-4.636650	-3.652823
104	1	0	-2.191473	-5.544134	-4.230169
105	6	0	6.671707	-3.169624	-2.641085
106	1	0	7.451941	-3.880760	-2.917739
107	1	0	6.126598	-2.860728	-3.538690
108	1	0	7.128911	-2.282410	-2.189892
109	6	0	5.204032	5.878784	0.726314
110	1	0	5.993254	6.631251	0.676105
111	1	0	4.253098	6.377285	0.935164
112	1	0	5.417592	5.178116	1.539905
113	6	0	6.622245	2.703922	-0.559247
114	6	0	7.058070	1.228493	-0.494711
115	1	0	6.820951	0.771957	0.472629
116	1	0	6.600766	0.623933	-1.285004
117	1	0	8.143070	1.172068	-0.626586
118	6	0	7.068757	3.258917	-1.926158
119	1	0	6.825770	4.318936	-2.028233
120	1	0	8.152663	3.144807	-2.040068
121	1	0	6.585678	2.714376	-2.744954
122	6	0	7.370113	3.441867	0.567137
123	1	0	7.309699	4.524758	0.459080
124	1	0	6.980721	3.163761	1.552285
125	1	0	8.430987	3.169312	0.538849

6a(S)2a

RwB97XD SCF energy -5021.644625 a.u.
 RwB97XD SCF enthalpy -5019.652560 a.u.
 RwB97XD SCF free energy -5019.898250 a.u.
 Three lowest frequencies (cm⁻¹) 15.5, 16.4, 20.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.053763	-0.874841	2.382480
2	6	0	0.781475	-0.715777	3.724705
3	6	0	0.970480	0.481078	4.407404
4	6	0	1.420253	1.609914	3.769201
5	6	0	1.700079	1.481934	2.401669
6	6	0	1.542011	0.280926	1.708560
7	1	0	1.570206	2.546767	4.292263
8	1	0	2.073425	2.357609	1.884768
9	6	0	0.876335	-2.229748	1.791552
10	6	0	-0.082215	-2.587763	0.806109
11	6	0	1.662003	-3.256951	2.267619
12	6	0	-0.144816	-3.892975	0.323014
13	6	0	1.585210	-4.559082	1.786854
14	6	0	0.701243	-4.909409	0.795875
15	1	0	-0.878848	-4.152385	-0.431677
16	1	0	0.639780	-5.920795	0.411523
17	8	0	0.640557	0.315707	5.714837
18	8	0	0.293328	-1.653108	4.585445
19	8	0	2.626527	-3.184697	3.228053
20	8	0	2.503855	-5.332316	2.436547
21	6	0	0.464846	-1.092658	5.887186
22	1	0	-0.424627	-1.278265	6.487295
23	1	0	1.364492	-1.514585	6.350069
24	6	0	2.923871	-4.543153	3.551522
25	1	0	2.352335	-4.836946	4.440561
26	1	0	3.996935	-4.657832	3.700588
27	15	0	-1.168124	-1.272939	0.141138
28	15	0	1.890147	0.271467	-0.092940
29	46	0	0.003429	0.243906	-1.300667
30	6	0	-1.956504	-0.533520	1.599230
31	6	0	-2.582348	-1.290893	2.580132
32	6	0	-1.923601	0.854534	1.721061
33	6	0	-3.175178	-0.699718	3.702456
34	1	0	-2.615479	-2.369514	2.464471
35	6	0	-2.451717	1.506535	2.830166
36	1	0	-1.448010	1.422256	0.932020
37	6	0	-3.008782	0.693882	3.847896
38	6	0	-2.438271	-2.112969	-0.857070
39	6	0	-3.776731	-2.234709	-0.493529
40	6	0	-2.041028	-2.507301	-2.130743
41	6	0	-4.710214	-2.814158	-1.356676
42	1	0	-4.090227	-1.862671	0.472864
43	6	0	-2.923292	-3.074233	-3.052501
44	1	0	-1.006634	-2.345686	-2.416433
45	6	0	-4.242263	-3.295642	-2.603717
46	6	0	2.914723	1.756148	-0.353147
47	6	0	4.303930	1.693408	-0.321496
48	6	0	2.293680	2.976984	-0.582369
49	6	0	5.087403	2.837855	-0.449190
50	1	0	4.782288	0.732517	-0.202483
51	6	0	3.015396	4.166857	-0.716930
52	1	0	1.212092	2.998958	-0.660302

126	6	0	2.204042	5.442652	-1.046915	199	8	0	-2.323370	4.255875	-2.092162
127	6	0	1.505585	5.944064	0.231072	200	6	0	-2.427210	5.415427	-2.754033
128	1	0	0.814643	5.188602	0.622412	201	8	0	-2.107678	5.528440	-3.919841
129	1	0	2.222897	6.180692	1.022060	202	6	0	-2.982173	6.518577	-1.860661
130	1	0	0.930128	6.851149	0.017373	203	6	0	-1.890759	6.908466	-0.848113
131	6	0	3.026780	6.583649	-1.673420	204	1	0	-1.017268	7.333078	-1.352215
132	1	0	2.333285	7.355638	-2.023744	205	1	0	-2.285125	7.662119	-0.158687
133	1	0	3.714825	7.060084	-0.976088	206	1	0	-1.567336	6.045314	-0.259330
134	1	0	3.601458	6.234674	-2.536800	207	6	0	-3.350698	7.723548	-2.728678
135	6	0	1.113080	5.090705	-2.085883	208	1	0	-4.130188	7.467332	-3.452837
136	1	0	0.615884	6.005825	-2.420988	209	1	0	-3.727742	8.530082	-2.092436
137	1	0	1.544583	4.601778	-2.966004	210	1	0	-2.483038	8.098216	-3.278730
138	1	0	0.336354	4.440622	-1.676511	211	6	0	-4.222824	5.996256	-1.115424
139	6	0	-6.212597	-2.815195	-0.992734	212	1	0	-4.671109	6.815164	-0.543957
140	6	0	-1.417430	-2.223340	-4.891520	213	1	0	-4.976702	5.617312	-1.813683
141	1	0	-1.924068	-1.252773	-4.849904	214	1	0	-3.966585	5.193866	-0.418235
142	1	0	-0.509008	-2.165704	-4.286121	215	1	0	0.843033	1.133596	-2.284374
143	1	0	-1.094814	-2.389611	-5.924174	216	1	0	-1.933103	0.598654	-3.363747
144	6	0	-6.956041	-1.919939	-2.003453	217	1	0	-1.953639	2.082884	-0.964188
145	1	0	-8.025984	-1.894694	-1.766387						
146	1	0	-6.577375	-0.892734	-1.962386						
147	1	0	-6.843942	-2.290969	-3.024968						
148	6	0	-6.839703	-4.223171	-0.987242						
149	1	0	-6.241107	-4.922671	-0.394027						
150	1	0	-7.834530	-4.170794	-0.531282						
151	1	0	-6.964055	-4.629093	-1.990342						
152	6	0	-6.446188	-2.235112	0.410069						
153	1	0	-6.057023	-1.218892	0.516399						
154	1	0	-7.522252	-2.194422	0.605978						
155	1	0	-5.992834	-2.864266	1.181678						
156	6	0	-2.512046	1.177665	6.082451						
157	1	0	-2.957466	1.693185	6.935475						
158	1	0	-2.348103	0.126782	6.340235						
159	1	0	-1.546729	1.632670	5.844894						
160	6	0	-3.994001	-1.632634	4.630118						
161	6	0	-3.047478	-2.573046	5.396381						
162	1	0	-3.629091	-3.287990	5.989195						
163	1	0	-2.404270	-3.141984	4.717568						
164	1	0	-2.406032	-2.015574	6.084819						
165	6	0	-4.922231	-0.924352	5.633592						
166	1	0	-5.570302	-1.680337	6.090539						
167	1	0	-4.391160	-0.426426	6.444690						
168	1	0	-5.565227	-0.190474	5.140091						
169	6	0	-4.928782	-2.485225	3.743164						
170	1	0	-5.602761	-1.842599	3.168165						
171	1	0	-4.388634	-3.129114	3.044324						
172	1	0	-5.541918	-3.136266	4.375077						
173	6	0	-2.520092	3.048760	2.861649						
174	6	0	-1.864491	3.669861	1.614948						
175	1	0	-1.941712	4.759082	1.686876						
176	1	0	-0.800451	3.417125	1.533583						
177	1	0	-2.369981	3.368964	0.692877						
178	6	0	-1.823502	3.666081	4.088800						
179	1	0	-0.814644	3.260529	4.217798						
180	1	0	-1.731560	4.748459	3.948277						
181	1	0	-2.385416	3.502607	5.008303						
182	6	0	-4.006291	3.459246	2.846252						
183	1	0	-4.503447	3.073456	1.949066						
184	1	0	-4.533600	3.078957	3.724534						
185	1	0	-4.096252	4.551651	2.839708						
186	8	0	-1.863794	0.685930	-2.403425						
187	6	0	-2.409203	1.933778	-1.944418						
188	6	0	-3.883548	1.875618	-1.756537						
189	6	0	-4.948570	2.328027	-2.471142						
190	8	0	-4.310587	1.326898	-0.584732						
191	6	0	-6.111019	2.039036	-1.687613						
192	1	0	-4.911254	2.827523	-3.429023						
193	6	0	-5.661303	1.434765	-0.557923						
194	1	0	-7.140407	2.257977	-1.931618						
195	1	0	-6.149695	1.053362	0.325508						
196	6	0	-1.977770	3.088259	-2.834300						
197	1	0	-2.492625	3.081530	-3.798979						
198	1	0	-0.897804	3.047700	-3.002623						

2.3. Catalytic cycle 2a – 1a (R).

3a(R)

RwB97XD SCF energy -5020.433606 a.u.

RwB97XD SCF enthalpy -5018.465266 a.u.

RwB97XD SCF free energy -5018.709479 a.u.

Three lowest frequencies (cm⁻¹) 8.0, 15.1, 19.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.853712	-0.699372	2.578883
2	6	0	0.458372	-0.391698	3.861194
3	6	0	0.795819	0.793010	4.505125
4	6	0	1.586014	1.737212	3.897360
5	6	0	2.010909	1.449487	2.591843
6	6	0	1.664776	0.270739	1.929139
7	1	0	1.866731	2.658028	4.394425
8	1	0	2.626082	2.187286	2.090861
9	6	0	0.412448	-2.006571	2.024299
10	6	0	-0.584561	-2.169530	1.028033
11	6	0	0.929106	-3.164183	2.562313
12	6	0	-0.957529	-3.445638	0.609384
13	6	0	0.543837	-4.431944	2.143681
14	6	0	-0.393999	-4.609603	1.156052
15	1	0	-1.715033	-3.558098	-0.158084
16	1	0	-0.696343	-5.956700	0.823128
17	8	0	0.266235	0.794930	5.757684
18	8	0	-0.290932	-1.165960	4.693895
19	8	0	1.874797	-3.274757	3.538698
20	8	0	1.240780	-5.369584	2.848559
21	6	0	-0.626508	-0.322960	5.795330
22	1	0	-1.652226	0.035164	5.672045
23	1	0	-0.490739	-0.866924	6.729872
24	6	0	1.852240	-4.650734	3.922272
25	1	0	1.245071	-4.763601	4.828300
26	1	0	2.871768	-5.006665	4.068824
27	15	0	-1.272551	-0.680735	0.216888
28	15	0	2.098371	0.112312	0.156855
29	46	0	0.318807	0.558885	-1.128025
30	6	0	-1.941065	0.378978	1.539941
31	6	0	-2.756289	-0.063933	2.582035
32	6	0	-1.668177	1.733963	1.423133
33	6	0	-3.292006	0.824438	3.515089
34	1	0	-2.968074	-1.122414	2.663134
35	6	0	-2.155680	2.681456	2.326970
36	1	0	-1.044400	2.062382	0.598438
37	6	0	-2.912406	2.188211	3.405537
38	6	0	-2.679067	-1.309356	-0.749915
39	6	0	-3.847706	-1.798038	-0.165558
40	6	0	-2.563352	-1.313160	-2.131670
41	6	0	-4.859338	-2.372964	-0.926860
42	1	0	-3.956404	-1.740595	0.907919
43	6	0	-3.566487	-1.819901	-2.967206
44	1	0	-1.668278	-0.893842	-2.576615
45	6	0	-4.660289	-2.440697	-2.330994
46	6	0	3.484639	1.272497	-0.078336
47	6	0	4.810294	0.866143	-0.011673
48	6	0	3.188893	2.595114	-0.398582
49	6	0	5.860612	1.770367	-0.190951
50	1	0	5.029976	-0.178147	0.156258
51	6	0	4.183266	3.553959	-0.571633
52	1	0	2.149744	2.864207	-0.535864
53	6	0	5.516544	3.130309	-0.355808
54	6	0	2.733411	-1.552896	-0.156452
55	6	0	2.289955	-2.206108	-1.296892
56	6	0	3.650841	-2.184714	0.685260
57	6	0	2.790571	-3.452103	-1.685405
58	1	0	1.523077	-1.729410	-1.899637
59	6	0	4.236223	-3.394940	0.325251
60	1	0	3.913383	-1.707938	1.621768
61	6	0	3.857898	-3.958514	-0.921339
62	6	0	2.090108	-4.135035	-2.884675
63	6	0	2.383298	-3.352076	-4.177647
64	1	0	1.862353	-3.816081	-5.022721
65	1	0	2.042159	-2.313578	-4.103997
66	1	0	3.453478	-3.339972	-4.407735
67	6	0	2.448506	-5.616358	-3.097016
68	1	0	2.330908	-6.194371	-2.176399
69	1	0	1.761508	-6.030890	-3.843006
70	1	0	3.461102	-5.767575	-3.472711
71	6	0	0.565066	-4.106785	-2.625976
72	1	0	0.316682	-4.662804	-1.716355
73	1	0	0.164638	-3.094339	-2.521330
74	1	0	0.043664	-4.579144	-3.465427
75	6	0	5.200701	-4.115115	1.290016
76	6	0	4.649376	-5.524865	1.582106
77	1	0	4.646067	-6.147390	0.685362
78	1	0	5.266187	-6.020383	2.340245
79	1	0	3.622952	-5.470084	1.957893
80	6	0	6.627533	-4.223642	0.719194
81	1	0	6.995663	-3.250062	0.375898
82	1	0	7.307648	-4.577614	1.502148
83	1	0	6.686476	-4.932065	-0.107773
84	6	0	5.305885	-3.368200	2.630012
85	1	0	5.767394	-2.380707	2.516155
86	1	0	4.331216	-3.241512	3.110658
87	1	0	5.939901	-3.947668	3.308371
88	8	0	4.565532	-5.047788	-1.367124
89	8	0	6.519936	4.073587	-0.361705
90	8	0	-3.321290	3.051715	4.393077
91	8	0	-5.604352	-3.118695	-3.064516
92	6	0	-5.194828	-4.419702	-3.479240
93	1	0	-6.085425	-4.919476	-3.864650
94	1	0	-4.441122	-4.376553	-4.270734
95	1	0	-4.787423	-4.992379	-2.639971
96	6	0	-3.374656	-1.606278	-4.488166
97	6	0	-4.670498	-1.710948	-5.312070
98	1	0	-4.461318	-1.373413	-6.332744
99	1	0	-5.063882	-2.724248	-5.382269
100	1	0	-5.454327	-1.065919	-4.901791
101	6	0	-2.322214	-2.594203	-5.025136
102	1	0	-2.163523	-2.430520	-6.097090
103	1	0	-1.360704	-2.452768	-4.518921
104	1	0	-2.623020	-3.636204	-4.883932
105	6	0	5.513624	-4.718214	-2.379675
106	1	0	6.038547	-5.642144	-2.628901
107	1	0	5.028111	-4.324923	-3.278108
108	1	0	6.232760	-3.974114	-2.020020
109	6	0	6.776463	4.604511	0.941955
110	1	0	7.575033	5.340017	0.828930
111	1	0	5.889592	5.089994	1.356781
112	1	0	7.094819	3.822957	1.636471
113	6	0	7.298862	1.231447	-0.379998
114	6	0	7.339129	-0.304400	-0.264574
115	1	0	7.060369	-0.647657	0.738118
116	1	0	6.688372	-0.797380	-0.994290
117	1	0	8.361127	-0.646043	-0.455203
118	6	0	7.750841	1.603699	-1.806763
119	1	0	7.786680	2.687548	-1.943252
120	1	0	8.752367	1.202350	-1.998577
121	1	0	7.068716	1.184908	-2.554856
122	6	0	8.319852	1.780714	0.631805
123	1	0	8.541756	2.834269	0.459684
124	1	0	7.972952	1.653055	1.662636
125	1	0	9.261412	1.230606	0.527977
126	6	0	8.311794	4.930592	-1.172507
127	6	0	2.291555	5.056225	-1.387697
128	1	0	1.896663	4.272781	-2.041392
129	1	0	1.738880	5.031142	-0.441432
130	1	0	2.081453	6.017524	-1.866711
131	6	0	4.240350	6.137552	-0.319524
132	1	0	3.797823	7.047836	-0.738455
133	1	0	3.889223	6.044697	0.713690
134	1	0	5.321728	6.277587	-0.316032
135	6	0	4.487061	5.021599	-2.556208
136	1	0	4.223774	5.967386	-3.043053
137	1	0	5.575979	4.974243	-2.469894
138	1	0	4.156499	4.203769	-3.205881
139	6	0	-6.150427	-2.871541	-0.239634
140	6	0	-2.841231	-0.173335	-4.730387
141	1	0	-3.497509	0.578984	-4.280211
142	1	0	-1.832601	-0.023733	-4.337593
143	1	0	-2.795965	0.016118	-5.807843
144	6	0	-7.368933	-2.111182	-0.795815
145	1	0	-8.288566	-2.516606	-0.358403
146	1	0	-7.315828	-1.050424	-0.529807
147	1	0	-7.442361	-2.197626	-1.881937
148	6	0	-6.358549	-4.386403	-0.429938
149	1	0	-5.446529	-4.946367	-0.196746
150	1	0	-7.145829	-4.734344	0.247853
151	1	0	-6.670462	-4.631056	-1.445371

152	6	0	-6.111519	-2.607821	1.275243	4	6	0	0.363719	4.130121	2.004770
153	1	0	-5.982430	-1.544350	1.503713	5	6	0	0.942332	3.038487	1.341135
154	1	0	-7.061592	-2.924452	1.716626	6	6	0	0.460392	1.735146	1.472139
155	1	0	-5.314188	-3.170418	1.773256	7	1	0	0.761201	5.132261	1.896920
156	6	0	-2.323301	3.251721	5.390675	8	1	0	1.809029	3.234537	0.722214
157	1	0	-2.726658	3.973625	6.103551	9	6	0	-1.303646	0.147529	2.536164
158	1	0	-2.092845	2.317798	5.913074	10	6	0	-2.013005	-0.631466	1.583156
159	1	0	-1.399522	3.649260	4.957148	11	6	0	-1.283045	-0.344922	3.823421
160	6	0	-4.412534	0.335910	4.466902	12	6	0	-2.612768	-1.830725	1.966711
161	6	0	-4.341686	0.822194	5.927763	13	6	0	-1.880877	-1.544168	4.193220
162	1	0	-5.165868	0.361399	6.482955	14	6	0	-2.553420	-2.319821	3.281001
163	1	0	-3.415504	0.517631	6.423314	15	1	0	-3.164356	-2.414897	1.239948
164	1	0	-4.447266	1.901932	6.016247	16	1	0	-3.032721	-3.250988	3.558900
165	6	0	-5.735366	0.845392	3.855538	17	8	0	-1.439178	4.694630	3.598296
166	1	0	-6.587857	0.503183	4.453523	18	8	0	-2.287499	2.578568	3.779456
167	1	0	-5.760205	1.939513	3.823324	19	8	0	-0.693980	0.219995	4.914924
168	1	0	-5.864288	0.469950	2.834532	20	8	0	-1.677340	-1.755099	5.525560
169	6	0	-4.462870	-1.200975	4.524463	21	6	0	-2.184089	3.827856	4.458613
170	1	0	-4.710728	-1.652390	3.560153	22	1	0	-3.176755	4.240174	4.628522
171	1	0	-3.512329	-1.623066	4.871565	23	1	0	-1.631328	3.688115	5.395819
172	1	0	-5.241020	-1.507825	5.229928	24	6	0	-1.235336	-0.491337	6.026998
173	6	0	-1.823452	4.160290	2.012862	25	1	0	-2.096117	0.060637	6.424077
174	6	0	-0.322585	4.405364	2.257565	26	1	0	-0.462805	-0.639886	6.779635
175	1	0	-0.067434	5.442900	2.012783	27	15	0	-2.028057	-0.109089	-0.173936
176	1	0	-0.053254	4.229407	3.303782	28	15	0	1.270920	0.382870	0.538212
177	1	0	0.296247	3.747267	1.637577	29	46	0	0.075787	-0.421649	-1.215872
178	6	0	-2.637781	5.205923	2.794006	30	6	0	-2.521941	1.633310	-0.205589
179	1	0	-2.375378	5.257663	3.850947	31	6	0	-3.585813	2.128735	0.549880
180	1	0	-2.433481	6.191248	2.360841	32	6	0	-1.854859	2.472277	-1.083657
181	1	0	-3.713002	5.023846	2.712717	33	6	0	-3.948202	3.470382	0.485549
182	6	0	-2.123825	4.424912	0.519296	34	1	0	-4.128741	1.446165	1.192292
183	1	0	-1.511229	3.816490	-0.150947	35	6	0	-2.173551	3.828556	-1.206746
184	1	0	-3.178206	4.235614	0.292908	36	1	0	-1.051726	2.058191	-1.685461
185	1	0	-1.912404	5.473841	0.286208	37	6	0	-3.158525	4.320583	-0.332089
186	8	0	-1.226853	1.562677	-2.298504	38	6	0	-3.383569	-1.041001	-0.949170
187	6	0	-1.300103	2.637134	-2.899859	39	6	0	-4.594602	-0.439913	-1.281627
188	1	0	1.433865	1.249767	-1.947366	40	6	0	-3.191086	-2.387232	-1.235684
189	6	0	-0.212622	3.207286	-3.659079	41	6	0	-5.653348	-1.177634	-1.804801
190	6	0	0.931788	2.681072	-4.203223	42	1	0	-4.710702	0.622708	-1.125911
191	8	0	-0.335223	4.519577	-4.023478	43	6	0	-4.213410	-3.191443	-1.751642
192	6	0	1.547000	3.732446	-4.928263	44	1	0	-2.219939	-2.826164	-1.034086
193	1	0	1.273985	1.661679	-4.104190	45	6	0	-5.468895	-2.575095	-1.940349
194	6	0	0.738496	4.821096	-4.772059	46	6	0	2.895970	1.053556	0.070526
195	1	0	2.468711	3.691676	-5.489158	47	6	0	4.047653	0.725758	0.773976
196	1	0	0.802240	5.840692	-5.122205	48	6	0	2.979725	1.914766	-1.017904
197	6	0	-2.598739	3.407135	-2.875601	49	6	0	5.280786	1.292591	0.453251
198	1	0	-2.933803	3.612556	-3.898056	50	1	0	3.981674	0.011767	1.582118
199	1	0	-2.440198	4.367696	-2.372768	51	6	0	4.176903	2.535349	-1.384203
200	8	0	-3.546226	2.610882	-2.193930	52	1	0	2.081065	2.108533	-1.592638
201	6	0	-4.702341	3.197366	-1.843597	53	6	0	5.309951	2.255021	-0.583624
202	8	0	-4.910183	4.379842	-2.021857	54	6	0	1.534640	-0.980693	1.703686
203	6	0	-5.676407	2.187580	-1.253903	55	6	0	1.179211	-2.261610	1.300958
204	6	0	-5.885839	1.081834	-2.306128	56	6	0	2.010985	-0.772028	2.995633
205	1	0	-4.978504	0.488488	-2.439386	57	6	0	1.278812	-3.362308	2.150985
206	1	0	-6.687798	0.414095	-1.982583	58	1	0	0.775968	-2.391816	0.304471
207	1	0	-6.172458	1.506634	-3.274531	59	6	0	2.188535	-1.833858	3.882392
208	6	0	-5.078550	1.586651	0.030224	60	1	0	2.233260	0.240649	3.308407
209	1	0	-4.940269	2.351116	0.802613	61	6	0	1.840197	-3.131520	3.426851
210	1	0	-5.763191	0.826482	0.421695	62	6	0	0.757380	-4.726232	1.642551
211	1	0	-4.116133	1.108823	-0.163041	63	6	0	1.926162	-5.580793	1.118048
212	6	0	-6.999479	2.888478	-0.944850	64	1	0	1.541009	-6.507295	0.676670
213	1	0	-7.702478	2.165601	-0.519071	65	1	0	2.476790	-5.043410	0.338841
214	1	0	-6.863508	3.698003	-0.221517	66	1	0	2.631908	-5.855554	1.903150
215	1	0	-7.450014	3.309195	-1.848843	67	6	0	-0.025078	-5.488833	2.728354
						68	1	0	-0.813083	-4.856347	3.152336
						69	1	0	-0.503667	-6.365739	2.279319
						70	1	0	0.607378	-5.832085	3.545774
						71	6	0	-0.221667	-4.528378	0.465648
						72	1	0	-1.043723	-3.856076	0.734860
						73	1	0	0.266054	-4.138867	-0.433118
						74	1	0	-0.651798	-5.497366	0.195098
						75	6	0	2.753576	-1.558009	5.293410
						76	6	0	1.985041	-2.326354	6.388985
						77	1	0	2.292193	-3.371764	6.457103
						78	1	0	2.169168	-1.861614	7.362459
						79	1	0	0.907347	-2.314367	6.201453
						80	6	0	4.246050	-1.938014	5.336624
						81	1	0	4.819287	-1.355718	4.607728
						82	1	0	4.654370	-1.728180	6.331913
						83	1	0	4.413854	-2.995198	5.127354
						84	6	0	2.662335	-0.059878	5.642071
						85	1	0	3.301209	0.558511	5.003184

TS1a(R)

RwB97XD SCF energy -5020.418735 a.u.

RwB97XD SCF enthalpy -5018.453084 a.u.

RwB97XD SCF free energy -5018.699158 a.u.

Three lowest frequencies (cm⁻¹) -135.3, 6.3, 10.5

Imaginary frequency (cm⁻¹) -135.3

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.674197	1.472078	2.287861
2	6	0	-1.208636	2.560520	2.943145
3	6	0	-0.704910	3.851018	2.820374

86	1	0	1.636594	0.314256	5.571053	168	1	0	-6.458272	3.645331	-0.593612
87	1	0	3.008290	0.086430	6.669859	169	6	0	-5.910219	2.829088	1.966225
88	8	0	1.966525	-4.175151	4.303466	170	1	0	-6.186634	1.988979	1.320004
89	8	0	6.516703	2.860648	-0.834903	171	1	0	-5.274437	2.452291	2.775310
90	8	0	-3.402351	5.670502	-0.263388	172	1	0	-6.831304	3.209378	2.418555
91	8	0	-6.563604	-3.322547	-2.303217	173	6	0	-1.423404	4.617255	-2.305067
92	6	0	-7.192329	-3.987886	-1.210320	174	6	0	0.043362	4.815529	-1.883188
93	1	0	-8.118971	-4.416917	-1.596096	175	1	0	0.598843	5.317630	-2.683216
94	1	0	-6.567128	-4.791985	-0.811837	176	1	0	0.128182	5.425539	-0.978376
95	1	0	-7.420593	-3.289061	-0.399340	177	1	0	0.529255	3.853790	-1.686130
96	6	0	-3.854033	-4.663221	-2.069145	178	6	0	-2.040304	5.977899	-2.672860
97	6	0	-4.801061	-5.358102	-3.063919	179	1	0	-1.922662	6.732875	-1.895556
98	1	0	-4.362574	-6.322815	-3.341112	180	1	0	-1.534448	6.353661	-3.568841
99	1	0	-5.790495	-5.557972	-2.655111	181	1	0	-3.105433	5.866481	-2.903701
100	1	0	-4.920833	-4.771456	-3.979918	182	6	0	-1.444884	3.781852	-3.606720
101	6	0	-3.790053	-5.472695	-0.760081	183	1	0	-0.926012	2.824575	-3.511453
102	1	0	-3.439841	-6.490765	-0.964887	184	1	0	-2.472881	3.579436	-3.926148
103	1	0	-3.095559	-5.014885	-0.048014	185	1	0	-0.945216	4.339306	-4.405761
104	1	0	-4.766987	-5.548138	-0.274239	186	8	0	-0.519832	-1.364744	-3.076545
105	6	0	3.133286	-4.988118	4.249714	187	6	0	0.747809	-1.462591	-3.186837
106	1	0	3.609748	-4.983824	5.235003	188	1	0	1.553188	-0.588226	-1.775985
107	1	0	2.848970	-6.017988	4.011313	189	6	0	1.384933	-2.764474	-2.873061
108	1	0	3.845752	-4.627339	3.502741	190	6	0	0.991416	-4.034134	-3.165129
109	6	0	6.679543	4.182611	-0.326748	191	8	0	2.621385	-2.771787	-2.309269
110	1	0	7.745850	4.325437	-0.138245	192	6	0	2.063044	-4.884555	-2.750719
111	1	0	6.357951	4.931476	-1.055328	193	1	0	0.069757	-4.319437	-3.649245
112	1	0	6.125121	4.322826	0.605941	194	6	0	3.016973	-0.065959	-2.236774
113	6	0	6.550206	0.815050	1.191014	195	1	0	2.110224	-5.961285	-2.821938
114	6	0	6.216467	-0.260711	2.239658	196	1	0	3.982208	-4.237475	-1.785439
115	1	0	5.570931	0.133046	3.032447	197	6	0	1.430001	-0.534593	-4.187570
116	1	0	5.733051	-1.140481	1.802082	198	1	0	1.023890	0.471693	-4.088710
117	1	0	7.144859	-0.598764	2.710256	199	1	0	1.214047	-0.929779	-5.185133
118	6	0	7.521083	0.184662	0.174322	200	8	0	2.829533	-0.444844	-3.977061
119	1	0	7.800916	0.894809	-0.606243	201	6	0	3.621569	-1.347413	-4.592988
120	1	0	8.435132	-0.138958	0.685252	202	8	0	3.180269	-2.197797	-5.336169
121	1	0	7.070901	-0.694753	-0.298541	203	6	0	5.095833	-1.123997	-4.292313
122	6	0	7.254876	1.960213	1.942978	204	6	0	5.308697	-0.612850	-2.861866
123	1	0	7.776200	2.637962	1.268715	205	1	0	4.931532	-1.325997	-2.121862
124	1	0	6.546209	2.540079	2.543801	206	1	0	6.379985	-0.472168	-2.688619
125	1	0	8.003173	1.542395	2.625413	207	1	0	4.812554	0.345029	-2.698596
126	6	0	4.158290	3.452400	-2.630477	208	6	0	5.840942	-2.445696	-4.501696
127	6	0	3.094417	2.959690	-3.637257	209	1	0	5.717863	-2.819560	-5.521367
128	1	0	3.241875	1.905704	-3.890377	210	1	0	6.909058	-2.295181	-4.317725
129	1	0	2.071598	3.090740	-3.273562	211	1	0	5.479624	-3.214060	-3.809999
130	1	0	3.175425	3.545294	-4.558224	212	6	0	5.588844	-0.070815	-5.305192
131	6	0	3.765914	4.881421	-2.208515	213	1	0	6.654669	0.117380	-5.141608
132	1	0	3.703141	5.531225	-3.088939	214	1	0	5.455766	-0.421093	-6.333740
133	1	0	2.788770	4.881081	-1.715730	215	1	0	5.052641	0.876034	-5.188030

4a(R)

RwB97XD SCF energy -5020.433579 a.u.
 RwB97XD SCF enthalpy -5018.463909 a.u.
 RwB97XD SCF free energy -5018.70027 a.u.
 Three lowest frequencies (cm⁻¹) -7.1, 17.3, 24.4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.406564	2.616971	1.052420
2	6	0	-2.178104	3.748234	0.905925
3	6	0	-1.807085	4.821034	0.099030
4	6	0	-0.644064	4.810385	-0.631300
5	6	0	0.165557	3.672188	-0.499016
6	6	0	-0.187864	2.601546	0.319477
7	1	0	-0.352335	5.643243	-1.259847
8	1	0	1.103653	3.651152	-1.040622
9	6	0	-1.832921	1.571311	2.019890
10	6	0	-2.127740	0.209775	1.727572
11	6	0	-1.943667	1.936856	3.344329
12	6	0	-2.471928	-0.672230	2.751454
13	6	0	-2.282476	1.045644	4.357054
14	6	0	-2.547230	-0.275659	4.093998
15	1	0	-2.703816	-1.704963	2.522635
16	1	0	-2.811908	-0.976616	4.876379
17	8	0	-2.757322	5.792258	0.182743
18	8	0	-3.380146	4.019766	1.489745
19	8	0	-1.701982	3.163203	3.883419

20	8	0	-2.268630	1.692577	5.552144	102	1	0	-1.914078	-6.137520	3.252639
21	6	0	-3.544571	5.427771	1.319897	103	1	0	-1.985576	-4.377893	3.058462
22	1	0	-4.591652	5.657041	1.132289	104	1	0	-3.479881	-5.315143	3.182681
23	1	0	-3.161004	5.946587	2.206676	105	6	0	4.315972	-0.494057	5.493869
24	6	0	-2.163751	3.082952	5.232944	106	1	0	4.782111	-0.682652	6.462674
25	1	0	-3.152994	3.548318	5.307131	107	1	0	4.441280	-1.372985	4.853682
26	1	0	-1.439126	3.555597	5.895772	108	1	0	4.804546	0.361730	5.015459
27	15	0	-1.962885	-0.420622	0.022727	109	6	0	6.424663	3.589707	-2.156045
28	15	0	0.860328	1.119829	0.403644	110	1	0	7.449328	3.703135	-2.514179
29	46	0	0.168295	-0.786410	-0.626715	111	1	0	5.740817	4.057608	-2.869659
30	6	0	-2.744712	0.795064	-1.060577	112	1	0	6.314869	4.091395	-1.189488
31	6	0	-4.012307	1.298379	-0.763720	113	6	0	6.147095	1.245030	0.709629
32	6	0	-2.103507	1.181786	-2.225640	114	6	0	5.765952	0.838068	2.146063
33	6	0	-4.623226	2.232876	-1.591264	115	1	0	5.266698	1.651221	2.684976
34	1	0	-4.517474	0.944037	0.126042	116	1	0	5.120443	-0.046637	2.176191
35	6	0	-2.657931	2.122698	-3.099074	117	1	0	6.679756	0.591914	2.695908
36	1	0	-1.133148	0.751192	-2.450331	118	6	0	6.887926	0.053089	0.074486
37	6	0	-3.874982	2.706451	-2.700886	119	1	0	7.185028	0.268554	-0.954242
38	6	0	-2.924771	-1.951523	-0.068988	120	1	0	7.791837	-0.177415	0.649797
39	6	0	-4.135600	-2.008019	-0.754485	121	1	0	6.252760	-0.839098	0.073093
40	6	0	-2.427942	-3.096570	0.540880	122	6	0	7.104475	2.446009	0.821683
41	6	0	-4.913377	-3.162446	-0.751398	123	1	0	7.621949	2.644762	-0.116820
42	1	0	-4.476434	-1.135944	-1.293419	124	1	0	6.574926	3.352601	1.133472
43	6	0	-3.155752	-4.288663	0.582400	125	1	0	7.868066	2.230219	1.576874
44	1	0	-1.449261	-3.054742	1.005084	126	6	0	3.770473	2.076978	-3.883716
45	6	0	-4.443948	-4.263361	0.006765	127	6	0	2.782765	1.054363	-4.493021
46	6	0	2.474395	1.482438	-0.342959	128	1	0	3.040186	0.032418	-4.200767
47	6	0	3.633157	1.380169	0.421765	129	1	0	1.742707	1.242496	-4.213992
48	6	0	2.575930	1.683971	-1.714616	130	1	0	2.826995	1.117128	-5.585191
49	6	0	4.893573	1.543292	-0.143386	131	6	0	3.251834	3.492305	-4.203837
50	1	0	3.546629	1.160372	1.475373	132	1	0	3.144148	3.618696	-5.287039
51	6	0	3.806435	1.886806	-2.346138	133	1	0	2.272276	3.665148	-3.745826
52	1	0	1.668101	1.686184	-2.307054	134	1	0	3.932308	4.268761	-3.841666
53	6	0	4.951938	1.885486	-1.517238	135	6	0	5.113416	1.845391	-4.599785
54	6	0	1.216194	0.761073	2.137191	136	1	0	4.928141	1.814343	-5.678821
55	6	0	1.349654	-0.570594	2.494966	137	1	0	5.841889	2.636587	-4.423450
56	6	0	1.471016	1.760744	3.075843	138	1	0	5.564926	0.892823	-4.311906
57	6	0	1.818976	-0.958662	3.752545	139	6	0	-6.189149	-3.226352	-1.618772
58	1	0	1.093020	-1.333882	1.766698	140	6	0	-0.987842	-5.543756	0.770275
59	6	0	1.971864	1.443939	4.335176	141	1	0	-0.930817	-5.566874	-0.322717
60	1	0	1.291993	2.793410	2.801864	142	1	0	-0.395187	-4.697154	1.125816
61	6	0	2.241532	0.076335	4.605325	143	1	0	-0.507074	-6.448651	1.155848
62	6	0	1.789767	-2.474154	4.052906	144	6	0	-6.009743	-4.339669	-2.669436
63	6	0	2.783378	-3.198426	3.127056	145	1	0	-6.897498	-4.397340	-3.309478
64	1	0	2.742048	-4.279423	3.300555	146	1	0	-5.145046	-4.133254	-3.309467
65	1	0	2.544317	-3.022053	2.073423	147	1	0	-5.865767	-5.315341	-2.199662
66	1	0	3.812680	-2.866888	3.300245	148	6	0	-7.462498	-3.492230	-0.793255
67	6	0	2.070149	-2.866943	5.512607	149	1	0	-7.541941	-2.797682	0.050084
68	1	0	1.432673	-2.316591	6.209819	150	1	0	-8.340350	-3.344594	-1.427973
69	1	0	1.851464	-3.934133	5.628453	151	1	0	-7.502710	-4.512680	-0.412718
70	1	0	3.110259	-2.720408	5.806006	152	6	0	-6.417646	-1.904383	-2.373898
71	6	0	0.364917	-2.987642	3.736653	153	1	0	-5.581450	-1.644312	-3.031293
72	1	0	-0.381247	-2.482562	4.359459	154	1	0	-7.307452	-2.004895	-3.002890
73	1	0	0.088625	-2.840581	2.688618	155	1	0	-6.594028	-1.067440	-1.688774
74	1	0	0.309383	-4.062207	3.939921	156	6	0	-3.789668	5.009226	-3.054246
75	6	0	2.144387	2.539494	5.407159	157	1	0	-4.272666	5.773692	-3.665481
76	6	0	1.295668	2.154909	6.635358	158	1	0	-3.944222	5.234972	-1.994714
77	1	0	1.664224	1.240368	7.104642	159	1	0	-2.714224	5.009075	-3.258033
78	1	0	1.328269	2.956687	7.381515	160	6	0	-6.094081	2.632537	-1.354526
79	1	0	0.250266	1.993070	6.353351	161	6	0	-6.282090	4.143926	-1.133526
80	6	0	3.612488	2.732986	5.830828	162	1	0	-7.295850	4.336510	-0.766237
81	1	0	4.259942	2.886165	4.960549	163	1	0	-5.578434	4.516148	-0.384197
82	1	0	3.693204	3.622715	6.465214	164	1	0	-6.149421	4.713783	-2.052934
83	1	0	3.991284	1.886580	6.403925	165	6	0	-6.914519	2.184877	-2.581041
84	6	0	1.638780	3.898689	4.895895	166	1	0	-7.972279	2.429535	-2.432783
85	1	0	2.245832	4.277659	4.066479	167	1	0	-6.574397	2.682120	-3.492731
86	1	0	0.595844	3.855576	4.568153	168	1	0	-6.836346	1.102116	-2.730337
87	1	0	1.701988	4.630547	5.707203	169	6	0	-6.671057	1.921476	-0.119088
88	8	0	2.938548	-0.222986	5.749706	170	1	0	-6.621788	0.830652	-0.204782
89	8	0	6.184370	2.188150	-2.040310	171	1	0	-6.157796	2.221425	0.801392
90	8	0	-4.390943	3.763840	-3.407234	172	1	0	-7.725806	2.192273	-0.011847
91	8	0	-5.284443	-5.340634	0.140524	173	6	0	-1.879275	2.390154	-4.409200
92	6	0	-5.963605	-5.380796	1.394054	174	6	0	-0.587626	3.164065	-4.090063
93	1	0	-6.707848	-6.176051	1.323362	175	1	0	0.005831	3.295699	-5.001693
94	1	0	-5.279275	-5.603572	2.217753	176	1	0	-0.797149	4.154923	-3.675398
95	1	0	-6.464240	-4.429727	1.602546	177	1	0	0.025026	2.620000	-3.364267
96	6	0	-2.459074	-5.501192	1.244417	178	6	0	-2.663691	3.137656	-5.501193
97	6	0	-3.058004	-6.870743	0.877738	179	1	0	-2.838317	4.187985	-5.267674
98	1	0	-2.384605	-7.650795	1.248794	180	1	0	-2.078345	3.106761	-6.426725
99	1	0	-4.036045	-7.051706	1.322482	181	1	0	-3.628339	2.663213	-5.701353
100	1	0	-3.145204	-6.993970	-0.205968	182	6	0	-1.492070	1.026321	-5.028664
101	6	0	-2.465131	-5.320143	2.773842	183	1	0	-0.838274	0.430347	-4.386128

184	1	0	-2.384312	0.429443	-5.247140
185	1	0	-0.956297	1.191573	-5.969103
186	8	0	0.077394	-2.604384	-1.566229
187	6	0	1.427547	-2.476625	-1.789560
188	6	0	2.286065	-3.406299	-0.979217
189	6	0	2.175728	-4.715770	-0.634755
190	8	0	3.497966	-2.921241	-0.587569
191	6	0	3.406933	-5.065789	0.009322
192	1	0	1.336508	-5.361448	-0.846583
193	6	0	4.168758	-3.943624	0.007507
194	1	0	3.680313	-6.026000	0.422688
195	1	0	5.149944	-3.707688	0.390251
196	6	0	1.732926	-2.540187	-3.295443
197	1	0	1.141670	-1.782822	-3.812608
198	1	0	1.490239	-3.534493	-3.675555
199	8	0	3.100627	-2.222211	-3.546199
200	6	0	3.993942	-3.218028	-3.685322
201	8	0	3.684777	-4.390824	-3.668384
202	6	0	5.401858	-2.677742	-3.902690
203	6	0	5.744937	-1.653157	-2.810214
204	1	0	5.752036	-2.127004	-1.824948
205	1	0	6.742709	-1.243856	-2.996511
206	1	0	5.032881	-0.824265	-2.787072
207	6	0	6.389661	-3.844448	-3.847891
208	1	0	6.185740	-4.581073	-4.630150
209	1	0	7.407956	-3.468542	-3.987815
210	1	0	6.340757	-4.352814	-2.879536
211	6	0	5.438116	-2.010753	-5.290482
212	1	0	6.449041	-1.640779	-5.489016
213	1	0	5.175599	-2.725377	-6.077576
214	1	0	4.747430	-1.164782	-5.346997
215	1	0	1.813074	-1.423062	-1.484481

5a(R)

RwB97XD SCF energy -5021.616218 a.u.
 RwB97XD SCF enthalpy -5019.628203 a.u.
 RwB97XD SCF free energy -5019.875590 a.u.
 Three lowest frequencies (cm⁻¹) 8.7, 13.2, 19.6

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.629149	-0.730629	2.430206
2	6	0	1.586743	-0.636471	3.804112
3	6	0	1.901116	0.531787	4.494134
4	6	0	2.243236	1.688712	3.840081
5	6	0	2.269006	1.629190	2.439045
6	6	0	1.977554	0.460343	1.738715
7	1	0	2.488368	2.599408	4.373043
8	1	0	2.541833	2.528286	1.899486
9	6	0	1.439589	-2.056892	1.788439
10	6	0	0.426349	-2.424371	0.859106
11	6	0	2.338802	-3.046658	2.121288
12	6	0	0.389373	-3.718610	0.340822
13	6	0	2.298871	-4.329360	1.586142
14	6	0	1.330816	-4.699394	0.685765
15	1	0	-0.397670	-4.006332	-0.343683
16	1	0	1.283236	-5.697774	0.267880
17	8	0	1.810070	0.304192	5.831279
18	8	0	1.263266	-1.613602	4.697363
19	8	0	3.400155	-2.943257	2.968353
20	8	0	3.331800	-5.058843	2.086835
21	6	0	1.699861	-1.115980	5.962943
22	1	0	0.962950	-1.354868	6.727707
23	1	0	2.685519	-1.535355	6.196076
24	6	0	3.845521	-4.283920	3.174426
25	1	0	3.430911	-4.664182	4.115330
26	1	0	4.934568	-4.313268	3.164911
27	15	0	-0.794488	-1.177753	0.310946
28	15	0	1.994135	0.481892	-0.081736
29	46	0	0.011006	0.261898	-1.251231
30	6	0	-1.353113	-0.360072	1.822763
31	6	0	-1.839628	-1.155165	2.861026
32	6	0	-1.372070	1.020742	1.939125

33	6	0	-2.295677	-0.591052	4.044674
34	1	0	-1.869577	-2.229110	2.724216
35	6	0	-1.808625	1.655321	3.108331
36	1	0	-1.021843	1.612147	1.101462
37	6	0	-2.166790	0.814956	4.182388
38	6	0	-2.221809	-2.057840	-0.372448
39	6	0	-3.489919	-1.894068	0.177802
40	6	0	-2.080472	-2.776842	-1.552806
41	6	0	-4.599230	-2.548570	-0.350605
42	1	0	-3.612484	-1.244823	1.032010
43	6	0	-3.152001	-3.446067	-2.145742
44	1	0	-1.114136	-2.794243	-2.043975
45	6	0	-4.381587	-3.408887	-1.452874
46	6	0	2.667216	2.102910	-0.532619
47	6	0	4.007340	2.275598	-0.856017
48	6	0	1.793540	3.180662	-0.609369
49	6	0	4.511046	3.529269	-1.195609
50	1	0	4.661638	1.414712	-0.841695
51	6	0	2.221488	4.459871	-0.970986
52	1	0	0.741167	3.009779	-0.403479
53	6	0	3.611364	4.624689	-1.173418
54	6	0	3.151451	-0.786422	-0.645962
55	6	0	2.815736	-1.498737	-1.787825
56	6	0	4.338525	-1.076820	0.026896
57	6	0	3.667768	-2.455868	-2.344897
58	1	0	1.853612	-1.308030	-2.253284
59	6	0	5.252883	-1.984401	-0.500334
60	1	0	4.542147	-0.576458	0.965968
61	6	0	4.935505	-2.584748	-1.746800
62	6	0	3.104501	-3.278178	-3.528296
63	6	0	2.969747	-2.375786	-4.768444
64	1	0	2.542532	-2.943517	-5.602438
65	1	0	2.309778	-1.524023	-4.570076
66	1	0	3.938658	-1.981688	-5.090647
67	6	0	3.913698	-4.535205	-3.891388
68	1	0	4.104786	-5.157131	-3.012320
69	1	0	3.326194	-5.129539	-4.599497
70	1	0	4.867943	-4.314028	-4.370186
71	6	0	1.695882	-3.785646	-3.136410
72	1	0	1.744576	-4.421779	-4.246551
73	1	0	0.989463	-2.974977	-2.937343
74	1	0	1.282735	-4.379587	-3.958270
75	6	0	6.516306	-2.371040	0.294881
76	6	0	6.522342	-3.898263	0.505567
77	1	0	6.635941	-4.432233	-0.439455
78	1	0	7.351884	-4.183734	1.161942
79	1	0	5.588863	-4.230535	0.970166
80	6	0	7.810778	-1.937711	-0.417600
81	1	0	7.776727	-0.876594	-0.689216
82	1	0	8.662640	-2.082881	0.255956
83	1	0	8.001636	-2.523158	-1.317385
84	6	0	6.521183	-1.710405	1.683623
85	1	0	6.598510	-0.619318	1.620428
86	1	0	5.628440	-1.962602	2.264737
87	1	0	7.393567	-2.065493	2.241031
88	8	0	5.913127	-3.327526	-2.360602
89	8	0	4.139338	5.869258	-1.409555
90	8	0	-2.438697	1.344585	5.418315
91	8	0	-5.432357	-4.188403	-1.868325
92	6	0	-5.324103	-5.547141	-1.451280
93	1	0	-6.228512	-6.051659	-1.795690
94	1	0	-4.448381	-6.037244	-1.888177
95	1	0	-5.256590	-5.621596	-0.360594
96	6	0	-2.883877	-4.089940	-3.527526
97	6	0	-4.142894	-4.492129	-4.315482
98	1	0	-3.840170	-4.759448	-5.333728
99	1	0	-4.658117	-5.356641	-3.896606
100	1	0	-4.855772	-3.665514	-4.385578
101	6	0	-1.970705	-5.317239	-3.355006
102	1	0	-1.724262	-5.745333	-4.333190
103	1	0	-1.031119	-5.046399	-2.860578
104	1	0	-2.451099	-6.098910	-2.757777
105	6	0	6.552218	-2.630567	-3.428428

106	1	0	7.344924	-3.283352	-3.797910	179	1	0	-2.445017	3.710229	5.173573
107	1	0	5.854950	-2.412852	-4.243249	180	1	0	-2.975389	4.856649	3.948305
108	1	0	6.986419	-1.687509	-3.079087	181	1	0	-3.819889	3.313326	4.131642
109	6	0	4.330233	6.668845	-0.244405	182	6	0	-2.447851	3.665212	1.728176
110	1	0	5.018675	7.468722	-0.523513	183	1	0	-1.745079	3.490944	0.909635
111	1	0	3.392791	7.115730	0.098188	184	1	0	-3.394186	3.170181	1.485219
112	1	0	4.762779	6.082788	0.572649	185	1	0	-2.626093	4.744346	1.761383
113	6	0	5.980696	3.660122	-1.651066	186	8	0	-1.684057	0.068518	-2.373923
114	6	0	6.692676	2.294002	-1.646971	187	6	0	-2.362712	1.254789	-2.631789
115	1	0	6.774328	1.874199	-0.637996	188	6	0	-3.663406	0.939981	-3.310223
116	1	0	6.195667	1.559521	-2.289631	189	6	0	-4.483147	-0.142503	-3.278704
117	1	0	7.709247	2.426128	-2.030222	190	8	0	-4.243215	1.942631	-4.027473
118	6	0	6.012593	4.191264	-3.097418	191	6	0	-5.654304	0.217650	-4.024198
119	1	0	5.535659	5.170186	-3.177269	192	1	0	-4.283650	-1.074221	-2.771685
120	1	0	7.050181	4.288705	-3.436179	193	6	0	-5.457062	1.490574	-4.447695
121	1	0	5.500463	3.500950	-3.776650	194	1	0	-6.524620	-0.394570	-4.214389
122	6	0	6.798382	4.591107	-0.735377	195	1	0	-6.039021	2.177573	-5.043243
123	1	0	6.542691	5.640916	-0.878599	196	6	0	-2.616669	1.992369	-1.305704
124	1	0	6.655420	4.336867	0.320187	197	1	0	-1.655609	2.260745	-0.863517
125	1	0	7.864456	4.480846	-0.962273	198	1	0	-3.171547	1.348731	-0.619682
126	6	0	1.128831	5.543678	-1.143879	199	8	0	-3.301175	3.229840	-1.508879
127	6	0	-0.134134	4.903043	-1.768945	200	6	0	-4.627728	3.264345	-1.312932
128	1	0	0.097389	4.370953	-2.698223	201	8	0	-5.267093	2.309175	-0.918616
129	1	0	-0.635016	4.212912	-1.086224	202	6	0	-5.207914	4.645791	-1.592901
130	1	0	-0.858905	5.688999	-2.002952	203	6	0	-4.651611	5.209443	-2.908757
131	6	0	0.722549	6.098558	0.234161	204	1	0	-4.898112	4.560142	-3.754318
132	1	0	-0.072894	6.844144	0.121486	205	1	0	-5.094836	6.193114	-3.094009
133	1	0	0.343190	5.297839	0.877705	206	1	0	-3.565816	5.327618	-2.870900
134	1	0	1.558670	6.574644	0.753647	207	6	0	-6.732048	4.532004	-1.672555
135	6	0	1.531565	6.694220	-2.084112	208	1	0	-7.156342	4.161870	-0.735349
136	1	0	0.642972	7.298072	-2.295878	209	1	0	-7.164490	5.516086	-1.878314
137	1	0	2.282066	7.360903	-1.661594	210	1	0	-7.032710	3.849951	-2.474603
138	1	0	1.911304	6.313836	-3.037837	211	6	0	-4.800407	5.556937	-0.418950
139	6	0	-6.004550	-2.257393	0.216053	212	1	0	-5.237221	6.550654	-0.561704
140	6	0	-2.148638	-3.054550	-4.412356	213	1	0	-5.164690	5.159910	0.534343
141	1	0	-2.730845	-2.132291	-4.508494	214	1	0	-3.713274	5.665964	-0.358920
142	1	0	-1.158452	-2.791118	-4.031522	215	1	0	-1.794616	1.945137	-3.284883
143	1	0	-2.003833	-3.474256	-5.413365	216	1	0	0.470257	1.673443	-2.495507
144	6	0	-6.894521	-1.696415	-0.911329	217	1	0	0.758972	1.043643	-2.840812
145	1	0	-7.904729	-1.512579	-0.528043						
146	1	0	-6.496595	-0.745430	-1.280741						
147	1	0	-6.971406	-2.391744	-1.750226						
148	6	0	-6.658471	-3.510727	0.826375						
149	1	0	-5.986946	-3.998864	1.540538						
150	1	0	-7.566840	-3.222718	1.367152						
151	1	0	-6.947422	-4.235179	0.064558						
152	6	0	-5.949672	-1.189178	1.321883						
153	1	0	-5.516502	-0.247990	0.967174						
154	1	0	-6.969276	-0.974942	1.657199						
155	1	0	-5.383100	-1.527927	2.196616						
156	6	0	-1.269661	1.633250	6.181317						
157	1	0	-1.603973	1.842014	7.199398						
158	1	0	-0.581688	0.782588	6.187253						
159	1	0	-0.741579	2.509614	5.793707						
160	6	0	-2.993271	-1.471243	5.103147						
161	6	0	-2.199433	-1.547212	6.418767						
162	1	0	-2.654802	-2.292332	7.080541						
163	1	0	-1.167627	-1.857169	6.226744						
164	1	0	-2.188024	-0.597490	6.953780						
165	6	0	-4.404841	-0.910788	5.367516						
166	1	0	-4.929003	-1.549858	6.086781						
167	1	0	-4.368009	0.101370	5.773942						
168	1	0	-4.993658	-0.891202	4.443682						
169	6	0	-3.164609	-2.913411	4.595592						
170	1	0	-3.720541	-2.957437	3.652428						
171	1	0	-2.203770	-3.420852	4.456827						
172	1	0	-3.730933	-3.484971	5.337356						
173	6	0	-1.892391	3.201861	3.094884						
174	6	0	-0.491139	3.816262	3.254467						
175	1	0	-0.557990	4.909163	3.208468						
176	1	0	-0.028679	3.547831	4.207712						
177	1	0	0.177571	3.483217	2.454032						
178	6	0	-2.835955	3.791104	4.159647						
179	1	0									
180	1	0									
181	1	0									
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190	8	0									
191	6	0									
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194	1	0									
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196	6	0									
197	1	0									
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199	8	0									
200	6	0									
201	8	0									
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212	1	0									
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217	1	0									

TS2a(R)

RwB97XD SCF energy	-5021.603774 a.u.
RwB97XD SCF enthalpy	-5019.618339 a.u.
RwB97XD SCF free energy	-5019.864415 a.u.
Three lowest frequencies (cm ⁻¹)	-1042, 8.2, 14.9
Imaginary frequency (cm ⁻¹)	-1042

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X	Coordinates Y	Coordinates Z (Angstroms)
1	6	0	1.443941	0.043852	2.567073
2	6	0	1.377158	0.569004	3.843141
3	6	0	1.788669	1.850475	4.163179
4	6	0	2.249337	2.721134	3.207029
5	6	0	2.313152	2.229546	1.895663
6	6	0	1.935879	0.927899	1.568476
7	1	0	2.565245	3.728153	3.451377
8	1	0	2.688318	2.892583	1.125733
9	6	0	1.111266	-1.387071	2.348771
10	6	0	0.096289	-1.901142	1.495906
11	6	0	1.853420	-2.324553	3.034896
12	6	0	-0.085182	-3.277833	1.371607
13	6	0	1.663223	-3.695641	2.902043
14	6	0	0.701414	-4.208492	2.066932
15	1	0	-0.867550	-3.664105	0.730170
16	1	0	0.544705	-5.274837	1.956013
17	8	0	1.648518	2.049681	5.499838
18	8	0	0.932943	-0.062923	4.972139
19	8	0	2.883416	-2.093648	3.895750
20	8	0	2.562835	-4.352944	3.684311
21	6	0	1.407385	0.749301	6.045895
22	1	0	0.648267	0.815049	6.823494
23	1	0	2.350015	0.336628	6.424649

24	6	0	3.118788	-3.347575	4.536628	106	1	0	7.152606	-4.821536	-2.029400
25	1	0	2.600433	-3.364527	5.502627	107	1	0	5.796958	-4.044547	-2.887766
26	1	0	4.190947	-3.507163	4.644184	108	1	0	6.891991	-3.060027	-1.890588
27	15	0	-0.917162	-0.749814	0.497070	109	6	0	5.398576	5.821090	-2.322709
28	15	0	2.059232	0.379939	-0.163350	110	1	0	6.392161	6.120780	-2.664279
29	46	0	0.165250	0.032258	-1.376295	111	1	0	4.707460	6.643644	-2.526341
30	6	0	-1.448068	0.555798	1.629497	112	1	0	5.430098	5.626019	-1.246693
31	6	0	-2.005787	0.212331	2.862368	113	6	0	6.506886	2.264332	-2.397570
32	6	0	-1.346976	1.889196	1.263840	114	6	0	6.986484	0.884544	-1.907093
33	6	0	-2.403712	1.186997	3.767819	115	1	0	6.967714	0.806267	-0.814269
34	1	0	-2.127915	-0.835904	3.105873	116	1	0	6.395109	0.062844	-2.325083
35	6	0	-1.718953	2.922182	2.133841	117	1	0	8.022328	0.738194	-2.228381
36	1	0	-0.949679	2.131105	0.282923	118	6	0	6.653551	2.278932	-3.931298
37	6	0	-2.143828	2.537357	3.419094	119	1	0	6.363653	3.241712	-4.355398
38	6	0	-2.397517	-1.668519	-0.007515	120	1	0	7.696052	2.082996	-4.206511
39	6	0	-3.655175	-1.400019	0.529636	121	1	0	6.032817	1.499019	-4.386333
40	6	0	-2.267175	-2.647105	-0.985118	122	6	0	7.445439	3.309511	-1.766498
41	6	0	-4.765655	-2.167625	0.187153	123	1	0	7.339895	4.291135	-2.225723
42	1	0	-3.765341	-0.581328	1.225601	124	1	0	7.263006	3.405814	-0.690678
43	6	0	-3.341771	-3.441960	-1.391567	125	1	0	8.486216	2.995845	-1.902863
44	1	0	-1.295402	-2.798270	-1.441050	126	6	0	2.042522	4.991722	-2.671242
45	6	0	-4.563411	-3.243020	-0.714393	127	6	0	0.576232	4.527722	-2.835585
46	6	0	2.986418	1.675748	-1.025351	128	1	0	0.499822	3.635127	-3.466912
47	6	0	4.334897	1.531724	-1.318252	129	1	0	0.085364	4.322805	-1.878954
48	6	0	2.299229	2.801352	-1.462511	130	1	0	0.003311	5.328060	-3.313819
49	6	0	5.031416	2.516312	-2.017310	131	6	0	2.035289	6.124214	-1.626349
50	1	0	4.843730	0.632301	-1.002361	132	1	0	1.362428	6.926568	-1.949679
51	6	0	2.927158	3.824057	-2.173332	133	1	0	1.676310	5.749764	-0.662297
52	1	0	1.237122	2.865688	-1.257077	134	1	0	3.022875	6.559340	-1.466761
53	6	0	4.321218	3.684227	-2.391150	135	6	0	2.474967	5.517937	-4.052522
54	6	0	3.055925	-1.126587	-0.203711	136	1	0	1.738901	6.249202	-4.402263
55	6	0	2.714206	-2.116211	-1.112733	137	1	0	3.448665	6.004017	-4.047803
56	6	0	4.157802	-1.304917	0.633670	138	1	0	2.509800	4.702244	-4.783096
57	6	0	3.483401	-3.271236	-1.276724	139	6	0	-6.159412	-1.786024	0.735858
58	1	0	1.817512	-1.986865	-1.709930	140	6	0	-2.209717	-3.747762	-3.624159
59	6	0	4.994886	-2.406664	0.485737	141	1	0	-2.705960	-2.850469	-4.005796
60	1	0	4.359638	-0.561340	1.394837	142	1	0	-1.214277	-3.466134	-3.272109
61	6	0	4.687549	-3.327155	-0.550121	143	1	0	-2.065445	-4.437982	-4.461726
62	6	0	2.906565	-4.357495	-2.214540	144	6	0	-7.096063	-1.451808	-0.442003
63	6	0	2.968358	-3.869313	-3.673311	145	1	0	-8.099023	-1.223890	-0.063225
64	1	0	2.531356	-4.621627	-4.339422	146	1	0	-6.738302	-0.571841	-0.986841
65	1	0	2.406787	-2.937764	-3.804652	147	1	0	-7.178949	-2.287676	-1.140296
66	1	0	3.998772	-3.690188	-3.996085	148	6	0	-6.783572	-2.908045	1.587677
67	6	0	3.579413	-5.736742	-2.104987	149	1	0	-6.078256	-3.273444	2.342039
68	1	0	3.627755	-6.079037	-1.067207	150	1	0	-7.661250	-2.517037	2.114014
69	1	0	2.976948	-6.457880	-2.667877	151	1	0	-7.116850	-3.750396	0.981626
70	1	0	4.585811	-5.762446	-2.523124	152	6	0	-6.086834	-0.536771	1.632194
71	6	0	1.422577	-4.583684	-1.838814	153	1	0	-5.682784	0.332624	1.105648
72	1	0	1.327538	-4.910317	-0.797770	154	1	0	-7.099003	-0.280563	1.961027
73	1	0	0.806490	-3.690372	-1.973801	155	1	0	-5.485425	-0.713115	2.530942
74	1	0	1.001669	-5.363759	-2.481619	156	6	0	-1.113775	3.879894	5.016590
75	6	0	6.155818	-2.641831	1.473655	157	1	0	-1.373611	4.628718	5.767260
76	6	0	5.965245	-4.019410	2.138972	158	1	0	-0.629279	3.026808	5.500397
77	1	0	6.073516	-4.831661	1.417893	159	1	0	-0.413047	4.315462	4.296340
78	1	0	6.711255	-4.161576	2.928809	160	6	0	-3.192299	0.796038	5.034458
79	1	0	4.969948	-4.097554	2.587571	161	6	0	-2.479815	1.194850	6.338201
80	6	0	7.533287	-2.578485	0.787501	162	1	0	-3.003976	0.749342	7.190827
81	1	0	7.639997	-1.660984	0.197831	163	1	0	-1.452202	0.819716	6.345396
82	1	0	8.320234	-2.578954	1.549939	164	1	0	-2.464437	2.274156	6.488696
83	1	0	7.709321	-3.434639	0.135955	165	6	0	-4.574712	1.475284	4.967247
84	6	0	6.157468	-1.583521	2.589908	166	1	0	-5.171428	1.194449	5.842455
85	1	0	6.359176	-0.577947	2.203838	167	1	0	-4.485925	2.564110	4.951349
86	1	0	5.211372	-1.562344	3.139820	168	1	0	-5.119466	1.160053	4.070290
87	1	0	6.951986	-1.823655	3.303284	169	6	0	-3.422535	-0.723139	5.098083
88	8	0	5.608373	-4.309185	-0.818050	170	1	0	-3.957270	-1.100476	4.220009
89	8	0	5.030976	4.653628	-3.054320	171	1	0	-2.481971	-1.276395	5.197525
90	8	0	-2.334464	3.488428	4.390495	172	1	0	-4.033663	-0.952303	5.976567
91	8	0	-5.627556	-4.080890	-0.942522	173	6	0	-1.652359	4.365757	1.577030
92	6	0	-5.556738	-5.312639	-0.226955	174	6	0	-0.186060	4.758399	1.326808
93	1	0	-6.533454	-5.789423	-0.329285	175	1	0	-0.141454	5.760481	0.885781
94	1	0	-4.791429	-5.977370	-0.637532	176	1	0	0.391517	4.771010	2.256289
95	1	0	-5.341659	-5.143255	0.832840	177	1	0	0.303326	4.063389	0.635572
96	6	0	-3.064917	-4.443274	-2.539364	178	6	0	-2.317817	5.449560	2.443517
97	6	0	-4.318897	-4.956578	-3.269136	179	1	0	-1.769998	5.669595	3.359967
98	1	0	-3.996763	-5.517398	-4.153232	180	1	0	-2.351539	6.375490	1.858816
99	1	0	-4.932032	-5.627465	-2.669012	181	1	0	-3.344594	5.183561	2.707721
100	1	0	-4.944350	-4.126862	-3.810795	182	6	0	-2.406373	4.395802	0.229120
101	6	0	-2.256818	-5.631627	-1.984770	183	1	0	-1.973365	3.724303	-0.514250
102	1	0	-1.998095	-6.323157	-2.794732	184	1	0	-3.456058	4.120675	0.369556
103	1	0	-1.324631	-5.288498	-1.523260	185	1	0	-2.369419	5.407919	-0.187343
104	1	0	-2.817293	-6.190947	-1.229731	186	8	0	-1.183642	-0.273298	-3.054521
105	6	0	6.398521	-4.034324	-1.973583	187	6	0	-2.226367	0.632800	-3.356115

188	6	0	-3.467677	-0.128679	-3.689747
189	6	0	-4.519180	-0.572559	-2.952593
190	8	0	-3.606044	-0.537373	-4.983640
191	6	0	-5.366733	-1.300768	-3.847024
192	1	0	-4.666942	-0.405070	-1.896629
193	6	0	-4.761156	-1.249377	-5.060819
194	1	0	-6.298712	-1.794724	-3.611623
195	1	0	-5.011312	-1.642069	-6.034805
196	6	0	-2.456309	1.571265	-2.172144
197	1	0	-1.553034	2.167802	-2.011522
198	1	0	-2.678991	0.995807	-1.272776
199	8	0	-3.528930	2.472794	-2.445160
200	6	0	-4.579763	2.474399	-1.610507
201	8	0	-4.610174	1.828367	-0.581189
202	6	0	-5.708578	3.355831	-2.125380
203	6	0	-6.248970	2.717144	-3.418767
204	1	0	-6.619731	1.703388	-3.234446
205	1	0	-7.079527	3.320180	-3.799417
206	1	0	-5.477792	2.665488	-4.192358
207	6	0	-6.813209	3.421322	-1.069129
208	1	0	-6.444233	3.852738	-0.133475
209	1	0	-7.631397	4.049169	-1.435333
210	1	0	-7.215922	2.428067	-0.850426
211	6	0	-5.168654	4.765276	-2.417661
212	1	0	-5.986140	5.397164	-2.779234
213	1	0	-4.758123	5.226792	-1.513583
214	1	0	-4.387766	4.746700	-3.182180
215	1	0	-1.953527	1.236883	-4.235060
216	1	0	0.940428	0.582988	-2.882169
217	1	0	0.111485	0.316427	-3.171876

6a(R)*2a

RwB97XD SCF energy -5021.645700 a.u.
 RwB97XD SCF enthalpy -5019.653781 a.u.
 RwB97XD SCF free energy -5019.902454 a.u.
 Three lowest frequencies (cm⁻¹) 11.0, 15.1, 18.0

Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.688650	2.111464	-1.190042
2	6	0	-1.915355	3.466590	-1.317884
3	6	0	-2.717127	4.197247	-0.447827
4	6	0	-3.314971	3.610259	0.638815
5	6	0	-3.086946	2.237397	0.809194
6	6	0	-2.308983	1.484630	-0.071720
7	1	0	-3.938347	4.171091	1.324765
8	1	0	-3.554897	1.754928	1.658877
9	6	0	-0.911763	1.453774	-2.279321
10	6	0	0.382674	0.875734	-2.171747
11	6	0	-1.449797	1.493209	-3.548066
12	6	0	1.018587	0.366559	-3.302322
13	6	0	-0.804120	0.985793	-4.668995
14	6	0	0.434760	0.401474	-4.578564
15	1	0	2.011119	-0.058036	-3.217174
16	1	0	0.947420	0.004059	-5.446626
17	8	0	-2.775807	5.491720	-0.860801
18	8	0	-1.422333	4.300072	-2.279269
19	8	0	-2.657737	2.007790	-3.917387
20	8	0	-1.592721	1.172806	-5.767018
21	6	0	-2.197477	5.493030	-2.168796
22	1	0	-1.553320	6.364000	-2.279703
23	1	0	-2.997034	5.476909	-2.919167
24	6	0	-2.603091	2.089667	-5.340945
25	1	0	-2.317386	3.107529	-5.633505
26	1	0	-3.564867	1.797527	-5.761515
27	15	0	1.148518	0.797003	-0.509048
28	15	0	-2.023582	-0.288062	0.316654
29	46	0	0.041185	-0.534997	1.152216
30	6	0	1.175597	2.526861	0.043877
31	6	0	1.689715	3.549494	-0.753741
32	6	0	0.729184	2.816661	1.322925
33	6	0	1.694085	4.869800	-0.318273
34	1	0	2.099602	3.292100	-1.723024
35	6	0	0.712278	4.120459	1.830498
36	1	0	0.368279	2.000992	1.941748
37	6	0	1.098174	5.140522	0.942120
38	6	0	2.898790	0.345231	-0.752801

39	6	0	3.915230	1.177072	-0.288824
40	6	0	3.239169	-0.894145	-1.285489
41	6	0	5.260055	0.856865	-0.456529
42	1	0	3.647965	2.100096	0.204568
43	6	0	4.569569	-1.279120	-1.492471
44	1	0	2.446847	-1.582281	-1.558378
45	6	0	5.561245	-0.332312	-1.161334
46	6	0	-3.394280	-0.712988	1.446242
47	6	0	-4.607932	-1.205369	0.972467
48	6	0	-3.240123	-0.499654	2.808814
49	6	0	-5.695710	-1.402305	1.819172
50	1	0	-4.707371	-1.435825	-0.077662
51	6	0	-4.282663	-0.693927	3.720086
52	1	0	-2.276579	-0.161186	3.173390
53	6	0	-5.536168	-1.043896	3.179590
54	6	0	-2.337069	-1.215782	-1.208328
55	6	0	-1.518020	-2.266846	-1.529678
56	6	0	-3.412327	-0.894821	-2.042105
57	6	0	-1.785425	-3.116841	-2.626010
58	1	0	-0.643815	-2.474701	-0.912136
59	6	0	-3.772190	-1.720812	-3.101622
60	1	0	-3.981654	0.004099	-1.837497
61	6	0	-2.993367	-2.887276	-3.307432
62	6	0	-0.695539	-4.146108	-3.001622
63	6	0	-0.542810	-5.186796	-1.878152
64	1	0	0.258385	-5.891776	-2.126109
65	1	0	-0.288280	-4.712087	-0.925188
66	1	0	-1.465643	-5.758272	-1.735058
67	6	0	-0.892920	-4.877615	-4.340456
68	1	0	-1.073133	-4.179789	-5.162054
69	1	0	0.029159	-5.425531	-4.564558
70	1	0	-1.701887	-5.608954	-4.321438
71	6	0	0.631730	-3.367743	-3.141977
72	1	0	0.565271	-2.619837	-3.939326
73	1	0	0.905926	-2.851889	-2.218826
74	1	0	1.441261	-4.062529	-3.387578
75	6	0	-4.915700	-1.324575	-4.057177
76	6	0	-4.333660	-1.198700	-5.478925
77	1	0	-3.970370	-2.160389	-5.848257
78	1	0	-5.101150	-0.835909	-6.172096
79	1	0	-3.496710	-0.494393	-5.494916
80	6	0	-6.071210	-2.343318	-4.059378
81	1	0	-6.415103	-2.557313	-3.041944
82	1	0	-6.919401	-1.927907	-4.614841
83	1	0	-5.792306	-3.281095	-4.540443
84	6	0	-5.514697	0.037516	-3.670236
85	1	0	-6.001919	0.006938	-2.688866
86	1	0	-4.762022	0.830763	-3.660505
87	1	0	-6.277861	0.311026	-4.405433
88	8	0	-3.447319	-3.804080	-4.223262
89	8	0	-6.654117	-1.062571	-3.978566
90	8	0	0.918063	6.458603	1.287720
91	8	0	6.873562	-0.554742	-1.502145
92	6	0	7.158355	-0.243860	-2.863938
93	1	0	8.227441	-0.411149	-3.006652
94	1	0	6.599216	-0.885179	-3.551768
95	1	0	6.917596	0.800179	-3.090566
96	6	0	4.806104	-2.708345	-2.041482
97	6	0	6.247517	-3.235169	-1.914498
98	1	0	6.241462	-4.306571	-2.144340
99	1	0	6.945222	-2.763413	-2.606987
100	1	0	6.630472	-3.111001	-0.898909
101	6	0	4.369296	-2.765483	-3.517320
102	1	0	4.474786	-3.785842	-3.903222
103	1	0	3.322859	-2.467158	-3.638711
104	1	0	4.978761	-2.107485	-4.144567
105	6	0	-4.051318	-4.939874	-3.608327
106	1	0	-4.369732	-5.602399	-4.415162
107	1	0	-3.347827	-5.471603	-2.959626
108	1	0	-4.922248	-4.648296	-3.010696
109	6	0	-7.202803	0.235617	4.196545
110	1	0	-8.140925	0.093395	4.736178
111	1	0	-6.534736	0.862495	4.795581
112	1	0	-7.399474	0.745596	3.247659
113	6	0	-6.982741	-2.057085	1.273647
114	6	0	-6.825287	-2.442404	-0.208418
115	1	0	-6.689273	-1.563488	-0.848062
116	1	0	-5.986672	-3.126682	-0.375815
117	1	0	-7.735067	-2.951580	-0.541467
118	6	0	-7.259540	-3.352066	2.061911
119	1	0	-7.408948	-3.151736	3.125012
120	1	0	-8.164373	-3.835289	1.676390

121	1	0	-6.429158	-4.059103	1.957373	203	6	0	5.310627	-5.636085	1.880808
122	6	0	-8.206217	-1.126247	1.365553	204	1	0	5.299205	-5.581371	0.787223
123	1	0	-8.533231	-0.977451	2.394753	205	1	0	5.677803	-6.626949	2.166729
124	1	0	-7.998449	-0.149057	0.916706	206	1	0	4.284099	-5.532981	2.243490
125	1	0	-9.044073	-1.572176	0.818228	207	6	0	7.653140	-4.722023	1.934601
126	6	0	-3.925323	-0.532669	5.216744	208	1	0	8.325395	-3.955332	2.330895
127	6	0	-2.634833	-1.340225	5.495819	209	1	0	8.045286	-5.702065	2.223553
128	1	0	-2.783390	-2.401313	5.267967	210	1	0	7.669796	-4.657467	0.842300
129	1	0	-1.772007	-0.989400	4.923395	211	6	0	6.234237	-4.661657	4.015307
130	1	0	-2.375379	-1.256050	6.556309	212	1	0	6.641598	-5.632435	4.314691
131	6	0	-3.655561	0.952699	5.520159	213	1	0	6.857544	-3.880160	4.462471
132	1	0	-3.371807	1.079805	6.570850	214	1	0	5.224016	-4.573335	4.424226
133	1	0	-2.840262	1.344293	4.902253	215	1	0	2.707664	-1.596832	3.987006
134	1	0	-4.542092	1.567607	5.334174	216	1	0	1.646226	0.069829	3.323294
135	6	0	-4.971150	-1.072768	6.208378	217	1	0	-0.729834	-1.382488	2.206130
136	1	0	-4.530537	-1.054964	7.211076						
137	1	0	-5.882730	-0.476610	6.250100						
138	1	0	-5.244456	-2.107527	5.983913						
139	6	0	6.345949	1.761537	0.164452						
140	6	0	3.933195	-3.696008	-1.235540						
141	1	0	4.185550	-3.665512	-0.171465						
142	1	0	2.863669	-3.504092	-1.340491						
143	1	0	4.107840	-4.715572	-1.594319						
144	6	0	7.208598	0.926552	1.130039						
145	1	0	7.978573	1.562791	1.581151						
146	1	0	6.598492	0.510363	1.938502						
147	1	0	7.705902	0.102092	0.616052						
148	6	0	7.249439	2.411088	-0.900625						
149	1	0	6.656391	2.892964	-1.685532						
150	1	0	7.869365	3.182522	-0.430806						
151	1	0	7.922561	1.688020	-1.362616						
152	6	0	5.719537	2.904790	0.982845						
153	1	0	5.064777	2.536332	1.780073						
154	1	0	6.520548	3.480900	1.456542						
155	1	0	5.144029	3.596645	0.357523						
156	6	0	-0.422839	6.899037	1.085912						
157	1	0	-0.440007	7.966096	1.316352						
158	1	0	-0.734506	6.741006	0.049061						
159	1	0	-1.124155	6.375172	1.743748						
160	6	0	2.415027	5.957934	-1.141059						
161	6	0	1.454440	7.040658	-1.662882						
162	1	0	1.988835	7.699805	-2.355917						
163	1	0	0.620470	6.588027	-2.208419						
164	1	0	1.056341	7.662531	-0.860754						
165	6	0	3.505178	6.603690	-0.263160						
166	1	0	4.049561	7.359793	-0.840145						
167	1	0	3.079473	7.089319	0.617114						
168	1	0	4.228689	5.852471	0.072926						
169	6	0	3.118099	5.350786	-2.367040						
170	1	0	3.839020	4.574894	-2.087735						
171	1	0	2.407544	4.924534	-3.083512						
172	1	0	3.669817	6.141139	-2.885892						
173	6	0	0.317837	4.276044	3.318414						
174	6	0	-1.181459	3.979401	3.498635						
175	1	0	-1.445988	4.024770	4.561288						
176	1	0	-1.803457	4.703851	2.964230						
177	1	0	-1.435168	2.980979	3.126578						
178	6	0	0.643264	5.644395	3.942258						
179	1	0	0.013612	6.450709	3.566130						
180	1	0	0.473791	5.578019	5.022480						
181	1	0	1.689614	5.920784	3.783628						
182	6	0	1.119371	3.236013	4.137494						
183	1	0	0.853481	2.203878	3.890671						
184	1	0	2.196722	3.357868	3.981806						
185	1	0	0.913157	3.374220	5.203879						
186	8	0	1.869860	-0.472766	2.465314						
187	6	0	2.509682	-1.691711	2.916147						
188	6	0	1.615312	-2.855457	2.684251						
189	6	0	1.417813	-3.697724	1.633339						
190	8	0	0.707725	-3.114935	3.665270						
191	6	0	0.306467	-4.527775	1.988054						
192	1	0	1.995324	-3.724513	0.720628						
193	6	0	-0.083501	-4.124856	3.224502						
194	1	0	-0.131667	-5.324573	1.404367						
195	1	0	-0.852361	-4.455295	3.906233						
196	6	0	3.820900	-1.767185	2.151589						
197	1	0	4.448696	-0.913891	2.416584						
198	1	0	3.641690	-1.756384	1.073144						
199	8	0	4.452898	-2.991228	2.525032						
200	6	0	5.703593	-3.187137	2.086620						
201	8	0	6.309029	-2.345171	1.454502						
202	6	0	6.233257	-4.559881	2.479708						

2.4. Catalytic cycle 2a –1b (S).

3a(S)-1b

RwB97XD SCF energy -5094.190888 a.u.

RwB97XD SCF enthalpy -5092.254020 a.u.

RwB97XD SCF free energy -5092.494971 a.u.

Three lowest frequencies (cm⁻¹) 16.7, 17.0, 22.7

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.093825	-0.596982	2.572418
2	6	0	0.328614	-1.473368	3.549850
3	6	0	-0.138481	-2.780533	3.661852
4	6	0	-1.074204	-3.283822	2.793810
5	6	0	-1.505419	-2.423625	1.774904
6	6	0	-1.040804	-1.113196	1.645088
7	1	0	-1.457454	-4.293480	2.880503
8	1	0	-2.224546	-2.813911	1.066257
9	6	0	0.439409	0.793514	2.636683
10	6	0	1.419588	1.346354	1.767963
11	6	0	0.061176	1.581052	3.701622
12	6	0	1.937354	2.616029	2.008868
13	6	0	0.578007	2.853289	3.928760
14	6	0	1.524789	3.401595	3.098268
15	1	0	2.694146	3.021461	1.347415
16	1	0	1.943449	4.385663	3.273527
17	8	0	0.436329	-3.376220	4.738242
18	8	0	1.206331	-1.223610	4.559405
19	8	0	-0.836567	1.276896	4.679640
20	8	0	0.005079	3.376334	5.048518
21	6	0	1.514487	-2.508782	5.094175
22	1	0	2.433781	-2.879374	4.630356
23	1	0	1.597499	-2.446116	6.178816
24	6	0	-0.621350	2.262657	5.687347
25	1	0	0.052360	1.856998	6.453265
26	1	0	-1.576432	2.568555	6.112968
27	15	0	1.911202	0.351383	0.311374
28	15	0	-1.557906	-0.138821	0.175349
29	46	0	0.133180	0.048862	-1.266854
30	6	0	2.646733	-1.153171	1.011744
31	6	0	3.628450	-1.086701	1.996282
32	6	0	2.305566	-2.381944	0.467453
33	6	0	4.295989	-2.224446	2.448728
34	1	0	3.891894	-0.114136	2.396427
35	6	0	2.893621	-3.572275	0.905870
36	1	0	1.551460	-2.405902	-0.314010
37	6	0	3.853753	-3.471944	1.937136
38	6	0	3.289179	1.218696	-0.504191
39	6	0	4.520951	0.603450	-0.715332
40	6	0	3.036155	2.444875	-1.108053
41	6	0	5.538952	1.236871	-1.425173
42	1	0	4.684196	-0.389795	-0.320504
43	6	0	4.013860	3.140969	-1.824777
44	1	0	2.043902	2.874182	-1.015337
45	6	0	5.296414	2.556331	-1.876386
46	6	0	-2.971046	-1.108972	-0.435995
47	6	0	-4.239502	-1.018879	0.134184
48	6	0	-2.716967	-2.115713	-1.356385
49	6	0	-5.206350	-1.996057	-0.089153
50	1	0	-4.464822	-0.186126	0.785195
51	6	0	-3.645704	-3.121170	-1.640181
52	1	0	-1.749490	-2.136590	-1.846652
53	6	0	-4.835436	-3.107154	-0.887278
54	6	0	-2.160165	1.457060	0.788346
55	6	0	-1.773424	2.640322	0.168814
56	6	0	-2.991167	1.505847	1.910196
57	6	0	-2.272317	3.883149	0.582807
58	1	0	-1.062034	2.592646	-0.651226
59	6	0	-3.585245	2.695957	2.313676
60	1	0	-3.178341	0.592659	2.461600
61	6	0	-3.294634	3.853947	1.552579

62	6	0	-1.621412	5.165217	0.004931
63	6	0	-2.000878	5.384007	-1.468836
64	1	0	-1.509950	6.290106	-1.842337
65	1	0	-1.673349	4.548974	-2.094257
66	1	0	-3.079266	5.517639	-1.601630
67	6	0	-1.930023	6.448597	0.798281
68	1	0	-1.765301	6.311129	1.870566
69	1	0	-1.249986	7.234441	0.451270
70	1	0	-2.947647	6.811697	0.651620
71	6	0	-0.088449	4.988303	0.073594
72	1	0	0.247185	4.847591	1.105415
73	1	0	0.265133	4.140286	-0.518203
74	1	0	0.395472	5.885431	-0.325669
75	6	0	-4.462412	2.747902	3.579501
76	6	0	-3.933805	3.849680	4.520285
77	1	0	-4.072114	4.842407	4.089845
78	1	0	-4.462550	3.810121	5.478850
79	1	0	-2.865173	3.712935	4.712146
80	6	0	-5.938949	3.019436	3.238311
81	1	0	-6.313502	2.296089	2.505154
82	1	0	-6.548309	2.924907	4.144138
83	1	0	-6.087030	4.025614	2.843328
84	6	0	-4.401147	1.417299	4.348015
85	1	0	-4.850463	0.592072	3.784741
86	1	0	-3.372318	1.144053	4.603814
87	1	0	-4.964788	1.518593	5.280750
88	8	0	-4.031070	4.979827	1.814998
89	8	0	-5.675419	-4.191868	-0.907075
90	8	0	4.398504	-4.626257	2.432527
91	8	0	6.356643	3.255317	-2.400276
92	6	0	6.921012	4.183144	-1.479643
93	1	0	7.805138	4.605917	-1.960590
94	1	0	6.222685	4.991259	-1.238791
95	1	0	7.214431	3.689116	-0.546803
96	6	0	3.569812	4.455606	-2.509569
97	6	0	4.529311	4.988110	-3.588600
98	1	0	4.031449	5.810130	-4.114778
99	1	0	5.461183	5.381477	-3.183035
100	1	0	4.776123	4.218109	-4.324817
101	6	0	3.355219	5.538983	-1.436565
102	1	0	2.963080	6.454322	-1.894283
103	1	0	2.638707	5.205841	-0.679432
104	1	0	4.290009	5.791034	-0.926201
105	6	0	-5.010191	5.251459	0.817911
106	1	0	-5.539913	6.150630	1.137548
107	1	0	-4.555014	5.429104	-0.161225
108	1	0	-5.723369	4.423556	0.729757
109	6	0	-5.214616	-5.251191	-0.072520
110	1	0	-5.983116	-6.025842	-0.095124
111	1	0	-4.268315	-5.669077	-0.431971
112	1	0	-5.070953	-4.909126	0.958387
113	6	0	-6.616399	-1.844443	0.519526
114	6	0	-6.801785	-0.449280	1.142657
115	1	0	-6.163941	-0.301263	2.020822
116	1	0	-6.596239	0.351851	0.424517
117	1	0	-7.839119	-0.341188	1.474568
118	6	0	-7.685086	-2.007508	-0.578827
119	1	0	-7.626599	-2.989818	-1.049830
120	1	0	-8.683129	-1.893781	-0.141157
121	1	0	-7.571444	-1.244184	-1.355015
122	6	0	-6.867786	-2.880948	1.631269
123	1	0	-6.977801	-3.888769	1.228758
124	1	0	-6.055379	-2.880725	2.365887
125	1	0	-7.796350	-2.635097	2.158754
126	6	0	-3.254672	-4.120967	-2.753185
127	6	0	-2.031528	-4.944015	-2.303319
128	1	0	-1.168607	-4.302419	-2.095185
129	1	0	-2.248949	-5.520195	-1.397588
130	1	0	-1.742325	-5.647954	-3.091523
131	6	0	-4.367810	-5.080511	-3.208383
132	1	0	-4.027742	-5.588835	-4.117245
133	1	0	-4.598774	-5.853582	-2.475052
134	1	0	-5.291020	-4.546462	-3.446545

135	6	0	-2.867383	-3.303095	-4.005956
136	1	0	-2.539094	-3.983103	-4.798582
137	1	0	-3.728187	-2.738556	-4.379374
138	1	0	-2.053345	-2.597737	-3.818951
139	6	0	6.836131	0.471858	-1.763514
140	6	0	2.223908	4.203577	-3.229620
141	1	0	2.320298	3.399919	-3.967931
142	1	0	1.410912	3.942121	-2.549073
143	1	0	1.917294	5.112473	-3.757890
144	6	0	7.029540	0.470163	-3.293240
145	1	0	7.936369	-0.087451	-3.554184
146	1	0	6.181654	-0.014769	-3.789953
147	1	0	7.127504	1.483909	-3.686006
148	6	0	8.074371	1.088608	-1.086475
149	1	0	7.913147	1.225097	-0.011781
150	1	0	8.933273	0.420389	-1.214112
151	1	0	8.338652	2.050676	-1.526120
152	6	0	6.752903	-0.999185	-1.318514
153	1	0	5.901220	-1.519512	-1.769581
154	1	0	7.662503	-1.516749	-1.638931
155	1	0	6.683544	-1.106441	-0.230978
156	6	0	3.736051	-5.140781	3.576528
157	1	0	4.121926	-6.149242	3.739041
158	1	0	3.945725	-4.537698	4.467930
159	1	0	2.650533	-5.187696	3.426151
160	6	0	5.470998	-2.006679	3.438069
161	6	0	4.927588	-1.727943	4.851607
162	1	0	5.745977	-1.421268	5.512766
163	1	0	4.181842	-0.926179	4.840762
164	1	0	4.469582	-2.619126	5.290507
165	6	0	6.479077	-3.168379	3.508845
166	1	0	7.348405	-2.836155	4.086986
167	1	0	6.077849	-4.054266	3.999722
168	1	0	6.828972	-3.459208	2.513985
169	6	0	6.284109	-0.769021	2.989944
170	1	0	6.633541	-0.875574	1.957814
171	1	0	5.724095	0.166419	3.064334
172	1	0	7.163480	-0.664557	3.633289
173	6	0	2.440881	-4.859448	0.172309
174	6	0	0.941331	-5.088192	0.443822
175	1	0	0.593158	-5.973529	-0.100560
176	1	0	0.758720	-5.252920	1.511020
177	1	0	0.330086	-4.237290	0.126379
178	6	0	3.187360	-6.155696	0.528849
179	1	0	2.985297	-6.494803	1.546074
180	1	0	2.837618	-6.941829	-0.150145
181	1	0	4.267368	-6.057106	0.404497
182	6	0	2.650772	-4.643175	-1.343260
183	1	0	2.084840	-3.791644	-1.727724
184	1	0	3.708986	-4.473380	-1.569667
185	1	0	2.326127	-5.535231	-1.890076
186	8	0	1.425082	0.031808	-3.069549
187	6	0	0.839795	-0.215992	-4.136698
188	1	0	-1.097603	-0.083935	-2.205403
189	6	0	0.710563	-1.554787	-4.635030
190	6	0	0.213135	-2.068032	-5.811976
191	8	0	1.133526	-2.575304	-3.834159
192	6	0	0.342151	-3.472853	-5.720595
193	1	0	-0.191422	-1.500742	-6.638236
194	6	0	0.899172	-3.715501	-4.495600
195	1	0	0.055723	-4.211087	-6.454186
196	1	0	1.176894	-4.627793	-3.988050
197	6	0	0.195743	0.905559	-4.946502
198	1	0	0.346525	0.765863	-6.017360
199	1	0	0.610086	1.861184	-4.625666
200	8	0	-1.213038	0.849369	-4.702661
201	6	0	-1.732382	1.766434	-3.858009
202	8	0	-1.119805	2.745518	-3.488501
203	6	0	-3.117632	1.431467	-3.439148
204	6	0	-3.753954	0.255716	-3.847820
205	6	0	-3.762324	2.303959	-2.558108
206	6	0	-5.038000	-0.037044	-3.380444
207	1	0	-3.247182	-0.427922	-4.518502

208	6	0	-5.034797	2.006565	-2.089014
209	1	0	-3.258549	3.207147	-2.240494
210	6	0	-5.670982	0.838131	-2.504141
211	1	0	-5.523560	-0.952759	-3.691712
212	1	0	-5.527361	2.684911	-1.399121
213	1	0	-6.668617	0.611663	-2.142307

TS1a (S) -1b

RwB97XD SCF energy -5094.180672 a.u.
 RwB97XD SCF enthalpy -5092.245983 a.u.
 RwB97XD SCF free energy -5092.484916 a.u.
 Three lowest frequencies (cm⁻¹) -617.5, 9.4, 16.7
 Imaginary frequency (cm⁻¹) -617.5

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.032458	-0.530011	2.523491
2	6	0	0.393322	-1.389045	3.515228
3	6	0	-0.042272	-2.707115	3.626414
4	6	0	-0.945483	-3.241143	2.742329
5	6	0	-1.384662	-2.395858	1.714256
6	6	0	-0.953863	-1.074469	1.585573
7	1	0	-1.303505	-4.260224	2.828179
8	1	0	-2.086198	-2.805606	0.998869
9	6	0	0.481364	0.867235	2.564591
10	6	0	1.391054	1.440056	1.634986
11	6	0	0.148490	1.657244	3.642179
12	6	0	1.874723	2.732698	1.817650
13	6	0	0.631634	2.951495	3.815115
14	6	0	1.496021	3.524271	2.913926
15	1	0	2.580881	3.148441	1.108406
16	1	0	1.884020	4.527270	3.046728
17	8	0	0.527074	-3.281181	4.717181
18	8	0	1.252149	-1.113100	4.532978
19	8	0	-0.673061	1.339910	4.679577
20	8	0	0.114290	3.473180	4.960782
21	6	0	1.576970	-2.386195	5.087660
22	1	0	2.513980	-2.740053	4.647423
23	1	0	1.634172	-2.310951	6.173174
24	6	0	-0.435105	2.351603	5.656144
25	1	0	0.295550	1.985759	6.388608
26	1	0	-1.375307	2.634098	6.128925
27	15	0	1.894211	0.416244	0.213885
28	15	0	-1.469812	-0.130924	0.093279
29	46	0	0.257030	-0.110960	-1.383684
30	6	0	2.638056	-1.063843	0.951096
31	6	0	3.578582	-0.949639	1.970130
32	6	0	2.376320	-2.306551	0.394739
33	6	0	4.287713	-2.054519	2.441385
34	1	0	3.787134	0.034332	2.375094
35	6	0	2.980286	-3.470422	0.877028
36	1	0	1.685763	-2.363452	-0.440960
37	6	0	3.908485	-3.323358	1.932975
38	6	0	3.254187	1.254760	-0.652991
39	6	0	4.479254	0.617444	-0.837768
40	6	0	3.011036	2.457538	-1.305614
41	6	0	5.503563	1.209799	-1.571269
42	1	0	4.630469	-0.361226	-0.405222
43	6	0	3.999609	3.114354	-2.045262
44	1	0	2.023052	2.899581	-1.233361
45	6	0	5.276386	2.514738	-2.070151
46	6	0	-2.945863	-1.058132	-0.440187
47	6	0	-4.184450	-0.858666	0.172447
48	6	0	-2.784875	-2.143125	-1.290945
49	6	0	-5.200850	-1.805149	0.083746
50	1	0	-4.344412	0.037896	0.753762
51	6	0	-3.774959	-3.122850	-1.441471
52	1	0	-1.840331	-2.257140	-1.814707
53	6	0	-4.915483	-2.995884	-0.627584

54	6	0	-2.027209	1.493860	0.677862	127	6	0	-2.277260	-5.053529	-2.054449
55	6	0	-1.697705	2.651573	-0.015929	128	1	0	-1.387771	-4.424931	-1.950361
56	6	0	-2.793315	1.582607	1.844163	129	1	0	-2.448940	-5.554760	-1.095684
57	6	0	-2.185931	3.906849	0.378219	130	1	0	-2.056050	-5.821336	-2.803815
58	1	0	-1.052668	2.576619	-0.886331	131	6	0	-4.675477	-5.193093	-2.764830
59	6	0	-3.377860	2.781635	2.232937	132	1	0	-4.411332	-5.797455	-3.639988
60	1	0	-2.942693	0.691695	2.441854	133	1	0	-4.877248	-5.885442	-1.947130
61	6	0	-3.140880	3.911475	1.412839	134	1	0	-5.598389	-4.655215	-2.994757
62	6	0	-1.594454	5.167719	-0.300252	135	6	0	-3.214897	-3.533576	-3.828964
63	6	0	-2.064793	5.292752	-1.759191	136	1	0	-2.948579	-4.280222	-4.584065
64	1	0	-1.613746	6.181273	-2.215921	137	1	0	-4.102478	-2.997668	-4.182334
65	1	0	-1.766202	4.422978	-2.350502	138	1	0	-2.389214	-2.822319	-3.765462
66	1	0	-3.151805	5.403278	-1.830660	139	6	0	6.790121	0.414867	-1.880556
67	6	0	-1.881315	6.490250	0.434667	140	6	0	2.235260	4.152871	-3.502502
68	1	0	-1.656100	6.418970	1.502301	141	1	0	2.331622	3.330306	-4.219764
69	1	0	-1.235770	7.264328	0.005127	142	1	0	1.412225	3.919652	-2.823371
70	1	0	-2.911764	6.829582	0.324592	143	1	0	1.944049	5.051266	-4.056786
71	6	0	-0.057495	5.019693	-0.304948	144	6	0	6.989749	0.361877	-3.408475
72	1	0	0.337030	4.969290	0.714770	145	1	0	7.888315	-0.218658	-3.646880
73	1	0	0.277305	4.128894	-0.840994	146	1	0	6.136315	-0.124533	-3.893898
74	1	0	0.388514	5.887088	-0.801766	147	1	0	7.106748	1.360596	-3.832999
75	6	0	-4.180709	2.879326	3.544863	148	6	0	8.034666	1.033484	-1.217227
76	6	0	-3.562138	3.982488	4.426630	149	1	0	7.872295	1.201599	-0.147125
77	1	0	-3.684551	4.967516	3.973178	150	1	0	8.884320	0.349873	-1.323405
78	1	0	-4.044600	3.992588	5.410162	151	1	0	8.313228	1.979253	-1.682960
79	1	0	-2.491444	3.809646	4.570640	152	6	0	6.681058	-1.040371	-1.390407
80	6	0	-5.667474	3.192455	3.291857	153	1	0	5.820899	-1.559543	-1.826537
81	1	0	-6.103949	2.487119	2.576546	154	1	0	7.582169	-1.582708	-1.693337
82	1	0	-6.223477	3.102366	4.231782	155	1	0	6.609439	-1.112923	-0.300095
83	1	0	-5.813992	4.206207	2.917499	156	6	0	3.860160	-4.952812	3.616083
84	6	0	-4.115926	1.560861	4.333431	157	1	0	4.254725	-5.957148	3.781848
85	1	0	-4.609218	0.737179	3.805045	158	1	0	4.088864	-4.335181	-4.492868
86	1	0	-3.084639	1.266238	4.549968	159	1	0	2.771888	-5.006430	3.493348
87	1	0	-4.635800	1.692105	5.287661	160	6	0	5.462089	-1.767230	3.414544
88	8	0	-3.865657	5.044027	1.678574	161	6	0	4.927613	-1.436432	4.819617
89	8	0	-5.789761	-0.447448	-0.499732	162	1	0	5.744468	-1.072471	5.452796
90	8	0	4.489454	-4.450985	2.447124	163	1	0	4.156016	-0.660337	4.783006
91	8	0	6.345696	3.183196	-2.612433	164	1	0	4.505473	-2.319913	5.307540
92	6	0	6.921134	4.131365	-1.718775	165	6	0	6.502447	-2.896358	3.528282
93	1	0	7.812160	4.525913	-2.210546	166	1	0	7.359959	-2.516568	4.094405
94	1	0	6.233742	4.956253	-1.504800	167	1	0	6.128406	-3.775091	4.052362
95	1	0	7.205148	3.662047	-0.770583	168	1	0	6.863398	-3.212966	2.545486
96	6	0	3.576731	4.410895	-2.775926	169	6	0	6.240009	-0.532778	2.897665
97	6	0	4.550258	4.901297	-3.862677	170	1	0	6.588408	-0.685474	1.870970
98	1	0	4.066224	5.716740	-4.411252	171	1	0	5.653977	0.389189	2.923650
99	1	0	5.485746	5.291174	-3.462536	172	1	0	7.118465	-0.369900	3.530035
100	1	0	4.789230	4.109733	-4.578282	173	6	0	2.655928	-4.766727	0.092927
101	6	0	3.368067	5.527860	-1.736553	174	6	0	1.127691	-4.908505	-0.077429
102	1	0	2.986895	6.433075	-2.222550	175	1	0	0.904487	-5.823900	-0.636506
103	1	0	2.646889	5.224448	-0.971829	176	1	0	0.631668	-4.981202	0.896371
104	1	0	4.303768	5.785637	-1.230781	177	1	0	0.677820	-4.075369	-0.624099
105	6	0	-4.916040	5.265167	0.742922	178	6	0	3.156785	-6.086642	0.696187
106	1	0	-5.439706	6.165534	1.068993	179	1	0	2.707719	-6.292485	1.671603
107	1	0	-4.530524	5.418501	-0.269715	180	1	0	2.857569	-6.901173	0.024548
108	1	0	-5.617135	4.422474	0.729737	181	1	0	4.241240	-6.116143	0.801611
109	6	0	-5.312635	-5.043989	0.398162	182	6	0	3.313435	-4.615853	-1.296326
110	1	0	-6.084877	-5.813587	0.448259	183	1	0	2.937915	-3.737588	-1.829251
111	1	0	-4.377211	-5.491670	0.046336	184	1	0	4.400113	-4.515650	-1.200212
112	1	0	-5.143583	-4.627975	1.397581	185	1	0	3.107238	-5.500676	-1.909480
113	6	0	-6.571633	-1.543339	0.741682	186	8	0	1.569864	-0.279629	-3.026169
114	6	0	-6.676340	-0.088767	1.233007	187	6	0	0.523178	-0.626157	-3.689766
115	1	0	-5.982802	0.119394	2.054561	188	1	0	-0.734190	-0.547613	-2.589860
116	1	0	-6.486608	0.631800	0.430645	189	6	0	0.369574	-2.041809	-4.071324
117	1	0	-7.688042	0.089154	1.610836	190	6	0	-0.102238	-2.646940	-5.198661
118	6	0	-7.698952	-1.770930	-0.283927	191	8	0	0.859346	-2.971234	-3.210800
119	1	0	-7.710364	-2.800893	-0.643420	192	6	0	0.120058	-4.045246	-5.019484
120	1	0	-8.668695	-1.558487	0.179690	193	1	0	-0.547016	-2.160663	-6.055082
121	1	0	-7.584228	-1.105909	-1.144761	194	6	0	0.695855	-4.179073	-3.795858
122	6	0	-6.801410	-2.455057	1.962174	195	1	0	-0.124882	-4.841033	-5.707219
123	1	0	-6.963866	-3.493983	1.672313	196	1	0	1.033417	-5.031595	-3.226270
124	1	0	-5.955586	-2.411844	2.657062	197	6	0	-0.104956	0.407226	-4.636633
125	1	0	-7.694731	-2.122394	2.502519	198	1	0	0.111989	0.129791	-5.669934
126	6	0	-3.507608	-4.231810	-2.483773	199	1	0	0.335244	1.378668	-4.416181

200	8	0	-1.522209	0.446558	-4.498656
201	6	0	-2.012164	1.439177	-3.723500
202	8	0	-1.343879	2.392216	-3.379905
203	6	0	-3.425764	1.227163	-3.332747
204	6	0	-4.127131	0.068351	-3.678293
205	6	0	-4.034249	2.205560	-2.541058
206	6	0	-5.435822	-0.100783	-3.239983
207	1	0	-3.646837	-0.696215	-4.277148
208	6	0	-5.341739	2.034823	-2.107158
209	1	0	-3.477663	3.093686	-2.271032
210	6	0	-6.044038	0.884673	-2.462922
211	1	0	-5.980073	-1.003592	-3.498946
212	1	0	-5.811922	2.797477	-1.494091
213	1	0	-7.069123	0.756692	-2.130266

54	6	0	-1.843271	1.216730	1.260840
55	6	0	-1.748592	2.426527	0.590986
56	6	0	-2.473445	1.161326	2.505794
57	6	0	-2.346608	3.593331	1.084274
58	1	0	-1.216891	2.455505	-0.353178
59	6	0	-3.131359	2.271130	3.026170
60	1	0	-2.459929	0.228360	3.056574
61	6	0	-3.134746	3.453086	2.241471
62	6	0	-2.060865	4.905643	0.317420
63	6	0	-2.800833	4.898374	-1.033006
64	1	0	-2.595783	5.828697	-1.575056
65	1	0	-2.473879	4.063893	-1.605675
66	1	0	-3.884336	4.819441	-1.032470
67	6	0	-2.405044	6.194474	1.084702
68	1	0	-1.968860	6.195584	2.087791
69	1	0	-1.982347	7.043437	0.536480
70	1	0	-3.476570	6.372127	1.175545
71	6	0	-0.543111	4.977594	0.036187
72	1	0	0.030965	4.967793	0.969203
73	1	0	-0.190092	4.157195	-0.593236
74	1	0	-0.316881	5.908855	-0.492883
75	6	0	-3.751798	2.221703	4.437450
76	6	0	-3.075301	3.302234	5.304280
77	1	0	-3.299845	4.305950	4.937463
78	1	0	-3.427870	3.230034	6.339335
79	1	0	-1.988234	3.178632	5.300916
80	6	0	-5.275430	2.448405	4.26424
81	1	0	-5.771306	1.780749	3.713613
82	1	0	-5.681379	2.233554	5.421113
83	1	0	-5.536044	3.478554	4.183308
84	6	0	-3.505479	0.859192	5.105831
85	1	0	-4.013222	0.043737	4.577965
86	1	0	-2.440618	0.618661	5.174195
87	1	0	-3.906752	0.887480	6.123747
88	8	0	-3.927122	4.490281	2.668014
89	8	0	-5.880604	-3.601123	-1.155710
90	8	0	4.330474	-4.719897	1.931795
91	8	0	5.862460	3.889932	-2.658529
92	6	0	6.330602	4.890994	-1.758020
93	1	0	7.125748	5.430464	-2.275877
94	1	0	5.538109	5.594193	-1.485316
95	1	0	6.730357	4.443341	-0.842056
96	6	0	2.943042	4.713251	-2.684080
97	6	0	3.784451	5.346111	-3.806974
98	1	0	3.167522	6.092128	-4.319418
99	1	0	4.674901	5.858762	-3.443872
100	1	0	4.029250	4.602252	-4.547222
101	6	0	2.644653	5.774151	-1.609252
102	1	0	2.110490	6.622070	-2.052604
103	1	0	2.022673	5.362569	-0.808946
104	1	0	3.562822	6.159360	-1.155269
105	6	0	-5.147986	4.604415	1.941072
106	1	0	-5.720549	5.402319	2.417234
107	1	0	-4.973613	6.692476	0.892506
108	1	0	-5.718296	3.669963	1.977910
109	6	0	-5.611745	-4.886077	-0.598537
110	1	0	-6.511796	-5.484253	-0.750859
111	1	0	-4.765581	-5.374897	-1.091002
112	1	0	-5.396592	-4.815386	0.472753
113	6	0	-6.407433	-1.531859	0.807032
114	6	0	-6.352587	-0.310660	1.743137
115	1	0	-5.656499	-0.460121	2.575813
116	1	0	-6.066547	0.604682	1.213330
117	1	0	-7.345248	-0.147428	2.174304
118	6	0	-7.515425	-1.266893	-0.229349
119	1	0	-7.624166	-2.099120	-0.926701
120	1	0	-8.473612	-1.122466	0.282041
121	1	0	-7.300800	-0.361653	-0.804387
122	6	0	-6.792671	-2.748609	1.670095
123	1	0	-7.091758	-3.603734	1.062937
124	1	0	-5.967188	-3.051441	2.323282
125	1	0	-7.644176	-2.487606	2.308543
126	6	0	-3.512403	-3.515157	-3.052571
127	6	0	-2.472467	-4.629608	-2.834447
128	1	0	-1.523940	-4.225513	-2.466900
129	1	0	-2.823532	-5.370962	-2.109280
130	1	0	-2.273604	-5.147194	-3.779437
131	6	0	-4.787162	-4.121141	-3.664248
132	1	0	-4.541347	-4.485095	-4.667898
133	1	0	-5.180821	-4.969121	-3.103654
134	1	0	-5.579312	-3.741192	-3.766229
135	6	0	-2.973583	-2.527885	-4.111133

4a(S) -1b

RwB97XD SCF energy -5094.196518 a.u.
RwB97XD SCF enthalpy -5092.257156 a.u.
RwB97XD SCF free energy -5092.496500 a.u.
Three lowest frequencies (cm⁻¹) 17.9, 18.5, 21.7

Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates X Y Z (Angstroms)
1	6	0	0.382735 -0.942133 2.648145
2	6	0	0.826744 -1.876768 3.559979
3	6	0	0.365772 -3.190834 3.587239
4	6	0	-0.547025 -3.657326 2.674487
5	6	0	-1.020793 -2.728448 1.736379
6	6	0	-0.593693 -1.401916 1.721082
7	1	0	-0.902402 -4.680789 2.689339
8	1	0	-1.758738 -3.065426 1.017428
9	6	0	0.857704 0.463991 2.752798
10	6	0	1.532406 1.209551 1.743021
11	6	0	0.614979 1.140417 3.928536
12	6	0	1.863816 2.547502 1.951223
13	6	0	0.949585 2.477117 4.124932
14	6	0	1.565683 3.217829 3.146519
15	1	0	2.387910 3.099832 1.180761
16	1	0	1.823324 4.259989 3.291983
17	8	0	0.958970 -3.856744 4.613616
18	8	0	1.742154 -1.703459 4.553126
19	8	0	-0.015284 0.666497 5.038091
20	8	0	0.545314 2.865941 5.363009
21	6	0	1.591174 -2.843587 5.398768
22	1	0	2.568316 -3.194364 5.728588
23	1	0	0.943257 -2.583937 6.244634
24	6	0	0.192172 1.658364 6.043986
25	1	0	1.021195 1.352991 6.692476
26	1	0	-0.731636 1.808091 6.602188
27	15	0	1.959454 0.411171 0.162858
28	15	0	-1.239436 -0.277397 0.434699
29	46	0	0.261424 0.018788 -1.264352
30	6	0	2.780803 -1.133711 0.611811
31	6	0	3.759230 -1.142751 1.602361
32	6	0	2.455104 -2.310221 -0.048425
33	6	0	4.387687 -2.324876 1.992094
34	1	0	4.039501 -0.206280 2.074751
35	6	0	3.004450 -3.536275 0.329898
36	1	0	1.741261 -2.269898 -0.865395
37	6	0	3.908885 -3.524273 1.412942
38	6	0	3.154070 1.453378 -0.710525
39	6	0	4.449789 1.004860 -0.954246
40	6	0	2.718609 2.644373 -1.281353
41	6	0	5.355292 1.779832 -1.675389
42	1	0	4.748829 0.036523 -0.577894
43	6	0	3.574257 3.467828 -2.016442
44	1	0	1.679620 2.929623 -1.156855
45	6	0	4.921855 3.056858 -2.105579
46	6	0	-2.726950 -1.107117 -0.201222
47	6	0	-3.956818 -0.964500 0.442186
48	6	0	-2.629058 -1.950213 -1.299291
49	6	0	-5.054973 -1.742151 0.092691
50	1	0	-4.047763 -0.245319 1.243418
51	6	0	-3.710660 -2.726907 -1.736481
52	1	0	-1.675705 -2.028370 -1.813527
53	6	0	-4.871901 -2.695226 -0.940398

136	1	0	-2.791119	-3.057159	-5.052127
137	1	0	-3.700419	-1.731859	-4.302449
138	1	0	-2.034139	-2.064458	-3.811704
139	6	0	6.733933	1.200997	-2.059949
140	6	0	1.610906	4.291771	-3.348143
141	1	0	1.779696	3.503870	-4.090095
142	1	0	0.863884	3.936353	-2.634636
143	1	0	1.173392	5.153569	-3.862708
144	6	0	6.847515	1.179118	-3.597387
145	1	0	7.813553	0.755023	-3.893662
146	1	0	6.058883	0.556146	-4.033636
147	1	0	6.769859	2.180730	-4.025287
148	6	0	7.903982	2.001783	-1.458564
149	1	0	7.773890	2.143104	-0.380211
150	1	0	8.839151	1.451723	-1.611329
151	1	0	8.021529	2.978711	-1.927996
152	6	0	6.885702	-0.248808	-1.569206
153	1	0	6.106025	-0.909088	-1.963739
154	1	0	7.849090	-0.639570	-1.911545
155	1	0	6.875656	-0.315959	-0.476448
156	6	0	3.526113	-5.135965	3.028534
157	1	0	3.930629	-6.088629	3.375861
158	1	0	3.563742	-4.403720	3.843214
159	1	0	2.481680	-5.272191	2.723676
160	6	0	5.571702	-2.187546	2.981366
161	6	0	5.068168	-1.640947	4.328405
162	1	0	5.916313	-1.468027	5.000212
163	1	0	4.531374	-0.694173	4.217072
164	1	0	4.399606	-2.358576	4.811286
165	6	0	6.374209	-3.469809	3.259328
166	1	0	7.256467	-3.195075	3.848689
167	1	0	5.814431	-4.204431	3.840340
168	1	0	6.722792	-3.946556	2.340067
169	6	0	6.572482	-1.179984	2.370395
170	1	0	6.963203	-1.553067	1.417939
171	1	0	6.129878	-0.195271	2.197018
172	1	0	7.418866	-1.042758	3.051874
173	6	0	2.615042	-4.751201	-0.545107
174	6	0	1.078919	-4.875205	-0.612357
175	1	0	0.803973	-5.717846	-1.256439
176	1	0	0.659224	-5.061010	0.381786
177	1	0	0.599708	-3.979678	-1.018600
178	6	0	3.164924	-6.119034	-0.112425
179	1	0	2.774301	-6.444599	0.854352
180	1	0	2.848508	-6.858615	-0.856876
181	1	0	4.255313	-6.133621	-0.068522
182	6	0	3.174285	-4.473088	-1.958048
183	1	0	2.775088	-3.550244	-2.387845
184	1	0	4.266098	-4.387415	-1.930025
185	1	0	2.916987	-5.296824	-2.633038
186	8	0	1.398325	0.055521	-2.966104
187	6	0	0.299764	-0.299399	-3.720428
188	6	0	0.446256	-1.618437	-4.416497
189	6	0	0.411123	-2.037549	-5.708385
190	8	0	0.584660	-2.689451	-3.585919
191	6	0	0.543300	-3.465439	-5.672438
192	1	0	0.295960	-1.418131	-6.586240
193	6	0	0.642141	-3.801894	-4.363255
194	1	0	0.559399	-4.144591	-6.512733
195	1	0	0.758831	-4.740449	-3.843979
196	6	0	-0.214370	0.831510	-4.631698
197	1	0	0.029846	0.675914	-5.681651
198	1	0	0.211262	1.774530	-4.288780
199	8	0	-1.650434	0.887679	-4.574730
200	6	0	-2.162842	1.473675	-3.486143
201	8	0	-1.470192	2.039279	-2.654729
202	6	0	-3.633254	1.339925	-3.375036
203	6	0	-4.421756	0.924609	-4.452337
204	6	0	-4.221703	1.621922	-2.138319
205	6	0	-5.796883	0.799299	-4.289041
206	1	0	-3.962576	0.707253	-5.410376
207	6	0	-5.595425	1.490978	-1.980582
208	1	0	-3.598644	1.929951	-1.305140
209	6	0	-6.382702	1.081177	-3.055811
210	1	0	-6.412657	0.481716	-5.124329
211	1	0	-6.051855	1.704345	-1.019063
212	1	0	-7.456302	0.977449	-2.931308
213	1	0	-0.594761	-0.495053	-3.025854

5a(S) -1b

RwB97XD SCF energy -5095.370706 a.u.
RwB97XD SCF enthalpy -5093.413666 a.u.
RwB97XD SCF free energy -5093.657583 a.u.
Three lowest frequencies (cm⁻¹) 14.9, 17.3, 19.1

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates		Z (Angstroms)
			X	Y	
1	6	0	-0.433387	-1.868167	-2.420776
2	6	0	-0.123413	-2.073826	-3.746720
3	6	0	-0.575776	-1.244410	-4.770004
4	6	0	-1.365973	-0.151611	-4.517830
5	6	0	-1.692557	0.06934	-3.174726
6	6	0	-1.247315	-0.735017	-2.142335
7	1	0	-1.729882	0.490186	-5.311014
8	1	0	-2.328591	0.934778	-2.953666
9	6	0	-0.039777	-2.889567	-1.415911
10	6	0	0.790995	-2.695011	-0.278523
11	6	0	-0.555043	-4.158475	-1.574054
12	6	0	1.015200	-3.743644	0.614769
13	6	0	-0.327600	-4.594081	-0.674242
14	6	0	0.450405	-5.015447	0.443164
15	1	0	1.657533	-3.594180	1.473201
16	1	0	0.632603	-5.814350	1.151922
17	8	0	-0.120970	-1.710763	-5.962964
18	8	0	0.630021	-3.075186	-4.278289
19	8	0	-1.383788	-4.594288	-2.562964
20	8	0	-1.000328	-6.303187	-1.083331
21	6	0	0.389179	-3.017039	-5.684950
22	1	0	1.322494	-3.168405	-6.224996
23	1	0	-0.364995	-3.765383	-5.954434
24	6	0	-1.420739	-6.014939	-2.419816
25	1	0	-0.716020	-6.467572	-3.127155
26	1	0	-2.439446	-6.371036	-2.569605
27	15	0	1.505264	-1.050890	0.073471
28	15	0	-1.672785	-0.341678	-0.413943
29	46	0	0.023659	0.447807	0.935842
30	6	0	2.193232	-0.419460	-1.474203
31	6	0	3.077221	-1.180599	-2.233407
32	6	0	1.841321	0.856851	-1.899125
33	6	0	3.590632	-0.706115	-3.442009
34	1	0	3.363714	-2.164973	-1.876424
35	6	0	2.304227	1.388155	-3.101344
36	1	0	1.174472	1.446012	-1.278637
37	6	0	3.107562	0.542872	-3.897713
38	6	0	2.820695	-1.306287	1.293518
39	6	0	4.169750	-1.123845	1.004260
40	6	0	2.427088	-1.549048	2.603957
41	6	0	5.142686	-1.267900	1.995122
42	1	0	4.459607	-0.859053	-0.003842
43	6	0	3.341805	-1.667550	3.649166
44	1	0	1.367689	-1.617098	2.823932
45	6	0	4.706939	-1.612381	3.298086
46	6	0	-2.928750	0.968378	-0.464622
47	6	0	-4.211677	0.743408	0.019298
48	6	0	-2.553112	2.253178	-0.838670
49	6	0	-5.153848	1.767424	0.078255
50	1	0	-4.473687	-0.245531	0.366293
51	6	0	-3.448651	3.324737	-0.823234
52	1	0	-1.526217	2.425322	-1.140961
53	6	0	-4.775812	3.035061	-0.428259
54	6	0	-2.504759	-1.776616	0.295509
55	6	0	-2.338452	-2.021507	1.648965
56	6	0	-3.382239	-2.562158	-0.452561
57	6	0	-3.096442	-2.985322	2.321981
58	1	0	-1.606404	-1.435695	2.197756
59	6	0	-4.190527	-3.512191	0.162811
60	1	0	-3.443271	-2.402905	-1.522137
61	6	0	-4.103070	-3.623667	1.574894
62	6	0	-2.724554	-3.250169	3.798021
63	6	0	-3.070739	-2.012397	4.646768
64	1	0	-2.790412	-2.182398	5.692186
65	1	0	-2.537483	-1.121986	4.296722
66	1	0	-4.143359	-1.794463	4.617732
67	6	0	-3.371400	-4.493425	4.432402
68	1	0	-3.224950	-5.385878	3.818221
69	1	0	-2.891512	-4.670892	5.401052
70	1	0	-4.438920	-4.375379	4.620854

71	6	0	-1.198118	-3.486609	3.865752	153	1	0	6.225389	0.233461	-0.137257
72	1	0	-0.908765	-4.363428	3.275863	154	1	0	7.873349	-0.365500	0.024842
73	1	0	-0.619427	-2.631888	3.506240	155	1	0	6.584613	-1.482026	-0.433497
74	1	0	-0.904731	-3.664022	4.905394	156	6	0	2.466017	0.492226	-6.124456
75	6	0	-5.080880	-4.464555	-0.680914	157	1	0	2.810880	0.836288	-7.101542
76	6	0	-4.673006	-5.903478	-0.384842	158	1	0	2.393185	-0.601874	-6.125943
77	1	0	-4.874069	-6.169861	0.654980	159	1	0	1.473701	0.913399	-5.921114
78	1	0	-5.236405	-6.588630	-1.028016	160	6	0	4.650891	-1.586141	-4.148262
79	1	0	-3.604838	-6.054143	-0.572542	161	6	0	3.993870	-2.880932	-4.653728
80	6	0	-6.581642	-4.258836	-0.390426	162	1	0	4.753838	-3.546964	-5.077771
81	1	0	-6.870890	-3.204495	-0.460352	163	1	0	3.480480	-3.422068	-3.853183
82	1	0	-7.168269	-4.814226	-1.130731	164	1	0	3.267639	-2.658274	-5.440543
83	1	0	-6.859896	-4.634365	0.594489	165	6	0	5.387010	-0.932836	-5.330482
84	6	0	-4.876847	-4.199240	-2.184890	166	1	0	6.208462	-1.595560	-5.625585
85	1	0	-5.219812	-3.204052	-2.489509	167	1	0	4.749411	-0.079781	-6.205184
86	1	0	-3.830538	-4.310752	-2.484086	168	1	0	5.819036	0.394945	-5.063370
87	1	0	-5.464009	-4.931476	-2.747867	169	6	0	5.738500	-1.940225	-3.110561
88	8	0	-5.042148	-4.397308	2.210600	170	1	0	6.214928	-1.032256	-2.726355
89	8	0	-5.747837	4.004002	-0.471482	171	1	0	5.347087	-2.506144	-2.261157
90	8	0	3.419084	0.942035	-5.169456	172	1	0	6.512534	-2.555124	-3.581781
91	8	0	5.671172	-1.852294	4.246384	173	6	0	1.879816	2.839714	-3.439112
92	6	0	5.891179	-3.236503	4.507141	174	6	0	0.378248	2.863873	-3.770220
93	1	0	6.735805	-3.293866	5.196230	175	1	0	0.052550	3.894743	-3.949270
94	1	0	5.019342	-3.706495	4.971397	176	1	0	0.159505	2.277790	-4.668273
95	1	0	6.130999	-3.779724	3.587426	177	1	0	-0.219192	2.455745	-2.948846
96	6	0	2.750660	-1.796576	5.074408	178	6	0	2.642597	3.502576	-4.599018
97	6	0	3.723174	-1.439320	6.212432	179	1	0	2.391843	3.077477	-5.571474
98	1	0	3.155677	-1.387171	7.147870	180	1	0	2.370251	4.563701	-4.623639
99	1	0	4.512057	-2.176358	6.358825	181	1	0	3.725817	3.439537	-4.463339
100	1	0	4.189509	-0.462796	6.050983	182	6	0	2.124464	3.735933	-2.203704
101	6	0	2.213128	-3.224613	5.277927	183	1	0	1.578877	3.405857	-1.315963
102	1	0	1.704746	-3.304150	6.245463	184	1	0	3.188879	3.774633	-1.949995
103	1	0	1.494842	-3.487956	4.495368	185	1	0	1.793750	4.755873	-2.426659
104	1	0	3.014081	-3.969755	5.259360	186	8	0	1.538550	1.216529	2.072959
105	6	0	-6.074702	-3.622809	2.818705	187	6	0	1.694218	2.588374	1.884155
106	1	0	-6.779378	-4.331950	3.256743	188	6	0	3.068821	2.904473	1.361205
107	1	0	-5.682311	-2.968651	3.603642	189	6	0	4.022902	3.825131	1.669777
108	1	0	-6.592894	-3.004931	2.076890	190	8	0	3.488746	2.145581	0.316317
109	6	0	-6.331088	4.215955	-1.755151	191	6	0	5.099804	3.619376	0.743589
110	1	0	-7.289669	4.711913	-1.589596	192	1	0	3.968795	4.566726	2.454271
111	1	0	-5.706763	4.861824	-2.379260	193	6	0	4.716654	2.588769	-0.051303
112	1	0	-6.495454	3.268170	-2.277405	194	1	0	6.030687	4.165231	0.684817
113	6	0	-6.516585	1.503295	0.754919	195	1	0	5.168529	2.086422	-0.893159
114	6	0	-6.605206	0.062938	1.296132	196	6	0	1.417511	3.328375	3.198494
115	1	0	-6.565953	-0.682702	0.493996	197	1	0	2.265632	3.274482	3.883231
116	1	0	-5.814222	-0.164190	2.019242	198	1	0	0.536401	2.895792	3.672853
117	1	0	-7.563039	-0.061323	1.810863	199	8	0	1.203546	4.725155	2.936355
118	6	0	-6.668801	2.455717	1.956964	200	6	0	-0.051695	5.106911	2.680846
119	1	0	-6.627697	3.502041	1.647801	201	8	0	-1.025149	4.399495	2.878065
120	1	0	-7.631964	2.283376	2.450749	202	6	0	-0.135331	6.474478	2.109298
121	1	0	-5.876632	2.281666	2.693804	203	6	0	0.969671	7.078131	1.502448
122	6	0	-7.698932	1.692994	-0.213601	204	6	0	-1.377001	7.115184	2.104160
123	1	0	-7.874128	2.743232	-0.446108	205	6	0	0.826052	8.319940	0.891661
124	1	0	-7.539113	1.147922	-1.149936	206	1	0	1.927614	6.569487	1.489521
125	1	0	-8.613651	1.303513	0.246629	207	6	0	-1.512625	8.360256	1.502859
126	6	0	-2.888969	4.712701	-1.219766	208	1	0	-2.229997	6.630012	2.566848
127	6	0	-2.880696	4.847951	-2.753974	209	6	0	-0.411708	8.960849	0.892372
128	1	0	-2.313561	4.029777	-3.210599	210	1	0	1.680396	8.785808	0.410928
129	1	0	-3.887145	4.833315	-3.179668	211	1	0	-2.476564	8.858918	1.502610
130	1	0	-2.405318	5.791684	-3.044495	212	1	0	-0.520182	9.929270	0.413471
131	6	0	-3.644988	5.891937	-0.581112	213	1	0	0.961122	2.976914	1.149897
132	1	0	-3.081206	6.812773	-0.763212	214	1	0	-1.188724	1.337181	2.132801
133	1	0	-4.644515	6.035800	-0.988990	215	1	0	-1.148540	1.874291	1.578250
134	1	0	-3.733591	5.763287	0.502272						
135	6	0	-1.424287	4.832100	-0.738422						
136	1	0	-1.077873	5.860799	-0.879376						
137	1	0	-1.336465	4.587119	0.323450						
138	1	0	-0.740573	4.192412	-1.302500						
139	6	0	6.619474	-0.935131	1.685783						
140	6	0	1.566483	-0.809120	5.216248						
141	1	0	1.876020	0.217471	4.993141						
142	1	0	0.718343	-1.056214	4.571945						
143	1	0	1.196219	-0.837215	6.246201						
144	6	0	7.004984	0.321850	2.491083						
145	1	0	8.048869	0.589360	2.290397						
146	1	0	6.375442	1.172370	2.204791						
147	1	0	6.896861	0.157997	3.566150						
148	6	0	7.588712	-2.086219	2.018977						
149	1	0	7.247037	-3.031577	1.583878						
150	1	0	8.572533	-1.864042	1.591593						
151	1	0	7.723092	-2.221045	3.091327						
152	6	0	6.822551	-0.619232	0.196232						

TS2a(S) -1b											
RwB97XD SCF energy		-5095.353354 a.u.									
RwB97XD SCF enthalpy		-5093.398981 a.u.									
RwB97XD SCF free energy		-5093.641841 a.u.									
Three lowest frequencies (cm ⁻¹)		-1069, 12.1, 15.5									
Imaginary frequency (cm ⁻¹)		-1069									
Cartesian coordinates:											
Standard orientation:											
Center	Atomic	Atomic	Coordinates								
Number	Number	Type	X	Y	Z	(Angstroms)					
1	6	0	0.915344	-1.938522	2.298039						
2	6	0	0.703226	-2.314126	3.605760						
3	6	0	1.003314	-1.493743	4.691319						
4	6	0	1.524820	-0.235478	4.525345						
5	6	0	1.741108	0.180810	3.203759						

6	6	0	1.451788	-0.633567	2.111033	88	8	0	5.916195	-2.999441	-2.482401
7	1	0	1.769241	0.400660	5.367424	89	8	0	4.565805	5.231944	0.581483
8	1	0	2.164431	1.165670	3.047942	90	8	0	-3.320023	-0.285673	5.357961
9	6	0	0.705584	-2.932732	1.212991	91	8	0	-5.131879	-2.898110	-4.246826
10	6	0	-0.185911	-2.814698	0.111328	92	6	0	-4.968199	-4.286177	-4.527093
11	6	0	1.463470	-4.084253	1.252361	93	1	0	-5.782279	-4.567380	-5.197535
12	6	0	-0.229811	-3.808623	-0.866457	94	1	0	-4.013700	-4.490448	-5.019926
13	6	0	1.414974	-5.064991	0.267702	95	1	0	-5.023542	-4.883732	-3.611442
14	6	0	0.580148	-4.952937	-0.816649	96	6	0	-2.364637	-2.019855	-5.124032
15	1	0	-0.920011	-3.720053	-1.696501	97	6	0	-3.432345	-1.902054	-6.226827
16	1	0	0.535453	-5.712096	-1.588463	98	1	0	-2.928976	-1.685863	-7.175217
17	8	0	0.706311	-2.146083	5.844894	99	1	0	-4.009549	-2.814850	-6.369962
18	8	0	0.200087	-3.494329	4.060213	100	1	0	-4.128571	-1.082677	-6.023630
19	8	0	2.387722	-4.432283	2.190180	101	6	0	-1.482603	-3.255071	-5.384912
20	8	0	2.306516	-6.049332	0.568700	102	1	0	-0.999978	-3.170852	-6.365108
21	6	0	0.479937	-3.504894	5.460360	103	1	0	-0.697911	-3.344054	-4.626864
22	1	0	-0.375511	-3.901502	6.004737	104	1	0	-2.060485	-4.183807	-5.376090
23	1	0	1.390060	-4.087802	5.644144	105	6	0	6.767744	-1.972949	-2.991014
24	6	0	2.686717	-5.803368	1.924980	106	1	0	7.603173	-2.474907	-3.482275
25	1	0	2.088433	-6.438986	2.588483	107	1	0	6.247279	-1.340261	-3.716863
26	1	0	3.756020	-5.973260	2.045670	108	1	0	7.146265	-1.338181	-2.182262
27	15	0	-1.198507	-1.302423	-0.081647	109	6	0	5.077471	5.661526	1.840795
28	15	0	1.757984	-0.012138	0.431293	110	1	0	5.967362	6.261380	1.637713
29	46	0	0.006699	0.453781	-0.933621	111	1	0	4.355448	6.288769	2.370634
30	6	0	-1.956628	-0.978113	1.527928	112	1	0	5.350361	4.810739	2.472720
31	6	0	-2.655757	-1.973451	2.204459	113	6	0	5.990146	3.005409	-0.586484
32	6	0	-1.839697	0.288915	2.090339	114	6	0	6.462026	1.633104	-1.107183
33	6	0	-3.212742	-1.744210	3.463820	115	1	0	6.604245	0.908376	-0.297800
34	1	0	-2.754624	-2.951383	1.743978	116	1	0	5.770438	1.202454	-1.840010
35	6	0	-2.375214	0.589272	3.342968	117	1	0	7.427892	1.759933	-1.606052
36	1	0	-1.303573	1.053309	1.537158	118	6	0	5.903911	3.946424	-1.804443
37	6	0	-2.973411	-0.478841	4.047973	119	1	0	5.597674	4.953815	-1.516186
38	6	0	-2.470141	-1.696033	-1.315504	120	1	0	6.881942	4.014523	-2.293890
39	6	0	-3.814819	-1.890414	-1.005607	121	1	0	5.185564	3.564735	-2.538649
40	6	0	-2.060267	-1.747764	-2.644771	122	6	0	7.066955	3.509125	0.392253
41	6	0	-4.737633	-2.233340	-1.993691	123	1	0	6.947790	4.566626	0.624358
42	1	0	-4.140749	-1.773412	0.019557	124	1	0	7.050956	2.941085	1.328574
43	6	0	-2.932181	-2.078717	-3.684102	125	1	0	8.057802	3.383373	-0.058128
44	1	0	-1.023196	-1.527518	-2.875215	126	6	0	1.645582	5.157383	1.388858
45	6	0	-4.250673	-2.413125	-3.311754	127	6	0	1.725931	5.328846	2.918533
46	6	0	2.647663	1.560522	0.574656	128	1	0	1.380406	4.418628	3.421127
47	6	0	3.954297	1.675356	0.120520	129	1	0	2.740098	5.534937	3.267740
48	6	0	1.946375	2.697786	0.957560	130	1	0	1.083090	6.156695	3.238658
49	6	0	4.597370	2.910224	0.073995	131	6	0	2.001641	6.469576	0.665560
50	1	0	4.467573	0.789115	-0.223594	132	1	0	1.238568	7.219160	0.899708
51	6	0	2.533405	3.963179	0.964053	133	1	0	2.966464	6.882440	0.954610
52	1	0	0.904220	2.589916	1.234461	134	1	0	2.005761	6.323044	-0.419858
53	6	0	3.893057	4.035187	0.569019	135	6	0	0.165041	4.877828	1.044280
54	6	0	2.885752	-1.152579	-0.390456	136	1	0	-0.425098	5.772953	1.264568
55	6	0	2.784493	-1.286237	-1.765857	137	1	0	0.035440	4.642247	-0.016769
56	6	0	3.900700	-1.813144	0.302158	138	1	0	-0.263463	4.068495	1.640204
57	6	0	3.724037	-2.005850	-2.508838	139	6	0	-6.243588	-2.319704	-1.661422
58	1	0	1.955307	-0.802277	-2.273577	140	6	0	-1.476004	-0.762458	-5.266171
59	6	0	4.890052	-2.511971	-0.382190	141	1	0	-2.031600	0.147239	-5.017405
60	1	0	3.920797	-1.754836	1.383759	142	1	0	-0.576971	-0.795798	-4.644899
61	6	0	4.835535	-2.498302	-1.800522	143	1	0	-1.136179	-0.679646	-6.303690
62	6	0	3.404741	-2.202703	-4.007457	144	6	0	-6.990697	-1.261460	-2.496521
63	6	0	3.466904	-0.846927	-4.735148	145	1	0	-8.059317	-1.277950	-2.253434
64	1	0	3.231539	-0.981316	-5.796762	146	1	0	-6.607818	-0.258520	-2.281607
65	1	0	2.746682	-0.132631	-4.321149	147	1	0	-6.883306	-1.447953	-3.567084
66	1	0	4.463253	-0.398644	-4.664446	148	6	0	-6.842318	-3.713183	-1.935910
67	6	0	4.297324	-3.212519	-4.747821	149	1	0	-6.223745	-4.505735	-1.501445
68	1	0	4.340151	-4.173360	-4.228086	150	1	0	-7.834657	-3.778703	-1.476519
69	1	0	3.865016	-3.386308	-5.739195	151	1	0	-6.964576	-3.907021	-3.001512
70	1	0	5.316255	-2.855511	-4.900070	152	6	0	-6.504668	-2.014056	-0.178357
71	6	0	1.963192	-2.754836	-4.110430	153	1	0	-6.131956	-1.029410	0.117729
72	1	0	1.872048	-3.713576	-3.588116	154	1	0	-7.584096	-2.024342	0.002527
73	1	0	1.215616	-2.071400	-3.697202	155	1	0	-6.055426	-2.769133	0.473363
74	1	0	1.709625	-2.915271	-5.163374	156	6	0	-2.264044	-0.617333	6.251330
75	6	0	5.941089	-3.335405	0.389116	157	1	0	-2.644028	-0.456426	7.261970
76	6	0	5.821208	-4.806855	-0.055542	158	1	0	-1.963015	-1.665306	6.134391
77	1	0	6.075549	-4.931698	-1.110354	159	1	0	-1.388906	0.022894	6.083888
78	1	0	6.497183	-5.434699	0.535830	160	6	0	-4.041142	-2.893126	4.088756
79	1	0	4.799585	-5.173083	0.091343	161	6	0	-3.108895	-4.061278	4.452679
80	6	0	7.378964	-2.835221	0.158524	162	1	0	-3.697126	-4.905901	4.828724
81	1	0	7.462607	-1.760940	0.355729	163	1	0	-2.531488	-4.409018	3.590665
82	1	0	8.057282	-3.352490	0.846095	164	1	0	-2.408378	-3.764528	5.238393
83	1	0	7.727403	-3.033072	-0.855246	165	6	0	-4.860975	-2.525503	5.337928
84	6	0	5.682940	-3.286760	1.903969	166	1	0	-5.518810	-3.369804	5.573106
85	1	0	5.812969	-2.278740	2.313040	167	1	0	-4.240293	-2.342635	6.215761
86	1	0	4.680427	-3.639210	2.163459	168	1	0	-5.490499	-1.647470	5.171611
87	1	0	6.404667	-3.938295	2.406519	169	6	0	-5.063911	-3.374894	3.036520

170	1	0	-5.739106	-2.561120	2.751830	25	1	0	-0.131914	-0.063474	6.871394
171	1	0	-4.592503	-3.762018	2.129520	26	1	0	1.507585	-0.823662	6.734519
172	1	0	-5.670126	-4.184280	3.456519	27	15	0	-1.857819	-0.139145	0.467045
173	6	0	-2.275355	2.060242	3.820640	28	15	0	1.567639	0.305135	0.291001
174	6	0	-0.804044	2.418932	4.089999	29	46	0	-0.053145	-0.367684	-1.097186
175	1	0	-0.726714	3.470167	4.389373	30	6	0	-2.378472	1.598510	0.547783
176	1	0	-0.388290	1.805034	4.894727	31	6	0	-3.220236	2.137291	1.516898
177	1	0	-0.182795	2.276886	3.200615	32	6	0	-1.900077	2.419386	-0.467004
178	6	0	-3.090232	2.413282	5.076888	33	6	0	-3.556073	3.494216	1.516848
179	1	0	-2.683741	1.967754	5.985722	34	1	0	-3.611154	1.486165	2.292620
180	1	0	-3.059735	3.501214	5.205038	35	6	0	-2.166748	3.786609	-0.512506
181	1	0	-4.138332	2.116870	4.984806	36	1	0	-1.265261	1.977287	-1.228916
182	6	0	-2.810543	2.974396	2.695569	37	6	0	-2.931101	4.314690	0.547440
183	1	0	-2.271954	2.853908	1.753167	38	6	0	-3.317773	-1.129590	0.018211
184	1	0	-3.870607	2.778700	2.502205	39	6	0	-4.621633	-0.639534	0.034785
185	1	0	-2.710393	4.022316	2.998010	40	6	0	-3.084950	-2.418083	-0.447822
186	8	0	-1.233347	1.327762	-2.494758	41	6	0	-5.704516	-1.448808	-0.311274
187	6	0	-1.945386	2.467259	-2.068523	42	1	0	-4.790093	0.389419	0.324417
188	6	0	-3.273738	2.109026	-1.483581	43	6	0	-4.118286	-3.275733	-0.833410
189	6	0	-4.571016	2.326222	-1.829920	44	1	0	-2.059060	-2.762647	-0.521578
190	8	0	-3.223171	1.444641	-0.298259	45	6	0	-5.432266	-2.795253	-0.655293
191	6	0	-5.369758	1.757224	-0.782519	46	6	0	3.066221	0.941028	-0.530206
192	1	0	-4.923028	2.841911	-2.712135	47	6	0	4.335823	0.710652	-0.015610
193	6	0	-4.497163	1.231197	0.113072	48	6	0	2.933184	1.652058	-1.715168
194	1	0	-6.447896	1.745544	-0.711086	49	6	0	5.478618	1.205130	-0.641364
195	1	0	-4.611350	0.707165	1.050087	50	1	0	4.437107	0.122780	0.884274
196	6	0	-2.081264	3.429271	-3.249809	51	6	0	4.028926	2.193287	-2.391096
197	1	0	-2.862388	3.120888	-3.946181	52	1	0	1.939449	1.777481	-2.125786
198	1	0	-1.127939	3.487976	-3.776165	53	6	0	5.300151	2.001149	-1.799182
199	8	0	-2.461759	4.727596	-2.774115	54	6	0	2.117968	-1.107184	1.287440
200	6	0	-1.473428	5.510522	-2.323283	55	6	0	1.802125	-2.380885	0.838416
201	8	0	-0.292940	5.231950	-2.442324	56	6	0	2.881141	-0.959472	2.447847
202	6	0	-1.971224	6.737766	-1.651930	57	6	0	2.290172	-3.533200	1.461189
203	6	0	-3.332728	6.946935	-1.412166	58	1	0	1.152368	-2.479887	-0.025425
204	6	0	-1.030891	7.677692	-1.220094	59	6	0	3.452751	-2.062782	3.076330
205	6	0	-3.746028	8.094576	-0.743864	60	1	0	3.040000	0.036135	2.844467
206	1	0	-4.060980	6.212999	-1.738781	61	6	0	3.221234	-3.336792	2.496705
207	6	0	-1.448762	8.821982	-0.551741	62	6	0	1.718849	-4.880807	0.965347
208	1	0	0.022621	7.502360	-1.408864	63	6	0	2.204830	-5.164908	-0.467667
209	6	0	-2.806771	9.030375	-0.313430	64	1	0	1.826788	-6.136446	-0.805929
210	1	0	-4.802421	8.257811	-0.555756	65	1	0	1.842150	-4.408269	-1.171284
211	1	0	-0.717144	9.550154	-0.216303	66	1	0	3.297699	-5.188382	-0.529831
212	1	0	-3.134028	9.923953	0.209502	67	6	0	2.030945	-6.093823	1.858988
213	1	0	-1.375549	2.995388	-1.283558	68	1	0	1.780535	-5.900193	2.905576
214	1	0	0.905748	1.726159	-1.788672	69	1	0	1.419121	-6.936139	1.518226
215	1	0	0.109778	1.681980	-2.262384	70	1	0	3.072754	-6.412005	1.808508

6b(S)»2a											
RwB97XD SCF energy			-5095.412238 a.u.								
RwB97XD SCF enthalpy			-5093.451140 a.u.								
RwB97XD SCF free energy			-5093.692322 a.u.								
Three lowest frequencies (cm ⁻¹)			11.3, 15.0, 18.5								
Cartesian coordinates:											

Center	Atomic	Atomic	Coordinates	(Angstroms)							
Number	Number	Type	X	Y	Z						

1	6	0	0.154338	1.387441	2.506835	71	6	0	0.177276	-4.761470	0.940276
2	6	0	-0.147877	2.474149	3.299758	72	1	0	-0.220128	-4.554233	1.940033
3	6	0	0.345678	3.754395	3.071446	73	1	0	-0.177518	-3.976267	0.266223
4	6	0	1.184270	4.021968	2.017713	74	1	0	-0.251524	-5.706461	0.591700
5	6	0	1.539717	2.929434	1.213138	75	6	0	4.232857	-1.898112	4.396946
6	6	0	1.060691	1.638269	1.439496	76	6	0	3.544596	-2.750880	5.481251
7	1	0	1.576502	5.014569	1.831090	77	1	0	3.620937	-3.817214	5.258688
8	1	0	2.228223	3.110506	0.396009	78	1	0	4.014041	-2.573195	6.455400
9	6	0	-0.434835	0.076463	2.897602	79	1	0	2.482425	-2.499889	5.560748
10	6	0	-1.399412	-0.666997	2.163170	80	6	0	5.709029	-2.318692	4.269437
11	6	0	-0.088956	-0.436902	4.129938	81	1	0	6.196989	-1.810641	3.430615
12	6	0	-1.900904	-1.862632	2.677318	82	1	0	6.245655	-2.040380	5.183420
13	6	0	-0.600651	-1.626501	4.633983	83	1	0	5.821727	-3.394886	4.138703
14	6	0	-1.506003	-2.375181	3.923127	84	6	0	4.223702	-0.435498	4.871095
15	1	0	-2.632558	-2.425205	2.108629	85	1	0	4.758155	0.223728	4.177603
16	1	0	-1.911361	-3.303843	4.307375	86	1	0	3.209482	-0.048508	5.004951
17	8	0	-0.137645	4.598229	4.027531	87	1	0	4.734692	-0.372750	5.837018
18	8	0	-0.951759	2.493753	4.401847	88	8	0	3.931207	-4.402546	2.993482
19	8	0	0.790338	0.091746	5.028484	89	8	0	6.431346	2.535563	-2.367827
20	8	0	-0.052614	-1.868541	5.861021	90	8	0	-3.063757	5.675470	0.649796
21	6	0	-0.639990	3.727491	5.044666	91	8	0	-6.510808	-3.626276	-0.848260
22	1	0	-1.538047	4.152141	5.487859	92	6	0	-6.775870	-4.498476	0.246657
23	1	0	0.143977	3.556902	5.793292	93	1	0	-7.762719	-4.931750	0.072058
24	6	0	0.557993	-0.632425	6.235950	94	1	0	-6.041909	-5.306806	0.309013
						95	1	0	-6.779390	-3.954574	1.196989
						96	6	0	-3.705884	-4.639042	-1.438871
						97	6	0	-4.792269	-5.310775	-2.297768
						98	1	0	-4.346543	-6.167749	-2.814125
						99	1	0	-5.635396	-5.685048	-1.718471
						100	1	0	-5.177827	-4.624931	-3.058764
						101	6	0	-3.261156	-5.589991	-0.313355
						102	1	0	-2.853858	-6.515074	-0.737213
						103	1	0	-2.482651	-5.126265	0.299945
						104	1	0	-4.087956	-5.860632	0.349408
						105	6	0	5.008487	-4.791094	2.144110
						106	1	0	5.527197	-5.608267	2.648807

107	1	0	4.651113	-5.139138	1.169738	189	6	0	-3.869316	-0.684128	-4.921061
108	1	0	5.704879	-3.960527	1.983936	190	8	0	-3.459671	0.677440	-3.203983
109	6	0	6.689169	3.915083	-2.118340	191	6	0	-5.093652	-0.048785	-4.531088
110	1	0	7.772444	4.038038	-2.044840	192	1	0	-3.726441	-1.401887	-5.716698
111	1	0	6.332659	4.538815	-2.943105	193	6	0	-4.783604	0.758253	-3.484845
112	1	0	6.224030	4.246824	-1.185424	194	1	0	-6.069576	-0.179499	-4.975815
113	6	0	6.866942	0.832458	-0.075927	195	1	0	-5.357571	1.432749	-2.867697
114	6	0	6.747264	-0.128397	1.122177	196	6	0	-0.806938	-1.169598	-5.053775
115	1	0	6.240713	0.333499	1.976913	197	1	0	-1.013635	-0.632788	-5.979079
116	1	0	6.219778	-1.052797	0.863184	198	1	0	-1.154201	-2.202428	-5.145298
117	1	0	7.753346	-0.406850	1.451539	199	8	0	0.624395	-1.134660	-4.915747
118	6	0	7.696832	0.104842	-1.150858	200	6	0	1.223552	-2.036057	-4.134334
119	1	0	7.804732	0.704935	-2.055725	201	8	0	0.619562	-2.914507	-3.533510
120	1	0	8.698064	-0.110660	-0.760433	202	1	0	-0.953114	0.505013	-3.733457
121	1	0	7.229519	-0.849207	-1.415905	203	1	0	1.175241	-0.480254	-2.044257
122	6	0	7.628879	2.073531	0.425000	204	1	0	-0.908189	-2.071812	-2.869001
123	1	0	7.976768	2.704878	-0.391602	205	6	0	2.685163	-1.810237	-4.041650
124	1	0	7.005676	2.679297	1.091633	206	6	0	3.330697	-2.123289	-2.841176
125	1	0	8.512474	1.756558	0.989954	207	6	0	3.398973	-1.237398	-5.097588
126	6	0	3.743922	2.954473	-3.707977	208	6	0	4.683157	-1.841528	-2.690583
127	6	0	3.493511	4.442110	-3.393793	209	1	0	2.767106	-2.553305	-2.019928
128	1	0	2.660884	4.548325	-2.690563	210	6	0	4.759642	-0.990810	-4.952062
129	1	0	4.363682	4.932106	-2.953051	211	1	0	2.894682	-0.996577	-6.027284
130	1	0	3.232326	4.981363	-4.311601	212	6	0	5.397332	-1.275743	-3.745825
131	6	0	4.861453	2.798192	-4.755557	213	1	0	5.177537	-2.060217	-1.749231
132	1	0	4.531284	3.248258	-5.697644	214	1	0	5.320668	-0.565290	-5.777663
133	1	0	5.796905	3.276953	-4.472503	215	1	0	6.454375	-1.058782	-3.629166
134	1	0	5.067446	1.739990	-4.943746						
135	6	0	2.459230	2.413951	-4.377288						
136	1	0	2.356817	2.867907	-5.368000						
137	1	0	2.494302	1.327275	-4.507209						
138	1	0	1.550033	2.669293	-3.824175						
139	6	0	-7.130575	-0.857990	-0.368347						
140	6	0	-2.500364	-4.423068	-2.384851						
141	1	0	-2.729259	-3.670691	-3.147011						
142	1	0	-1.591273	-4.119493	-1.857722						
143	1	0	-2.268202	-5.363576	-2.894515						
144	6	0	-7.711363	-1.049420	-1.782586						
145	1	0	-8.710245	-0.602077	-1.838635						
146	1	0	-7.078811	-0.560055	-2.529363						
147	1	0	-7.796047	-2.105664	-2.044008						
148	6	0	-8.071892	-1.501723	0.667518						
149	1	0	-7.627067	-1.490979	1.668390						
150	1	0	-9.007722	-0.933259	0.713018						
151	1	0	-8.327642	-2.529535	0.410007						
152	6	0	-7.117100	0.651091	-0.076022						
153	1	0	-6.466994	1.205768	-0.760664						
154	1	0	-8.130707	1.047243	-0.193597						
155	1	0	-6.801437	0.861842	0.950163						
156	6	0	-2.041696	6.264774	1.443894						
157	1	0	-2.243318	7.337434	1.474778						
158	1	0	-2.048446	5.863883	2.464121						
159	1	0	-1.051006	6.096187	1.003906						
160	6	0	-4.581926	3.970317	2.573927						
161	6	0	-3.936087	3.919091	3.967785						
162	1	0	-4.669341	4.192426	4.734836						
163	1	0	-3.551080	2.922612	4.202340						
164	1	0	-3.107283	4.631024	4.025692						
165	6	0	-5.156755	5.382480	2.364073						
166	1	0	-5.979679	5.522136	3.074262						
167	1	0	-4.427291	6.170589	2.552559						
168	1	0	-5.559201	5.517695	1.356303						
169	6	0	-5.794415	3.014576	2.539489						
170	1	0	-6.279213	3.042911	1.558221						
171	1	0	-5.532162	1.976938	2.761449						
172	1	0	-6.530693	3.329141	3.286659						
173	6	0	-1.577001	4.563116	-1.713139						
174	6	0	-0.043088	4.608777	-1.579989						
175	1	0	0.389407	5.121929	-2.446228						
176	1	0	0.262787	5.149143	-0.678046						
177	1	0	0.387889	3.602543	-1.530928						
178	6	0	-2.094642	5.999077	-1.898800						
179	1	0	-1.750870	6.681744	-1.120737						
180	1	0	-1.715753	6.378242	-2.854724						
181	1	0	-3.186762	6.038232	-1.933321						
182	6	0	-1.935964	3.802030	-3.010484						
183	1	0	-1.491564	2.804043	-3.054358						
184	1	0	-3.020533	3.693787	-3.119287						
185	1	0	-1.561657	4.358424	-3.876494						
186	8	0	-1.305523	-1.205708	-2.659455						
187	6	0	-1.460909	-0.453426	-3.883875						
188	6	0	-2.911975	-0.203319	-4.086465						

2.5. Catalytic cycle 2a + 1b (R)

3a(R) -1b

RwB97XD SCF energy -5094.188846 a.u.
 RwB97XD SCF enthalpy -5092.251307 a.u.
 RwB97XD SCF free energy -5092.493311 a.u.
 Three lowest frequencies (cm⁻¹) 10.0, 13.8, 17.7

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.901914	0.449851	2.610320
2	6	0	-0.473916	0.111580	3.875940
3	6	0	-0.751608	-1.108679	4.482095
4	6	0	-1.514084	-2.064041	3.856450
5	6	0	-1.984054	-1.742467	2.575559
6	6	0	-1.700570	-0.525880	1.952157
7	1	0	-1.744688	-3.013445	4.324762
8	1	0	-2.584500	-2.482563	2.058822
9	6	0	-0.515686	1.792773	2.095945
10	6	0	0.405865	2.038016	1.042371
11	6	0	-1.011519	2.907099	2.736011
12	6	0	0.721762	3.344597	0.676784
13	6	0	-0.674852	4.205660	2.373611
14	6	0	0.179432	4.462529	1.330230
15	1	0	1.421154	3.521163	-0.131741
16	1	0	0.437897	5.473089	1.036329
17	8	0	-0.199103	-1.133196	5.725441
18	8	0	0.250429	0.887130	4.729659
19	8	0	-1.894540	2.939238	3.774712
20	8	0	-1.328723	5.085992	3.183231
21	6	0	0.669369	0.001929	5.766194
22	1	0	1.689723	-0.325872	5.555417
23	1	0	0.581221	0.498246	6.731910
24	6	0	-1.896524	4.293528	4.229005
25	1	0	-1.273993	4.376222	5.127318
26	1	0	-2.922439	4.614141	4.412840
27	15	0	1.147152	0.608872	0.168801
28	15	0	-2.179609	-0.345381	0.195130
29	46	0	-0.381154	-0.864900	-1.034400
30	6	0	2.045689	-0.284327	1.484333
31	6	0	2.778861	0.351656	2.488550
32	6	0	2.025254	-1.669102	1.435805
33	6	0	3.484847	-0.369852	3.452246
34	1	0	2.787363	1.433847	2.511520
35	6	0	2.698767	-2.462442	2.370870
36	1	0	1.457589	-2.148069	0.644383
37	6	0	3.370110	-1.785919	3.409131
38	6	0	2.408778	1.341431	-0.922578
39	6	0	3.566320	1.949262	-0.431917
40	6	0	2.204835	1.284477	-2.294442
41	6	0	4.470848	2.583387	-1.276403
42	1	0	3.747584	1.937783	0.634097
43	6	0	3.097590	1.861129	-3.208619
44	1	0	1.326686	0.766719	-2.665925
45	6	0	4.169069	2.593380	-2.663015
46	6	0	-3.653688	-1.409363	-0.004897
47	6	0	-4.938477	-0.909613	0.183352
48	6	0	-3.496314	-2.740051	-0.385489
49	6	0	-6.066489	-1.727298	0.094094
50	1	0	-5.070767	0.142532	0.385367
51	6	0	-4.577620	-3.614627	-0.483041
52	1	0	-2.500679	-3.092993	-0.618691
53	6	0	-5.843019	-3.104902	-0.114466
54	6	0	-2.749767	1.350768	-0.097883
55	6	0	-2.326771	1.994142	-1.251111
56	6	0	-3.622363	2.007339	0.773388
57	6	0	-2.811305	3.253963	-1.620661
58	1	0	-1.585108	1.502476	-1.874072
59	6	0	-4.197157	3.227553	0.431698
60	1	0	-3.860875	1.540160	1.721037

61	6	0	-3.843604	3.783166	-0.825169
62	6	0	-2.126448	3.932210	-2.831419
63	6	0	-2.428215	3.137510	-4.115320
64	1	0	-1.926025	3.602353	-4.971174
65	1	0	-2.075928	2.102675	-4.042767
66	1	0	-3.502100	3.112968	-4.328027
67	6	0	-2.488483	5.410494	-3.059340
68	1	0	-2.366639	6.001114	-2.147661
69	1	0	-1.805347	5.814821	-3.814491
70	1	0	-3.502293	5.556883	-3.433629
71	6	0	-0.601754	3.914999	-2.577520
72	1	0	-0.354452	4.496906	-1.684150
73	1	0	-0.199333	2.907170	-2.446341
74	1	0	-0.082983	4.365759	-3.429874
75	6	0	-5.122023	3.964305	1.423308
76	6	0	-4.508065	5.341237	1.742191
77	1	0	-4.453639	5.969795	0.850644
78	1	0	-5.120456	5.861245	2.487769
79	1	0	-3.496875	5.234933	2.146053
80	6	0	-6.547980	4.155657	0.871367
81	1	0	-6.957946	3.217131	0.483877
82	1	0	-7.206826	4.496569	1.677853
83	1	0	-6.583622	4.960709	0.082187
84	6	0	-5.249503	3.189415	2.745190
85	1	0	-5.745294	2.221437	2.609072
86	1	0	-4.279234	3.016469	3.219436
87	1	0	-5.860229	3.774464	3.439928
88	8	0	-4.537748	4.889202	-1.249952
89	8	0	-6.902879	-3.976643	-0.004839
90	8	0	3.966207	-2.512498	4.412414
91	8	0	4.989038	3.331658	-3.481731
92	6	0	4.427170	4.582640	-3.869960
93	1	0	5.182580	5.091892	-4.471061
94	1	0	3.520407	4.451133	-4.467308
95	1	0	4.180745	5.194635	-2.995857
96	6	0	2.828427	1.600539	-4.711621
97	6	0	4.019969	1.878008	-5.646274
98	1	0	3.780061	1.475712	-6.636315
99	1	0	4.233024	2.938769	-5.775848
100	1	0	4.930196	1.382412	-5.296955
101	6	0	1.607329	2.416202	-5.175141
102	1	0	1.400132	2.213025	-6.232011
103	1	0	0.714232	2.148283	-4.600820
104	1	0	1.768488	3.492693	-5.065015
105	6	0	-5.519575	4.582333	-2.237005
106	1	0	-6.018042	5.520995	-2.485190
107	1	0	-5.067533	4.161867	-3.140968
108	1	0	-6.255325	3.866946	-1.853134
109	6	0	-7.032418	-4.509784	1.316624
110	1	0	-7.852702	-5.229011	1.284002
111	1	0	-6.116854	-5.015180	1.634641
112	1	0	-7.263036	-3.726195	2.042987
113	6	0	-7.474519	-1.089484	0.061254
114	6	0	-7.388148	0.445746	0.137442
115	1	0	-6.980099	0.789899	1.094318
116	1	0	-6.780816	0.867822	-0.670233
117	1	0	-8.395419	0.863119	0.042349
118	6	0	-8.125324	-1.448586	-1.289672
119	1	0	-8.254401	-2.528165	-1.397342
120	1	0	-9.112152	-0.978657	-1.367103
121	1	0	-7.514333	-1.088732	-2.124674
122	6	0	-8.395783	-1.546418	1.205924
123	1	0	-8.720578	-2.580358	1.083293
124	1	0	-7.908482	-1.439835	2.180860
125	1	0	-9.297277	-0.923625	1.216003
126	6	0	-4.387807	-4.999886	-1.143463
127	6	0	-2.929732	-5.208417	-1.591616
128	1	0	-2.593854	-4.436297	-2.292657
129	1	0	-2.234226	-5.234892	-0.745150
130	1	0	-2.852922	-6.170545	-2.107506
131	6	0	-4.755516	-6.187928	-0.236545
132	1	0	-4.426846	-7.118834	-0.711123
133	1	0	-4.259743	-6.118400	0.737407

134	1	0	-5.831853	-6.268069	-0.080264
135	6	0	-5.267234	-5.039173	-2.410049
136	1	0	-5.143262	-6.001165	-2.920213
137	1	0	-6.325590	-4.918395	-2.166821
138	1	0	-4.980133	-4.246380	-3.109542
139	6	0	5.788233	3.157272	-0.710873
140	6	0	2.492367	0.102634	-4.890263
141	1	0	3.278160	-0.532896	-4.468652
142	1	0	1.541976	-0.161394	-4.422319
143	1	0	2.396941	-0.129408	-5.955888
144	6	0	6.959733	2.357976	-1.314158
145	1	0	7.911355	2.724578	-0.912558
146	1	0	6.873783	1.294402	-1.065911
147	1	0	6.989259	2.455625	-2.402289
148	6	0	5.977521	4.656664	-1.011388
149	1	0	5.093052	5.235572	-0.724052
150	1	0	6.825303	5.037097	-0.431220
151	1	0	6.193355	4.843643	-2.062939
152	6	0	5.853779	3.006664	0.818643
153	1	0	5.793934	1.962846	1.139223
154	1	0	6.810819	3.398712	1.176655
155	1	0	5.058509	3.570201	1.319458
156	6	0	3.069170	-2.918380	5.443110
157	1	0	3.593416	-3.864734	6.043179
158	1	0	2.794901	-2.077551	6.087012
159	1	0	2.154174	-3.356452	5.033103
160	6	0	4.469962	0.378790	4.389931
161	6	0	4.434984	-0.018763	5.878027
162	1	0	5.135330	0.623385	6.422701
163	1	0	3.451470	0.133187	6.330485
164	1	0	4.745944	-1.049858	6.038234
165	6	0	5.893618	0.095714	3.868255
166	1	0	6.634133	0.576643	4.517522
167	1	0	6.103645	-0.977882	3.848788
168	1	0	6.026848	0.494914	2.858860
169	6	0	4.234692	1.898562	4.339792
170	1	0	4.424288	2.322581	3.349000
171	1	0	3.212796	2.158021	4.639586
172	1	0	4.923201	2.390430	5.033612
173	6	0	2.611762	-3.992425	2.138814
174	6	0	1.159318	-4.442333	2.392319
175	1	0	1.063104	-5.520769	2.222301
176	1	0	0.851501	-4.233603	3.422226
177	1	0	0.458146	-3.933019	1.721982
178	6	0	3.559687	-4.863403	2.981346
179	1	0	3.280303	-4.917060	4.033344
180	1	0	3.159521	-5.885496	2.588571
181	1	0	4.594791	-4.519265	2.911386
182	6	0	2.982311	-4.299463	0.669357
183	1	0	2.383995	-3.747874	-0.059983
184	1	0	4.036473	-4.071574	0.486953
185	1	0	2.830216	-5.366584	0.474987
186	8	0	1.171830	-1.811119	-2.205221
187	6	0	1.263692	-2.527229	-3.207078
188	1	0	-1.424544	-1.770516	-1.725409
189	6	0	0.206517	-2.721834	-4.164531
190	6	0	-0.985887	-2.085612	-4.410751
191	8	0	0.411784	-3.692177	-5.106837
192	6	0	-1.543440	-2.713323	-5.551797
193	1	0	-1.393352	-1.256596	-3.851248
194	6	0	-0.653843	-3.680256	-5.922323
195	1	0	-2.478381	-2.480345	-6.039317
196	1	0	-0.650395	-4.411456	-6.717335
197	6	0	2.573302	-3.242160	-3.467765
198	1	0	2.880151	-3.123555	-4.510982
199	1	0	2.447254	-4.312255	-3.264385
200	8	0	3.517447	-2.659974	-2.596327
201	6	0	4.651154	-3.323999	-2.344815
202	8	0	4.949514	-4.364965	-2.895638
203	6	0	5.447646	-2.637404	-1.298181
204	6	0	6.660896	-3.200339	-0.896341
205	6	0	4.952722	-1.497410	-0.657392
206	6	0	7.377663	-2.623361	0.146277

207	1	0	7.029210	-4.091207	-1.394664
208	6	0	5.663796	-0.937995	0.394660
209	1	0	4.009594	-1.060833	-0.965733
210	6	0	6.876608	-1.496166	0.795828
211	1	0	8.320957	-3.058734	0.460039
212	1	0	5.257513	-0.071920	0.904594
213	1	0	7.429359	-1.054584	1.619342

TS1a(R) -1b

RwB97XD SCF energy	-5094.176478 a.u.
RwB97XD SCF enthalpy	-5092.242672 a.u.
RwB97XD SCF free energy	-5092.484306 a.u.
Three lowest frequencies (cm ⁻¹)	-618.9, 9.0, 11.4
Imaginary frequency (cm ⁻¹)	-618.9

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates		Z (Angstroms)
			X	Y	
1	6	0	0.759524	1.001259	2.450487
2	6	0	0.626386	1.993481	3.397272
3	6	0	1.203220	3.252507	3.273738
4	6	0	1.942567	3.597290	2.169516
5	6	0	2.101445	2.605148	1.190839
6	6	0	1.537356	1.334575	1.307650
7	1	0	2.394320	4.576001	2.060695
8	1	0	2.697094	2.851850	0.320566
9	6	0	0.134982	-0.315455	2.743568
10	6	0	-0.909030	-0.936755	2.008358
11	6	0	0.553628	-0.986140	3.873906
12	6	0	-1.414575	-2.173612	2.410037
13	6	0	0.038120	-2.214930	4.269441
14	6	0	-0.944006	-2.847763	3.546938
15	1	0	-2.211628	-2.638209	1.840278
16	1	0	-1.351687	-3.806266	3.845538
17	8	0	0.890332	3.999672	4.369249
18	8	0	-0.084053	1.936789	4.560203
19	8	0	1.513926	-0.596739	4.761259
20	8	0	0.662970	-2.614565	5.415343
21	6	0	0.366874	3.059696	5.313646
22	1	0	-0.469773	3.502214	5.851183
23	1	0	1.169463	2.745986	5.991944
24	6	0	1.305562	-1.432936	5.898067
25	1	0	0.640070	-0.922312	6.605372
26	1	0	2.263376	-1.687805	6.348094
27	15	0	-1.511692	-0.187916	0.450796
28	15	0	1.794677	0.125095	-0.044881
29	46	0	0.008238	-0.533431	-1.303969
30	6	0	-1.736483	1.588325	0.768570
31	6	0	-2.392593	2.057908	1.906137
32	6	0	-1.251437	2.497747	-0.161489
33	6	0	-2.549236	3.420646	2.143011
34	1	0	-2.763476	1.337922	2.624426
35	6	0	-1.387760	3.880660	-0.001072
36	1	0	-0.727074	2.117028	-1.032655
37	6	0	-1.973166	4.316279	1.204620
38	6	0	-3.154928	-0.922153	0.176238
39	6	0	-4.327037	-0.337851	0.659287
40	6	0	-3.235624	-2.118619	-0.526078
41	6	0	-5.552393	-0.990951	0.572507
42	1	0	-4.277836	0.639472	1.117284
43	6	0	-4.443348	-2.812481	-0.674103
44	1	0	-2.334635	-2.527411	-0.968371
45	6	0	-5.557500	-2.287709	0.004506
46	6	0	3.151596	0.848921	-1.007257
47	6	0	4.477300	0.633443	-0.647879
48	6	0	2.853801	1.675384	-2.087781
49	6	0	5.522065	1.310382	-1.275846
50	1	0	4.698418	-0.081424	0.131787
51	6	0	3.849292	2.410464	-2.735651
52	1	0	1.821980	1.749591	-2.412679
53	6	0	5.160841	2.296606	-2.220457
54	6	0	2.433063	-1.373960	0.758563
55	6	0	1.993075	-2.611301	0.311174
56	6	0	3.323041	-1.310557	1.830941
57	6	0	2.442870	-3.810677	0.870166
58	1	0	1.258329	-2.641222	-0.485858

59	6	0	3.871526	-2.465680	2.380878	141	1	0	-4.479124	-2.776437	-3.400550
60	1	0	3.591293	-0.339960	2.228914	142	1	0	-2.838064	-3.186781	-2.887864
61	6	0	3.469986	-3.709873	1.830025	143	1	0	-3.840871	-4.406506	-3.677506
62	6	0	1.764470	-5.114220	0.390812	144	6	0	-7.863742	-0.291168	-0.130819
63	6	0	2.407447	-5.576630	-0.928397	145	1	0	-8.773241	0.241104	0.170157
64	1	0	1.881057	-6.454429	-1.320336	146	1	0	-7.449359	0.215474	-1.008130
65	1	0	2.350330	-4.783967	-1.680071	147	1	0	-8.143891	-1.305134	-0.421612
66	1	0	3.460476	-5.841264	-0.804850	148	6	0	-7.469746	-0.967093	2.264566
67	6	0	1.796943	-6.243771	1.436356	149	1	0	-6.728379	-1.093399	3.061203
68	1	0	1.415824	-5.895036	2.402118	150	1	0	-8.278272	-0.340637	2.657962
69	1	0	1.147478	-7.057055	1.095689	151	1	0	-7.896874	-1.942097	2.026245
70	1	0	2.788859	-6.663872	1.595503	152	6	0	-6.580332	1.179013	1.398497
71	6	0	0.265650	-4.845428	0.114249	153	1	0	-6.112569	1.729598	0.575927
72	1	0	-0.235369	-4.434135	0.997180	154	1	0	-7.531155	1.670078	1.627721
73	1	0	0.097986	-4.162001	-0.722516	155	1	0	-5.945258	1.270550	2.285352
74	1	0	-0.223637	-5.789454	-0.145789	156	6	0	-0.800617	6.169958	2.026750
75	6	0	4.846347	-2.368344	3.572682	157	1	0	-0.974153	7.226522	2.238794
76	6	0	4.347058	-3.253623	4.732425	158	1	0	-0.519199	5.653233	2.948634
77	1	0	4.450666	-4.315048	4.506297	159	1	0	0.019092	6.080347	1.308296
78	1	0	4.918910	-3.039738	5.642052	160	6	0	-3.436441	3.896311	3.314300
79	1	0	3.290112	-3.059726	4.937168	161	6	0	-2.775060	4.953448	4.218172
80	6	0	6.270720	-2.786137	3.160839	162	1	0	-3.367699	5.070443	5.131608
81	1	0	6.606642	-2.224028	2.282308	163	1	0	-1.768062	4.647361	4.512374
82	1	0	6.968252	-2.574465	3.979043	164	1	0	-2.711828	5.929628	3.738772
83	1	0	6.343633	-3.850531	2.936769	165	6	0	-4.724961	4.484574	2.704684
84	6	0	4.936277	-0.926044	4.101594	166	1	0	-5.400678	4.820342	3.499632
85	1	0	5.367635	-0.239535	3.364681	167	1	0	-4.503495	5.342128	2.062635
86	1	0	3.959838	-0.538567	4.408219	168	1	0	-5.253017	3.733714	2.106370
87	1	0	5.592119	-0.910538	4.977748	169	6	0	-3.830667	2.723500	4.228763
88	8	0	4.093979	-4.833604	2.310454	170	1	0	-4.400101	1.950045	3.604846
89	8	0	6.133887	3.148688	-2.690169	171	1	0	-2.952125	2.255978	4.687257
90	8	0	-2.021678	5.656774	1.496694	172	1	0	-4.468709	3.099686	5.034202
91	8	0	-6.702140	-3.037785	0.132672	173	6	0	-0.892111	4.772521	-1.169151
92	6	0	-6.591773	-4.020827	1.159687	174	6	0	0.647576	4.790239	-1.193495
93	1	0	-7.549406	-4.542892	1.199635	175	1	0	0.996626	5.392689	-2.039930
94	1	0	-5.793591	-4.739914	0.946995	176	1	0	1.070418	5.217643	-0.279416
95	1	0	-6.390224	-3.555105	2.130726	177	1	0	1.053711	3.779961	-1.308891
96	6	0	-4.429989	-4.040766	-1.614598	178	6	0	-1.420216	6.219064	-1.158385
97	6	0	-5.803118	-4.657818	-1.929478	179	1	0	-0.978827	6.838662	-0.378563
98	1	0	-5.667644	-5.402140	-2.722173	180	1	0	-1.166033	6.682674	-2.117600
99	1	0	-6.252637	-5.173910	-1.080360	181	1	0	-2.508110	6.251715	-1.050778
100	1	0	-6.511466	-3.909229	-2.293818	182	6	0	-1.379646	4.168538	-2.505827
101	6	0	-3.514525	-5.132546	-1.032420	183	1	0	-0.972405	3.174022	-2.703714
102	1	0	-3.453525	-5.980505	-1.723891	184	1	0	-2.471690	4.100479	-2.535504
103	1	0	-2.497331	-4.761150	-0.870235	185	1	0	-1.059957	4.814733	-3.329807
104	1	0	-3.895091	-5.504521	-0.074945	186	8	0	-1.129195	-1.625013	-2.721851
105	6	0	5.076171	-5.411918	1.454497	187	6	0	-0.135929	-1.426871	-3.509614
106	1	0	5.812139	-5.899856	2.097733	188	1	0	1.027724	-0.688458	-2.554464
107	1	0	4.637679	-6.167487	0.796219	189	6	0	0.719036	-2.567947	-3.864376
108	1	0	5.573525	-4.649903	0.846270	190	6	0	0.582094	-3.905880	-3.657004
109	6	0	6.252411	4.328440	-1.888794	191	8	0	1.831914	-2.307906	-4.600640
110	1	0	7.033963	4.937541	-2.346124	192	6	0	1.694416	-4.516736	-4.314791
111	1	0	5.315424	4.890836	-1.866672	193	1	0	-0.218475	-4.392630	-3.118863
112	1	0	6.530167	4.086899	-0.859798	194	6	0	2.416918	-3.503770	-4.859889
113	6	0	6.980648	0.855492	-1.042464	195	1	0	1.923343	-5.570920	-4.368816
114	6	0	7.041696	-0.319150	-0.048649	196	1	0	3.327632	-3.467621	-5.438208
115	1	0	6.701168	-0.028475	0.951588	197	6	0	-0.304104	-0.336615	-4.580409
116	1	0	6.450250	-1.178555	-0.381150	198	1	0	-0.472173	-0.829288	-5.541897
117	1	0	8.079687	-0.653258	0.043136	199	1	0	0.565070	0.312175	-4.654287
118	6	0	7.525874	0.352785	-2.395040	200	8	0	-1.409931	0.473131	-4.226009
119	1	0	7.540588	1.152471	-3.140141	201	6	0	-2.629389	-0.072372	-4.450535
120	1	0	8.549568	-0.018682	-2.272481	202	8	0	-2.801597	-1.018581	-5.190764
121	1	0	6.912521	-0.468042	-2.782304	203	6	0	-3.710658	0.630456	-3.721565
122	6	0	7.915728	1.950444	-0.498852	204	6	0	-5.025805	0.508450	-4.179160
123	1	0	8.130372	2.716490	-1.244867	205	6	0	-3.434272	1.370657	-2.572260
124	1	0	7.500901	2.428500	0.394689	206	6	0	-6.050890	1.160526	-3.504502
125	1	0	8.871332	1.495314	-0.217248	207	1	0	-5.233400	-0.081972	-5.065800
126	6	0	3.527009	3.185677	-4.033131	208	6	0	-4.462522	2.012271	-1.891749
127	6	0	2.059958	2.986175	-4.446397	209	1	0	-2.417260	1.430106	-2.209349
128	1	0	1.820616	1.928252	-4.587222	210	6	0	-5.768678	1.917845	-2.366339
129	1	0	1.358150	3.410681	-3.720922	211	1	0	-7.071458	1.080798	-3.865075
130	1	0	1.888860	3.488528	-5.403314	212	1	0	-4.240793	2.582480	-0.993969
131	6	0	3.760881	4.703663	-3.924807	213	1	0	-6.573133	2.427919	-1.844989
132	1	0	3.315219	5.199069	-4.794157						
133	1	0	3.289276	5.119598	-3.028027						
134	1	0	4.821655	4.957852	-3.917551						
135	6	0	4.404193	2.612741	-5.164699						
136	1	0	4.177836	3.124064	-6.107056						
137	1	0	5.467585	2.746613	-4.954138						
138	1	0	4.211474	1.543478	-5.305926						
139	6	0	-6.848700	-0.289613	1.029026						
140	6	0	-3.856786	-3.569114	-2.971151						

4a(R) -1b

RwB97XD SCF energy -5094.196376 a.u.

RwB97XD SCF enthalpy -5092.256638 a.u.

RwB97XD SCF free energy -5092.498130 a.u.

Three lowest frequencies (cm⁻¹) 9.8, 14.8, 19.4

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)								
			X	Y	Z						
						79	1	0	-3.877900	-5.079236	-2.551831
						80	6	0	-6.836303	-3.620109	-1.441067
						81	1	0	-7.130060	-2.640794	-1.046924
						82	1	0	-7.490836	-3.849246	-2.289455
						83	1	0	-7.020858	-4.373827	-0.675235
						84	6	0	-5.304082	-2.768543	-3.190370
						85	1	0	-5.668046	-1.748120	-3.026842
						86	1	0	-4.290701	-2.713696	-3.600580
						87	1	0	-5.946279	-3.223794	-3.950574
						88	8	0	-5.018462	-4.797128	0.700173
						89	8	0	-5.832684	4.426411	1.041375
						90	8	0	2.763452	3.476666	-4.203656
						91	8	0	5.587792	-3.613351	2.414701
						92	6	0	5.241235	-4.991397	2.294746
						93	1	0	6.076703	-5.560245	2.706338
						94	1	0	4.330176	-5.231370	2.852019
						95	1	0	5.090376	-5.269006	1.246234
						96	6	0	3.218547	-2.815962	4.135241
						97	6	0	4.457865	-3.267553	4.927686
						98	1	0	4.195036	-3.283525	5.991130
						99	1	0	4.800916	-4.269303	4.668164
						100	1	0	5.291516	-2.571415	4.801756
						101	6	0	2.110015	-3.873826	4.274718
						102	1	0	1.927008	-4.088016	5.333682
						103	1	0	1.170260	-3.520232	3.839874
						104	1	0	2.379964	-4.812876	3.780304
						105	6	0	-5.984588	-4.440118	1.686657
						106	1	0	-6.611525	-5.320219	1.839622
						107	1	0	-5.512253	-4.161107	2.633815
						108	1	0	-6.605286	-3.603326	1.348201
						109	6	0	-6.067712	5.110347	-0.194427
						110	1	0	-6.754652	5.928014	0.029575
						111	1	0	-5.140327	5.512412	-0.610137
						112	1	0	-6.517345	4.446786	-0.937207
						113	6	0	-6.923680	1.695181	0.814351
						114	6	0	-7.137966	0.198369	0.522779
						115	1	0	-6.941927	-0.045141	-0.527609
						116	1	0	-6.513761	-0.445188	1.151528
						117	1	0	-8.181873	-0.055709	0.730429
						118	6	0	-7.266220	1.939200	2.298040
						119	1	0	-7.147699	2.992443	2.564858
						120	1	0	-8.305991	1.654045	2.493664
						121	1	0	-6.621477	1.341235	2.951321
						122	6	0	-7.920850	2.468973	-0.065913
						123	1	0	-8.018837	3.510480	0.241698
						124	1	0	-7.638741	2.432843	-1.123395
						125	1	0	-8.910726	2.009668	0.028676
						126	6	0	-3.042496	4.899983	1.830957
						127	6	0	-1.533795	4.781167	2.102210
						128	1	0	-1.292872	3.870603	2.655693
						129	1	0	-0.945092	4.798146	1.178887
						130	1	0	-1.211977	5.631276	2.711373
						131	6	0	-3.261438	6.208322	1.051488
						132	1	0	-2.698516	7.013852	1.535483
						133	1	0	-2.902552	6.126131	0.019827
						134	1	0	-4.309227	6.510765	1.039157
						135	6	0	-3.747828	4.995757	3.199191
						136	1	0	-3.354271	5.851788	3.758589
						137	1	0	-4.825628	5.130587	3.085564
						138	1	0	-3.568642	4.093527	3.793627
						139	6	0	6.258814	-2.273338	-0.057149
						140	6	0	2.744100	-1.510287	4.814018
						141	1	0	3.498369	-0.723434	4.708293
						142	1	0	1.805426	-1.132469	4.402381
						143	1	0	2.585845	-1.690583	5.882751
						144	6	0	7.311853	-1.618235	0.856296
						145	1	0	8.295973	-1.648904	0.374730
						146	1	0	7.061650	-0.569563	1.045968
						147	1	0	7.387558	-2.134664	1.816062
						148	6	0	6.671881	-3.723808	-0.373076
						149	1	0	5.867013	-4.264913	-0.882548
						150	1	0	7.540828	-3.716938	-1.040426
						151	1	0	6.954220	-4.275496	0.523505
						152	6	0	6.257210	-1.509610	-1.391823
						153	1	0	6.005285	-0.453155	-1.626701
						154	1	0	7.258782	-1.555629	-1.830660
						155	1	0	5.561810	-1.952734	-2.113003
						156	6	0	1.609294	3.795724	-4.982116
						157	1	0	1.926759	4.532877	-5.721490
						158	1	0	1.218323	2.910998	-5.492534
						159	1	0	0.813428	4.222463	-4.364460
						160	6	0	3.782661	0.796959	-4.663862

161	6	0	3.267038	1.266462	-6.036542	15	1	0	1.265719	3.476171	0.954297
162	1	0	3.818775	0.747795	-6.827869	16	1	0	0.140790	4.972851	2.557777
163	1	0	2.207242	1.032221	-6.162593	17	8	0	-0.716686	-2.748430	5.262992
164	1	0	3.406595	2.336890	-6.185554	18	8	0	-0.071120	-0.577589	4.939731
165	6	0	5.175312	1.407919	-4.409840	19	8	0	-2.049982	1.663292	4.455433
166	1	0	5.847915	1.165774	-5.240571	20	8	0	-1.636337	3.917742	4.465731
167	1	0	5.123878	2.496955	-4.320894	21	6	0	-0.409940	-1.529189	5.946870
168	1	0	5.616967	1.004282	-3.491653	22	1	0	0.437934	-1.680307	6.611970
169	6	0	3.946355	-0.729367	-4.746722	23	1	0	-1.301032	-1.184606	6.485615
170	1	0	4.393474	-1.150555	-3.841113	24	6	0	-2.113938	2.834492	5.269502
171	1	0	2.990085	-1.231532	-4.930695	25	1	0	-1.455583	2.709743	6.137044
172	1	0	4.616410	-0.970362	-5.577505	26	1	0	-3.146728	3.021549	5.560373
173	6	0	1.654450	4.406354	-1.534435	27	15	0	1.144573	0.636770	0.365806
174	6	0	0.134089	4.655292	-1.544092	28	15	0	-1.995022	-0.243707	0.042568
175	1	0	-0.083675	5.661247	-1.168074	29	46	0	-0.219542	0.158799	-1.396432
176	1	0	-0.282832	4.573688	-2.553064	30	6	0	1.689860	-0.904743	1.137378
177	1	0	-0.390059	3.934607	-0.906348	31	6	0	2.378761	-0.912266	2.350014
178	6	0	2.359101	5.514114	-2.336043	32	6	0	1.430652	-2.101495	0.485451
179	1	0	1.942483	5.660479	-3.332360	33	6	0	2.763887	-2.107413	2.949559
180	1	0	2.234037	6.458842	-1.795947	34	1	0	2.598314	0.033652	2.829041
181	1	0	3.431573	5.324415	-2.431384	35	6	0	1.791817	-3.339220	1.024391
182	6	0	2.169798	4.555001	-0.084010	36	1	0	0.919219	-2.070802	-0.470408
183	1	0	1.697385	3.863512	0.618647	37	6	0	2.378890	-3.317435	2.306052
184	1	0	3.251669	4.395651	-0.034715	38	6	0	2.594479	1.593931	-0.145318
185	1	0	1.961522	5.569402	0.271744	39	6	0	3.875944	1.312204	0.322831
186	8	0	1.183652	0.742719	2.629808	40	6	0	2.400334	2.658754	-1.015954
187	6	0	1.026640	1.994361	3.215982	41	6	0	4.946716	2.160228	0.039661
188	6	0	-0.161629	2.018982	4.141351	42	1	0	4.035491	0.428997	0.926056
189	6	0	-1.177815	1.137240	4.353541	43	6	0	3.439892	3.514842	-1.382844
190	8	0	-0.374895	3.151593	4.864627	44	1	0	1.410181	2.819901	-1.426139
191	6	0	-2.083211	1.776241	5.266639	45	6	0	4.679905	3.308155	-0.744337
192	1	0	-1.270920	0.152360	3.915265	46	6	0	-3.131803	-1.381612	-0.795070
193	6	0	-1.546294	2.989889	5.540711	47	6	0	-4.508942	-1.270136	-0.649655
194	1	0	-3.002832	1.374695	5.667669	48	6	0	-2.599995	-2.371508	-1.618444
195	1	0	-1.845163	3.813150	6.171617	49	6	0	-5.379000	-2.193317	-1.231560
196	6	0	2.317183	2.356087	3.946752	50	1	0	-4.907204	-0.441687	-0.080119
197	1	0	2.604556	1.563881	4.641147	51	6	0	-3.411021	-3.330065	-2.223699
198	1	0	2.234280	3.306201	4.480782	52	1	0	-1.529111	-2.383130	-1.790238
199	8	0	3.302695	2.500306	2.917675	53	6	0	-4.789245	-3.285555	-1.907689
200	6	0	4.525954	2.004459	3.099773	54	6	0	-2.912050	1.276954	0.379418
201	8	0	4.947774	1.596403	4.166110	55	6	0	-2.679681	2.359304	-0.455784
202	6	0	5.311308	2.043614	1.837226	56	6	0	-3.850948	1.385504	1.406341
203	6	0	6.704466	2.109800	1.898534	57	6	0	-3.418187	3.542170	-0.363229
204	6	0	4.663330	2.025771	0.599593	58	1	0	-1.898320	2.280108	-1.204773
205	6	0	7.443642	2.187572	0.721812	59	6	0	-4.652647	2.517375	1.523787
206	1	0	7.200031	2.116302	2.864234	60	1	0	-3.953309	0.566455	2.107846
207	6	0	5.404971	2.094480	-0.573693	61	6	0	-4.483993	3.541547	0.555463
208	1	0	3.583145	1.954831	0.557104	62	6	0	-2.957930	4.715862	-1.258539
209	6	0	6.795278	2.183329	-0.512715	63	6	0	-3.267245	4.398848	-2.733041
210	1	0	8.526080	2.252968	0.768275	64	1	0	-2.908656	5.210330	-3.376094
211	1	0	4.894690	2.081231	-1.531916	65	1	0	-2.772632	3.475058	-3.053191
212	1	0	7.373649	2.243366	-1.429891	66	1	0	-4.341550	4.281884	-2.906139
213	1	0	0.866268	2.786050	2.457127	67	6	0	-3.551386	6.086815	-0.891225
						68	1	0	-3.409488	6.312681	0.169602
						69	1	0	-3.026765	6.855125	-1.469516
						70	1	0	-4.612544	6.178253	-1.122802
						71	6	0	-1.425292	4.864144	-1.104022
						72	1	0	-1.151214	5.044271	-0.059007
						73	1	0	-0.875833	3.985860	-1.454892
						74	1	0	-1.082122	5.717167	-1.698346
						75	6	0	-5.620507	2.670499	2.715031
						76	6	0	-5.250732	3.954717	3.484375
						77	1	0	-5.437158	4.849814	2.887595
						78	1	0	-5.843342	4.027464	4.403284
						79	1	0	-4.191023	3.948909	3.759082
						80	6	0	-7.094907	2.732000	2.274570
						81	1	0	-7.350525	1.891738	1.619320
						82	1	0	-7.741288	2.673963	3.157432
						83	1	0	-7.330882	3.662534	1.758184
						84	6	0	-5.491251	1.489969	3.692263
						85	1	0	-5.802632	0.543297	3.237079
						86	1	0	-4.470772	1.373878	4.069781
						87	1	0	-6.145750	1.669063	4.550856
						88	8	0	-5.399428	4.565164	0.548726
						89	8	0	-5.593486	-4.324376	-2.316773
						90	8	0	2.634327	-4.489824	2.964225
						91	8	0	5.692086	4.224185	-0.893898
						92	6	0	5.537989	5.381985	-0.077640
						93	1	0	6.444619	5.975707	-0.207223
						94	1	0	4.671542	5.979660	-0.376535
						95	1	0	5.424405	5.112145	0.977540
						96	6	0	3.120690	4.568813	-2.470275

5a(R) -1b

RwB97XD SCF energy -5095.379436 a.u.

RwB97XD SCF enthalpy -5093.422731 a.u.

RwB97XD SCF free energy -5093.666336 a.u.

Three lowest frequencies (cm⁻¹) 13.6, 15.9, 18.9

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		Z
			X	Y	
1	6	0	-0.956418	-0.337917	2.657804
2	6	0	-0.709739	-1.028763	3.822544
3	6	0	-1.087498	-2.354146	4.012810
4	6	0	-1.718489	-3.072062	3.026138
5	6	0	-1.989973	-2.389045	1.830909
6	6	0	-1.633404	-1.054742	1.637378
7	1	0	-2.008837	-4.106480	3.166054
8	1	0	-2.506150	-2.928605	1.045678
9	6	0	-0.577452	1.092575	2.575449
10	6	0	0.331022	1.665307	1.645215
11	6	0	-1.150164	1.962558	3.477742
12	6	0	0.565970	3.041663	1.656885
13	6	0	-0.905749	3.330905	3.479606
14	6	0	-0.055758	3.907429	2.567599

97	6	0	4.349138	5.217642	-3.131929
98	1	0	4.005877	5.805711	-3.989998
99	1	0	4.893728	5.894980	-2.474566
100	1	0	5.049916	4.463941	-3.502906
101	6	0	2.212337	5.661941	-1.878814
102	1	0	1.916846	6.372692	-2.658823
103	1	0	1.300704	5.228804	-1.455121
104	1	0	2.714760	6.223406	-1.084828
105	6	0	-6.372800	4.429037	-0.485310
106	1	0	-7.092590	5.237922	-0.348151
107	1	0	-5.921785	4.514520	-1.478723
108	1	0	-6.887353	3.464606	-0.416611
109	6	0	-5.700265	-5.352081	-1.326144
110	1	0	-6.358721	-6.117095	-1.741281
111	1	0	-4.725759	-5.792108	-1.101130
112	1	0	-6.128706	-4.967893	-0.397174
113	6	0	-6.897847	-1.903705	-1.251773
114	6	0	-7.220780	-0.581260	-0.531719
115	1	0	-6.983799	-0.628090	0.537227
116	1	0	-6.694535	0.274108	-0.967872
117	1	0	-8.293355	-0.383820	-0.621285
118	6	0	-7.323385	-1.751082	-2.726013
119	1	0	-7.137830	-2.668526	-3.290461
120	1	0	-8.394738	-1.528510	-2.785176
121	1	0	-6.779841	-0.931332	-3.208349
122	6	0	-7.760253	-2.992652	-0.589425
123	1	0	-7.800784	-3.906207	-1.183764
124	1	0	-7.398322	-3.236192	0.415014
125	1	0	-8.787128	-2.624481	-0.490059
126	6	0	-8.822345	-4.268057	-3.301961
127	6	0	-1.330602	-3.976060	-3.540344
128	1	0	-1.148362	-2.935822	-3.828347
129	1	0	-0.719638	-4.210368	-2.662235
130	1	0	-0.974806	-4.606329	-4.361336
131	6	0	-2.934345	-5.763184	-2.955953
132	1	0	-2.324582	-6.343183	-3.656974
133	1	0	-2.561666	-5.967762	-1.946346
134	1	0	-3.958380	-6.129363	-3.038468
135	6	0	-3.563197	-3.988941	-4.625544
136	1	0	-3.159443	-4.625624	-5.420659
137	1	0	-4.633005	-4.192841	-4.538065
138	1	0	-3.433790	-2.944297	-4.929626
139	6	0	6.369914	1.803688	0.520705
140	6	0	2.354036	3.862821	-3.613886
141	1	0	2.940380	3.033257	-4.022852
142	1	0	1.383614	3.471536	-3.298654
143	1	0	2.165614	4.578118	-4.421391
144	6	0	7.291399	1.673286	-0.708140
145	1	0	8.281234	1.317146	-0.400216
146	1	0	6.883996	0.957946	-1.428900
147	1	0	7.415913	2.632504	-1.214934
148	6	0	6.945512	2.852497	1.491240
149	1	0	6.245585	3.063422	2.307175
150	1	0	7.868260	2.464761	1.937239
151	1	0	7.194150	3.788188	0.990840
152	6	0	6.382786	0.459059	1.266203
153	1	0	5.994090	-0.355705	0.652929
154	1	0	7.414287	0.210026	1.533226
155	1	0	5.804125	0.501373	2.196166
156	6	0	1.492148	-5.036157	3.623498
157	1	0	1.829825	-5.944014	4.126353
158	1	0	1.088530	-4.338056	4.362379
159	1	0	0.699789	-5.291875	2.914568
160	6	0	3.664513	-2.082600	4.204019
161	6	0	3.103636	-2.900937	5.381451
162	1	0	3.655158	-2.649907	6.293824
163	1	0	2.049555	-2.670347	5.554268
164	1	0	3.201571	-3.974577	5.222581
165	6	0	5.047278	-2.639148	3.811403
166	1	0	5.709457	-2.645311	4.684879
167	1	0	4.973071	-3.663760	3.436105
168	1	0	5.513290	-2.019537	3.037613
169	6	0	3.864927	-0.646486	4.716335
170	1	0	4.335670	0.003040	3.971261
171	1	0	2.918983	-0.189956	5.028761
172	1	0	4.527161	-0.668987	5.587173
173	6	0	1.504092	-4.588241	0.151736
174	6	0	-0.012380	-4.859832	0.137541
175	1	0	-0.226036	-5.748707	-0.466820
176	1	0	-0.407345	-5.032276	1.143084
177	1	0	-0.561113	-4.017021	-0.296552
178	6	0	2.255513	-5.864576	0.571589

179	1	0	1.870286	-6.319569	1.483864
180	1	0	2.145466	-6.605625	-0.227696
181	1	0	3.324476	-5.675816	0.704153
182	6	0	1.953443	-4.317976	-1.302855
183	1	0	1.495085	-3.431649	-1.749203
184	1	0	3.039442	-4.203430	-1.363911
185	1	0	1.673707	-5.173660	-1.926316
186	8	0	1.401250	0.427136	-2.583637
187	6	0	1.527311	-0.445419	-3.665058
188	6	0	0.667332	-0.042786	-4.830965
189	6	0	0.481249	1.131635	-5.491491
190	8	0	-0.192843	-0.982740	-5.314836
191	6	0	-0.564420	0.900349	-6.445164
192	1	0	1.019238	2.052925	-5.317329
193	6	0	-0.934102	-0.395790	-6.292024
194	1	0	-0.975850	1.606767	-7.152242
195	1	0	-1.661010	-1.028250	-6.778976
196	6	0	2.999327	-0.464088	-4.063275
197	1	0	3.365594	0.555877	-4.207607
198	1	0	3.168759	-1.047464	-4.973750
199	8	0	3.697241	-1.090190	-2.976991
200	6	0	5.016876	-0.924775	-2.897496
201	8	0	5.660693	-0.257633	-3.687431
202	6	0	5.607966	-1.677783	-1.759000
203	6	0	6.995609	-1.827625	-1.699862
204	6	0	4.801896	-2.244543	-0.769181
205	6	0	7.572155	-2.548947	-0.659882
206	1	0	7.613701	-1.381704	-2.472229
207	6	0	5.380302	-2.978378	0.259861
208	1	0	3.728939	-2.103358	-0.800445
209	6	0	6.764503	-3.129416	0.317317
210	1	0	8.650386	-2.664449	-0.614574
211	1	0	4.748350	-3.423753	1.019959
212	1	0	7.213803	-3.695569	1.127770
213	1	0	1.247948	-1.482417	-3.409125
214	1	0	-1.375485	0.396851	-2.896823
215	1	0	-1.332468	-0.377284	-2.887933

TS2a(R) -1b

RwB97XD SCF energy -5095.359187 a.u.
RwB97XD SCF enthalpy -5093.404003 a.u.
RwB97XD SCF free energy -5093.646900 a.u.
Three lowest frequencies (cm⁻¹) -1095, 5.8, 12.0
Imaginary frequency (cm⁻¹) -1095

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates		Z (Angstroms)
			X	Y	
1	6	0	1.022497	-1.415205	2.452721
2	6	0	0.880406	-1.568339	3.830846
3	6	0	1.350939	-0.639597	4.769196
4	6	0	2.000264	0.520127	4.381653
5	6	0	2.181173	0.698276	2.995724
6	6	0	1.725063	-0.230995	2.039480
7	1	0	2.367246	1.246855	5.100886
8	1	0	2.719364	1.581635	2.665146
9	6	0	0.524802	-2.500491	1.561105
10	6	0	-0.439167	-2.362192	0.505283
11	6	0	0.981780	-3.799674	1.784011
12	6	0	-0.819229	-3.483018	-0.258938
13	6	0	0.583337	-4.904555	1.021090
14	6	0	-0.311802	-4.777431	-0.026728
15	1	0	-1.548279	-3.361878	-1.054469
16	1	0	-0.622024	-5.626352	-0.629548
17	8	0	1.034493	-1.058921	6.039796
18	8	0	0.235459	-2.594908	4.487849
19	8	0	1.910685	-4.201251	2.720756
20	8	0	1.235507	-6.034812	1.457749
21	6	0	0.615084	-2.439593	5.876713
22	1	0	-0.248779	-2.635385	6.512559
23	1	0	1.465021	-3.099616	6.095905
24	6	0	1.843428	-5.648710	2.717046
25	1	0	1.201914	-5.982211	3.543793
26	1	0	2.852699	-6.058289	2.773343
27	15	0	-1.188477	-0.728220	0.090161
28	15	0	2.061021	0.106969	0.265216
29	46	0	0.272105	0.705587	-1.022058

30	6	0	-1.857310	-0.030212	1.647943	112	1	0	6.927593	3.687512	2.276228
31	6	0	-2.446816	-0.830052	2.642238	113	6	0	6.982528	2.093606	-0.598023
32	6	0	-1.831430	1.362740	1.808471	114	6	0	7.139001	0.648791	-1.130150
33	6	0	-2.991606	-0.263069	3.806975	115	1	0	7.064511	-0.096108	-0.326252
34	1	0	-2.475557	-1.906510	2.502674	116	1	0	6.395310	0.406363	-1.901042
35	6	0	-2.355190	2.001770	2.951196	117	1	0	8.133593	0.548680	-1.584244
36	1	0	-1.391199	1.958436	1.011866	118	6	0	7.188519	3.054717	-1.801156
37	6	0	-2.883308	1.152812	3.968591	119	1	0	7.122538	4.103243	-1.489777
38	6	0	-2.613835	-1.180779	-0.985886	120	1	0	8.182495	2.888559	-2.240327
39	6	0	-3.827410	-1.630473	-0.429150	121	1	0	6.437367	2.873778	-2.582192
40	6	0	-2.454455	-1.192803	-2.380544	122	6	0	8.124467	2.321540	0.424996
41	6	0	-4.818250	-2.230202	-1.222506	123	1	0	8.256511	3.380603	0.664946
42	1	0	-3.983091	-1.540449	0.641097	124	1	0	7.953323	1.762689	1.354805
43	6	0	-3.434222	-1.740639	-3.239943	125	1	0	9.068123	1.963669	-0.010297
44	1	0	-1.544516	-0.772921	-2.805394	126	6	0	3.157486	5.368647	0.524257
45	6	0	-4.539868	-2.374345	-2.614327	127	6	0	1.611690	5.395827	0.534462
46	6	0	3.256698	1.507859	0.239205	128	1	0	1.180733	4.880772	-0.332592
47	6	0	4.611708	1.284085	-0.051184	129	1	0	1.200604	4.951158	1.450395
48	6	0	2.802490	2.826120	0.435617	130	1	0	1.278894	6.441390	0.495512
49	6	0	5.553654	2.330457	-0.033389	131	6	0	3.624992	6.200140	1.746165
50	1	0	4.937124	0.280617	-0.302380	132	1	0	3.061715	7.143644	1.768731
51	6	0	3.696063	3.911345	0.496925	133	1	0	3.432444	5.748899	2.691406
52	1	0	1.734810	2.999794	0.542663	134	1	0	4.687189	6.453779	1.688432
53	6	0	5.084224	3.607245	0.380662	135	6	0	3.629601	6.079001	-0.774424
54	6	0	2.969241	-1.324315	-0.418554	136	1	0	3.243211	7.108112	-0.793321
55	6	0	2.810600	-1.638191	-1.774505	137	1	0	4.723224	6.123522	-0.829709
56	6	0	3.882249	-2.057776	0.364204	138	1	0	3.255210	5.559208	-1.666787
57	6	0	3.592659	-2.625816	-2.408711	139	6	0	-6.168743	-2.671956	-0.600386
58	1	0	2.056303	-1.097722	-2.345453	140	6	0	-2.929498	-0.057062	-5.037722
59	6	0	4.719088	-3.026389	-0.213819	141	1	0	-3.773456	0.569811	-4.719300
60	1	0	3.952394	-1.848605	1.427541	142	1	0	-2.028770	0.292566	-4.522551
61	6	0	4.618086	-3.220941	-1.625581	143	1	0	-2.779515	0.095479	-6.115693
62	6	0	3.221913	-2.979419	-3.877538	144	6	0	-7.333394	-1.956650	-1.337005
63	6	0	3.612556	-1.807056	-4.814987	145	1	0	-8.291201	-2.255878	-0.887774
64	1	0	3.309638	-2.036024	-5.846502	146	1	0	-7.243332	-0.866163	-1.246729
65	1	0	3.113863	-0.875584	-4.513787	147	1	0	-7.357464	-2.216923	-2.400545
66	1	0	4.695739	-1.627624	-4.811551	148	6	0	-6.380945	-4.207083	-0.672415
67	6	0	3.827175	-4.296433	-4.423764	149	1	0	-5.523443	-4.748449	-0.249946
68	1	0	3.634629	-5.141067	-3.750955	150	1	0	-7.269557	-4.475156	-0.083228
69	1	0	3.341229	-4.515718	-5.385085	151	1	0	-6.545548	-4.551513	-1.697061
70	1	0	4.903028	-4.239405	-4.610561	152	6	0	-6.255386	-2.275899	0.891792
71	6	0	1.679130	-3.169808	-3.955366	153	1	0	-6.125862	-1.196011	1.039090
72	1	0	1.346442	-3.975261	-3.286630	154	1	0	-7.249007	-2.548397	1.271549
73	1	0	1.128283	-2.258803	-3.696454	155	1	0	-5.511289	-2.805902	1.501500
74	1	0	1.401989	-3.441872	-4.982718	156	6	0	-2.473151	2.113255	6.165442
75	6	0	5.642418	-3.896030	0.680092	157	1	0	-2.933526	1.879774	7.131258
76	6	0	5.218998	-5.382380	0.523768	158	1	0	-1.514724	1.589746	6.077503
77	1	0	5.365312	-5.731563	-0.504493	159	1	0	-2.317009	3.196536	6.105891
78	1	0	5.824808	-6.012898	1.190233	160	6	0	-3.730328	-1.165116	4.831383
79	1	0	4.162231	-5.520603	0.787848	161	6	0	-3.127438	-1.064453	6.258925
80	6	0	7.146550	-3.756894	0.327865	162	1	0	-3.492809	-1.905246	6.865246
81	1	0	7.464102	-2.705572	0.332529	163	1	0	-2.031620	-1.114828	6.236761
82	1	0	7.740445	-4.287286	1.085827	164	1	0	-3.422651	-0.142361	6.764938
83	1	0	7.384431	-4.194161	-0.645219	165	6	0	-5.228527	-0.759819	4.878562
84	6	0	5.499412	-3.518596	2.173728	166	1	0	-5.758619	-1.386441	5.610202
85	1	0	5.829345	-2.488932	2.370860	167	1	0	-5.349325	0.288738	5.172364
86	1	0	4.469675	-3.629197	2.535887	168	1	0	-5.705672	-0.906264	3.899845
87	1	0	6.135638	-4.188393	2.767337	169	6	0	-3.666289	-2.657090	4.424274
88	8	0	5.545978	-4.070062	-2.217545	170	1	0	-4.124133	-2.844302	3.444235
89	8	0	6.014447	4.619271	0.613298	171	1	0	-2.635083	-3.034908	4.405145
90	8	0	-3.407535	1.673557	5.145916	172	1	0	-4.223926	-3.245577	5.164717
91	8	0	-5.424958	-3.141790	-3.364248	173	6	0	-2.315106	3.563130	3.001135
92	6	0	-4.903724	-4.456770	-3.686193	174	6	0	-1.015956	4.035789	3.705081
93	1	0	-5.696046	-4.963257	-4.245509	175	1	0	-0.966471	5.133762	3.681855
94	1	0	-3.999033	-4.391732	-4.302670	176	1	0	-0.952407	3.718955	4.750518
95	1	0	-4.674869	-5.018869	-2.771456	177	1	0	-0.132939	3.643091	3.183237
96	6	0	-3.226776	-1.560764	-4.772156	178	6	0	-3.568418	4.173059	3.675083
97	6	0	-4.447041	-1.901579	-5.663432	179	1	0	-3.667694	3.920318	4.732704
98	1	0	-4.220721	-1.557728	-6.682928	180	1	0	-3.510842	5.267044	3.590582
99	1	0	-4.660702	-2.972548	-5.723184	181	1	0	-4.483415	3.846129	3.162212
100	1	0	-5.353456	-1.382692	-5.329155	182	6	0	-2.278190	4.153318	1.566865
101	6	0	-2.006810	-2.390390	-5.247519	183	1	0	-1.336577	3.942006	1.045655
102	1	0	-1.839185	-2.225371	-6.321364	184	1	0	-3.109507	3.791091	0.948507
103	1	0	-1.094217	-2.095542	-4.714164	185	1	0	-2.363111	5.245526	1.642226
104	1	0	-2.160660	-3.466229	-5.090190	186	8	0	-0.905764	1.719539	-2.639587
105	6	0	6.589786	-3.368093	-2.941401	187	6	0	-1.227233	3.115713	-2.555513
106	1	0	7.260329	-4.143461	-3.323777	188	6	0	-0.249058	3.925811	-3.370212
107	1	0	6.179168	-2.789241	-3.777227	189	6	0	0.439924	3.687053	-4.534351
108	1	0	7.140751	-2.694277	-2.272874	190	8	0	0.020235	5.206457	-2.924469
109	6	0	6.471308	4.643017	1.996278	191	6	0	1.185459	4.880308	-4.824835
110	1	0	7.215659	5.443175	2.049283	192	1	0	0.414709	2.772760	-5.115403
111	1	0	5.642882	4.857592	2.680294	193	6	0	0.896702	5.770231	-3.827944

194	1	0	1.846220	5.050818	-5.666774	48	6	0	-2.732882	-2.572331	-1.362856
195	1	0	1.200278	6.785144	-3.608551	49	6	0	-5.448580	-2.490227	-0.661368
196	6	0	-2.632505	3.335197	-3.128738	50	1	0	-4.992426	-0.544338	0.114053
197	1	0	-2.743242	2.822120	-4.088962	51	6	0	-3.530258	-3.667139	-1.692942
198	1	0	-2.824216	4.406912	-3.262015	52	1	0	-1.694266	-2.548220	-1.666494
199	8	0	-3.608538	2.816820	-2.173303	53	6	0	-4.859338	-3.650257	-1.212736
200	6	0	-4.904115	2.951361	-2.569468	54	6	0	-3.016712	1.372981	-0.057117
201	8	0	-5.213901	3.364886	-3.688651	55	6	0	-2.762335	2.344446	-1.013022
202	6	0	-5.886072	2.587626	-1.512272	56	6	0	-3.978354	1.612073	0.926586
203	6	0	-7.254937	2.727854	-1.817290	57	6	0	-3.494682	3.534496	-1.076373
204	6	0	-5.495182	2.159787	-0.227903	58	1	0	-1.963452	2.169072	-1.726325
205	6	0	-8.222188	2.451132	-0.846363	59	6	0	-4.790208	2.740872	0.877891
206	1	0	-7.542423	3.060453	-2.812532	60	1	0	-4.095814	0.893269	1.728440
207	6	0	-6.467761	1.889847	0.742495	61	6	0	-4.589974	3.642394	-0.199173
208	1	0	-4.441427	2.043477	0.008971	62	6	0	-2.993202	4.602475	-2.075530
209	6	0	-7.829899	2.036319	0.436312	63	6	0	-3.250652	4.131999	-3.518495
210	1	0	-9.278267	2.563159	-1.085528	64	1	0	-2.866885	4.873106	-4.229684
211	1	0	-6.162739	1.568216	1.736835	65	1	0	-2.747934	3.180152	-3.722180
212	1	0	-8.582904	1.828529	1.194873	66	1	0	-4.318480	3.994758	-3.715075
213	1	0	-1.214385	3.486804	-1.520116	67	6	0	-3.588470	6.007192	-1.880636
214	1	0	1.322685	1.672882	-2.036130	68	1	0	-3.485116	6.347983	-0.846365
215	1	0	0.494139	1.773560	-2.473245	69	1	0	-3.034185	6.704665	-2.517994
						70	1	0	-4.639077	6.078568	-2.162129
						71	6	0	-1.466924	4.764214	-1.878036
						72	1	0	-1.234123	5.069483	-0.852467
						73	1	0	-0.910580	3.847770	-2.093616
						74	1	0	-1.093794	5.537237	-2.557889
						75	6	0	-5.816003	3.011374	1.998038
						76	6	0	-5.571026	4.416788	2.583523
						77	1	0	-5.841957	5.199475	1.873661
						78	1	0	-6.167945	4.555889	3.491451
						79	1	0	-4.516149	4.552593	2.840858
						80	6	0	-7.265939	2.903564	1.490611
						81	1	0	-7.440335	1.940723	0.997502
						82	1	0	-7.956936	2.971966	2.338505
						83	1	0	-7.522691	3.703117	0.795259
						84	6	0	-5.662983	1.996872	3.144324
						85	1	0	-5.909291	0.976438	2.830394
						86	1	0	-4.651988	1.996953	3.562406
						87	1	0	-6.357565	2.263327	3.947118
						88	8	0	-5.502136	4.657452	-0.353750
						89	8	0	-5.619004	-4.792576	-1.329174
						90	8	0	2.922110	-3.600388	3.815022
						91	8	0	5.684020	4.002300	-1.940850
						92	6	0	5.541215	5.343480	-1.480208
						93	1	0	6.454204	5.870224	-1.764085
						94	1	0	4.682880	5.842204	-1.940570
						95	1	0	5.420603	5.378904	-0.392442
						96	6	0	3.087551	3.885348	-3.513265
						97	6	0	4.305388	4.314127	-4.351247
						98	1	0	3.949700	4.627704	-5.338759
						99	1	0	4.849211	5.156440	-3.925062
						100	1	0	5.007598	3.487979	-4.496149
						101	6	0	2.194809	5.108404	-3.235225
						102	1	0	1.885707	5.573802	-4.177886
						103	1	0	1.290491	4.820584	-2.689102
						104	1	0	2.716153	5.865543	-2.641710
						105	6	0	-6.434977	4.417883	-1.404469
						106	1	0	-7.186491	5.207215	-1.342942
						107	1	0	-5.956319	4.455435	-2.387800
						108	1	0	-6.918578	3.441726	-1.288796
						109	6	0	-5.499753	-5.642187	-0.184354
						110	1	0	-6.084665	-6.538573	-0.397907
						111	1	0	-4.458355	-5.918069	0.000205
						112	1	0	-5.890275	-5.158013	0.714518
						113	6	0	-6.977382	-2.300283	-0.532931
						114	6	0	-7.320307	-0.882109	-0.039356
						115	1	0	-6.956329	-0.701842	0.978261
						116	1	0	-6.918044	-0.103666	-0.696125
						117	1	0	-8.408396	-0.765413	-0.022786
						118	6	0	-7.593783	-2.464773	-1.936592
						119	1	0	-7.413909	-3.465018	-2.338180
						120	1	0	-8.677239	-2.307665	-1.888328
						121	1	0	-7.176925	-1.731928	-2.636129
						122	6	0	-7.652443	-3.290717	0.432322
						123	1	0	-7.683330	-4.301469	0.023262
						124	1	0	-7.147312	-3.314173	1.403558
						125	1	0	-8.688370	-2.978527	0.604011
						126	6	0	-2.995651	-4.736058	-2.673259
						127	6	0	-1.595838	-4.358777	-3.191321
						128	1	0	-1.583276	-3.370614	-3.663351
						129	1	0	-0.838922	-4.378685	-2.399340

6b(R)*2a

RwB97XD SCF energy -5095.406432 a.u.
RwB97XD SCF enthalpy -5093.447145 a.u.
RwB97XD SCF free energy -5093.695537 a.u.
Three lowest frequencies (cm⁻¹) 9.3, 13.7, 18.1
Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X	Coordinates Y	Coordinates Z (Angstroms)
1	6	0	-1.066326	0.273892	2.494410
2	6	0	-0.798623	-0.202128	3.759047
3	6	0	-1.094926	-1.496959	4.169117
4	6	0	-1.679791	-2.400516	3.317135
5	6	0	-1.979988	-1.938568	2.026897
6	6	0	-1.694869	-0.639332	1.604092
7	1	0	-1.908677	-3.415038	3.620711
8	1	0	-2.460734	-2.630801	1.345996
9	6	0	-0.705033	1.685174	2.202563
10	6	0	0.307054	2.103536	1.299375
11	6	0	-1.335764	2.683845	2.912261
12	6	0	0.572423	3.460977	1.123734
13	6	0	-1.062216	4.034138	2.731365
14	6	0	-0.116230	4.459983	1.830781
15	1	0	1.341115	3.773539	0.426000
16	1	0	0.101854	5.510951	1.681510
17	8	0	-0.697600	-1.660061	5.463106
18	8	0	-0.193678	0.466831	4.782615
19	8	0	-2.307318	2.541092	3.858003
20	8	0	-1.866130	4.768946	3.555099
21	6	0	-0.457639	-0.330213	5.935095
22	1	0	0.407618	-0.321782	6.595475
23	1	0	-1.360199	0.041713	6.435304
24	6	0	-2.398932	3.821488	4.482846
25	1	0	-1.790411	3.823436	5.395628
26	1	0	-3.443008	4.052027	4.689917
27	15	0	1.150030	0.845087	0.267302
28	15	0	-2.083628	-0.177545	-0.131673
29	46	0	-0.272247	-0.007904	-1.445676
30	6	0	1.740825	-0.460203	1.378365
31	6	0	2.383746	-0.217655	2.587432
32	6	0	1.521040	-1.768560	0.970080
33	6	0	2.793610	-1.265825	3.408624
34	1	0	2.547529	0.809784	2.886220
35	6	0	1.912227	-2.872875	1.730358
36	1	0	1.025124	-1.922048	0.019782
37	6	0	2.510707	-2.589971	2.980927
38	6	0	2.600329	1.692901	-0.425806
39	6	0	3.885496	1.578009	0.097584
40	6	0	2.397713	2.456616	-1.569106
41	6	0	4.950727	2.302462	-0.435699
42	1	0	4.050470	0.915575	0.936460
43	6	0	3.426658	3.180408	-2.177919
44	1	0	1.400996	2.491140	-1.999451
45	6	0	4.673723	3.170260	-1.520404
46	6	0	-3.236155	-1.483522	-0.658049
47	6	0	-4.592351	-1.430947	-0.356965

130	1	0	-1.292448	-5.087889	-3.948777	212	1	0	7.506659	-2.906009	2.283781
131	6	0	-2.888090	-6.143926	-2.061007	213	1	0	1.422827	-2.265192	-2.535589
132	1	0	-2.322103	-6.791887	-2.739196	214	1	0	-1.290481	-0.471470	-2.543759
133	1	0	-2.358641	-6.124897	-1.102234	215	1	0	1.604830	0.418669	-3.454046
134	1	0	-3.866242	-6.604822	-1.915008						
135	6	0	-3.934728	-4.778028	-3.895763						
136	1	0	-3.571145	-5.516040	-4.619658						
137	1	0	-4.953116	-5.053709	-3.612528						
138	1	0	-3.967138	-3.803507	-4.395085						
139	6	0	6.380878	2.087904	0.104932						
140	6	0	2.293806	2.900255	-4.405261						
141	1	0	2.864961	1.980655	-4.579497						
142	1	0	1.318304	2.635737	-3.985664						
143	1	0	2.102850	3.363103	-5.378661						
144	6	0	7.276419	1.599573	-1.051265						
145	1	0	8.274005	1.349148	-0.673037						
146	1	0	6.857034	0.703610	-1.518791						
147	1	0	7.386011	2.364861	-1.822286						
148	6	0	6.980960	3.365728	0.720796						
149	1	0	6.299633	3.810119	1.454508						
150	1	0	7.912215	3.115619	1.241331						
151	1	0	7.221004	4.114648	-0.033834						
152	6	0	6.402933	1.010828	1.202875						
153	1	0	5.996250	0.058314	0.854946						
154	1	0	7.438426	0.836211	1.510392						
155	1	0	5.844229	1.322604	2.092852						
156	6	0	1.920456	-4.286201	4.564010						
157	1	0	2.309444	-4.444804	5.572240						
158	1	0	0.997805	-3.702129	4.625842						
159	1	0	1.709225	-5.263097	4.120053						
160	6	0	3.584432	-0.956480	4.697795						
161	6	0	3.008047	-1.680752	5.933856						
162	1	0	3.266604	-1.130169	6.844343						
163	1	0	1.919180	-1.760840	5.884984						
164	1	0	3.415044	-2.686736	6.038426						
165	6	0	5.052659	-1.380381	4.500323						
166	1	0	5.631529	-1.143327	5.400724						
167	1	0	5.136574	-2.455593	4.322119						
168	1	0	5.507398	-0.851491	3.655275						
169	6	0	3.576326	0.551601	5.006586						
170	1	0	4.065534	1.142540	4.225663						
171	1	0	2.559530	0.934533	5.147313						
172	1	0	4.129658	0.726293	5.934213						
173	6	0	1.668151	-4.280670	1.129034						
174	6	0	0.319216	-4.844672	1.618125						
175	1	0	0.161061	-5.843074	1.194002						
176	1	0	0.252784	-4.927188	2.703263						
177	1	0	-0.501971	-4.203893	1.280871						
178	6	0	2.820855	-5.257298	1.426816						
179	1	0	2.967133	-5.452321	2.487273						
180	1	0	2.618843	-6.213369	0.932452						
181	1	0	3.763125	-4.869137	1.025470						
182	6	0	1.565610	-4.213846	-0.411815						
183	1	0	0.671190	-3.682096	-0.751678						
184	1	0	2.443309	-3.744462	-0.867187						
185	1	0	1.492644	-5.233177	-0.804391						
186	8	0	1.433697	-0.267382	-2.793239						
187	6	0	1.689137	-1.561408	-3.330633						
188	6	0	0.835249	-1.823035	-4.531902						
189	6	0	-0.019801	-1.054639	-5.255090						
190	8	0	0.867202	-3.088525	-5.024336						
191	6	0	-0.559897	-1.913026	-6.270475						
192	1	0	-0.247048	-0.011698	-5.085337						
193	6	0	0.010640	-3.127524	-6.082039						
194	1	0	-1.278144	-1.650830	-7.033672						
195	1	0	-0.076818	-4.079603	-6.582461						
196	6	0	3.171204	-1.703299	-3.631363						
197	1	0	3.532660	-0.840302	-4.197645						
198	1	0	3.362170	-2.615035	-4.204166						
199	8	0	3.841640	-1.796308	-2.370302						
200	6	0	5.177666	-1.704154	-2.387537						
201	8	0	5.806941	-1.424345	-3.390230						
202	6	0	5.792108	-2.013054	-1.070788						
203	6	0	7.186456	-1.996638	-0.971151						
204	6	0	5.017816	-2.350520	0.042209						
205	6	0	7.801534	-2.310223	0.235099						
206	1	0	7.779872	-1.738663	-1.841909						
207	6	0	5.638013	-2.681031	1.241449						
208	1	0	3.937044	-2.354764	-0.025031						
209	6	0	7.027556	-2.656499	1.341813						
210	1	0	8.884002	-2.289750	0.311234						
211	1	0	5.033276	-2.962043	2.095849						

2.6. Catalytic cycle 2a – 1c (S)

3a(S) -1c

RwB97XD SCF energy -4902.505584 a.u.
 RwB97XD SCF enthalpy -4900.627323 a.u.
 RwB97XD SCF free energy -4900.865109 a.u.
 Three lowest frequencies (cm⁻¹) 13.2, 14.0, 18.4

Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.183389	-0.363954	2.579650
2	6	0	0.315453	-1.113821	3.622487
3	6	0	-0.043544	-2.437371	3.857376
4	6	0	-0.949477	-3.089926	3.058857
5	6	0	-1.478031	-2.354148	1.988734
6	6	0	-1.121375	-1.028445	1.740063
7	1	0	-1.240101	-4.117711	3.240467
8	1	0	-2.185236	-2.850461	1.333853
9	6	0	0.274983	1.050039	2.464387
10	6	0	1.144173	1.559861	1.461424
11	6	0	-0.083963	1.936910	3.454672
12	6	0	1.538452	2.895022	1.479966
13	6	0	0.317489	3.267913	3.467433
14	6	0	1.119527	3.787172	2.481128
15	1	0	2.210250	3.267242	0.714955
16	1	0	1.435465	4.823754	2.484292
17	8	0	0.603115	-2.892515	4.964470
18	8	0	1.197792	-0.708342	4.577206
19	8	0	-0.870477	1.689191	4.539855
20	8	0	-0.215486	3.886946	4.561071
21	6	0	1.597625	-1.904543	5.245741
22	1	0	2.553884	-2.241063	4.837886
23	1	0	1.645480	-1.725314	6.319333
24	6	0	-0.701589	2.826547	5.387099
25	1	0	0.043232	2.594224	6.157474
26	1	0	-1.662626	3.107105	5.817719
27	15	0	1.686098	0.396476	0.158627
28	15	0	-1.724767	-0.260752	0.194676
29	46	0	-0.074699	-0.280285	-1.312174
30	6	0	2.541000	-0.913148	1.081211
31	6	0	3.481731	-0.599731	2.058598
32	6	0	2.367187	-2.232815	0.697866
33	6	0	4.274245	-1.576181	2.659287
34	1	0	3.626704	0.442179	2.319563
35	6	0	3.075952	-3.275656	1.304284
36	1	0	1.664500	-2.448456	-0.101860
37	6	0	3.997143	-2.925256	2.315138
38	6	0	3.014975	1.204209	-0.792890
39	6	0	4.284235	0.634977	-0.876794
40	6	0	2.713921	2.298315	-1.596669
41	6	0	5.290645	1.202353	-1.653399
42	1	0	4.488625	-0.272021	-0.326902
43	6	0	3.679235	2.924002	-2.394247
44	1	0	1.697110	2.677265	-1.602830
45	6	0	4.992660	2.416645	-2.315364
46	6	0	-3.219383	-1.208451	-0.255053
47	6	0	-4.467955	-0.889468	0.277640
48	6	0	-3.122493	-2.247693	-1.167768
49	6	0	-5.603542	-1.632394	-0.030706
50	1	0	-4.555733	-0.038809	0.937151
51	6	0	-4.226494	-3.019560	-1.543574
52	1	0	-2.157002	-2.453479	-1.615723
53	6	0	-5.437567	-2.757092	-0.876183
54	6	0	-2.315893	1.408227	0.583527
55	6	0	-2.095052	2.424351	-0.333843
56	6	0	-3.033646	1.676171	1.752433
57	6	0	-2.639400	3.703587	-0.162966
58	1	0	-1.482931	2.212088	-1.205798
59	6	0	-3.860060	2.903533	1.946646
60	1	0	-3.113469	0.899826	2.503677
61	6	0	-3.523875	3.870782	0.918112
62	6	0	-2.177262	4.796829	-1.153226
63	6	0	-2.717291	4.493420	-2.562870
64	1	0	-2.396024	5.274356	-3.261524
65	1	0	-2.339292	3.538180	-2.940153
66	1	0	-3.811609	4.459194	-2.576904

67	6	0	-2.550811	6.238885	-0.768480
68	1	0	-2.269221	6.469998	0.262354
69	1	0	-2.000280	6.919617	-1.426967
70	1	0	-3.611883	6.457868	-0.893563
71	6	0	-0.632670	4.763649	-1.199645
72	1	0	-0.205508	4.996714	-0.218003
73	1	0	-0.241624	3.794533	-1.517550
74	1	0	-0.273505	5.510229	-1.915507
75	6	0	-4.396216	3.209820	3.267942
76	6	0	-3.728184	4.431285	3.929751
77	1	0	-3.858087	5.333887	3.328823
78	1	0	-4.171551	4.612365	4.915516
79	1	0	-2.654746	4.265797	4.061570
80	6	0	-5.896731	3.490971	3.062807
81	1	0	-6.376789	2.691752	2.488067
82	1	0	-6.391593	3.540389	4.039147
83	1	0	-6.074388	4.441718	2.560701
84	6	0	-4.294769	2.029332	4.248046
85	1	0	-4.805378	1.137178	3.868254
86	1	0	-3.257634	1.765589	4.472222
87	1	0	-4.779652	2.307188	5.189068
88	8	0	-4.281063	5.012579	1.015136
89	8	0	-6.516453	-3.589252	-1.050842
90	8	0	4.679678	-3.932709	2.947943
91	8	0	6.033946	3.085685	-2.915387
92	6	0	6.514319	4.185546	-2.147508
93	1	0	7.402349	4.559558	-2.660508
94	1	0	5.772518	4.987686	-2.080535
95	1	0	6.781786	3.874964	-1.131574
96	6	0	3.191521	4.077496	-3.302941
97	6	0	4.159173	4.481658	-4.429710
98	1	0	3.634357	5.172171	-5.098811
99	1	0	5.051674	4.995088	-4.073113
100	1	0	4.472744	3.617216	-5.022345
101	6	0	2.872702	5.310754	-2.438323
102	1	0	2.453283	6.110075	-3.059837
103	1	0	2.142633	5.069739	-1.659438
104	1	0	3.769749	5.701629	-1.947574
105	6	0	-5.417241	4.998528	0.154197
106	1	0	-5.961115	5.927036	0.337212
107	1	0	-5.127709	4.952609	-0.900196
108	1	0	-6.067453	4.144555	0.373790
109	6	0	-6.432728	-4.776332	-0.266111
110	1	0	-7.362982	-5.324249	-0.426167
111	1	0	-5.587236	-5.403356	-0.567457
112	1	0	-6.326126	-4.540708	0.798147
113	6	0	-6.988859	-1.158596	0.457965
114	6	0	-6.881246	0.150359	1.260649
115	1	0	-6.313954	0.020235	2.189089
116	1	0	-6.419235	0.956446	0.680872
117	1	0	-7.888059	0.480126	1.535489
118	6	0	-7.871171	-0.871826	-0.773335
119	1	0	-8.020773	-1.769927	-1.376646
120	1	0	-8.854035	-0.508260	-0.452542
121	1	0	-7.416895	-0.101626	-1.406373
122	6	0	-7.684277	-2.189952	1.366696
123	1	0	-8.016285	-3.067565	0.810428
124	1	0	-7.023235	-2.515860	2.175868
125	1	0	-8.570891	-1.736071	1.822106
126	6	0	-3.992267	-4.029373	-2.691974
127	6	0	-3.081640	-5.166259	-2.193250
128	1	0	-2.132643	-4.778674	-1.807582
129	1	0	-3.561397	-5.735785	-1.390254
130	1	0	-2.853411	-5.859485	-3.010638
131	6	0	-5.262522	-4.634090	-3.314912
132	1	0	-4.971532	-5.186709	-4.215184
133	1	0	-5.776832	-5.337722	-2.660015
134	1	0	-5.973895	-3.860150	-3.615650
135	6	0	-3.281369	-3.276160	-3.842340
136	1	0	-3.093726	-3.965883	-4.671937
137	1	0	-3.910672	-2.461209	-4.216163
138	1	0	-2.318371	-2.852612	-3.548835
139	6	0	6.640126	0.470294	-1.817138
140	6	0	1.893525	3.622850	-4.009487
141	1	0	2.061663	2.705202	-4.583317
142	1	0	1.071086	3.442235	-3.315530
143	1	0	1.561864	4.402250	-4.703437
144	6	0	6.921721	0.251336	-3.316826
145	1	0	7.865458	-0.291428	-3.441755
146	1	0	6.125933	-0.344447	-3.777617
147	1	0	7.006632	1.197265	-3.855275
148	6	0	7.803923	1.245536	-1.173582

149	1	0	7.582167	1.496407	-0.130461	10	6	0	1.156347	1.607754	1.416703
150	1	0	8.707438	0.625145	-1.181225	11	6	0	-0.007683	1.980280	3.444890
151	1	0	8.035911	2.165437	-1.711771	12	6	0	1.561632	2.939527	1.422987
152	6	0	6.603212	-0.921314	-1.159682	13	6	0	0.412104	3.307974	3.452208
153	1	0	5.803599	-1.550307	-1.565809	14	6	0	1.183006	3.828719	2.441474
154	1	0	7.553249	-1.429553	-1.352902	15	1	0	2.212940	3.306691	0.637872
155	1	0	6.479628	-0.868317	-0.072707	16	1	0	1.507109	4.862627	2.440263
156	6	0	4.106887	-4.362708	4.174475	17	8	0	0.536202	-2.851498	4.954806
157	1	0	4.589242	-5.307155	4.434310	18	8	0	1.181170	-0.683098	4.574014
158	1	0	4.292464	-3.640572	4.977589	19	8	0	-0.770708	1.742718	4.546062
159	1	0	3.026182	-4.520889	4.078691	20	8	0	-0.072955	3.926146	4.562978
160	6	0	5.411461	-1.085093	3.593835	21	6	0	1.553014	-1.888834	5.238565
161	6	0	4.855380	-0.744226	4.989059	22	1	0	2.503377	-2.247555	4.831738
162	1	0	5.632153	-0.255879	5.588514	23	1	0	1.607227	-1.714451	6.312788
163	1	0	4.003050	-0.059616	4.920385	24	6	0	-0.553610	2.868147	5.395498
164	1	0	4.536447	-1.638134	5.532612	25	1	0	0.208962	2.617003	6.143171
165	6	0	6.581258	-2.074206	3.741158	26	1	0	-1.494764	3.164336	5.859011
166	1	0	7.399452	-1.570304	4.267244	27	15	0	1.707308	0.450530	0.124954
167	1	0	6.322478	-2.963966	4.314003	28	15	0	-1.632275	-0.201467	0.119549
168	1	0	6.960895	-2.395128	2.765688	29	46	0	0.078712	-0.334957	-1.367159
169	6	0	6.020771	0.209729	3.004407	30	6	0	2.554432	-0.865501	1.041076
170	1	0	6.321562	0.072692	1.960241	31	6	0	3.465298	-0.537632	2.041580
171	1	0	5.338165	1.062072	3.052318	32	6	0	2.422648	-2.184709	0.638482
172	1	0	6.911076	0.484833	3.578748	33	6	0	4.276010	-1.498197	2.643124
173	6	0	2.823539	-4.684103	0.711526	34	1	0	3.573138	0.503616	2.321267
174	6	0	1.311383	-4.988757	0.754657	35	6	0	3.147315	-3.214160	1.248546
175	1	0	1.121599	-5.978217	0.323493	36	1	0	1.742164	-2.411354	-0.177140
176	1	0	0.946654	-4.995956	1.787498	37	6	0	4.045691	-2.850427	2.276874
177	1	0	0.713890	-4.263616	0.193693	38	6	0	3.014113	1.246789	-0.860007
178	6	0	3.536527	-5.866632	1.385855	39	6	0	4.291599	0.693566	-0.920585
179	1	0	3.208068	-6.020570	2.416109	40	6	0	2.683764	2.285888	-1.722798
180	1	0	3.283176	-6.774795	0.826826	41	6	0	5.276181	1.221330	-1.751114
181	1	0	4.621953	-5.759662	1.377531	42	1	0	4.518402	-0.170412	-0.313430
182	6	0	3.305123	-4.651813	-0.755624	43	6	0	3.622115	2.858337	-2.588443
183	1	0	2.804986	-3.875412	-1.340262	44	1	0	1.662426	2.653156	-1.730424
184	1	0	4.383598	-4.464156	-0.803334	45	6	0	4.944542	2.374302	-2.501295
185	1	0	3.110533	-5.616130	-1.238638	46	6	0	-3.140889	-1.120334	-0.342125
186	8	0	1.276885	-0.506124	-3.068705	47	6	0	-4.383540	-0.740285	0.167445
187	6	0	0.754308	-1.125706	-4.012262	48	6	0	-3.063964	-2.245499	-1.151756
188	1	0	-1.280699	-0.645925	-2.224506	49	6	0	-5.520606	-1.518032	-0.021230
189	6	0	0.542970	-2.543166	-3.974935	50	1	0	-4.462719	0.179897	0.726868
190	6	0	0.127858	-3.446389	-4.925396	51	6	0	-4.172522	-3.068934	-1.391246
191	8	0	0.772263	-3.193235	-2.795264	52	1	0	-2.111105	-2.497970	-1.606632
192	6	0	0.106260	-4.711142	-4.293178	53	6	0	-5.362280	-2.743529	-0.713061
193	1	0	-0.127710	-3.222040	-5.951466	54	6	0	-2.203521	1.474579	0.510708
194	6	0	0.498938	-4.489696	-3.003257	55	6	0	-2.009288	2.492800	-0.409802
195	1	0	-0.169470	-5.660542	-4.726972	56	6	0	-2.899491	1.734704	1.694707
196	1	0	0.628258	-5.145062	-2.154449	57	6	0	-2.542819	3.774277	-0.213087
197	6	0	0.247825	-0.366374	-5.229962	58	1	0	-1.437236	2.280408	-1.307302
198	1	0	0.429680	-0.907830	-6.157804	59	6	0	-3.523350	2.958287	1.910572
199	1	0	0.714673	0.617593	-5.262528	60	1	0	-2.966343	0.951917	2.440139
200	8	0	-1.177245	-0.261048	-5.095702	61	6	0	-3.397464	3.939320	0.893227
201	6	0	-1.660824	0.809797	-4.431274	62	6	0	-2.113731	4.879127	-1.206361
202	8	0	-0.957808	1.722159	-4.049423	63	6	0	-2.790425	4.658147	-2.571163
203	6	0	-3.133916	0.694167	-4.203399	64	1	0	-2.428452	5.401255	-3.291087
204	1	0	-3.626472	0.172283	-5.025012	65	1	0	-2.570391	3.662697	-2.967725
205	1	0	-3.281650	0.114695	-3.283902	66	1	0	-3.877913	4.762240	-2.504470
206	1	0	-3.565499	1.686074	-4.063826	67	6	0	-2.371670	6.319876	-0.728786

TS1a(S) -1c

RWB97XD SCF energy -4902.496336 a.u.
 RWB97XD SCF enthalpy -4900.619680 a.u.
 RWB97XD SCF free energy -4900.855354 a.u.
 Three lowest frequencies (cm⁻¹) -455.7, 11.2, 13.7
 Imaginary frequency (cm⁻¹) -455.7
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X Y (Angstroms)		Z
1	6	0	-0.155995	-0.315953	2.549660
2	6	0	0.312359	-1.071465	3.603977
3	6	0	-0.074787	-2.390059	3.834055
4	6	0	-0.973088	-3.030031	3.017078
5	6	0	-1.462607	-2.290762	1.930971
6	6	0	-1.080250	-0.972078	1.685890
7	1	0	-1.287262	-4.051539	3.195105
8	1	0	-2.161526	-2.780072	1.262770
9	6	0	0.315135	1.094096	2.441297

10	6	0	1.156347	1.607754	1.416703
11	6	0	-0.007683	1.980280	3.444890
12	6	0	1.561632	2.939527	1.422987
13	6	0	0.412104	3.307974	3.452208
14	6	0	1.183006	3.828719	2.441474
15	1	0	2.212940	3.306691	0.637872
16	1	0	1.507109	4.862627	2.440263
17	8	0	0.536202	-2.851498	4.954806
18	8	0	1.181170	-0.683098	4.574014
19	8	0	-0.770708	1.742718	4.546062
20	8	0	-0.072955	3.926146	4.562978
21	6	0	1.553014	-1.888834	5.238565
22	1	0	2.503377	-2.247555	4.831738
23	1	0	1.607227	-1.714451	6.312788
24	6	0	-0.553610	2.868147	5.395498
25	1	0	0.208962	2.617003	6.143171
26	1	0	-1.494764	3.164336	5.859011
27	15	0	1.707308	0.450530	0.124954
28	15	0	-1.632275	-0.201467	0.119549
29	46	0	0.078712	-0.334957	-1.367159
30	6	0	2.554432	-0.865501	1.041076
31	6	0	3.465298	-0.537632	2.041580
32	6	0	2.422648	-2.184709	0.638482
33	6	0	4.276010	-1.498197	2.643124
34	1	0	3.573138	0.503616	2.321267
35	6	0	3.147315	-3.214160	1.248546
36	1	0	1.742164	-2.411354	-0.177140
37	6	0	4.045691	-2.850427	2.276874
38	6	0	3.014113	1.246789	-0.860007
39	6	0	4.291599	0.693566	-0.920585
40	6	0	2.683764	2.285888	-1.722798
41	6	0	5.276181	1.221330	-1.751114
42	1	0	4.518402	-0.170412	-0.313430
43	6	0	3.622115	2.858337	-2.588443
44	1	0	1.662426	2.653156	-1.730424
45	6	0	4.944542	2.374302	-2.501295
46	6	0	-3.140889	-1.120334	-0.342125
47	6	0	-4.383540	-0.740285	0.167445
48	6	0	-3.063964	-2.245499	-1.151756
49	6	0	-5.520606	-1.518032	-0.021230
50	1	0	-4.462719	0.179897	0.726868
51	6	0	-4.172522	-3.068934	-1.391246
52	1	0	-2.111105	-2.497970	-1.606632
53	6	0	-5.362280	-2.743529	-0.713061
54	6	0	-2.203521	1.474579	0.510708
55	6	0	-2.009288	2.492800	-0.409802
56	6	0	-2.899491	1.734704	1.694707
57	6	0	-2.542819	3.774277	-0.213087
58	1	0	-1.437236	2.280408	-1.307302
59	6	0	-3.523350	2.958287	1.910572
60	1	0	-2.966343	0.951917	2.440139
61	6	0	-3.397464	3.939320	0.893227
62	6	0	-2.113731	4.879127	-1.206361
63	6	0	-2.790425	4.658147	-2.571163
64	1	0	-2.428452	5.401255	-3.291087
65	1	0	-2.570391	3.662697	-2.967725
66	1	0	-3.877913	4.762240	-2.504470
67	6	0	-2.371670	6.319876	-0.728786
68	1	0	-1.971784	6.487334	0.275423
69	1	0	-1.857636	7.003668	-1.413153
70	1	0	-3.425995	6.595012	-0.726134
71	6	0	-0.584821	4.774173	-1.401254
72	1	0	-0.056389	4.911069	-0.451263
73	1	0	-0.279993	3.814987	-1.824788
74	1	0	-0.251873	5.552933	-2.094490
75	6	0	-4.248122	3.247598	3.242479
76	6	0	-3.560534	4.444971	3.926944
77	1	0	-3.676339	5.357269	3.337926
78	1	0	-4.0029		

92	6	0	6.435773	4.169718	-2.527455
93	1	0	7.303393	4.514934	-3.092804
94	1	0	5.680966	4.962144	-2.509569
95	1	0	6.735248	3.953099	-1.496198
96	6	0	3.098496	3.922402	-3.582805
97	6	0	4.037248	4.244405	-4.759694
98	1	0	3.488505	4.873609	-5.468904
99	1	0	4.931720	4.792634	-4.465339
100	1	0	4.349827	3.338156	-5.285902
101	6	0	2.776968	5.220532	-2.820160
102	1	0	2.323288	5.954151	-3.496109
103	1	0	2.076121	5.036324	-2.000764
104	1	0	3.679594	5.669202	-2.393608
105	6	0	-5.283061	5.132349	0.203263
106	1	0	-5.822219	6.045903	0.460631
107	1	0	-5.020259	5.160046	-0.858209
108	1	0	-5.929654	4.265914	0.379472
109	6	0	-6.264783	-4.676305	0.217568
110	1	0	-7.138016	-5.321786	0.108882
111	1	0	-5.356923	-5.257463	0.024514
112	1	0	-6.218894	-4.292303	1.242516
113	6	0	-6.897241	-1.004543	0.449360
114	6	0	-6.786227	0.402658	1.060827
115	1	0	-6.186760	0.406266	1.978112
116	1	0	-6.355782	1.126994	0.361103
117	1	0	-7.788046	0.755977	1.324086
118	6	0	-7.829777	-0.910181	-0.774277
119	1	0	-7.970355	-1.886710	-1.242827
120	1	0	-8.811818	-0.533127	-0.467035
121	1	0	-7.422651	-0.219853	-1.521483
122	6	0	-7.536339	-1.913886	1.515594
123	1	0	-7.869310	-2.862781	1.094291
124	1	0	-6.838914	-2.115286	2.335829
125	1	0	-8.414883	-1.415860	1.940344
126	6	0	-3.971273	-4.216146	-2.409101
127	6	0	-2.930194	-5.208555	-1.857849
128	1	0	-1.969807	-4.724075	-1.654718
129	1	0	-3.281820	-5.668019	-0.927762
130	1	0	-2.751324	-6.008730	-2.584554
131	6	0	-5.231448	-5.002383	-2.811567
132	1	0	-4.966858	-5.649005	-3.655833
133	1	0	-5.608807	-5.650635	-2.020412
134	1	0	-6.039217	-4.342036	-3.134480
135	6	0	-3.445155	-3.583224	-3.715373
136	1	0	-3.202113	-4.370300	-4.437062
137	1	0	-4.208842	-2.938649	-4.162408
138	1	0	-2.544567	-2.985905	-3.567332
139	6	0	6.635876	0.502883	-1.886818
140	6	0	1.797748	3.386503	-4.227480
141	1	0	1.979627	2.434455	-4.737875
142	1	0	0.990804	3.239293	-3.506814
143	1	0	1.434900	4.105800	-4.969009
144	6	0	6.873856	0.151176	-3.368866
145	1	0	7.828137	-0.376724	-3.476657
146	1	0	6.081422	-0.505812	-3.744331
147	1	0	6.906260	1.046864	-3.991681
148	6	0	7.803267	1.361927	-1.366727
149	1	0	7.606489	1.729686	-0.353938
150	1	0	8.716797	0.757728	-1.331233
151	1	0	8.000816	2.215108	-2.016240
152	6	0	6.651870	-0.819248	-1.098497
153	1	0	5.858332	-1.503007	-1.418458
154	1	0	7.608940	-1.321902	-1.269841
155	1	0	6.555555	-0.664360	-0.018588
156	6	0	4.187059	-4.307586	4.114464
157	1	0	4.706581	-5.231928	4.374351
158	1	0	4.327875	-3.584647	4.926089
159	1	0	3.115829	-4.513581	4.005021
160	6	0	5.379845	-0.985213	3.606372
161	6	0	4.786984	-0.682855	4.995483
162	1	0	5.536406	-0.179068	5.616320
163	1	0	3.914340	-0.025800	4.918492
164	1	0	4.486999	-1.594165	5.520164
165	6	0	6.578272	-1.939277	3.759754
166	1	0	7.370910	-1.416537	4.306089
167	1	0	6.338719	-2.845357	4.314685
168	1	0	6.981391	-2.234772	2.786325
169	6	0	5.959569	0.337832	3.050829
170	1	0	6.298492	0.224471	2.015745
171	1	0	5.246883	1.165430	3.087826
172	1	0	6.821123	0.635293	3.656834
173	6	0	2.933617	-4.625726	0.646627

174	6	0	1.428746	-4.966698	0.678819
175	1	0	1.267039	-5.962465	0.250944
176	1	0	1.055336	-4.978291	1.708488
177	1	0	0.819356	-4.260211	0.107462
178	6	0	3.670588	-5.792689	1.322947
179	1	0	3.324875	-5.966607	2.344381
180	1	0	3.457019	-6.702440	0.750366
181	1	0	4.751100	-5.647617	1.342536
182	6	0	3.421532	-4.579855	-0.817969
183	1	0	2.901495	-3.820015	-1.406899
184	1	0	4.494958	-4.364848	-0.860545
185	1	0	3.254833	-5.550193	-1.299312
186	8	0	1.400031	-0.672472	-2.974254
187	6	0	0.369686	-1.155884	-3.572147
188	1	0	-0.913966	-0.944780	-2.493784
189	6	0	0.250216	-2.617813	-3.714522
190	6	0	-0.182948	-3.411007	-4.734195
191	8	0	0.700733	-3.380222	-2.685051
192	6	0	0.020352	-4.756644	-4.302217
193	1	0	-0.601300	-3.076548	-5.672505
194	6	0	0.548679	-4.672323	-3.052627
195	1	0	-0.204995	-5.662361	-4.845765
196	1	0	0.858826	-5.409088	-2.327472
197	6	0	-0.281982	-0.304558	-6.60590
198	1	0	0.130717	-0.605462	-5.627040
199	1	0	-0.045316	0.741214	-4.467240
200	8	0	-1.689482	-0.509568	-4.722078
201	6	0	-2.465090	0.434678	-4.141202
202	8	0	-2.017663	1.457326	-3.671712
203	6	0	-3.907609	0.037936	-4.134490
204	1	0	-4.173314	-0.514830	-5.036706
205	1	0	-4.077446	-0.614142	-3.270444
206	1	0	-4.528766	0.927446	-4.030349

4a(S) -1c

RwB97XD SCF energy -4902.511949 a.u.
 RwB97XD SCF enthalpy -4900.629224 a.u.
 RwB97XD SCF free energy -4900.864894 a.u.
 Three lowest frequencies (cm⁻¹) 11.0, 16.4, 20.2

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates		(Angstroms)
			X	Y	Z
1	6	0	0.193429	-2.256732	1.912154
2	6	0	-0.288129	-2.834816	3.065387
3	6	0	0.043766	-2.372441	4.336834
4	6	0	0.855737	-1.280972	4.527965
5	6	0	1.339469	-0.652423	3.371120
6	6	0	1.031768	-1.123057	2.098045
7	1	0	1.119670	-0.929908	5.518372
8	1	0	1.987693	0.208971	3.486546
9	6	0	-0.060682	-2.905107	0.595625
10	6	0	-0.745399	-2.347281	-0.523015
11	6	0	0.449655	-4.172133	0.412184
12	6	0	-0.853813	-3.065634	-1.712761
13	6	0	0.344864	-4.873996	-0.784832
14	6	0	-0.301236	-4.344541	-1.874254
15	1	0	-1.392868	-2.644030	-2.551649
16	1	0	-0.392308	-4.884778	-2.808845
17	8	0	-0.545589	-3.160576	5.271447
18	8	0	-1.115337	-3.908587	3.173725
19	8	0	1.159073	-4.910956	1.308769
20	8	0	0.981153	-6.068890	-0.664812
21	6	0	-1.098613	-4.269517	4.556180
22	1	0	-2.115476	-4.453401	4.901557
23	1	0	-0.455767	-5.145576	4.695091
24	6	0	1.261592	-6.213338	0.730555
25	1	0	0.511926	-6.872060	1.183555
26	1	0	2.274268	-6.593248	0.863891
27	15	0	-1.423609	-0.656458	-0.413649
28	15	0	1.610355	-0.242451	0.628356
29	46	0	0.126136	0.949168	-0.589415
30	6	0	-2.321134	-0.618376	1.155232
31	6	0	-3.277289	-1.595578	1.398931
32	6	0	-2.070331	0.364864	2.108163
33	6	0	-3.996976	-1.636848	2.596413
34	1	0	-3.472933	-2.340190	0.634380
35	6	0	-2.703808	0.344211	3.348222

36	1	0	-1.345812	1.131757	1.867782	118	6	0	6.289534	3.482046	-0.784134
37	6	0	-3.611824	-0.716322	3.594126	119	1	0	6.153220	4.412763	-0.229092
38	6	0	-2.589498	-0.402965	-1.773689	120	1	0	7.254003	3.532754	-1.301869
39	6	0	-3.920057	-0.059778	-1.543822	121	1	0	5.502246	3.414467	-1.543232
40	6	0	-2.076772	-0.338349	-3.064334	122	6	0	7.424638	2.332658	1.149749
41	6	0	-4.775914	0.239634	-2.602834	123	1	0	7.478158	3.301374	1.646770
42	1	0	-4.284542	-0.016615	-0.526365	124	1	0	7.349247	1.549799	1.912118
43	6	0	-2.875654	-0.037587	-4.167265	125	1	0	8.370877	2.186715	0.617254
44	1	0	-1.014260	-0.497506	-3.213689	126	6	0	2.301791	4.536147	2.692264
45	6	0	-4.250637	0.145328	-3.914771	127	6	0	2.069530	4.235171	4.183989
46	6	0	2.734568	1.094098	1.098367	128	1	0	1.485507	3.317160	4.310908
47	6	0	4.038557	1.118720	0.608969	129	1	0	3.010189	4.111695	4.728691
48	6	0	2.227851	2.207295	1.762867	130	1	0	1.514949	5.056689	4.651183
49	6	0	4.876510	2.203889	0.838156	131	6	0	3.029688	5.882422	2.528961
50	1	0	4.395989	0.275013	0.036592	132	1	0	2.359449	6.679362	2.868485
51	6	0	3.013360	3.333005	2.025822	133	1	0	3.944994	5.959835	3.114647
52	1	0	1.190542	2.196667	2.080813	134	1	0	3.271918	6.074640	1.479142
53	6	0	4.367701	3.265164	1.629396	135	6	0	0.922691	4.733949	2.022928
54	6	0	2.570796	-1.374687	-0.394870	136	1	0	0.433760	5.614143	2.452460
55	6	0	2.543347	-1.183173	-1.767712	137	1	0	1.040645	4.895248	0.949069
56	6	0	3.391953	-2.359317	0.154355	138	1	0	0.242804	3.893135	2.170611
57	6	0	3.390074	-1.886864	-2.628987	139	6	0	-6.200282	0.767555	-2.327661
58	1	0	1.851190	-0.454316	-2.179843	140	6	0	-0.907947	1.012628	-5.321723
59	6	0	4.275594	-3.076742	-0.645853	141	1	0	-1.197719	1.999988	-4.946769
60	1	0	3.341060	-2.549934	1.219666	142	1	0	-0.174558	0.591358	-4.629853
61	6	0	4.334430	-2.733804	-2.021804	143	1	0	-0.399109	1.148687	-6.281883
62	6	0	3.162486	-1.670991	-4.142122	144	6	0	-6.294719	2.201322	-2.887053
63	6	0	3.508641	-0.217516	-4.514902	145	1	0	-7.291825	2.614328	-2.696413
64	1	0	3.323144	-0.050224	-5.581709	146	1	0	-5.559698	2.852974	-2.401138
65	1	0	2.899912	0.499774	-3.954205	147	1	0	-6.118094	2.224452	-3.964984
66	1	0	4.562244	0.004875	-4.316345	148	6	0	-7.302641	-0.110172	-2.950167
67	6	0	3.929317	-2.622967	-5.074853	149	1	0	-7.166626	-1.165295	-2.689411
68	1	0	3.769749	-3.670821	-4.807158	150	1	0	-8.277650	0.205002	-2.562192
69	1	0	3.550872	-2.477975	-6.092784	151	1	0	-7.338980	-0.018849	-4.035763
70	1	0	5.002496	-2.431072	-5.101053	152	6	0	-6.487683	0.842550	-0.820034
71	6	0	1.662806	-1.916402	-4.428819	153	1	0	-5.778383	1.489638	-0.295609
72	1	0	1.387155	-2.952419	-4.203322	154	1	0	-7.486227	1.264689	-0.669309
73	1	0	1.007803	-1.259619	-3.850581	155	1	0	-6.472965	-0.146345	-0.350855
74	1	0	1.459148	-1.732100	-5.488655	156	6	0	-3.547372	-1.827340	5.654471
75	6	0	5.078414	-4.256623	-0.062440	157	1	0	-4.039393	-1.785194	6.627745
76	6	0	4.708827	-5.526298	-0.856202	158	1	0	-3.695454	-2.819694	5.219634
77	1	0	5.022156	-5.520211	-1.899941	159	1	0	-2.475195	-1.655064	5.778053
78	1	0	5.197404	-6.402250	-0.414997	160	6	0	-5.151968	-2.665492	2.673383
79	1	0	3.626572	-5.693233	-0.838190	161	6	0	-4.575606	-4.091207	2.743308
80	6	0	6.600386	-4.030071	-0.116156	162	1	0	-5.389360	-4.824694	2.722709
81	1	0	6.873843	-3.073045	0.341091	163	1	0	-3.911402	-4.301115	1.898822
82	1	0	7.105885	-4.823740	0.445453	164	1	0	-4.008652	-4.250257	3.665342
83	1	0	6.986197	-4.054549	-1.135290	165	6	0	-6.147091	-2.461617	3.830532
84	6	0	4.710198	-4.503640	1.409599	166	1	0	-6.999332	-3.129660	3.665868
85	1	0	5.009594	-3.670318	2.054989	167	1	0	-5.735444	-2.704155	4.809622
86	1	0	3.638384	-4.676495	1.545618	168	1	0	-6.528194	-1.436985	3.859627
87	1	0	5.238530	-5.394885	1.762294	169	6	0	-6.000536	-2.535753	1.387033
88	8	0	5.355390	-3.267464	-2.768672	170	1	0	-6.447197	-1.538367	1.322626
89	8	0	5.240019	4.266777	1.972390	171	1	0	-5.436423	-2.718270	0.469288
90	8	0	-4.146087	-0.810063	4.854292	172	1	0	-6.814483	-3.267518	1.414934
91	8	0	-5.128837	0.279839	-4.961569	173	6	0	-2.469784	1.487572	4.360707
92	6	0	-5.499476	-0.966103	-5.546874	174	6	0	-1.915375	0.990106	5.709222
93	1	0	-6.219823	-0.738842	-6.334626	175	1	0	-1.560031	1.846918	6.291986
94	1	0	-4.637397	-1.479865	-5.983382	176	1	0	-2.674806	0.482757	6.304489
95	1	0	-5.962418	-1.628943	-4.808224	177	1	0	-1.069248	0.311562	5.564987
96	6	0	-2.149827	0.111930	-5.525867	178	6	0	-3.800175	2.226590	4.601732
97	6	0	-2.966695	0.788126	-6.641073	179	1	0	-4.569591	1.550877	4.981926
98	1	0	-2.294944	0.984209	-7.483883	180	1	0	-3.653883	3.024079	5.339338
99	1	0	-3.782744	0.171875	-7.018427	181	1	0	-4.167082	2.688385	3.679530
100	1	0	-3.379650	1.746527	-6.314213	182	6	0	-1.459960	2.507971	3.810835
101	6	0	-1.681124	-1.273823	-6.006861	183	1	0	-0.473558	2.054600	3.659928
102	1	0	-1.108047	-1.175790	-6.935741	184	1	0	-1.792060	2.952976	2.867678
103	1	0	-1.040894	-1.758851	-5.262886	185	1	0	-1.341391	3.322605	4.532033
104	1	0	-2.527622	-1.939144	-6.205040	186	8	0	-0.897073	2.193730	-1.815348
105	6	0	6.420485	-2.339700	-2.973943	187	6	0	-0.941604	3.487501	-1.287788
106	1	0	7.190440	-2.867075	-3.539996	188	6	0	-2.289248	3.768243	-0.689990
107	1	0	6.088809	-1.464232	-3.541489	189	6	0	-3.274802	4.681603	-0.898862
108	1	0	6.837679	-2.001171	-2.019108	190	8	0	-2.676911	2.892600	0.277525
109	6	0	5.742906	4.161904	3.302879	191	6	0	-4.343323	4.339533	-0.002516
110	1	0	6.496882	4.943260	3.412567	192	1	0	-3.248259	5.501563	-1.602717
111	1	0	4.956422	4.316366	4.047407	193	6	0	-3.924979	3.244130	0.679280
112	1	0	6.120214	3.182864	3.476473	194	1	0	-5.294958	4.839697	0.107729
113	6	0	6.257291	2.255208	1.048574	195	1	0	-4.371477	2.617318	1.436061
114	6	0	6.495726	1.006185	-0.722406	196	6	0	-0.589207	4.475359	-2.402895
115	1	0	6.535327	0.087783	-0.125779	197	1	0	-1.416625	4.594785	-3.104783
116	1	0	5.731827	0.883116	-1.497907	198	1	0	0.286793	4.098777	-2.932907
117	1	0	7.460355	1.110001	-1.228688	199	8	0	-0.320664	5.788789	-1.887526

200	6	0	0.916443	6.014987	-1.424284
201	8	0	1.804860	5.183442	-1.454870
202	1	0	-0.182036	3.620235	-0.494041
203	6	0	1.048903	7.390170	-0.845921
204	1	0	2.099437	7.614399	-0.663682
205	1	0	0.610854	8.133811	-1.515501
206	1	0	0.500784	7.425099	0.101247

61	6	0	4.085872	-3.664866	-0.433147
62	6	0	2.509861	-4.293434	-2.458433
63	6	0	2.737867	-3.567911	-3.797341
64	1	0	2.360426	-4.180515	-4.623681
65	1	0	2.213895	-2.606417	-3.828566
66	1	0	3.801283	-3.379144	-3.976565
67	6	0	3.135391	-5.696715	-2.532852
68	1	0	3.056615	-6.224534	-1.578429
69	1	0	2.585513	-6.276508	-3.282221
70	1	0	4.182395	-5.688149	-2.837004
71	6	0	0.991686	-4.517446	-2.271260
72	1	0	0.785287	-5.037621	-1.329784
73	1	0	0.425524	-3.582689	-2.271923
74	1	0	0.609921	-5.131780	-3.092974
75	6	0	5.268848	-3.435204	1.860799
76	6	0	4.887109	-4.877156	2.251541
77	1	0	5.060561	-5.573899	1.428850
78	1	0	5.485040	-5.206105	3.108809
79	1	0	3.829515	-4.938709	2.526997
80	6	0	6.736902	-3.393123	1.396700
81	1	0	6.997964	-2.408480	0.993158
82	1	0	7.394459	-3.589111	2.250977
83	1	0	6.951633	-4.148436	0.640656
84	6	0	5.172027	-2.565167	3.125154
85	1	0	5.493454	-1.534304	2.939475
86	1	0	4.158389	-2.542305	3.536717
87	1	0	5.834457	-2.978739	3.891862
88	8	0	4.994231	-4.645065	-0.748620
89	8	0	5.687838	4.301372	-1.437210
90	8	0	-2.972779	3.151313	4.486870
91	8	0	-5.933752	-3.095443	-2.863547
92	6	0	-6.189652	-4.432840	-2.442384
93	1	0	-7.075132	-4.767939	-2.985592
94	1	0	-5.353196	-5.098334	-2.675921
95	1	0	-6.382704	-4.480601	-1.365669
96	6	0	-3.087079	-3.541597	-3.816250
97	6	0	-4.147791	-3.708529	-4.919336
98	1	0	-3.656679	-4.112953	-5.810938
99	1	0	-4.946342	-4.399677	-4.652520
100	1	0	-4.598398	-2.749795	-5.192617
101	6	0	-2.565327	-4.926178	-3.389659
102	1	0	-2.137167	-5.449145	-4.252249
103	1	0	-1.785690	-4.836689	-2.626122
104	1	0	-3.362646	-5.553705	-2.980032
105	6	0	5.945329	-4.217917	-1.722663
106	1	0	6.645154	-5.044053	-1.860544
107	1	0	5.466685	-3.984234	-2.678917
108	1	0	6.489138	-3.330572	-1.379602
109	6	0	6.077237	5.047343	-0.286279
110	1	0	6.968280	5.612450	-0.566373
111	1	0	5.297414	5.747722	0.026302
112	1	0	6.311808	4.385808	0.553822
113	6	0	6.612913	1.557070	-1.409390
114	6	0	6.762237	0.028056	-1.293052
115	1	0	6.635923	-0.324216	-0.262999
116	1	0	6.053774	-0.509291	-1.932632
117	1	0	7.770714	-0.253703	-1.611574
118	6	0	6.903229	1.934752	-2.875089
119	1	0	6.843247	3.013499	-3.031899
120	1	0	7.910526	1.604863	-3.153206
121	1	0	6.190910	1.447783	-3.550160
122	6	0	7.676308	2.183957	-0.488418
123	1	0	7.806928	3.250071	-0.674811
124	1	0	7.422924	2.039960	0.567333
125	1	0	8.643331	1.700227	-0.666028
126	6	0	2.752299	5.080442	-1.428283
127	6	0	2.432432	5.819676	-0.115062
128	1	0	1.783509	5.215921	0.527369
129	1	0	3.337754	6.053997	0.452442
130	1	0	1.916071	6.762583	-0.327815
131	6	0	3.624457	5.972615	-2.330354
132	1	0	3.028684	6.837552	-2.641717
133	1	0	4.515289	6.356167	-1.834277
134	1	0	3.937443	5.440985	-3.234269
135	6	0	1.428567	4.875009	-2.202420
136	1	0	1.023068	5.853365	-2.479864
137	1	0	1.591873	4.303954	-3.121158
138	1	0	0.655619	4.371472	-1.615899
139	6	0	-6.671086	-1.059967	-0.967276
140	6	0	-1.921030	-2.765447	-4.474710
141	1	0	-2.212296	-1.736507	-4.710208
142	1	0	-1.021155	-2.730725	-3.855069

5a(S) -1c

RwB97XD SCF energy -4903.694458 a.u.
 RwB97XD SCF enthalpy -4901.794956 a.u.
 RwB97XD SCF free energy -4902.032167 a.u.
 Three lowest frequencies (cm⁻¹) 11.0, 16.4, 20.2
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X	Coordinates Y	Coordinates Z (Angstroms)
1	6	0	0.659438	-0.401367	2.691802
2	6	0	0.443453	-0.046224	4.005357
3	6	0	0.939415	1.128113	4.563993
4	6	0	1.650294	2.038093	3.821161
5	6	0	1.865558	1.714604	2.473337
6	6	0	1.399595	0.527455	1.911070
7	1	0	2.044436	2.949047	4.255401
8	1	0	2.439420	2.409416	1.872010
9	6	0	0.241817	-1.750647	2.229060
10	6	0	-0.668417	-2.053895	1.178695
11	6	0	0.809666	-2.834182	2.864113
12	6	0	-0.922691	-3.381281	0.832773
13	6	0	0.555692	-4.152768	2.503529
14	6	0	-0.306716	-4.462102	1.480740
15	1	0	-1.632204	-3.609382	0.047531
16	1	0	-0.515417	-5.486116	1.195084
17	8	0	0.609726	1.177466	5.880317
18	8	0	-0.234873	-0.747302	4.954308
19	8	0	1.714815	-2.810552	3.880800
20	8	0	1.291268	-4.985142	3.289067
21	6	0	0.087485	-0.116356	6.194472
22	1	0	-0.813418	-0.008941	6.797814
23	1	0	0.857694	-0.701369	6.710023
24	6	0	1.795447	-4.159185	4.342790
25	1	0	1.163339	-4.277867	5.230254
26	1	0	2.836130	-4.412071	4.543995
27	15	0	-1.462323	-0.699431	0.241231
28	15	0	1.709088	0.170653	0.150997
29	46	0	-0.088986	0.297140	-1.287616
30	6	0	-2.050514	0.482841	1.475723
31	6	0	-2.841644	0.067927	2.539102
32	6	0	-1.704168	1.826275	1.354048
33	6	0	-3.273021	0.963382	3.524302
34	1	0	-3.128755	-0.976805	2.603383
35	6	0	-2.062149	2.760209	2.318812
36	1	0	-1.132327	2.134068	0.489306
37	6	0	-2.768929	2.278995	3.447223
38	6	0	-2.864446	-1.418325	-0.652778
39	6	0	-4.185274	-1.061446	-0.395895
40	6	0	-2.571206	-2.226437	-1.745379
41	6	0	-5.229706	-1.580792	-1.162808
42	1	0	-4.396321	-0.363153	0.403016
43	6	0	-3.563114	-2.762251	-2.565593
44	1	0	-1.530631	-2.418083	-1.983091
45	6	0	-4.897051	-2.495307	-2.191371
46	6	0	2.920316	1.404055	-0.405381
47	6	0	4.248529	1.060679	-0.631866
48	6	0	2.490165	2.696579	-0.682376
49	6	0	5.180405	2.007191	-1.049561
50	1	0	4.558000	0.036865	-0.478085
51	6	0	3.369757	3.698913	-1.100254
52	1	0	1.436859	2.928002	-0.562297
53	6	0	4.735281	3.344959	-1.184297
54	6	0	2.546349	-1.426713	0.048909
55	6	0	2.275390	-2.238285	-1.041185
56	6	0	3.504036	-1.819030	0.985622
57	6	0	3.001539	-3.407766	-1.290955
58	1	0	1.479784	-1.948485	-1.720888
59	6	0	4.287089	-2.949325	0.775605
60	1	0	3.644702	-1.213732	1.872769

143	1	0	-1.640158	-3.262854	-5.408658	1	6	0	0.980307	-0.858541	2.490991
144	6	0	-7.074337	-0.298992	-2.245866	2	6	0	0.986353	-0.724569	3.862247
145	1	0	-8.080199	0.121875	-2.132858	3	6	0	1.660963	0.298549	4.525071
146	1	0	-6.380528	0.526984	-2.437818	4	6	0	2.356133	1.265517	3.844316
147	1	0	-7.076974	-0.957264	-3.118465	5	6	0	2.354928	1.164680	2.445786
148	6	0	-7.697198	-2.173956	-0.682653	6	6	0	1.694150	0.139603	1.771676
149	1	0	-7.358765	-2.835160	0.122349	7	1	0	2.887351	2.059486	4.355091
150	1	0	-8.640466	-1.718789	-0.361511	8	1	0	2.904394	1.911582	1.885924
151	1	0	-7.910619	-2.775917	-1.565235	9	6	0	0.363714	-2.070625	1.890547
152	6	0	-6.755326	-0.077629	0.211402	10	6	0	-0.706526	-2.114503	0.954333
153	1	0	-6.108348	0.793732	0.077250	11	6	0	0.877714	-3.292008	2.274052
154	1	0	-7.782225	0.291600	0.296121	12	6	0	-1.157597	-3.339699	0.463230
155	1	0	-6.500621	-0.564222	1.157740	13	6	0	0.418354	-4.506622	1.776643
156	6	0	-2.075780	2.935182	5.574008	14	6	0	-0.599428	-4.564941	0.857169
157	1	0	-2.365572	3.633151	6.361524	15	1	0	-1.978673	-3.369353	-0.242085
158	1	0	-2.140157	1.910034	5.952275	16	1	0	-0.967013	-5.504738	0.462802
159	1	0	-1.042426	3.132475	5.275199	17	8	0	1.507199	0.144694	5.866683
160	6	0	-4.297905	0.425069	4.552649	18	8	0	0.385034	-1.531658	4.779727
161	6	0	-3.639030	-0.632482	5.454442	19	8	0	1.903568	-3.521263	3.140921
162	1	0	-4.387275	-1.070053	6.124856	20	8	0	1.139662	-5.521481	2.328425
163	1	0	-3.191659	-1.445085	4.873731	21	6	0	0.972897	-1.171829	6.029239
164	1	0	-2.857381	-0.186146	6.075629	22	1	0	0.211859	-1.164903	6.807539
165	6	0	-4.967008	1.485558	5.445046	23	1	0	1.788783	-1.867543	6.259007
166	1	0	-5.783539	1.001456	5.992007	24	6	0	1.848666	-4.920635	3.415439
167	1	0	-4.292210	1.912616	6.187594	25	1	0	1.293334	-5.085367	4.346550
168	1	0	-5.397469	2.300466	4.857175	26	1	0	2.859053	-5.324618	3.464594
169	6	0	-5.449022	-0.236303	3.761220	27	15	0	-1.428124	-0.557349	0.312926
170	1	0	-5.933961	0.495472	3.106856	28	15	0	1.770069	0.091476	-0.047333
171	1	0	-5.118575	-1.078137	3.146964	29	46	0	-0.105575	0.437658	-1.285933
172	1	0	-6.202000	-0.618429	4.458588	30	6	0	-1.752463	0.486735	1.753959
173	6	0	-1.761212	4.257878	2.093657	31	6	0	-2.453007	-0.003371	2.852295
174	6	0	-0.821812	4.845403	3.162370	32	6	0	-1.283980	1.796304	1.763773
175	1	0	-0.497539	5.844992	2.851636	33	6	0	-2.660217	0.776413	3.991350
176	1	0	-1.313342	4.948317	4.130294	34	1	0	-2.830368	-1.020663	2.824307
177	1	0	0.073781	4.228136	3.285427	35	6	0	-1.452745	2.630475	2.869142
178	6	0	-3.088263	5.041727	2.088263	36	1	0	-0.754718	2.163577	0.891027
179	1	0	-3.624961	4.928650	3.032808	37	6	0	-2.061705	2.057317	4.007370
180	1	0	-2.888945	6.108351	1.934933	38	6	0	-2.989055	-1.019686	-0.490318
181	1	0	-3.739361	4.703302	1.275063	39	6	0	-4.244161	-0.756609	0.054603
182	6	0	-1.087079	4.481610	0.729717	40	6	0	-2.898996	-1.654669	-1.725584
183	1	0	-0.111425	3.987074	0.675706	41	6	0	-5.408079	-1.203543	-0.571855
184	1	0	-1.706088	4.125613	-0.100217	42	1	0	-4.309221	-0.203335	0.981673
185	1	0	-0.920449	5.553006	0.581866	43	6	0	-4.022576	-2.124843	-2.408016
186	8	0	-1.653702	0.454580	-2.585612	44	1	0	-1.918042	-1.796326	-2.163993
187	6	0	-1.863641	1.756311	-3.043407	45	6	0	-5.264477	-1.964579	-1.758142
188	6	0	-3.155053	2.302746	-2.502360	46	6	0	2.964639	1.377782	-0.498902
189	6	0	-4.281222	2.846407	-3.037975	47	6	0	4.327072	1.101523	-0.577559
190	8	0	-3.268825	2.262406	-1.148918	48	6	0	2.503714	2.659068	-0.771991
191	6	0	-5.145025	3.160498	-1.934334	49	6	0	5.252591	2.108258	-0.835532
192	1	0	-4.474698	3.014957	-4.087847	50	1	0	4.666687	0.085632	-0.427134
193	6	0	-4.478294	2.779140	-0.815930	51	6	0	3.375774	3.708608	-1.075487
194	1	0	-6.130096	3.602815	-1.977474	52	1	0	1.433375	2.841171	-0.765440
195	1	0	-4.707748	2.802047	0.238927	53	6	0	4.755029	3.426696	-0.985839
196	6	0	-1.848034	1.756866	-4.575182	54	6	0	2.480912	-1.508260	-0.505724
197	1	0	-2.776915	1.357585	-4.986921	55	6	0	2.022294	-2.134338	-1.655098
198	1	0	-1.007889	1.150892	-4.917504	56	6	0	3.479645	-2.115190	0.258655
199	8	0	-1.730850	3.093244	-5.088777	57	6	0	2.590535	-3.319427	-2.130872
200	6	0	-0.492814	3.600461	-5.166842	58	1	0	1.192782	-1.691964	-2.197534
201	8	0	0.509074	2.956376	-4.916180	59	6	0	4.118388	-3.269127	-0.184508
202	1	0	-1.055384	2.438108	-2.717979	60	1	0	3.761127	-1.664136	1.202260
203	1	0	1.088814	0.501484	-2.795036	61	6	0	3.723658	-3.790086	-1.443645
204	1	0	0.984176	1.249158	-2.629099	62	6	0	1.877386	-3.991052	-3.326150
205	6	0	-0.509842	5.043557	-5.566453	63	6	0	2.005068	-3.100159	-4.575368
206	1	0	0.493913	5.364001	-5.844066	64	1	0	1.490632	-3.566275	-5.423094
207	1	0	-1.207344	5.208770	-6.390454	65	1	0	1.555790	-2.113970	-4.414878
208	1	0	-0.855395	5.635601	-4.712665	66	1	0	3.052717	-2.951393	-4.855811
						67	6	0	2.350821	-5.413005	-3.672523
						68	1	0	2.350397	-6.067614	-2.796889
						69	1	0	1.652129	-5.834466	-4.403670
						70	1	0	3.342737	-5.440793	-4.125158
						71	6	0	0.379896	-4.123589	-2.963520
						72	1	0	0.245579	-4.762610	-2.084012
						73	1	0	-0.095096	-3.160661	-2.756690

TS2a(S)-1c

RwB97XD SCF energy -4903.675113 a.u.
 RwB97XD SCF enthalpy -4901.778009 a.u.
 RwB97XD SCF free energy -4902.015600 a.u.
 Three lowest frequencies (cm⁻¹) -1046, 6.6, 8.6
 Imaginary frequency (cm⁻¹) -1046
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X Y Z	(Angstroms)	
71	6	0	0.379896	-4.123589	-2.963520
72	1	0	0.245579	-4.762610	-2.084012
73	1	0	-0.095096	-3.160661	-2.756690

74	1	0	-0.156188	-4.579785	-3.801983	147	1	0	-7.773994	-0.675352	-1.964160
75	6	0	5.146868	-3.988571	0.710990	148	6	0	-7.601324	-2.047149	0.459854
76	6	0	4.666510	-5.436099	0.938038	149	1	0	-7.001468	-2.691749	1.111368
77	1	0	4.674753	-6.010720	0.009984	150	1	0	-8.470841	-1.710422	1.035178
78	1	0	5.318970	-5.941008	1.658945	151	1	0	-7.975472	-2.642265	-0.372601
79	1	0	3.645143	-5.446656	1.331637	152	6	0	-6.661830	0.104458	1.214007
80	6	0	6.558711	-3.993635	0.096113	153	1	0	-6.095034	1.013250	0.992264
81	1	0	6.871191	-2.981187	-0.183282	154	1	0	-7.661683	0.409591	1.538775
82	1	0	7.276598	-4.372195	0.832386	155	1	0	-6.186537	-0.405775	2.056587
83	1	0	6.623643	-4.634317	-0.783869	156	6	0	-0.909213	2.476937	5.974417
84	6	0	5.255241	-3.313201	2.088435	157	1	0	-1.025268	3.028861	6.909076
85	1	0	5.666651	-2.299947	2.019608	158	1	0	-0.832762	1.404621	6.188614
86	1	0	4.289090	-3.261340	2.599423	159	1	0	0.009151	2.803626	5.471133
87	1	0	5.933809	-3.898234	2.717152	160	6	0	-3.524295	0.161631	5.119011
88	8	0	4.479946	-4.801956	-1.981097	161	6	0	-2.759222	-0.996081	5.781986
89	8	0	5.673265	4.443612	-1.070770	162	1	0	-3.396220	-1.486562	6.526551
90	8	0	-2.056376	2.761383	5.181840	163	1	0	-2.445020	-1.749922	5.054023
91	8	0	-6.404265	-2.519163	-2.286941	164	1	0	-1.869036	-0.622511	6.296052
92	6	0	-6.582200	-3.905172	-2.006697	165	6	0	-3.974213	1.133708	6.224012
93	1	0	-7.632611	-4.129593	-2.202747	166	1	0	-4.706125	0.614948	6.853256
94	1	0	-5.963326	-4.533309	-2.653322	167	1	0	-3.155751	1.451616	6.871036
95	1	0	-6.348352	-4.133916	-0.962133	168	1	0	-4.457353	2.025012	5.814860
96	6	0	-3.787548	-2.777538	-3.791231	169	6	0	-4.821464	-0.386946	4.485993
97	6	0	-5.016642	-2.757524	-4.718431	170	1	0	-5.385542	0.419704	4.005990
98	1	0	-4.702070	-3.067997	-5.720660	171	1	0	-4.638611	-1.166674	3.741945
99	1	0	-5.810653	-3.434234	-4.406399	172	1	0	-5.455364	-0.824823	5.264148
100	1	0	-5.437643	-1.750381	-4.799932	173	6	0	-0.950086	4.089882	2.739539
101	6	0	-3.297116	-4.224252	-3.590490	174	6	0	0.586938	4.101962	2.717350
102	1	0	-3.064743	-4.683160	-4.558120	175	1	0	0.952013	5.128593	2.601300
103	1	0	-2.390075	-4.245256	-2.977818	176	1	0	0.989828	3.698803	3.647113
104	1	0	-4.045268	-4.848510	-3.094643	177	1	0	0.981145	3.507689	1.886729
105	6	0	5.355317	-4.346778	-3.010989	178	6	0	-1.426762	5.052918	3.840135
106	1	0	5.911409	-5.219893	-3.356503	179	1	0	-0.954035	4.862272	4.804238
107	1	0	4.803347	-3.912951	-3.850869	180	1	0	-1.160513	6.072800	3.540312
108	1	0	6.055384	-3.594748	-2.630386	181	1	0	-2.511293	5.016967	3.975138
109	6	0	5.812191	5.176910	0.144515	182	6	0	-1.467277	4.675910	1.407073
110	1	0	6.604887	5.908748	-0.020397	183	1	0	-1.143723	4.108035	0.531147
111	1	0	4.888277	5.699537	0.411005	184	1	0	-2.561498	4.719002	1.395189
112	1	0	6.090539	4.517116	0.973184	185	1	0	-1.088907	5.696962	1.289144
113	6	0	6.741987	1.754205	-1.027372	186	8	0	-1.430234	0.831616	-2.948453
114	6	0	6.972438	0.235395	-0.923511	187	6	0	-1.981088	2.126564	-3.041691
115	1	0	6.750609	-0.146888	0.078931	188	6	0	-3.146782	2.321260	-2.125218
116	1	0	6.377332	-0.328203	-1.649881	189	6	0	-4.485361	2.482345	-2.303836
117	1	0	8.026464	0.023324	-1.128070	190	8	0	-2.847031	2.425070	-0.801136
118	6	0	7.180288	2.192537	-2.438582	191	6	0	-5.043876	2.705499	-1.002850
119	1	0	7.049016	3.266743	-2.584810	192	1	0	-5.012712	2.469046	-3.246969
120	1	0	8.239168	1.955545	-2.591468	193	6	0	-4.006567	2.647219	-0.131447
121	1	0	6.602288	1.667166	-3.206912	194	1	0	-6.080101	2.884787	-0.755413
122	6	0	7.645402	2.421470	0.026804	195	1	0	-3.925055	2.736943	0.941115
123	1	0	7.740809	3.495280	-0.135953	196	6	0	-2.372431	2.341024	-4.504631
124	1	0	7.266666	2.251012	1.040184	197	1	0	-3.214291	1.703212	-4.780707
125	1	0	8.650816	1.990307	-0.031089	198	1	0	-1.516608	2.106984	-5.140073
126	6	0	2.728405	5.038573	-1.531578	199	8	0	-2.810402	3.684973	-4.742486
127	6	0	2.035866	5.718943	-0.337275	200	6	0	-1.860356	4.612440	-4.936628
128	1	0	1.260957	5.073514	0.086717	201	8	0	-0.672970	4.355305	-4.959246
129	1	0	2.746112	5.963351	0.458760	202	1	0	-1.222867	2.882188	-2.777181
130	1	0	1.556539	6.649705	-0.660763	203	1	0	0.823042	1.101605	-2.637196
131	6	0	3.688348	6.035835	-2.203640	204	1	0	-0.029999	1.024997	-2.991831
132	1	0	3.091413	6.847646	-2.632875	205	6	0	-2.457356	5.975024	-5.113190
133	1	0	4.398138	6.490025	-1.512060	206	1	0	-1.677770	6.690499	-5.372810
134	1	0	4.249770	5.569232	-3.018140	207	1	0	-3.223134	5.952427	-5.892609
135	6	0	1.651511	4.708787	-2.592804	208	1	0	-2.940891	6.279823	-4.180230
136	1	0	1.220397	5.637776	-2.978884						
137	1	0	2.083844	4.161291	-3.436879						
138	1	0	0.824318	4.117009	-2.190490						
139	6	0	-6.794316	-0.819810	-0.007142						
140	6	0	-2.681811	-2.006448	-4.547806						
141	1	0	-2.932170	-0.946206	-4.652350						
142	1	0	-1.701368	-2.080879	-4.070835						
143	1	0	-2.573863	-2.431180	-5.551070						
144	6	0	-7.589722	-0.056399	-1.084492						
145	1	0	-8.557879	0.257038	-0.677470						
146	1	0	-7.050991	0.841422	-1.402433						

6c(S)*2a				
RwB97XD SCF energy			-4903.694458	a.u.
RwB97XD SCF enthalpy			-4901.815530	a.u.
RwB97XD SCF free energy			-4902.052870	a.u.
Three lowest frequencies (cm ⁻¹)			10.8, 18.4, 20.8	
Cartesian coordinates:				
Center	Atomic	Atomic	Coordinates	(Angstroms)

Number	Number	Type	X	Y	Z	81	1	0	-6.747232	3.243604	0.070300
1	6	0	-0.897433	0.645784	2.417459	82	1	0	-7.099168	4.517630	1.246817
2	6	0	-0.883177	0.401263	3.774450	83	1	0	-6.427524	4.946377	-0.324384
3	6	0	-1.614257	-0.616581	4.379575	84	6	0	-5.123219	3.230514	2.363531
4	6	0	-2.381438	-1.482771	3.643684	85	1	0	-5.568760	2.247751	2.173815
5	6	0	-2.393777	-1.278538	2.256602	86	1	0	-4.161462	3.085335	2.864829
6	6	0	-1.687463	-0.246512	1.638301	87	1	0	-5.784978	3.757342	3.058047
7	1	0	-2.956301	-2.276857	4.104752	88	8	0	-4.240474	5.202848	-1.468463
8	1	0	-2.998837	-1.949276	1.659540	89	8	0	-6.097856	-4.074288	-1.132229
9	6	0	-0.223111	1.882564	1.932931	90	8	0	2.107209	-3.118411	5.001621
10	6	0	0.888038	1.972673	1.050472	91	8	0	6.609838	2.409630	-2.185714
11	6	0	-0.694682	3.079699	2.432834	92	6	0	6.832700	3.765973	-1.809785
12	6	0	1.409632	3.221019	0.711934	93	1	0	7.884823	3.977367	-2.011770
13	6	0	-0.164715	4.316887	2.087521	94	1	0	6.217673	4.454892	-2.395878
14	6	0	0.889715	4.423966	1.215130	95	1	0	6.625323	3.924181	-0.746590
15	1	0	2.260442	3.283637	0.044267	96	6	0	3.987563	2.865109	-3.643839
16	1	0	1.314726	5.382066	0.940041	97	6	0	5.212827	2.873525	-4.576394
17	8	0	-1.435100	-0.565211	5.727143	98	1	0	4.899804	3.242240	-5.559182
18	8	0	-0.209121	1.097278	4.734572	99	1	0	6.017504	3.521887	-4.232184
19	8	0	-1.729996	3.262897	3.303045	100	1	0	5.619282	1.866437	-4.712237
20	8	0	-0.858109	5.300070	2.734130	101	6	0	3.531151	4.307992	-3.357949
21	6	0	-0.806910	0.697013	5.965456	102	1	0	3.323879	4.833144	-4.297431
22	1	0	-0.041762	0.586160	6.732228	103	1	0	2.616011	4.313444	-2.756861
23	1	0	-1.568816	1.431258	6.253829	104	1	0	4.289042	4.878301	-2.813857
24	6	0	-1.591466	4.610952	3.748112	105	6	0	-5.152998	4.961695	-2.537052
25	1	0	-1.018949	4.626036	4.684072	106	1	0	-5.708358	5.889367	-2.686578
26	1	0	-2.575457	5.062183	3.865791	107	1	0	-4.633557	4.698186	-3.463827
27	15	0	1.552591	0.438575	0.281807	108	1	0	-5.849022	4.153824	-2.286425
28	15	0	-1.821028	-0.058330	-0.180533	109	6	0	-6.237420	-4.816388	0.077618
29	46	0	0.044339	-0.353392	-1.393855	110	1	0	-7.073510	-5.502121	-0.070309
30	6	0	1.871182	-0.673874	1.679623	111	1	0	-5.334220	-5.390775	0.307019
31	6	0	2.593433	-0.265312	2.796300	112	1	0	-6.451308	-4.154657	0.923723
32	6	0	1.351819	-1.963549	1.636016	113	6	0	-6.962840	-1.307918	-0.958140
33	6	0	2.773847	-1.102418	3.898814	114	6	0	-7.075237	0.215512	-0.762910
34	1	0	3.011338	0.736571	2.811604	115	1	0	-6.783527	0.521184	0.248136
35	6	0	1.491605	-2.855432	2.701050	116	1	0	-6.471263	0.776778	-1.483460
36	1	0	0.805190	-2.269143	0.750179	117	1	0	-8.118107	0.514506	-0.907200
37	6	0	2.130338	-2.360691	3.859361	118	6	0	-7.477693	-1.633853	-2.374059
38	6	0	3.144668	0.929948	-0.454209	119	1	0	-7.448547	-2.707450	-2.573607
39	6	0	4.393208	0.569644	0.046443	120	1	0	-8.514215	-1.295089	-2.483415
40	6	0	3.076003	1.660739	-1.636317	121	1	0	-6.875148	-1.124744	-3.134286
41	6	0	5.571154	1.007018	-0.562807	122	6	0	-7.882488	-1.961313	0.090342
42	1	0	4.442871	-0.059239	0.925301	123	1	0	-8.057213	-3.017278	-0.116041
43	6	0	4.211288	2.124692	-2.303193	124	1	0	-7.466786	-1.862142	1.098854
44	1	0	2.098345	1.880496	-2.050915	125	1	0	-8.856311	-1.459664	0.081762
45	6	0	5.451844	1.862754	-1.684971	126	6	0	-3.222857	-4.864722	-1.738052
46	6	0	-3.146036	-1.220261	-0.626725	127	6	0	-2.504167	-5.583282	-0.580698
47	6	0	-4.487812	-0.851785	-0.607112	128	1	0	-1.661510	-4.991048	-0.210128
48	6	0	-2.798156	-2.518098	-0.972698	129	1	0	-3.180364	-5.772146	0.259337
49	6	0	-5.496924	-1.780555	-0.848546	130	1	0	-2.110163	-6.547317	-0.921953
50	1	0	-4.743940	0.177266	-0.398333	131	6	0	-4.277963	-5.805986	-2.345067
51	6	0	-3.757249	-3.498799	-1.241518	132	1	0	-3.757512	-6.653316	-2.804697
52	1	0	-1.744789	-2.770353	-1.040371	133	1	0	-4.969274	-6.215856	-1.608671
53	6	0	-5.106260	-3.125053	-1.067881	134	1	0	-4.860277	-5.310008	-3.126706
54	6	0	-2.456215	1.618104	-0.453553	135	6	0	-2.194638	-4.602088	-2.864124
55	6	0	-1.965843	2.353557	-1.520464	136	1	0	-1.821899	-5.556495	-3.250454
56	6	0	-3.413049	2.186005	0.389808	137	1	0	-2.653166	-4.057475	-3.696158
57	6	0	-2.455072	3.626865	-1.834567	138	1	0	-1.325486	-4.033376	-2.524039
58	1	0	-1.171127	1.928056	-2.123285	139	6	0	6.943315	0.510062	-0.054743
59	6	0	-3.984767	3.420711	0.099423	140	6	0	2.862402	2.161885	-4.438684
60	1	0	-3.719683	1.642225	1.274971	141	1	0	3.094389	1.105254	-4.606783
61	6	0	-3.554473	4.077834	-1.081791	142	1	0	1.887166	2.227407	-3.948842
62	6	0	-1.704938	4.397571	-2.944909	143	1	0	2.755837	2.646400	-5.414547
63	6	0	-1.960486	3.730181	-4.308121	144	6	0	7.682364	-0.200773	-1.205978
64	1	0	-1.403016	4.252990	-5.093529	145	1	0	8.637982	-0.598647	-0.845653
65	1	0	-1.637735	2.683238	-4.307464	146	1	0	7.090226	-1.039091	-1.586165
66	1	0	-3.021626	3.754206	-4.575471	147	1	0	7.886545	0.480149	-2.034177
67	6	0	-2.038708	5.896323	-3.041217	148	6	0	7.815673	1.655933	0.493343
68	1	0	-1.938544	6.395369	-2.073161	149	1	0	7.264943	2.258768	1.223664
69	1	0	-1.326772	6.361661	-3.731768	150	1	0	8.691489	1.236190	1.000851
70	1	0	-3.038585	6.092626	-3.429101	151	1	0	8.181408	2.312747	-0.295552
71	6	0	-0.190051	4.324053	-2.638680	152	6	0	6.781436	-0.506301	1.086948
72	1	0	0.035907	4.780593	-1.668969	153	1	0	6.167685	-1.365033	0.798650
73	1	0	0.196778	3.300883	-2.627923	154	1	0	7.768835	-0.885565	1.368426
74	1	0	0.361938	4.870446	-3.410573	155	1	0	6.341820	-0.048079	1.977300
75	6	0	-4.985766	4.066021	1.079461	156	6	0	0.976715	-2.825167	5.813462
76	6	0	-4.457366	5.456397	1.485937	157	1	0	1.083005	-3.407805	6.730658
77	1	0	-4.470215	6.154312	0.646878	158	1	0	0.934778	-1.757650	6.060074
78	1	0	-5.075649	5.874469	2.288017	159	1	0	0.044242	-3.107232	5.308872
79	1	0	-3.426755	5.387097	1.847238	160	6	0	3.671390	-0.567376	5.041529
80	6	0	-6.393675	4.200810	0.470460	161	6	0	2.979032	0.622372	5.728079
						162	1	0	3.648248	1.061719	6.476521

163	1	0	2.705398	1.406541	5.016047
164	1	0	2.071745	0.293746	6.242521
165	6	0	4.059822	-1.583326	6.129079
166	1	0	4.806484	-1.113748	6.779646
167	1	0	3.218468	-1.875200	6.758961
168	1	0	4.506547	-2.487480	5.707452
169	6	0	4.998871	-0.086755	4.415813
170	1	0	5.512241	-0.917543	3.919932
171	1	0	4.860092	0.713965	3.684352
172	1	0	5.660620	0.299342	5.198387
173	6	0	0.931662	-4.286873	2.504363
174	6	0	-0.604420	-4.236339	2.461679
175	1	0	-1.008310	-5.240216	2.287347
176	1	0	-1.013306	-3.867074	3.406902
177	1	0	-0.965397	-3.582406	1.661549
178	6	0	1.350983	-5.316260	3.567950
179	1	0	0.881122	-5.141831	4.536645
180	1	0	1.034553	-6.307829	3.224572
181	1	0	2.434766	-5.342332	3.710142
182	6	0	1.442939	-4.836663	1.154084
183	1	0	1.148923	-4.220763	0.300582
184	1	0	2.534884	-4.920139	1.151015
185	1	0	1.029781	-5.837908	0.991085
186	8	0	1.520402	-0.643872	-3.026511
187	6	0	1.896656	-2.021537	-3.252007
188	6	0	3.056084	-2.344648	-2.381211
189	6	0	4.381749	-2.544720	-2.607412
190	8	0	2.781006	-2.518362	-1.059803
191	6	0	4.960392	-2.866305	-1.338511
192	1	0	4.888899	-2.486395	-3.559739
193	6	0	3.946282	-2.822638	-0.438094
194	1	0	5.994986	-3.095201	-1.129449
195	1	0	3.888809	-2.975078	0.628802
196	6	0	2.211487	-2.219676	-4.733463
197	1	0	3.158924	-1.754467	-5.007740
198	1	0	1.410646	-1.795402	-5.345029
199	8	0	2.350969	-3.611947	-5.015703
200	6	0	1.212514	-4.306111	-5.208460
201	8	0	0.112855	-3.792564	-5.174602
202	1	0	1.046833	-2.656622	-2.978458
203	1	0	-1.038588	-0.752626	-2.457904
204	1	0	1.000630	-0.336449	-3.782824
205	6	0	1.493021	-5.755442	-5.452509
206	1	0	0.569075	-6.271603	-5.711002
207	1	0	2.227110	-5.867555	-6.254223
208	1	0	1.919495	-6.195601	-4.546053

2.7. Catalytic cycle 2a-1c (R)

3a(R) -1c

RwB97XD SCF energy -4902.509297 a.u.
 RwB97XD SCF enthalpy -4900.630657 a.u.
 RwB97XD SCF free energy -4900.867181 a.u.
 Three lowest frequencies (cm⁻¹) 8.5, 15.2, 19.2

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates		Z (Angstroms)
			X	Y	
1	6	0	-0.774756	-0.145635	2.565142
2	6	0	-0.359745	-0.791056	3.709851
3	6	0	-0.658301	-2.118127	3.996195
4	6	0	-1.444615	-2.871741	3.159925
5	6	0	-1.903368	-2.236966	1.996936
6	6	0	-1.586864	-0.913404	1.685022
7	1	0	-1.693756	-3.903234	3.378214
8	1	0	-2.516029	-2.816869	1.315868
9	6	0	-0.324519	1.262543	2.389059
10	6	0	0.655576	1.686843	1.452997
11	6	0	-0.785135	2.225521	3.257988
12	6	0	1.068934	3.015991	1.415944
13	6	0	-0.357619	3.547872	3.220971
14	6	0	0.562663	3.983027	2.299458
15	1	0	1.813256	3.325497	0.691129
16	1	0	0.895146	5.013799	2.263122
17	8	0	-0.093658	-2.463658	5.184413
18	8	0	0.381064	-0.262291	4.722705
19	8	0	-1.705460	2.072534	4.252014
20	8	0	-0.997026	4.256111	4.195148
21	6	0	0.776514	-1.378052	5.518613
22	1	0	1.803174	-1.646690	5.256701
23	1	0	0.667929	-1.135534	6.575402
24	6	0	-1.642075	3.278495	5.015125
25	1	0	-1.042040	3.107527	5.916385
26	1	0	-2.652574	3.610491	5.254078
27	15	0	1.320156	0.452909	0.283039
28	15	0	-2.033209	-0.311773	0.012438
29	46	0	-0.215003	-0.638711	-1.248750
30	6	0	2.165588	-0.774640	1.338582
31	6	0	2.985629	-0.432210	2.415841
32	6	0	2.010512	-2.112657	1.007583
33	6	0	3.643874	-1.403068	3.170538
34	1	0	3.108226	0.615313	2.661674
35	6	0	2.629202	-3.142944	1.724229
36	1	0	1.380476	-2.365281	0.162493
37	6	0	3.382780	-2.762628	2.851955
38	6	0	2.598408	1.332061	-0.675096
39	6	0	3.855189	1.652510	-0.160554
40	6	0	2.314564	1.642803	-1.998829
41	6	0	4.797550	2.345688	-0.914731
42	1	0	4.094699	1.358730	0.851904
43	6	0	3.229877	2.299071	-2.830567
44	1	0	1.353429	1.348794	-2.408086
45	6	0	4.426430	2.731024	-2.228053
46	6	0	-3.537944	-1.243323	-0.445448
47	6	0	-4.809354	-0.751833	-0.166113
48	6	0	-3.415045	-2.457801	-1.116698
49	6	0	-5.961640	-1.484603	-0.455901
50	1	0	-4.908766	0.230553	0.269418
51	6	0	-4.523054	-3.242763	-1.433799
52	1	0	-2.426112	-2.784632	-1.408624
53	6	0	-5.779373	-2.783211	-0.978486
54	6	0	-2.524396	1.428681	0.128663
55	6	0	-2.031566	2.316481	-0.815478
56	6	0	-3.405633	1.889642	1.111079
57	6	0	-2.466838	3.645384	-0.882552
58	1	0	-1.279893	1.961644	-1.514991
59	6	0	-3.926635	3.178899	1.061560
60	1	0	-3.692639	1.215737	1.909361
61	6	0	-3.515386	4.003795	-0.017074
62	6	0	-1.716030	4.573953	-1.866339
63	6	0	-1.949604	4.102687	-3.313213
64	1	0	-1.379235	4.729713	-4.007712
65	1	0	-1.630206	3.065755	-3.461510
66	1	0	-3.007765	4.171052	-3.587287

67	6	0	-2.060009	6.070447	-1.770733	149	1	0	5.891788	4.657456	0.186199
68	1	0	-1.965966	6.444830	-0.747997	150	1	0	7.581440	4.139084	0.234350
69	1	0	-1.348839	6.622819	-2.395007	151	1	0	6.812833	4.453530	-1.318884
70	1	0	-3.059170	6.310103	-2.135917	152	6	0	6.355249	2.030640	1.074607
71	6	0	-0.210408	4.473363	-1.533772	153	1	0	6.135230	0.961519	1.149087
72	1	0	-0.020828	4.827071	-0.515613	154	1	0	7.386021	2.172811	1.413606
73	1	0	0.180274	3.456168	-1.616700	155	1	0	5.702801	2.570005	1.770289
74	1	0	0.364820	5.100687	-2.222730	156	6	0	3.011461	-4.268709	4.613986
75	6	0	-4.851891	3.697826	2.181963	157	1	0	3.480758	-5.160864	5.033155
76	6	0	-4.200631	4.937731	2.824741	158	1	0	2.816137	-3.558900	5.423715
77	1	0	-4.109331	5.756830	2.108172	159	1	0	2.060194	-4.540875	4.146995
78	1	0	-4.809556	5.287331	3.666199	160	6	0	4.744626	-0.976121	4.172081
79	1	0	-3.200281	4.704513	3.201167	161	6	0	4.649093	-1.608273	5.572604
80	6	0	-6.257731	4.064968	1.669553	162	1	0	5.412413	-1.156950	6.215680
81	1	0	-6.694508	3.249701	1.083656	163	1	0	3.679908	-1.420585	6.043902
82	1	0	-6.917623	4.250348	2.524400	164	1	0	4.831351	-2.681839	5.553852
83	1	0	-6.251853	4.970028	1.061461	165	6	0	6.096506	-1.378902	3.547376
84	6	0	-5.036612	2.640436	3.282702	166	1	0	6.920085	-1.082215	4.206977
85	1	0	-5.563168	1.752926	2.914157	167	1	0	6.158325	-2.460344	3.394306
86	1	0	-4.083883	2.321307	3.715125	168	1	0	6.243864	-0.884693	2.581305
87	1	0	-5.641414	3.068483	4.088204	169	6	0	4.750458	0.548119	4.375422
88	8	0	-4.174983	5.195155	-0.196931	170	1	0	4.957988	1.092653	3.449739
89	8	0	-6.873513	-3.609460	-1.100103	171	1	0	3.799582	0.907340	4.785190
90	8	0	3.927011	-3.729831	3.662874	172	1	0	5.539279	0.810869	5.086915
91	8	0	5.298543	3.531844	-2.924919	173	6	0	2.421972	-4.574887	1.169167
92	6	0	4.904173	4.901111	-2.950906	174	6	0	0.953935	-4.986332	1.388447
93	1	0	5.681021	5.440743	-3.495669	175	1	0	0.778995	-5.986792	0.976484
94	1	0	3.945154	5.037442	-3.459968	176	1	0	0.703023	-5.009949	2.453868
95	1	0	4.818397	5.308537	-1.937791	177	1	0	0.264847	-4.292952	0.894314
96	6	0	2.851546	2.418495	-4.328527	178	6	0	3.338482	-5.662525	1.754913
97	6	0	4.008141	2.795260	-5.271721	179	1	0	3.102439	-5.916518	2.787855
98	1	0	3.662615	2.663089	-6.302858	180	1	0	3.204899	-6.575145	1.163718
99	1	0	4.329789	3.832022	-5.172689	181	1	0	4.393475	-5.381015	1.698434
100	1	0	4.877649	2.148718	-5.124688	182	6	0	2.714118	-4.570215	-0.349837
101	6	0	1.701312	3.425910	-4.504043	183	1	0	2.095020	-3.866590	-0.910524
102	1	0	1.412612	3.484632	-5.559649	184	1	0	3.765992	-4.335633	-0.542560
103	1	0	0.819201	3.121259	-3.932792	185	1	0	2.519715	-5.568290	-0.756678
104	1	0	1.985143	4.431300	-4.177635	186	8	0	1.547669	-1.362548	-2.273271
105	6	0	-5.130582	5.133282	-1.254171	187	6	0	2.084343	-1.950626	-3.210966
106	1	0	-5.618198	6.108742	-1.295684	188	1	0	-1.216669	-1.302062	-2.234787
107	1	0	-4.654219	4.924756	-2.217614	189	6	0	1.393512	-2.297778	-4.427889
108	1	0	-5.880635	4.358053	-1.062755	190	6	0	0.127421	-2.023594	-4.886132
109	6	0	-7.073974	-4.423823	0.058975	191	8	0	2.098369	-2.969138	-5.380057
110	1	0	-7.974012	-5.012459	-0.127031	192	6	0	0.053412	-2.580893	-6.187127
111	1	0	-6.227926	-5.095100	0.227031	193	1	0	-0.642997	-1.487223	-4.350553
112	1	0	-7.212948	-3.815261	0.955917	194	6	0	1.276241	-3.138361	-6.427873
113	6	0	-7.347246	-0.805767	-0.352977	195	1	0	-0.789851	-2.569525	-6.861636
114	6	0	-7.215682	0.656233	0.111061	196	1	0	1.688751	-3.688650	-7.273433
115	1	0	-6.815550	0.730823	1.128324	197	6	0	3.542780	-2.329367	-3.094330
116	1	0	-6.581394	1.251199	-0.554515	198	1	0	4.105049	-1.923924	-3.941960
117	1	0	-8.208232	1.117001	0.114444	199	1	0	3.639678	-3.420916	-3.114335
118	6	0	-7.971000	-0.788102	-1.763405	200	8	0	4.017840	-1.796656	-1.870842
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121	1	0	-7.331708	-0.241391	-2.465044	203	6	0	5.546697	-1.704390	-0.090603
122	6	0	-8.317470	-1.496565	0.622385	204	1	0	5.159933	-2.418243	0.645139
123	1	0	-8.679267	-2.450811	0.237470	205	1	0	6.628028	-1.634067	0.028730
124	1	0	-7.855299	-1.659557	1.601735	206	1	0	5.068827	-0.740829	0.087029
125	1	0	-9.192933	-0.855417	0.772190						
126	6	0	-4.364800	-4.438281	-2.402020						
127	6	0	-2.900284	-4.609829	-2.844118						
128	1	0	-2.501629	-3.711821	-3.327986						
129	1	0	-2.242589	-4.875038	-2.008600						
130	1	0	-2.846524	-5.422419	-3.575229						
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132	1	0	-4.514860	-6.592724	-2.501355						
133	1	0	-4.359183	-5.984888	-0.848565						
134	1	0	-5.904235	-5.847725	-1.718775						
135	6	0	-5.192999	-4.122343	-3.664524						
136	1	0	-5.093302	-4.934924	-4.393105						
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138	1	0	-4.842613	-3.198777	-4.138130						
139	6	0	6.222778	2.562822	-0.362302						
140	6	0	2.356388	1.034698	-4.808957						
141	1	0	3.128663	0.271447	-4.660985						
142	1	0	1.446042	0.710148	-4.300103						
143	1	0	2.128582	1.077217	-5.879315						
144	6	0	7.202299	1.768040	-1.248834						
145	1	0	8.224407	1.873387	-0.867503						
146	1	0	6.949410	0.701664	-1.248718						
147	1	0	7.185685	2.125260	-2.281561						
148	6	0	6.643152	4.044542	-0.323311						
149	1	0	5.891788	4.657456	0.186199						
150	1	0	7.581440	4.139084	0.234350						
151	1	0	6.812833	4.453530	-1.318884						
152	6	0	6.355249	2.030640	1.074607						
153	1	0	6.135230	0.961519	1.149087						
154	1	0	7.386021	2.172811	1.413606						
155	1	0	5.702801	2.570005	1.770289						
156	6	0	3.011461	-4.268709	4.613986						
157	1	0	3.480758	-5.160864	5.033155						
158	1	0	2.816137	-3.558900	5.423715						
159	1	0	2.060194	-4.540875	4.146995						
160	6	0	4.744626	-0.976121	4.172081						
161	6	0	4.649093	-1.608273	5.572604						
162	1	0	5.412413	-1.156950	6.215680						
163	1	0	3.679908	-1.420585	6.043902						
164	1	0	4.831351	-2.681839	5.553852						
165	6	0	6.096506	-1.378902	3.547376						
166	1	0	6.920085	-1.082215	4.206977						
167	1	0	6.158325	-2.460344	3.394306						
168	1	0	6.243864	-0.884693	2.581305						
169	6	0	4.750458	0.548119	4.375422						
170	1	0	4.957988	1.092653	3.449739						
171	1	0	3.799582	0.907340	4.785190						
172	1	0	5.539279	0.810869	5.086915						
173	6	0	2.421972	-4.574887	1.169167						
174	6	0	0.953935	-4.986332	1.388447						
175	1	0	0.778995	-5.986792	0.976484						
176	1	0	0.703023	-5.009949	2.453868						
177	1	0	0.264847	-4.292952	0.894314						
178	6	0	3.338482	-5.662525	1.754913						
179	1	0	3.102439	-5.916518	2.787855						
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181	1	0	4.393475	-5.381015	1.698434						
182	6	0	2.714118	-4.570215	-0.349837						
183	1	0	2.095020	-3.866590	-0.910524						
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10	6	0	-1.226762	-0.785680	1.960620	92	6	0	-7.349959	-3.366537	0.357546
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12	6	0	-1.816803	-1.955391	2.439515	94	1	0	-6.697313	-4.205898	0.616242
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14	6	0	-1.446606	-2.542959	3.658652	96	6	0	-4.385431	-4.325466	-1.273268
15	1	0	-2.609024	-2.431256	1.874046	97	6	0	-5.626306	-4.898161	-1.980343
16	1	0	-1.922594	-3.447348	4.018492	98	1	0	-5.358863	-5.869906	-2.409305
17	8	0	0.573807	4.227931	4.132804	99	1	0	-6.469459	-5.064885	-1.310355
18	8	0	-0.476242	2.209835	4.360089	100	1	0	-5.958245	-4.252276	-2.798292
19	8	0	1.053519	-0.307975	4.812417	101	6	0	-4.025727	-5.209249	-0.064332
20	8	0	0.062141	-2.218793	5.590576	102	1	0	-3.867628	-6.244869	-0.386061
21	6	0	-0.006988	3.339055	5.091979	103	1	0	-3.104757	-4.862147	0.416444
22	1	0	-0.841028	3.827015	5.592261	104	1	0	-4.817561	-5.208407	0.691035
23	1	0	0.766461	3.018731	5.800768	105	6	0	4.648627	-5.426371	1.668455
24	6	0	0.771238	-1.046643	5.999985	106	1	0	5.147691	-6.192927	2.264211
25	1	0	0.129710	-0.444766	6.655347	107	1	0	4.247845	-5.886668	0.760972
26	1	0	1.703658	-1.330298	6.486423	108	1	0	5.372304	-4.656181	1.381734
27	15	0	-1.689643	-0.121522	0.320949	109	6	0	6.353714	4.077788	-1.813029
28	15	0	1.631240	0.122840	-0.033010	110	1	0	7.181727	4.629865	-2.260794
29	46	0	-0.111907	-0.518940	-1.346783	111	1	0	5.437865	4.670296	-1.878942
30	6	0	-1.957432	1.659504	0.528524	112	1	0	6.566299	3.890490	-0.757544
31	6	0	-2.724826	2.160915	1.580060	113	6	0	6.889599	0.634813	-0.715148
32	6	0	-1.412072	2.534109	-0.400642	114	6	0	6.841526	-0.482063	0.343991
33	6	0	-2.898139	3.529403	1.755874	115	1	0	6.450439	-0.121648	1.302198
34	1	0	-3.183637	1.459726	2.266168	116	1	0	6.240269	-1.338983	0.022375
35	6	0	-1.545764	3.922848	-0.285228	117	1	0	7.858387	-0.846110	0.520334
36	1	0	-0.848441	2.122193	-1.232443	118	6	0	7.500838	0.035201	-1.998125
37	6	0	-2.211745	4.392842	0.862245	119	1	0	7.593270	0.787586	-2.785568
38	6	0	-3.288180	-0.860340	-0.114225	120	1	0	8.500507	-0.361007	-1.787710
39	6	0	-4.459531	-0.109693	-0.169599	121	1	0	6.883634	-0.786584	-2.376949
40	6	0	-3.318919	-2.200089	-0.482690	122	6	0	7.827390	1.726551	-0.170589
41	6	0	-5.682166	-0.697393	-0.483230	123	1	0	8.112130	2.445563	-0.939154
42	1	0	-4.411967	0.950580	0.034383	124	1	0	7.373868	2.262893	0.669685
43	6	0	-4.510254	-2.854052	-0.809130	125	1	0	8.748112	1.258658	0.194365
44	1	0	-2.385730	-2.752792	-0.508523	126	6	0	3.715486	2.907739	-4.052585
45	6	0	-5.695587	-2.097013	-0.700735	127	6	0	2.277139	2.703441	-4.556375
46	6	0	3.069086	0.757729	-0.937755	128	1	0	2.042251	1.641271	-4.673221
47	6	0	4.359683	0.525661	-0.475091	129	1	0	1.531098	3.158996	-3.896197
48	6	0	2.873208	1.526293	-2.081288	130	1	0	2.173319	3.172088	-5.539653
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50	1	0	4.503538	-0.146700	0.358532	132	1	0	3.584961	4.890165	-4.909786
51	6	0	3.933940	2.191692	-2.700326	133	1	0	3.440162	4.886156	-3.146930
52	1	0	1.869920	1.608244	-2.483148	134	1	0	5.024888	4.666418	-3.924575
53	6	0	5.204924	2.066528	-2.093761	135	6	0	4.656122	2.277792	-5.099279
54	6	0	2.165476	-1.377089	0.839880	136	1	0	4.497105	2.751887	-6.074398
55	6	0	1.731828	-2.602130	0.355256	137	1	0	5.705843	2.407120	-4.828254
56	6	0	2.964431	-1.336678	1.983552	138	1	0	4.456595	1.206154	-5.209753
57	6	0	2.097713	-3.813457	0.947150	139	6	0	-6.936783	0.186315	-0.650929
58	1	0	1.067991	-2.614890	-0.502979	140	6	0	-3.231126	-4.419999	-2.298710
59	6	0	3.432989	-2.507512	2.573558	141	1	0	-3.390505	-3.739824	-3.141932
60	1	0	3.224017	-0.373193	2.404876	142	1	0	-2.259508	-4.192569	-1.854527
61	6	0	3.047992	-3.739563	1.983466	143	1	0	-3.173234	-5.441184	-2.689575
62	6	0	1.385600	-5.083091	0.424144	144	6	0	-7.488183	0.006563	-2.078756
63	6	0	1.976576	-5.495001	-0.935404	145	1	0	-8.383123	0.624523	-2.213280
64	1	0	1.402814	-6.326592	-1.360044	146	1	0	-6.748189	0.318574	-2.823855
65	1	0	1.940468	-4.663168	-1.645225	147	1	0	-7.758935	-1.032585	-2.276818
66	1	0	3.018479	-5.816609	-0.850145	148	6	0	-8.038029	-0.146308	0.373275
67	6	0	1.421791	-6.274932	1.396401	149	1	0	-7.637722	-0.172063	1.392587
68	1	0	1.074129	-5.986227	2.393392	150	1	0	-8.812032	0.628186	0.339288
69	1	0	0.746948	-7.051133	1.019877	151	1	0	-8.522299	-1.100330	0.162703
70	1	0	2.409901	-6.723714	1.496658	152	6	0	-6.596819	1.677052	-0.472669
71	6	0	-0.114247	-4.755252	0.212777	153	1	0	-5.827110	2.017259	-1.173750
72	1	0	-0.567091	-4.370456	1.133446	154	1	0	-7.497545	2.269487	-0.661223
73	1	0	-0.285082	-4.023270	-0.582262	155	1	0	-6.263463	1.902978	0.546532
74	1	0	-0.646280	-5.667754	-0.075152	156	6	0	-1.040566	6.200124	1.766504
75	6	0	4.270068	-2.446161	3.868175	157	1	0	-1.172502	7.270638	1.933987
76	6	0	3.553958	-3.257887	4.966049	158	1	0	-0.877417	5.698080	2.724673
77	1	0	3.541796	-4.324377	4.734729	159	1	0	-0.162297	6.039340	1.133602
78	1	0	4.062696	-3.122442	5.927027	160	6	0	-3.892763	4.055557	2.810885
79	1	0	2.516710	-2.927972	5.077074	161	6	0	-3.254510	5.017448	3.829737
80	6	0	5.697151	-2.987456	3.661601	162	1	0	-3.952973	5.187402	4.656306
81	1	0	6.184918	-2.501614	2.808933	163	1	0	-2.337544	4.593410	4.247612
82	1	0	6.298852	-2.777963	4.553189	164	1	0	-3.021818	5.987408	3.390796
83	1	0	5.712659	-4.065876	3.503845	165	6	0	-5.033615	4.780898	2.069423
84	6	0	4.408715	-1.000721	4.375619	166	1	0	-5.773376	5.148966	2.789375
85	1	0	4.979070	-0.373221	3.681605	167	1	0	-4.659346	5.636034	1.501131
86	1	0	3.437678	-0.529892	4.553526	168	1	0	-5.543798	4.102505	1.376448
87	1	0	4.952806	-1.010646	5.325229	169	6	0	-4.514924	2.899559	3.611725
88	8	0	3.615905	-4.883398	2.487623	170	1	0	-5.053874	2.191623	2.973184
89	8	0	6.237132	2.855095	-2.547624	171	1	0	-3.760883	2.348010	4.184443
90	8	0	-2.234553	5.737666	1.137426	172	1	0	-5.237420	3.307910	4.325177
91	8	0	-6.919659	-2.707755	-0.831200	173	6	0	-0.967238	4.778416	-1.441240

174	6	0	0.570999	4.709318	-1.424471	37	6	0	-3.552224	3.501572	1.373059
175	1	0	0.975566	5.280703	-2.267678	38	6	0	-2.694788	-1.570030	-0.429275
176	1	0	0.985462	5.130074	-0.503185	39	6	0	-4.067633	-1.365315	-0.319914
177	1	0	0.928990	3.678249	-1.514296	40	6	0	-2.217917	-2.654110	-1.155303
178	6	0	-1.400383	6.255595	-1.457068	41	6	0	-4.976758	-2.292946	-0.823729
179	1	0	-0.948318	6.849183	-0.662707	42	1	0	-4.430523	-0.474817	0.173455
180	1	0	-1.076551	6.693747	-2.407531	43	6	0	-3.076078	-3.595425	-1.726556
181	1	0	-2.486462	6.363016	-1.393259	44	1	0	-1.147505	-2.759028	-1.294409
182	6	0	-1.466618	4.188382	-2.778815	45	6	0	-4.449777	-3.451077	-1.442907
183	1	0	-1.154076	3.154187	-2.939009	46	6	0	2.881953	1.500817	-0.426187
184	1	0	-2.559354	4.225240	-2.835003	47	6	0	4.199443	1.057671	-0.421053
185	1	0	-1.066178	4.780196	-3.608671	48	6	0	2.483173	2.472403	-1.344605
186	8	0	-1.288066	-1.563142	-2.756202	49	6	0	5.158446	1.603678	-1.274078
187	6	0	-0.306299	-1.355286	-3.560624	50	1	0	4.471505	0.245966	0.237545
188	1	0	0.895671	-0.693766	-2.615660	51	6	0	3.391055	3.065259	-2.219307
189	6	0	0.512753	-2.503977	-3.976560	52	1	0	1.430944	2.727527	-1.401913
190	6	0	0.378417	-3.841280	-3.764178	53	6	0	4.748467	2.685089	-2.083690
191	8	0	1.616646	-2.247487	-4.728370	54	6	0	2.468931	-0.868242	1.148393
192	6	0	1.481231	-4.455440	-4.434091	55	6	0	2.493082	-2.011333	0.365158
193	1	0	-0.412635	-4.325180	-3.210246	56	6	0	3.192292	-0.822908	2.338910
194	6	0	2.196520	-3.444620	-4.992812	57	6	0	3.289032	-3.113732	0.686777
195	1	0	1.707852	-5.510220	-4.488176	58	1	0	1.883838	-2.036185	-0.533565
196	1	0	3.097712	-3.411182	-5.861119	59	6	0	4.025790	-1.876498	2.705219
197	6	0	-0.466497	-0.214926	-4.572726	60	1	0	3.108160	0.056516	2.965831
198	1	0	-0.859553	-0.647218	-5.497348	61	6	0	4.133210	-2.969238	1.804223
199	1	0	0.473034	0.292646	-4.777639	62	6	0	3.128698	-4.361075	-0.211797
200	8	0	-1.363226	0.746185	-4.041783	63	6	0	3.744199	-4.086964	-1.596915
201	6	0	-2.683669	0.448139	-4.135752	64	1	0	3.579196	-4.945679	-2.257236
202	8	0	-3.104499	-0.445632	-4.836201	65	1	0	3.288769	-3.209867	-2.070505
203	6	0	-3.525549	1.373363	-3.315397	66	1	0	4.823097	-3.913967	-1.534562
204	1	0	-3.068613	1.553093	-2.340256	67	6	0	3.718418	-5.658879	0.365958
205	1	0	-3.613173	2.332816	-3.834224	68	1	0	3.353535	-5.847840	1.379703
206	1	0	-4.518404	0.939346	-3.197634	69	1	0	3.399473	-6.494561	-0.266153
						70	1	0	4.808248	-5.666575	0.386421
						71	6	0	1.616584	-4.628736	-0.399445
						72	1	0	1.115777	-4.760658	0.566168
						73	1	0	1.105549	-3.826952	-0.940583
						74	1	0	1.480954	-5.545754	-0.981542
						75	6	0	4.727136	-1.874675	4.079309
						76	6	0	4.232776	-3.099214	4.874415
						77	1	0	4.514330	-4.034717	4.385955
						78	1	0	4.669382	-3.094224	5.879436
						79	1	0	3.142564	-3.083124	4.975937
						80	6	0	6.262973	-1.913796	3.971742
						81	1	0	6.634935	-1.138386	3.293454
						82	1	0	6.700178	-1.728397	4.959111
						83	1	0	6.628348	-2.882457	3.631008
						84	6	0	4.368084	-0.616967	4.887930
						85	1	0	4.750476	0.295882	4.417872
						86	1	0	3.289742	-0.505493	5.030989
						87	1	0	4.828317	-0.692378	5.878138
						88	8	0	5.090411	-3.917162	2.069056
						89	8	0	5.698601	3.356986	-2.816607
						90	8	0	-4.072560	4.701209	1.789694
						91	8	0	-5.334923	-4.442982	-1.788763
						92	6	0	-5.319198	-5.553345	-0.895902
						93	1	0	-6.134043	-6.212735	-1.200495
						94	1	0	-4.375601	-6.104648	-0.948977
						95	1	0	-5.476947	-5.232581	0.139356
						96	6	0	-2.427169	-4.655531	-2.647934
						97	6	0	-3.406511	-5.393851	-3.576863
						98	1	0	-2.822581	-5.990714	-4.285863
						99	1	0	-4.071177	-6.079023	-3.051263
						100	1	0	-4.018448	-4.693162	-4.152706
						101	6	0	-1.649386	-5.675332	-1.798199
						102	1	0	-1.087072	-6.357480	-2.445750
						103	1	0	-0.936538	-5.171293	-1.138920
						104	1	0	-2.314217	-6.278066	-1.171850
						105	6	0	6.262005	-3.770987	1.268693
						106	1	0	6.971229	-4.525924	1.612967
						107	1	0	6.052127	-3.935413	0.207694
						108	1	0	6.703489	-2.776152	1.390596
						109	6	0	6.251135	4.468858	-2.105277
						110	1	0	7.002435	4.913975	-2.759826
						111	1	0	5.484597	5.211517	-1.869647
						112	1	0	6.720193	4.150566	-1.170953
						113	6	0	6.520717	0.889304	-1.436868
						114	6	0	6.603959	-0.355531	-0.532775
						115	1	0	6.572047	-0.097306	0.531567
						116	1	0	5.804194	-1.075146	-0.738256
						117	1	0	7.555225	-0.863657	-0.718484
						118	6	0	6.621423	0.402230	-2.897179

4a(R) -1c

RwB97XD SCF energy -4902.523889 a.u.

RwB97XD SCF enthalpy -4900.641546 a.u.

RwB97XD SCF free energy -4900.873138 a.u.

Three lowest frequencies (cm⁻¹) 19.0, 22.7, 24.8

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.057030	0.992989	2.746118
2	6	0	-0.483145	1.849688	3.677821
3	6	0	-0.223792	3.217795	3.689406
4	6	0	0.593273	3.807265	2.755329
5	6	0	1.172249	2.954204	1.802962
6	6	0	0.925673	1.582883	1.789156
7	1	0	0.796164	4.871522	2.761128
8	1	0	1.840751	3.388513	1.068197
9	6	0	-0.238540	-0.459414	2.831213
10	6	0	-0.912053	-1.226209	1.841768
11	6	0	0.174773	-1.148691	3.949454
12	6	0	-1.080890	-2.601005	2.008379
13	6	0	-0.007236	-2.518288	4.109260
14	6	0	-0.621202	-3.280824	3.145486
15	1	0	-1.596392	-3.178096	1.250189
16	1	0	-0.760344	-4.348963	3.261122
17	8	0	-0.898748	3.790267	4.724324
18	8	0	-1.338176	1.542096	4.692888
19	8	0	0.844352	-0.651526	5.025196
20	8	0	0.529243	-2.909444	5.295265
21	6	0	-1.312685	2.690915	5.540340
22	1	0	-2.308248	2.877711	5.937231
23	1	0	-0.576483	2.536678	6.338417
24	6	0	0.828127	-1.698820	5.997257
25	1	0	0.038289	-1.499089	6.730062
26	1	0	1.809621	-1.781173	6.463774
27	15	0	-1.493873	-0.432883	0.305796
28	15	0	1.607646	0.533659	0.453524
29	46	0	0.121010	-0.004623	-1.190100
30	6	0	-2.337500	1.099434	0.751364
31	6	0	-3.289645	1.147177	1.770054
32	6	0	-2.067147	2.235146	0.005058
33	6	0	-3.942196	2.335159	2.084075
34	1	0	-3.514187	0.238529	2.314841
35	6	0	-2.685193	3.460500	0.264820
36	1	0	-1.337015	2.169960	-0.794521

119	1	0	6.592530	1.237046	-3.601656
120	1	0	7.564697	-0.135235	-3.045946
121	1	0	5.800085	-0.281784	-3.138811
122	6	0	7.739939	1.768496	-1.107194
123	1	0	7.916071	2.531162	-1.866976
124	1	0	7.631786	2.255885	-0.132572
125	1	0	8.637912	1.142235	-1.066093
126	6	0	2.874357	3.908628	-3.408835
127	6	0	1.345286	4.068548	-3.357726
128	1	0	0.825093	3.105330	-3.370746
129	1	0	1.020326	4.629212	-2.476139
130	1	0	1.016211	4.624020	-2.41417
131	6	0	3.469553	5.324777	-3.492459
132	1	0	2.935809	5.893601	-4.261436
133	1	0	3.358154	5.862950	-2.545181
134	1	0	4.523425	5.311992	-3.771495
135	6	0	3.214197	3.135093	-4.699113
136	1	0	2.855121	3.690648	-5.572836
137	1	0	4.291659	2.989633	-4.810324
138	1	0	2.730019	2.152309	-4.701988
139	6	0	-6.492221	-2.011985	-0.743050
140	6	0	-1.427204	-3.932630	-3.582522
141	1	0	-1.924031	-3.130123	-4.137025
142	1	0	-0.576532	-3.499933	-3.049061
143	1	0	-1.021212	-4.649385	-4.304195
144	6	0	-7.098077	-2.054660	-2.159128
145	1	0	-8.156926	-1.775189	-2.120741
146	1	0	-6.582396	-1.355524	-2.824176
147	1	0	-7.024228	-3.050936	-2.598260
148	6	0	-7.221155	-3.024336	0.160314
149	1	0	-6.733005	-3.109388	1.137236
150	1	0	-8.250221	-2.687726	0.329309
151	1	0	-7.272532	-4.014942	-0.292625
152	6	0	-6.765957	-0.613176	-0.162687
153	1	0	-6.268820	0.180264	-0.745246
154	1	0	-7.844377	-0.427361	-0.176603
155	1	0	-6.435103	-0.527150	0.878234
156	6	0	-3.174389	5.442292	2.615296
157	1	0	-3.703039	6.348099	2.917557
158	1	0	-2.889201	4.870981	3.504013
159	1	0	-2.264957	5.720242	2.073486
160	6	0	-5.131243	2.324184	3.069244
161	6	0	-4.990531	3.329443	4.226794
162	1	0	-5.760295	3.125532	4.978796
163	1	0	-4.017111	3.234763	4.715048
164	1	0	-5.117772	4.359911	3.897263
165	6	0	-6.404958	2.650207	2.263228
166	1	0	-7.280364	2.638107	2.922532
167	1	0	-6.341604	3.639152	1.801598
168	1	0	-6.566755	1.909774	1.471854
169	6	0	-5.313703	0.935517	3.704280
170	1	0	-5.511066	0.156479	2.960645
171	1	0	-4.437990	0.640399	4.293607
172	1	0	-6.174006	0.962123	4.380017
173	6	0	-2.340463	4.617732	-0.702810
174	6	0	-0.907832	5.105072	-0.419420
175	1	0	-0.630635	5.888636	-1.133430
176	1	0	-0.810435	5.519522	0.588499
177	1	0	-0.185626	4.287041	-0.516169
178	6	0	-3.304827	5.815691	-0.658281
179	1	0	-3.224833	6.398210	0.259086
180	1	0	-3.060140	6.484874	-1.490165
181	1	0	-4.345499	5.500231	-0.777594
182	6	0	-2.394920	4.085497	-2.155419
183	1	0	-1.662244	3.299607	-2.357568
184	1	0	-3.388006	3.690731	-2.392791
185	1	0	-2.179507	4.904883	-2.849091
186	8	0	-1.199061	-0.268032	-2.717333
187	6	0	-0.715077	0.435213	-3.826378
188	1	0	-0.664791	1.520131	-3.612717
189	6	0	0.680375	-0.013224	-4.138534
190	6	0	1.402450	-0.533043	-5.157939
191	8	0	1.478236	0.056747	-3.017336
192	6	0	2.718969	-0.806318	-4.639302
193	1	0	1.049057	-0.705892	-6.164538
194	6	0	2.713639	-0.439532	-3.338066
195	1	0	3.559448	-1.218635	-5.179019
196	1	0	3.445148	-0.432727	-2.544856
197	6	0	-1.694390	0.286737	-4.981234
198	1	0	-1.892370	-0.761536	-5.212619
199	1	0	-1.349522	0.811944	-5.873933
200	8	0	-2.894445	0.949472	-4.560364

201	6	0	-3.850498	0.226647	-3.951290
202	8	0	-3.933841	-0.982573	-4.013915
203	6	0	-4.780306	1.117335	-3.182944
204	1	0	-4.333458	1.287024	-2.196378
205	1	0	-4.899763	2.084450	-3.674185
206	1	0	-5.749038	0.636001	-3.053465

5a(R) -1c

RwB97XD SCF energy -4903.694786 a.u.
 RwB97XD SCF enthalpy -4901.794460 a.u.
 RwB97XD SCF free energy -4902.028199 a.u.
 Three lowest frequencies (cm⁻¹) 7.3, 19.1, 21.9

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.717470	-1.356410	2.327656
2	6	0	-0.589974	-2.445858	3.159067
3	6	0	-1.183775	-3.675670	2.894797
4	6	0	-1.920439	-3.890632	1.755160
5	6	0	-2.075606	-2.793593	0.894274
6	6	0	-1.505942	-1.549366	1.163587
7	1	0	-2.376659	-4.849372	1.539271
8	1	0	-2.671553	-2.931370	-0.000160
9	6	0	-0.094194	-0.070815	2.718959
10	6	0	0.869126	0.653543	1.966293
11	6	0	-0.477805	0.495209	3.916316
12	6	0	1.327684	1.889828	2.425647
13	6	0	-0.006237	1.723174	4.365424
14	6	0	0.890054	2.459073	3.629429
15	1	0	2.063457	2.440716	1.853780
16	1	0	1.259796	3.420244	3.966088
17	8	0	-0.880066	-4.543382	3.899879
18	8	0	0.123176	-2.529645	4.317885
19	8	0	-1.377135	0.003568	4.813713
20	8	0	-0.589772	2.021119	5.558307
21	6	0	-0.357382	-3.716934	4.945280
22	1	0	0.464729	-4.226110	5.445115
23	1	0	-1.166339	-3.459628	5.639550
24	6	0	-1.198219	0.798995	5.985415
25	1	0	-0.521926	0.280836	6.675596
26	1	0	-2.166687	1.005826	6.438770
27	15	0	1.472959	0.039638	0.347085
28	15	0	-1.749212	-0.176809	-0.012872
29	46	0	0.025392	0.519191	-1.347613
30	6	0	1.715073	-1.750097	0.458422
31	6	0	2.370498	-2.331431	1.544116
32	6	0	1.275224	-2.549475	-0.586587
33	6	0	2.543390	-3.708885	1.626232
34	1	0	2.736817	-1.689766	2.335810
35	6	0	1.414158	-3.941037	-0.569235
36	1	0	0.789536	-2.078824	-1.435247
37	6	0	1.972524	-4.501129	0.595408
38	6	0	3.093516	0.814842	0.125798
39	6	0	4.275134	0.117338	0.367383
40	6	0	3.151338	2.143521	-0.273547
41	6	0	5.510793	0.757550	0.330406
42	1	0	4.227122	-0.938221	0.593053
43	6	0	4.359806	2.837324	-0.364466
44	1	0	2.228056	2.649403	-0.528922
45	6	0	5.516263	2.145959	0.051273
46	6	0	-3.076384	-0.740100	-1.111647
47	6	0	-4.411641	-0.494896	-0.816549
48	6	0	-2.736250	-1.378841	-2.300154
49	6	0	-5.435495	-0.955073	-1.645263
50	1	0	-4.653090	0.074800	0.069885
51	6	0	-3.707677	-1.862496	-3.174399
52	1	0	-1.685621	-1.485087	-2.545564
53	6	0	-5.053681	-1.742153	-2.755846
54	6	0	-2.394693	1.239704	0.909140
55	6	0	-2.009894	2.504484	0.491096
56	6	0	-3.266067	1.105996	1.990525
57	6	0	-2.517336	3.668411	1.073232
58	1	0	-1.285522	2.591147	-0.311030
59	6	0	-3.849081	2.223501	2.580953
60	1	0	-3.489904	0.112584	2.360193
61	6	0	-3.528087	3.494729	2.036853
62	6	0	-1.886352	5.001076	0.607452
63	6	0	-2.353352	5.320870	-0.823980

64	1	0	-1.857765	6.228470	-1.186696	146	1	0	7.084570	-0.326071	-1.648506
65	1	0	-2.109259	4.501589	-1.509031	147	1	0	7.914244	1.094083	-0.994743
66	1	0	-3.433978	5.487287	-0.873666	148	6	0	7.652513	0.406882	1.705321
67	6	0	-2.168711	6.203653	1.524411	149	1	0	7.049544	0.463417	2.618177
68	1	0	-1.931883	5.978189	2.568407	150	1	0	8.456743	-0.315307	1.884560
69	1	0	-1.530512	7.036115	1.208995	151	1	0	8.118448	1.377019	1.532150
70	1	0	-3.200609	6.552488	1.475914	152	6	0	6.504735	-1.551480	0.730817
71	6	0	-0.346255	4.833454	0.587183	153	1	0	5.933269	-1.993792	-0.091041
72	1	0	0.031167	4.537718	1.571948	154	1	0	7.449464	-2.099193	0.804487
73	1	0	-0.004543	4.096707	-0.146041	155	1	0	5.957232	-1.718730	1.664768
74	1	0	0.116206	5.788306	0.317172	156	6	0	0.767934	-6.404864	1.229328
75	6	0	-4.736731	2.070110	3.833344	157	1	0	0.933356	-7.474079	1.373277
76	6	0	-4.125040	2.906208	4.974455	158	1	0	0.476179	-5.951726	2.180714
77	1	0	-4.175750	3.975441	4.760594	159	1	0	-0.040201	-6.260528	0.506104
78	1	0	-4.663880	2.720076	5.910234	160	6	0	3.424006	-4.309114	2.742418
79	1	0	-3.073281	2.644593	5.126545	161	6	0	2.714092	-5.399164	3.566396
80	6	0	-6.189453	2.513258	3.581441	162	1	0	3.284322	-5.596088	4.480521
81	1	0	-6.808426	2.018251	2.698077	163	1	0	1.711152	-5.081077	3.660561
82	1	0	-6.809349	2.238642	4.442446	164	1	0	2.631484	-6.339778	3.022495
83	1	0	-6.274162	3.591897	3.449330	165	6	0	4.680207	-4.907640	2.078524
84	6	0	-4.785518	0.606488	4.303118	166	1	0	5.336974	-5.342180	2.840702
85	1	0	-5.276286	-0.045381	3.571838	167	1	0	4.414985	-5.695278	1.368206
86	1	0	-3.788700	0.206104	4.510388	168	1	0	5.246293	-4.136156	1.544538
87	1	0	-5.365920	0.551063	5.229451	169	6	0	3.880571	-3.226260	3.733716
88	8	0	-4.229099	4.578322	2.504619	170	1	0	4.459790	-2.431956	3.252063
89	8	0	-6.030611	-2.374486	-3.489351	171	1	0	3.031262	-2.769705	4.254357
90	8	0	2.000847	-5.863918	0.754922	172	1	0	4.526779	-3.684977	4.488187
91	8	0	6.711908	2.811630	0.170112	173	6	0	0.929670	-4.699802	-1.829272
92	6	0	6.816643	3.570970	1.371809	174	6	0	-0.609546	-4.664334	-1.879307
93	1	0	7.817652	4.005738	1.381224	175	1	0	-0.965916	-5.191195	-2.771707
94	1	0	6.075054	4.374582	1.409246	176	1	0	-1.053950	-5.146031	-1.002778
95	1	0	6.686143	2.935394	2.254018	177	1	0	-0.984314	-3.636306	-1.922666
96	6	0	4.290157	4.267252	-0.952967	178	6	0	1.410155	-6.157642	-1.948183
97	6	0	5.640143	4.856171	-1.397366	179	1	0	0.928705	-6.835027	-1.243247
98	1	0	5.446181	5.784296	-1.945911	180	1	0	1.167384	-6.515232	-2.954709
99	1	0	6.302379	5.106956	-0.568843	181	1	0	2.492845	-6.237921	-1.818272
100	1	0	6.172096	4.176175	-2.068859	182	6	0	1.480630	-3.988712	-3.086424
101	6	0	3.623860	5.213030	0.062311	183	1	0	1.196392	-2.935939	-3.159589
102	1	0	3.517658	6.215117	-0.368611	184	1	0	2.572926	-4.047329	-3.113373
103	1	0	2.623030	4.859573	0.335139	185	1	0	1.096503	-4.489338	-3.981392
104	1	0	4.210303	5.301544	0.982521	186	8	0	1.600637	1.074333	-2.508851
105	6	0	-5.246923	5.018698	1.608918	187	6	0	1.378517	1.260779	-3.870846
106	1	0	-5.805841	5.798552	2.129424	188	1	0	0.584940	0.590967	-4.245996
107	1	0	-4.824984	5.435066	0.689473	189	6	0	1.010139	2.689151	-4.191132
108	1	0	-5.923210	4.198748	1.343943	190	6	0	1.368499	3.553569	-5.176883
109	6	0	-6.293934	-3.701714	-3.022996	191	8	0	0.172875	3.316680	-3.317167
110	1	0	-7.026881	-4.130894	-3.708358	192	6	0	0.716874	4.800224	-4.887254
111	1	0	-5.386980	-4.311979	-3.023901	193	1	0	2.029380	3.343902	-6.005711
112	1	0	-6.702707	-3.693806	-2.009297	194	6	0	0.012899	4.598028	-3.747860
113	6	0	-6.879966	-0.449704	-1.421928	195	1	0	0.778667	5.721541	-5.448922
114	6	0	-6.958624	0.486617	-0.200911	196	1	0	-0.617697	5.227269	-3.138800
115	1	0	-6.714007	-0.033183	0.732174	197	6	0	2.658696	0.910786	-4.648286
116	1	0	-6.299586	1.355885	-0.297435	198	1	0	3.429371	1.666919	-4.494323
117	1	0	-7.981964	0.863047	-0.108144	199	1	0	2.453946	0.803303	-5.715458
118	6	0	-7.278657	0.371053	-2.665360	200	8	0	3.137721	-0.357519	-4.194378
119	1	0	-7.278261	-0.245684	-3.568010	201	6	0	4.142555	-0.348196	-3.300426
120	1	0	-8.285269	0.784426	-2.536106	202	8	0	4.779161	0.644507	-3.011224
121	1	0	-6.586799	1.206437	-2.818634	203	6	0	4.368887	-1.710978	-2.722870
122	6	0	-7.915582	-1.566536	-1.200882	204	1	0	3.618772	-1.885532	-1.943706
123	1	0	-8.115551	-2.124823	-2.116032	205	1	0	4.252225	-2.481260	-3.487303
124	1	0	-7.596904	-2.264790	-0.419891	206	1	0	5.362718	-1.766988	-2.279603
125	1	0	-8.862558	-1.119328	-0.880049	207	1	0	-1.196955	1.437915	-2.475683
126	6	0	-3.296076	-2.334580	-4.587346	208	1	0	-1.171261	0.739781	-2.815362
127	6	0	-1.786524	-2.135695	-4.817392						
128	1	0	-1.475911	-1.096015	-4.662927						
129	1	0	-1.177832	-2.779564	-4.173038						
130	1	0	-1.551086	-2.395306	-5.854129						
131	6	0	-3.601750	-3.817360	-4.863716						
132	1	0	-3.101033	-4.122838	-5.788822						
133	1	0	-3.231821	-4.460718	-4.058222						
134	1	0	-4.668502	-3.998930	-5.000560						
135	6	0	-4.034855	-1.457883	-5.619101						
136	1	0	-3.733521	-1.741785	-6.633592						
137	1	0	-5.117850	-1.575354	-5.541697						
138	1	0	-3.791321	-0.399122	-5.477084						
139	6	0	6.808762	-0.059704	0.503552						
140	6	0	3.415657	4.219699	-2.227985						
141	1	0	3.803795	3.481142	-2.935619						
142	1	0	2.371771	3.975304	-2.020441						
143	1	0	3.425100	5.200068	-2.715320						
144	6	0	7.641811	0.056664	-0.787911						
145	1	0	8.565894	-0.524573	-0.691667						

TS2a(R) -1c					

RwB97XD SCF energy					-4903.677710 a.u.
RwB97XD SCF enthalpy					-4901.782482 a.u.
RwB97XD SCF free energy					-4902.026212 a.u.
Three lowest frequencies (cm ⁻¹)					-1181, 5.2, 10.9
Imaginary frequency (cm ⁻¹)					-1181
Cartesian coordinates:					

Center	Atomic	Atomic	Coordinates		(Angstroms)
Number	Number	Type	X	Y	Z

1	6	0	0.980307	-0.858541	2.490991
2	6	0	0.986353	-0.724569	3.862247
3	6	0	1.660963	0.298549	4.525071
4	6	0	2.356133	1.265517	3.844316
5	6	0	2.354928	1.164680	2.445786

6	6	0	1.694150	0.139603	1.771676	88	8	0	4.479946	-4.801956	-1.981097
7	1	0	2.887351	2.059486	4.355091	89	8	0	5.673265	4.443612	-1.070770
8	1	0	2.904394	1.911582	1.885924	90	8	0	-2.056376	2.761383	5.181840
9	6	0	0.363714	-2.070625	1.890547	91	8	0	-6.404265	-2.519163	-2.286941
10	6	0	-0.706526	-2.114503	0.954333	92	6	0	-6.582200	-3.905172	-2.006697
11	6	0	0.877714	-3.292008	2.274052	93	1	0	-7.632611	-4.129593	-2.202747
12	6	0	-1.157597	-3.339699	0.463230	94	1	0	-5.963326	-4.533309	-2.653322
13	6	0	0.418354	-4.506622	1.776643	95	1	0	-6.348352	-4.133916	-0.962133
14	6	0	-0.599428	-4.564941	0.857169	96	6	0	-3.787548	-2.777538	-3.791231
15	1	0	-1.978673	-3.369353	-0.242085	97	6	0	-5.016642	-2.757524	-4.718431
16	1	0	-0.967013	-5.504738	0.462802	98	1	0	-4.702070	-3.067997	-5.720660
17	8	0	1.507199	0.144694	5.866683	99	1	0	-5.810653	-3.434234	-4.406399
18	8	0	0.385034	-1.531658	4.779727	100	1	0	-5.437643	-1.750381	-4.799932
19	8	0	1.903568	-3.521263	3.140921	101	6	0	-3.297116	-4.224252	-3.590490
20	8	0	1.139662	-5.521481	2.328425	102	1	0	-3.064743	-4.683160	-4.558120
21	6	0	0.972897	-1.171829	6.029239	103	1	0	-2.390075	-4.245256	-2.977818
22	1	0	0.211859	-1.164903	6.807539	104	1	0	-4.045268	-4.848510	-3.094643
23	1	0	1.788783	-1.867543	6.259007	105	6	0	5.355317	-4.346778	-3.010989
24	6	0	1.848666	-4.920635	3.415439	106	1	0	5.911409	-5.219893	-3.356503
25	1	0	1.293334	-5.085367	4.346550	107	1	0	4.803347	-3.912951	-3.850869
26	1	0	2.859053	-5.324618	3.464594	108	1	0	6.055384	-3.594748	-2.630386
27	15	0	-1.428124	-0.557349	0.312926	109	6	0	5.812191	5.176910	0.144515
28	15	0	1.770069	0.091476	-0.047333	110	1	0	6.604887	5.908748	-0.020397
29	46	0	-0.105575	0.437658	-1.285933	111	1	0	4.888277	5.695377	0.411005
30	6	0	-1.752463	0.486735	1.753959	112	1	0	6.090539	4.517116	0.973184
31	6	0	-2.453007	-0.003371	2.852295	113	6	0	6.741987	1.754205	-1.027372
32	6	0	-1.283980	1.796304	1.763773	114	6	0	6.972438	0.235395	-0.923511
33	6	0	-2.660217	0.776413	3.991350	115	1	0	6.750609	-0.146888	0.078931
34	1	0	-2.830368	-1.020663	2.824307	116	1	0	6.377332	-0.328203	-1.649881
35	6	0	-1.452745	2.630475	2.869142	117	1	0	8.026464	0.023324	-1.128070
36	1	0	-0.754718	2.163577	0.891027	118	6	0	7.180288	2.192537	-2.438582
37	6	0	-2.061705	2.057317	4.007370	119	1	0	7.049016	3.266743	-2.584810
38	6	0	-2.989055	-1.019686	-0.0490318	120	1	0	8.239168	1.955545	-2.591468
39	6	0	-4.244161	-0.756609	0.054603	121	1	0	6.602288	1.667166	-3.206912
40	6	0	-2.899896	-1.654669	-1.725584	122	6	0	7.645402	2.421470	0.026804
41	6	0	-5.408079	-1.203543	-0.571855	123	1	0	7.740809	3.495280	-0.135953
42	1	0	-4.309221	-0.203335	0.981673	124	1	0	7.266666	2.251012	1.040184
43	6	0	-4.022576	-2.124843	-2.408016	125	1	0	8.650816	1.990307	-0.031089
44	1	0	-1.918042	-1.796326	-2.163993	126	6	0	2.728405	5.038573	-1.531578
45	6	0	-5.264477	-1.964579	-1.758142	127	6	0	2.035866	5.718943	-0.337275
46	6	0	2.964639	1.377782	-0.498902	128	1	0	1.260957	5.073514	0.086717
47	6	0	4.327072	1.101523	-0.577559	129	1	0	2.746112	5.963351	0.458760
48	6	0	2.503714	2.659068	-0.771991	130	1	0	1.556539	6.649705	-0.660763
49	6	0	5.252591	2.108258	-0.835532	131	6	0	3.688348	6.035835	-2.203640
50	1	0	4.666687	0.085632	-0.427134	132	1	0	3.091413	6.847646	-2.632875
51	6	0	3.375774	3.708608	-1.075487	133	1	0	4.398138	6.490025	-1.512060
52	1	0	1.433375	2.841171	-0.765440	134	1	0	4.249770	5.569232	-3.018140
53	6	0	4.755029	3.426696	-0.985839	135	6	0	1.651511	4.708787	-2.592804
54	6	0	2.480912	-1.508260	-0.505724	136	1	0	1.220397	5.637776	-2.978884
55	6	0	2.022294	-2.134338	-1.655098	137	1	0	2.083844	4.616291	-3.436879
56	6	0	3.479645	-2.115190	0.258655	138	1	0	0.824318	4.117009	-2.190490
57	6	0	2.590535	-3.319427	-2.130872	139	6	0	-6.794316	-0.819810	-0.007142
58	1	0	1.192782	-1.691964	-2.197534	140	6	0	-2.681811	-2.006448	-4.547806
59	6	0	4.118388	-3.269127	-0.184508	141	1	0	-2.932170	-0.946206	-4.652350
60	1	0	3.761127	-1.664136	1.202260	142	1	0	-1.701368	-2.080879	-4.070835
61	6	0	3.723658	-3.790086	-1.443645	143	1	0	-2.573863	-2.431180	-5.551070
62	6	0	1.877386	-3.991052	-3.326150	144	6	0	-7.589722	-0.056399	-1.084492
63	6	0	2.005068	-3.100159	-4.575368	145	1	0	-8.557879	0.257038	-0.677470
64	1	0	1.490632	-3.566275	-5.423094	146	1	0	-7.050991	0.841422	-1.402433
65	1	0	1.555790	-2.113970	-4.414878	147	1	0	-7.773994	-0.675352	-1.964160
66	1	0	3.052717	-2.951393	-4.855811	148	6	0	-7.601324	-2.047149	0.459854
67	6	0	2.350821	-5.413005	-3.672523	149	1	0	-7.001468	-2.691749	1.111368
68	1	0	2.350397	-6.067614	-2.796889	150	1	0	-8.470841	-1.710422	1.035178
69	1	0	1.652129	-5.834466	-4.403670	151	1	0	-7.975472	-2.642265	-0.372601
70	1	0	3.342737	-5.440793	-4.125158	152	6	0	-6.661830	0.104458	1.214007
71	6	0	0.379896	-4.123589	-2.963520	153	1	0	-6.095034	1.013250	0.992264
72	1	0	0.245579	-4.762610	-2.084012	154	1	0	-7.661683	0.409591	1.538775
73	1	0	-0.095096	-3.180661	-2.756690	155	1	0	-6.186537	-0.405775	2.056587
74	1	0	-0.156188	-4.579785	-3.801983	156	6	0	-0.909213	2.476937	5.974417
75	6	0	5.146868	-3.988571	0.710990	157	1	0	-1.025268	3.028861	6.909076
76	6	0	4.666510	-5.436099	0.938038	158	1	0	-0.832762	1.404621	6.188614
77	1	0	4.674753	-6.010720	0.009984	159	1	0	0.009151	2.803626	5.471133
78	1	0	5.318970	-5.941008	1.658945	160	6	0	-3.524295	0.161631	5.119011
79	1	0	3.645143	-5.446656	1.331637	161	6	0	-2.759222	-0.996081	5.781986
80	6	0	6.558711	-3.993635	0.096113	162	1	0	-3.396220	-1.486562	6.526551
81	1	0	6.871191	-2.981187	-0.183282	163	1	0	-2.445020	-1.749922	5.054023
82	1	0	7.276598	-4.372195	0.832386	164	1	0	-1.869036	-0.622511	6.296052
83	1	0	6.623643	-4.634317	-0.783869	165	6	0	-3.974213	1.133708	6.224012
84	6	0	5.255241	-3.313201	2.088435	166	1	0	-4.706125	0.614948	6.853256
85	1	0	5.666651	-2.299947	2.019608	167	1	0	-3.155751	1.451616	6.871036
86	1	0	4.289090	-3.261340	2.599423	168	1	0	-4.457353	2.025012	5.814860
87	1	0	5.933809	-3.898234	2.717152	169	6	0	-4.821464	-0.386946	4.485993

170	1	0	-5.385542	0.419704	4.005990	29	46	0	-0.033553	-0.041149	-1.473582
171	1	0	-4.638611	-1.166674	3.741945	30	6	0	1.770954	-1.062445	1.265587
172	1	0	-5.455364	-0.824823	5.264148	31	6	0	2.420787	-1.099819	2.498757
173	6	0	-0.950086	4.089882	2.739539	32	6	0	1.339107	-2.250669	0.689124
174	6	0	0.586938	4.101962	2.717350	33	6	0	2.611945	-2.300518	3.178464
175	1	0	0.952013	5.128593	2.601300	34	1	0	2.768958	-0.169645	2.930068
176	1	0	0.998928	3.698803	3.647113	35	6	0	1.486382	-3.491578	1.315918
177	1	0	0.981145	3.507689	1.866729	36	1	0	0.854573	-2.205151	-0.280644
178	6	0	-1.426762	5.052918	3.840135	37	6	0	2.058487	-3.473922	2.602416
179	1	0	-0.954035	4.862272	4.804238	38	6	0	3.076158	1.120637	-0.229818
180	1	0	-1.160513	6.072800	3.540312	39	6	0	4.275574	0.845327	0.422483
181	1	0	-2.511293	5.016967	3.975138	40	6	0	3.091810	1.912722	-1.371124
182	6	0	-1.467277	4.675910	1.407073	41	6	0	5.481756	1.395434	-0.005041
183	1	0	-1.143723	4.108035	0.531147	42	1	0	4.261871	0.191268	1.282404
184	1	0	-2.561498	4.719002	1.395189	43	6	0	4.270164	2.466969	-1.883618
185	1	0	-1.088907	5.696962	1.289144	44	1	0	2.151911	2.103800	-1.878922
186	8	0	-1.430234	0.831616	-2.948453	45	6	0	5.443610	2.259786	-1.128200
187	6	0	-1.981088	2.126564	-3.041691	46	6	0	-3.243089	-1.011377	-0.795493
188	6	0	-3.146782	2.321260	-2.125218	47	6	0	-4.570691	-0.678549	-0.556886
189	6	0	-4.485361	2.482345	-2.303836	48	6	0	-2.942344	-2.172973	-1.500403
190	8	0	-2.847031	2.425070	-0.801136	49	6	0	-5.613815	-1.528645	-0.928926
191	6	0	-5.043876	2.705499	-1.002850	50	1	0	-4.797443	0.266774	-0.084180
192	1	0	-5.012712	2.469046	-3.246969	51	6	0	-3.931956	-3.077013	-1.882467
193	6	0	-4.006567	2.647219	-0.131447	52	1	0	-1.907230	-2.366959	-1.750324
194	1	0	-6.080101	2.884787	-0.755413	53	6	0	-5.252816	-2.781999	-1.472413
195	1	0	-3.925055	2.736943	0.941115	54	6	0	-2.475986	1.700953	0.006095
196	6	0	-2.372431	2.341024	-4.504631	55	6	0	-1.985138	2.657429	-0.869706
197	1	0	-3.214291	1.703212	-4.780707	56	6	0	-3.399988	2.075458	0.983960
198	1	0	-1.516608	2.106984	-5.140073	57	6	0	-2.438749	3.979623	-0.861138
199	8	0	-2.810402	3.684973	-4.742486	58	1	0	-1.216906	2.362635	-1.577446
200	6	0	-1.860356	4.612440	-4.936628	59	6	0	-3.945827	3.355760	1.000958
201	8	0	-0.672970	4.355305	-4.959246	60	1	0	-3.697209	1.346540	1.727828
202	1	0	-1.222867	2.882188	-2.777181	61	6	0	-3.515517	4.263273	-0.001521
203	1	0	0.823042	1.101605	-2.637196	62	6	0	-1.675922	4.977010	-1.764055
204	1	0	-0.029999	1.024997	-2.991831	63	6	0	-1.963027	4.670641	-3.244968
205	6	0	-2.457356	5.975024	-5.113190	64	1	0	-1.374594	5.336285	-3.886410
206	1	0	-1.677770	6.690499	-5.372810	65	1	0	-1.696835	3.638626	-3.498149
207	1	0	-3.223134	5.952427	-5.892609	66	1	0	-3.020320	4.814360	-3.488389
208	1	0	-2.940891	6.279823	-4.180230	67	6	0	-1.964523	6.461772	-1.483402
						68	1	0	-1.841235	6.700762	-0.423259
						69	1	0	-1.245895	7.065107	-2.048710
						70	1	0	-2.960840	6.777205	-1.793957
						71	6	0	-0.161291	4.789417	-1.507633
						72	1	0	0.084110	4.978033	-0.457340
						73	1	0	0.194870	3.787390	-1.764401
						74	1	0	0.400617	5.500841	-2.121669
						75	6	0	-4.920327	3.776644	2.120097
						76	6	0	-4.356978	5.023318	2.831380
						77	1	0	-4.363127	5.896159	2.176311
						78	1	0	-4.958437	5.256741	3.717058
						79	1	0	-3.324815	4.853622	3.152477
						80	6	0	-6.329942	4.077914	1.577660
						81	1	0	-6.707688	3.246406	0.972028
						82	1	0	-7.021734	4.220195	2.415486
						83	1	0	-6.354806	4.987659	0.976627
						84	6	0	-5.069485	2.666534	3.174288
						85	1	0	-5.532624	1.763952	2.760259
						86	1	0	-4.109262	2.390541	3.620001
						87	1	0	-5.721389	3.026114	3.976422
						88	8	0	-4.176116	5.463299	-0.096488
						89	8	0	-6.229564	-3.735681	-1.652032
						90	8	0	2.114236	-4.629763	3.342632
						91	8	0	6.616380	2.879695	-1.486133
						92	6	0	6.703002	4.238603	-1.064503
						93	1	0	7.715585	4.574539	-1.295355
						94	1	0	5.988093	4.874179	-1.594207
						95	1	0	6.522863	4.334499	0.010728
						96	6	0	4.161098	3.224403	-3.231340
						97	6	0	5.491648	3.397197	-3.987694
						98	1	0	5.271052	3.775138	-4.991564
						99	1	0	6.171627	4.108371	-3.520933
						100	1	0	6.015797	2.443148	-4.098265
						101	6	0	3.508025	4.598999	-2.997023
						102	1	0	3.365751	5.116712	-3.952399
						103	1	0	2.527102	4.486623	-2.523436
						104	1	0	4.118147	5.240376	-2.354347
						105	6	0	-5.093213	5.515362	-1.186170
						106	1	0	-5.602604	6.478142	-1.117387
						107	1	0	-4.582541	5.444359	-2.151343
						108	1	0	-5.830148	4.707007	-1.123291
						109	6	0	-6.371163	-4.594462	-0.516375
						110	1	0	-7.126125	-5.336256	-0.782425

6c(R)*2a

RwB97XD SCF energy -4903.726097 a.u.
 RwB97XD SCF enthalpy -4901.822114 a.u.
 RwB97XD SCF free energy -4902.058888 a.u.
 Three lowest frequencies (cm⁻¹) 14.2, 17.6, 20.0

Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.859476	0.056645	2.499473
2	6	0	-0.709023	-0.560051	3.722282
3	6	0	-1.243794	-1.806676	4.024283
4	6	0	-1.958627	-2.520161	3.094387
5	6	0	-2.137409	-1.911949	1.842813
6	6	0	-1.616582	-0.655260	1.528819
7	1	0	-2.379748	-3.494047	3.313429
8	1	0	-2.714531	-2.455698	1.105328
9	6	0	-0.249660	1.402157	2.343461
10	6	0	0.837756	1.722593	1.490994
11	6	0	-0.705440	2.419882	3.153939
12	6	0	1.350373	3.019543	1.465224
13	6	0	-0.181491	3.706053	3.127528
14	6	0	0.845521	4.045000	2.280293
15	1	0	2.174567	3.258522	0.802470
16	1	0	1.259800	5.045876	2.250489
17	8	0	-0.919901	-2.136350	5.306218
18	8	0	-0.016042	-0.093919	4.801930
19	8	0	-1.710540	2.358814	4.073111
20	8	0	-0.850805	4.482293	4.029974
21	6	0	-0.447510	-0.914825	5.883885
22	1	0	0.389927	-1.119518	6.548118
23	1	0	-1.276294	-0.422857	6.407764
24	6	0	-1.577744	3.555331	4.840147
25	1	0	-1.004632	3.340529	5.750485
26	1	0	-2.564335	3.959038	5.063952
27	15	0	1.469636	0.463151	0.320850
28	15	0	-1.869144	0.003068	-0.169657

111	1	0	-5.430903	-5.097225	-0.276072
112	1	0	-6.699170	-4.040230	0.366650
113	6	0	-7.071447	-1.014247	-0.881166
114	6	0	-7.131274	0.435572	-0.365305
115	1	0	-6.802956	0.515039	0.677102
116	1	0	-6.528633	1.118599	-0.973060
117	1	0	-8.167450	0.784804	-0.410525
118	6	0	-7.613862	-1.017169	-2.324730
119	1	0	-7.627094	-2.026213	-2.744322
120	1	0	-8.638130	-0.627554	-2.341961
121	1	0	-6.999521	-0.382970	-2.973151
122	6	0	-8.005474	-1.848888	0.012968
123	1	0	-8.229671	-2.821709	-0.425842
124	1	0	-7.578959	-1.997369	1.010661
125	1	0	-8.957475	-1.320711	0.134265
126	6	0	-3.577537	-4.243583	-2.833268
127	6	0	-2.100194	-4.178271	-3.263869
128	1	0	-1.844343	-3.222467	-3.732680
129	1	0	-1.415628	-4.350071	-2.425632
130	1	0	-1.912850	-4.964625	-4.002040
131	6	0	-3.803900	-5.635961	-2.218330
132	1	0	-3.357981	-6.395336	-2.869897
133	1	0	-3.330898	-5.722685	-1.234051
134	1	0	-4.863529	-5.876638	-2.123950
135	6	0	-4.433310	-4.105664	-4.108307
136	1	0	-4.174007	-4.899328	-4.817815
137	1	0	-5.499764	-4.184567	-3.885612
138	1	0	-4.253004	-3.142514	-4.598440
139	6	0	6.801989	0.972839	0.679051
140	6	0	3.246562	2.426503	-4.191083
141	1	0	3.620578	1.406733	-4.338594
142	1	0	2.207426	2.385670	-3.849774
143	1	0	3.228685	2.918454	-5.168311
144	6	0	7.630346	0.163694	-0.337767
145	1	0	8.564073	-0.176999	0.124172
146	1	0	7.079475	-0.718531	-0.680376
147	1	0	7.885648	0.767243	-1.212916
148	6	0	7.637621	2.161536	1.192598
149	1	0	7.030504	2.843939	1.797185
150	1	0	8.442909	1.783934	1.832097
151	1	0	8.101951	2.724414	0.383759
152	6	0	6.538285	0.074126	1.899824
153	1	0	5.996023	-0.839828	1.644807
154	1	0	7.496938	-0.229804	2.331293
155	1	0	5.980727	0.605875	2.678830
156	6	0	0.892967	-4.924386	4.018169
157	1	0	1.065219	-5.838201	4.589955
158	1	0	0.609191	-4.115223	4.697452
159	1	0	0.074150	-5.094794	3.312920
160	6	0	3.519316	-2.341727	4.427185
161	6	0	2.879171	-3.019107	5.653248
162	1	0	3.501598	-2.832861	6.535102
163	1	0	1.885328	-2.611348	5.856898
164	1	0	2.792767	-4.098287	5.532602
165	6	0	4.800740	-3.104162	4.033041
166	1	0	5.496023	-3.139366	4.879758
167	1	0	4.577080	-4.132124	3.734393
168	1	0	5.309966	-2.606514	3.199383
169	6	0	3.926938	-0.925713	4.865888
170	1	0	4.479372	-0.390382	4.087828
171	1	0	3.057016	-0.323721	5.152165
172	1	0	4.585335	-0.997828	5.736812
173	6	0	1.012610	-4.738969	0.525612
174	6	0	-0.527349	-4.781830	0.501082
175	1	0	-0.864554	-5.651760	-0.074453
176	1	0	-0.953107	-4.859451	1.505727
177	1	0	-0.939781	-3.882580	0.030485
178	6	0	1.553084	-6.084449	1.043853
179	1	0	1.105720	-6.396126	1.987128
180	1	0	1.314476	-6.856489	0.304435
181	1	0	2.639625	-6.063679	1.167263
182	6	0	1.496799	-4.630256	-0.937596
183	1	0	1.059454	-3.779540	-1.464019
184	1	0	2.585869	-4.544638	-0.998357
185	1	0	1.197856	-5.531485	-1.482820
186	8	0	1.617441	-0.324513	-2.854299
187	6	0	1.883715	-1.593729	-3.483634
188	1	0	1.262277	-2.314645	-2.948353
189	6	0	1.491275	-1.569174	-4.915730
190	6	0	2.163108	-1.327440	-6.072938
191	8	0	0.164219	-1.744634	-5.175510
192	6	0	1.185949	-1.362054	-7.119210

193	1	0	3.224522	-1.148307	-6.172764
194	6	0	-0.002453	-1.615516	-6.515763
195	1	0	1.352909	-1.219285	-8.176903
196	1	0	-1.010961	-1.738403	-6.880920
197	6	0	3.346242	-1.942643	-3.283765
198	1	0	3.996113	-1.147901	-3.661083
199	1	0	3.586575	-2.880491	-3.791845
200	8	0	3.535127	-2.098541	-1.872889
201	6	0	4.769766	-2.429487	-1.468303
202	8	0	5.709680	-2.499238	-2.235309
203	6	0	4.820206	-2.743876	-0.004315
204	1	0	4.217613	-2.042179	0.574079
205	1	0	4.404265	-3.745074	0.149704
206	1	0	5.855898	-2.738370	0.334281
207	1	0	-1.075902	-0.338392	-2.608554
208	1	0	1.811306	0.393225	-3.471421

2.8. Catalytic cycle 2b–1a (S)

1a^{2b}

RwB97XD SCF energy -3304.679746
 RwB97XD SCF enthalpy -3303.806043
 RwB97XD SCF free energy -3303.950296
 Three lowest frequencies (cm⁻¹) 12.9, 25.0, 31.5

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.941906	-0.127433	0.046451
2	6	0	-4.089045	-0.842060	-0.221302
3	6	0	-4.781872	-0.753832	-1.423275
4	6	0	-4.377950	0.096585	-2.422785
5	6	0	-3.227687	0.859391	-2.170157
6	6	0	-2.512737	0.765129	-0.977293
7	1	0	-4.916994	0.180221	-3.358935
8	1	0	-2.901503	1.544345	-2.943367
9	6	0	-2.282967	-0.331576	1.366753
10	6	0	-1.066501	-1.037981	1.572950
11	6	0	-2.903660	0.150035	2.498017
12	6	0	-0.553493	-1.192915	2.858385
13	6	0	-2.365140	0.016638	3.772462
14	6	0	-1.189467	-0.657934	3.989979
15	1	0	0.369194	-1.739978	3.010360
16	1	0	-0.769369	-0.773249	4.982223
17	8	0	-5.845941	-1.596196	-1.401009
18	8	0	-4.705682	-1.734222	0.598259
19	8	0	-4.066444	0.851558	2.560708
20	8	0	-3.164656	0.648552	4.672759
21	6	0	-5.801058	-2.276903	-0.142327
22	1	0	-5.633830	-3.344043	-0.313668
23	1	0	-6.731472	-2.097221	0.401200
24	6	0	-4.315363	1.091132	3.948197
25	1	0	-5.190376	0.513745	4.263934
26	1	0	-4.459996	2.160554	4.113926
27	15	0	-0.129275	-1.609641	0.104362
28	15	0	-0.932604	1.680593	-0.798665
29	46	0	0.763029	0.224480	-1.180917
30	6	0	-1.307848	-2.664904	-0.797717
31	6	0	-2.099520	-3.610331	-0.136773
32	6	0	-1.471515	-2.461809	-2.171476
33	6	0	-3.040552	-4.347201	-0.848095
34	1	0	-1.989759	-3.761461	0.933355
35	6	0	-2.425981	-3.189206	-2.877485
36	1	0	-0.868843	-1.713111	-2.680359
37	6	0	-3.211724	-4.129550	-2.215066
38	6	0	1.179980	-2.694817	0.760695
39	6	0	1.172584	-4.080958	0.594827
40	6	0	2.277349	-2.081359	1.380849
41	6	0	2.243892	-4.844113	1.055467
42	6	0	3.333284	-2.848171	1.858451
43	1	0	2.311007	-0.999199	1.486837
44	6	0	3.319395	-4.231851	1.691063
45	6	0	-1.030343	3.048488	-2.013793
46	6	0	-1.382410	4.350788	-1.653779
47	6	0	-0.735317	2.764176	-3.354367
48	6	0	-1.442994	5.351444	-2.622739
49	1	0	-1.596238	4.602349	-0.621376
50	6	0	-0.815247	3.760033	-4.319918
51	1	0	-0.441792	1.758259	-3.643107
52	6	0	-1.166906	5.058903	-3.954113
53	6	0	-1.002221	2.425281	0.858399
54	6	0	0.082224	2.283900	1.726902
55	6	0	-2.161150	3.079751	1.292716
56	6	0	0.008381	2.787342	3.022222
57	1	0	0.972458	1.758960	1.395818
58	6	0	-2.224149	3.596520	2.581948
59	1	0	-3.022907	3.162763	0.636953
60	6	0	-1.143837	3.443459	3.449543
61	8	0	5.662737	-2.646129	-0.410591
62	6	0	5.382618	-1.509710	-0.750428
63	1	0	1.267309	1.524218	-1.862141
64	6	0	4.144563	-1.215720	-1.478694
65	6	0	3.711112	-0.142318	-2.195170
66	8	0	3.239274	-2.238605	-1.570188
67	6	0	2.446045	-0.518073	-2.764270
68	1	0	4.223957	0.798859	-2.323683
69	6	0	2.222767	-1.808279	-2.326075

70	1	0	1.920802	-0.018649	-3.566429
71	1	0	1.455182	-2.532773	-2.555318
72	6	0	6.364505	-0.370987	-0.514467
73	1	0	6.928759	-0.198297	-1.434219
74	1	0	7.046327	-0.672437	0.282942
75	8	0	5.745611	0.878809	-0.212213
76	6	0	5.067159	0.921957	0.949060
77	8	0	4.969322	-0.054604	1.663957
78	6	0	4.456799	2.287470	1.220192
79	6	0	3.471191	2.604856	0.083540
80	1	0	2.728111	1.807396	-0.027512
81	1	0	2.938438	3.534629	0.308185
82	1	0	3.983719	2.728449	-0.874283
83	6	0	3.719827	2.239506	2.560672
84	1	0	4.407371	2.025494	3.384190
85	1	0	3.248778	3.208579	2.750166
86	1	0	2.941122	1.471162	2.561475
87	6	0	5.575877	3.340819	1.266239
88	1	0	5.138645	4.320067	1.484762
89	1	0	6.304468	3.109388	2.049857
90	1	0	6.103060	3.407862	0.310861
91	1	0	-0.593349	3.524918	-5.356139
92	1	0	-1.216744	5.840409	-4.705939
93	1	0	-1.705171	6.363246	-2.329633
94	1	0	0.846812	2.658183	3.699573
95	1	0	-1.203575	3.832140	4.461401
96	1	0	-3.124253	4.103476	2.914667
97	1	0	-3.650485	-5.082654	-0.332780
98	1	0	-3.960482	-4.693429	-2.762991
99	1	0	-2.562342	-3.014736	-3.940114
100	1	0	0.341105	-4.572651	0.100933
101	1	0	2.233524	-5.920595	0.914549
102	1	0	4.152751	-4.829465	2.047485
103	1	0	4.177683	-2.361044	2.333129

3b(S)₉₈

RwB97XD SCF energy -3304.683413 a.u.
 RwB97XD SCF enthalpy -3303.809924 a.u.
 RwB97XD SCF free energy -3303.954702 a.u.
 Three lowest frequencies (cm⁻¹) 17.5, 19.0, 27.5

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.502710	-0.810336	0.834009
2	6	0	-3.643587	-0.613644	1.579986
3	6	0	-3.651320	-0.594123	2.970448
4	6	0	-2.508213	-0.812766	3.699609
5	6	0	-1.334884	-1.051761	2.968638
6	6	0	-1.312198	-1.055665	1.574925
7	1	0	-2.508798	-0.802322	4.783190
8	1	0	-0.422063	-1.236399	3.522802
9	6	0	-2.613106	-0.755842	-0.650838
10	6	0	-2.148688	0.316417	-1.462171
11	6	0	-3.250430	-1.783001	-1.310418
12	6	0	-2.315994	0.275864	-2.843948
13	6	0	-3.393734	-1.822305	-2.692388
14	6	0	-2.937937	-0.803675	-3.492403
15	1	0	-1.958196	1.096879	-3.454973
16	1	0	-3.055175	-0.826681	-4.569480
17	8	0	-4.905360	-0.328735	3.416319
18	8	0	-4.895494	-0.371869	1.110577
19	8	0	-3.788958	-2.902749	-0.759499
20	8	0	-4.017585	-2.975774	-3.053431
21	6	0	-5.738318	-0.228941	2.256541
22	1	0	-6.216879	0.752868	2.236661
23	1	0	-6.476554	-1.035891	2.266824
24	6	0	-4.355214	-3.651022	-1.838696
25	1	0	-5.443337	-3.679187	-1.725962
26	1	0	-3.927015	-4.655623	-1.850161
27	15	0	-1.167001	1.648220	-0.672474
28	15	0	0.288969	-1.235407	0.709995
29	46	0	0.970749	0.753480	-0.055132
30	6	0	-2.227468	2.299490	0.655561
31	6	0	-3.596654	2.520897	0.471930
32	6	0	-1.652069	2.511807	1.912365
33	6	0	-4.379961	2.951703	1.537798
34	1	0	-4.054577	2.337561	-0.495935

35	6	0	-2.441698	2.931312	2.979595	1	6	0	-2.445148	0.709042	-1.055839
36	1	0	-0.590377	2.327467	2.059262	2	6	0	-3.573729	0.394979	-1.780415
37	6	0	-3.805249	3.147176	2.793148	3	6	0	-3.537636	0.030884	-3.122392
38	6	0	-1.002137	2.952829	-1.937788	4	6	0	-2.361427	0.000763	-3.830580
39	6	0	-1.813065	4.089766	-1.977300	5	6	0	-1.197613	0.345936	-3.127723
40	6	0	0.011074	2.795795	-2.894205	6	6	0	-1.218882	0.690666	-1.777564
41	6	0	-1.618167	5.052011	-2.965499	7	1	0	-2.330120	-0.274428	-4.878082
42	6	0	0.193784	3.752591	-3.886909	8	1	0	-0.257900	0.334639	-3.667693
43	1	0	0.657338	1.921312	-2.862954	9	6	0	-2.590118	1.020255	0.393005
44	6	0	-0.620326	4.883523	-3.921898	10	6	0	-2.194523	0.149541	1.445476
45	6	0	1.433476	-1.956795	1.941304	11	6	0	-3.174996	2.205454	0.778437
46	6	0	1.664712	-3.329627	2.040786	12	6	0	-2.386101	0.512574	2.775826
47	6	0	2.124269	-1.078424	2.785664	13	6	0	-3.340153	2.568810	2.110909
48	6	0	2.582695	-3.814915	2.970714	14	6	0	-2.962197	1.739843	3.138495
49	1	0	1.156488	-0.280044	1.385431	15	1	0	-2.083227	-0.161697	3.568475
50	6	0	3.025959	-1.567201	3.722951	16	1	0	-3.100946	2.015263	4.177200
51	1	0	1.963639	-0.007429	2.697303	17	8	0	-4.790752	-0.267100	-3.547923
52	6	0	3.260777	-2.938715	3.812589	18	8	0	-4.852772	0.344859	-1.325017
53	6	0	0.011147	-2.465394	-0.597825	19	8	0	-3.639063	3.194478	-0.029350
54	6	0	0.468634	-2.200417	-1.892406	20	8	0	-3.906585	3.800949	2.180413
55	6	0	-0.711388	-3.635397	-0.338966	21	6	0	-5.662776	-0.061962	-2.314722
56	6	0	0.199995	-3.098345	-2.921500	22	1	0	-6.169227	-0.999705	-2.190228
57	1	0	1.017824	-1.284872	-2.095593	23	1	0	-6.375942	0.731236	-2.670853
58	6	0	-0.962066	-4.537036	-1.367869	24	6	0	-4.106430	4.236458	0.832324
59	1	0	-1.101587	-3.831114	0.655527	25	1	0	-5.173011	4.399353	0.657147
60	6	0	-0.514797	-4.265335	-2.659697	26	1	0	-3.527525	5.146362	0.654621
61	8	0	2.066303	2.746253	-0.233028	27	15	0	-1.281857	-1.374655	1.024317
62	6	0	3.225214	2.354950	0.004492	28	15	0	0.362923	0.945058	-0.897688
63	1	0	2.293453	-0.022477	0.209156	29	46	0	0.899779	-0.936734	0.260160
64	6	0	3.722802	2.224707	1.350375	30	6	0	-2.344269	-2.288279	-0.130330
65	6	0	4.939484	1.847139	1.860475	31	6	0	-3.726257	-2.380957	0.067772
66	8	0	2.847374	2.463076	2.370506	32	6	0	-1.762778	-2.847893	-1.272026
67	6	0	4.800377	1.856563	3.270797	33	6	0	-4.517998	-3.032722	-0.871624
68	1	0	5.820867	1.593806	1.288272	34	1	0	-4.184864	-1.928859	0.942444
69	6	0	3.512027	2.235312	3.516424	35	6	0	-2.562099	-3.485851	-2.216422
70	1	0	5.550962	1.616176	4.008727	36	1	0	-0.689735	-2.764936	-1.428832
71	1	0	2.952826	2.385968	4.428088	37	6	0	-3.938141	-3.575286	-2.017808
72	6	0	4.180645	2.078987	-1.148288	38	6	0	-1.155643	-2.326013	2.573000
73	1	0	5.038411	2.751419	-1.073107	39	6	0	-2.021209	-3.374128	2.894800
74	1	0	3.651889	2.250473	-2.084994	40	6	0	-0.132557	-1.974110	3.464790
75	8	0	4.698042	0.751464	-1.085117	41	6	0	-1.868688	-4.055535	4.100425
76	6	0	4.115608	-0.182762	-1.863402	42	6	0	0.008142	-2.649903	4.671281
77	8	0	3.199774	0.072663	-2.619073	43	1	0	0.553274	-1.167637	3.215877
78	6	0	4.731826	-1.561189	-1.657193	44	6	0	-0.860185	-3.692938	4.989286
79	6	0	4.136073	-2.146159	-0.361531	45	6	0	1.595639	1.296941	-2.200319
80	1	0	3.057323	-2.293339	-0.461014	46	6	0	1.909020	2.597998	-2.600542
81	1	0	4.593889	-3.121030	-0.165310	47	6	0	2.255398	0.216538	-2.797707
82	1	0	4.323755	-1.499237	0.501534	48	6	0	2.879812	2.812075	-3.575744
83	6	0	4.356110	-2.452386	-2.844631	49	1	0	1.424785	3.452395	-2.141587
84	1	0	4.740301	-2.044814	-3.785092	50	6	0	3.214155	0.433265	-3.781508
85	1	0	4.790415	-3.446777	-2.702629	51	1	0	2.020482	-0.799143	-2.493167
86	1	0	3.272181	-2.565017	-2.934704	52	6	0	3.532785	1.733768	-4.166856
87	6	0	6.258575	-1.455314	-1.532282	53	6	0	0.150368	2.449251	0.096791
88	1	0	6.682001	-2.460713	-1.444152	54	6	0	0.570035	2.443274	1.429836
89	1	0	6.699191	-0.978281	-2.413621	55	6	0	-0.467499	3.586466	-0.435991
90	1	0	6.554462	-0.886419	-0.647396	56	6	0	0.367563	3.566039	2.227693
91	1	0	3.555922	-0.876031	4.370913	57	1	0	1.043976	1.558106	1.843728
92	1	0	3.976937	-3.321278	4.533273	58	6	0	-0.650584	4.711457	0.360640
93	1	0	2.767937	-4.882727	3.031363	59	1	0	-0.827715	3.587633	-1.460619
94	1	0	0.543524	-2.881771	-3.928128	60	6	0	-0.242345	4.698891	1.693695
95	1	0	-0.728086	-4.963076	-3.463566	61	8	0	1.846981	-2.743110	0.856017
96	1	0	-1.519520	-5.445563	-1.162866	62	6	0	2.914307	-2.161317	0.428734
97	1	0	-5.441754	3.123208	1.390928	63	1	0	2.447832	-0.632774	-0.082501
98	1	0	-4.422959	3.466456	3.627026	64	6	0	3.476969	-2.549572	-0.875276
99	1	0	-1.993128	3.079592	3.956910	65	6	0	4.702040	-2.370981	-1.445004
100	1	0	-2.593865	4.234851	-1.237972	66	8	0	2.633311	-3.158639	-1.750352
101	1	0	-2.249902	5.934717	-2.986382	67	6	0	4.609593	-2.919954	-2.759366
102	1	0	-0.473345	5.635214	-4.691446	68	1	0	5.561832	-1.906564	-0.983673
103	1	0	0.976755	3.619177	-4.626974	69	6	0	3.335751	-3.376505	-2.888310
						70	1	0	5.387878	-2.967898	-3.506872
						71	1	0	2.801858	-3.870562	-3.685943
						72	6	0	3.895163	-1.676153	1.495668
						73	1	0	4.678230	-2.432036	1.599088
						74	1	0	3.351125	-1.576644	2.433773
						75	8	0	4.540564	-0.458778	1.148419
						76	6	0	4.111234	0.663156	1.762662
						77	8	0	3.230735	0.655252	2.598991
						78	6	0	4.826425	1.904706	1.251818
						79	6	0	4.190589	2.248306	-0.108357
						80	1	0	3.122212	2.450281	0.007465
						81	1	0	4.663869	3.148368	-0.513378
						82	1	0	4.318096	1.438461	-0.833661

TS1b(S)_{eq}

RwB97XD SCF energy -3304.675698 a.u.
 RwB97XD SCF enthalpy -3303.804219 a.u.
 RwB97XD SCF free energy -3303.949629 a.u.
 Three lowest frequencies (cm⁻¹) -600.5, 13.4, 15.7
 Imaginary frequency (cm⁻¹) -600.5
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

83	6	0	4.590355	3.052904	2.236279
84	1	0	5.012335	2.827693	3.220719
85	1	0	5.072735	3.959282	1.858198
86	1	0	3.523506	3.260199	2.358379
87	6	0	6.329329	1.641927	1.084116
88	1	0	6.819486	2.564481	0.758042
89	1	0	6.787763	1.328687	2.027657
90	1	0	6.525280	0.872442	0.333383
91	1	0	3.714737	-0.415440	-4.236697
92	1	0	4.291220	1.905710	-4.924367
93	1	0	3.127403	3.827800	-3.867697
94	1	0	0.682134	3.551214	3.266437
95	1	0	-0.403723	5.573342	2.316435
96	1	0	-1.125158	5.593797	-0.056812
97	1	0	-5.589320	-3.107645	-0.714200
98	1	0	-4.561546	-4.067899	-2.757688
99	1	0	-2.110909	-3.906482	-3.109536
100	1	0	-2.810862	-3.666963	2.210688
101	1	0	-2.543424	-4.870179	4.344189
102	1	0	-0.747162	-4.224738	5.929007
103	1	0	0.798913	-2.366750	5.358772

4b(S)_{MS}

RwB97XD SCF energy -3304.684477 a.u.

RwB97XD SCF enthalpy -3303.808844 a.u.

RwB97XD SCF free energy -3303.952127 a.u.

Three lowest frequencies (cm⁻¹) 17.9, 22.9, 28.5

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.393057	1.317000	-0.424487
2	6	0	2.519935	2.592357	-0.929098
3	6	0	2.576952	2.873371	-2.289289
4	6	0	2.543169	1.875046	-3.231237
5	6	0	2.430830	0.562261	-2.748382
6	6	0	2.353467	0.268727	-1.387872
7	1	0	2.598162	2.084991	-4.292779
8	1	0	2.405365	-0.239387	-3.476865
9	6	0	2.335651	1.154016	1.055367
10	6	0	1.169987	0.824182	1.800265
11	6	0	3.478075	1.387985	1.788713
12	6	0	1.228018	0.729810	3.188251
13	6	0	3.532229	1.254629	3.170808
14	6	0	2.417768	0.933943	3.905627
15	1	0	0.334223	0.490622	3.751622
16	1	0	2.451053	0.842147	4.984895
17	8	0	2.672552	4.214670	-2.475441
18	8	0	2.588473	3.749420	-0.218505
19	8	0	4.702965	1.733921	1.311380
20	8	0	4.799761	1.488008	3.603269
21	6	0	2.624531	4.811189	-1.174774
22	1	0	1.716271	5.414100	-1.084449
23	1	0	3.524682	5.409479	-1.017098
24	6	0	5.565797	1.838342	2.446923
25	1	0	5.917240	2.869870	2.540810
26	1	0	6.398233	1.139163	2.337283
27	15	0	-0.343298	0.367172	0.869409
28	15	0	2.073112	-1.463526	-0.855896
29	46	0	-0.041853	-1.793781	-0.161338
30	6	0	-0.667032	1.809575	-0.194268
31	6	0	-0.674373	3.107924	0.327911
32	6	0	-0.817440	1.616255	-1.570156
33	6	0	-0.841187	4.198192	-0.520056
34	1	0	-0.535323	3.267756	1.393558
35	6	0	-0.962897	2.709724	-2.418490
36	1	0	-0.778027	0.612948	-1.983728
37	6	0	-0.974576	4.000112	-1.893987
38	6	0	-1.684754	0.282029	2.105661
39	6	0	-2.738911	1.195940	2.159423
40	6	0	-1.676176	-0.804753	2.992688
41	6	0	-3.756489	1.038523	3.099905
42	1	0	-2.775521	2.035974	1.474957
43	6	0	-2.682085	-0.947816	3.940814
44	1	0	-0.880266	-1.543629	2.940727
45	6	0	-3.727458	-0.026130	3.994111
46	6	0	2.542958	-2.478098	-2.302991
47	6	0	3.824081	-3.009796	-2.464011
48	6	0	1.573836	-2.705528	-3.288604
49	6	0	4.130116	-3.759573	-3.598258

50	1	0	4.587235	-2.859405	-1.708575
51	6	0	1.888535	-3.438881	-4.426707
52	1	0	0.570376	-2.306938	-3.163701
53	6	0	3.168076	-3.970322	-4.581269
54	6	0	3.303259	-1.754416	0.453645
55	6	0	2.910826	-2.373457	1.644280
56	6	0	4.618591	-1.298671	0.307642
57	6	0	3.825088	-2.526706	2.682877
58	1	0	1.885677	-2.714717	1.764541
59	6	0	5.532765	-1.470930	1.340971
60	1	0	4.924419	-0.787028	-0.600226
61	6	0	5.134174	-2.074868	2.532302
62	8	0	-2.042352	-2.446771	0.401301
63	6	0	-3.120350	-1.998289	-0.020138
64	1	0	0.263531	-3.221542	-0.724236
65	6	0	-4.327823	-2.249962	0.712371
66	6	0	-4.555347	-2.861154	1.921364
67	8	0	-5.512086	-1.821919	0.181052
68	6	0	-5.951269	-2.795427	2.142158
69	1	0	-3.803033	-3.296044	2.562723
70	6	0	-6.473538	-2.155993	1.053187
71	1	0	-6.502421	-3.171015	2.991277
72	1	0	-7.482393	-1.886826	0.776828
73	6	0	-3.196527	-1.207569	-1.307188
74	1	0	-3.785746	-1.767812	-2.039979
75	1	0	-2.188325	-1.054169	-1.697983
76	8	0	-3.797611	0.052625	-1.037323
77	6	0	-4.819508	0.445762	-1.828605
78	8	0	-5.180799	-0.195095	-2.790798
79	6	0	-5.436010	1.749840	-1.342081
80	6	0	-6.066609	1.492504	0.038293
81	1	0	-5.321284	1.149946	0.760496
82	1	0	-6.507581	2.422025	0.412259
83	1	0	-6.859096	0.740102	-0.024077
84	6	0	-4.342532	2.824402	-1.232889
85	1	0	-3.875290	3.007941	-2.204963
86	1	0	-4.790884	3.761348	-0.887741
87	1	0	-3.561189	2.536835	-0.525744
88	6	0	-6.509820	2.194406	-2.337263
89	1	0	-6.967114	3.124401	-1.986063
90	1	0	-6.082807	2.375914	-3.328239
91	1	0	-7.298160	1.442823	-2.437347
92	1	0	1.131834	-3.603265	-5.187388
93	1	0	3.411602	-4.552156	-5.464960
94	1	0	5.124675	-4.180059	-3.709351
95	1	0	6.552069	-1.117690	1.221124
96	1	0	5.845613	-2.190011	3.344232
97	1	0	3.511619	-2.993561	3.611225
98	1	0	-1.061533	2.553271	-3.487942
99	1	0	-1.085329	4.853162	-2.556322
100	1	0	-0.850892	5.203061	-0.109768
101	1	0	-4.568975	1.757905	3.130666
102	1	0	-4.519033	-0.143200	4.727797
103	1	0	-2.657229	-1.785205	4.631113

5b(S)_{MS}

RwB97XD SCF energy -3305.860132 a.u.

RwB97XD SCF enthalpy -3304.965278 a.u.

RwB97XD SCF free energy -3305.112224 a.u.

Three lowest frequencies (cm⁻¹) 7.8, .9, 7 26.2

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.045898	-0.261908	0.945545
2	6	0	3.667164	-0.929924	1.975843
3	6	0	3.700609	-0.446730	3.280439
4	6	0	3.136271	0.758612	3.619919
5	6	0	2.500430	1.465859	2.588517
6	6	0	2.442129	0.978904	1.285631
7	1	0	3.175693	1.144881	4.631346
8	1	0	2.045627	2.418436	2.832307
9	6	0	3.088391	-0.838068	-0.425687
10	6	0	1.979296	-1.359202	-1.150533
11	6	0	4.304169	-0.883043	-1.070935
12	6	0	2.157724	-1.878508	-2.431570
13	6	0	4.463650	-1.373546	-2.362217
14	6	0	3.406905	-1.892947	-3.069056
15	1	0	1.316167	-2.295978	-2.969249
16	1	0	3.527429	-2.295236	-4.067791

17	8	0	4.362667	-1.325687	4.073511
18	8	0	4.315420	-2.121533	1.910411
19	8	0	5.498645	-0.448245	-0.593770
20	8	0	5.760047	-1.251266	-2.739733
21	6	0	4.697499	-2.447731	3.249902
22	1	0	4.138097	-3.326067	3.585516
23	1	0	5.775445	-2.617707	3.287912
24	6	0	6.452804	-0.650538	-1.639666
25	1	0	7.234822	-1.328932	-1.289970
26	1	0	6.863527	0.313163	-1.952046
27	15	0	0.301085	-1.227321	-0.439683
28	15	0	1.497877	1.862176	0.004917
29	46	0	-0.522798	0.900691	-0.633734
30	6	0	0.468238	-1.826391	1.265876
31	6	0	1.102572	-3.052253	1.499053
32	6	0	0.028946	-1.051162	2.340598
33	6	0	1.279327	-3.503322	2.802299
34	1	0	1.467986	-3.648156	0.667518
35	6	0	0.221382	-1.500501	3.643215
36	1	0	-0.444421	-0.091496	2.159583
37	6	0	0.844384	-2.725368	3.874234
38	6	0	-0.758253	-2.389891	-1.350649
39	6	0	-1.281567	-3.535916	-0.750351
40	6	0	-1.100210	-2.084451	-2.675984
41	6	0	-2.121360	-4.378877	-1.476150
42	1	0	-1.058877	-3.773058	0.283404
43	6	0	-1.921546	-2.937778	-3.399631
44	1	0	-0.731444	-1.173729	-3.138303
45	6	0	-2.435655	-4.086866	-2.798622
46	6	0	1.108005	3.499624	0.698136
47	6	0	1.780518	4.656799	0.300763
48	6	0	0.071587	3.585379	1.638401
49	6	0	1.424709	5.887896	0.848613
50	1	0	2.575539	4.608729	-0.435987
51	6	0	-0.207035	4.814347	2.189452
52	1	0	-0.467226	2.690721	1.941770
53	6	0	0.405869	5.967734	1.793149
54	6	0	2.660562	2.083280	-1.371398
55	6	0	2.241502	1.814543	-2.677276
56	6	0	3.990338	2.441001	-1.121260
57	6	0	3.154033	1.885185	-3.726113
58	1	0	1.210088	1.529337	-2.868663
59	6	0	4.893955	2.521877	-2.174641
60	1	0	4.323673	2.635934	-0.106602
61	6	0	4.479549	2.231651	-3.474045
62	8	0	-2.315389	0.192592	-1.264010
63	6	0	-3.390860	0.333999	-0.379259
64	6	0	-3.668071	-0.942438	0.362162
65	6	0	-4.538592	-1.974144	0.191633
66	8	0	-2.849316	-1.206137	1.416663
67	6	0	-4.232309	-2.937509	1.209362
68	1	0	-5.309982	-2.041011	-0.562893
69	6	0	-3.196033	-2.421526	1.916060
70	1	0	-4.718731	-3.887122	1.381597
71	1	0	-2.619883	-2.768110	2.761056
72	6	0	-4.606337	0.745137	-1.205719
73	1	0	-4.861986	-0.032074	-1.930863
74	1	0	-4.393921	1.674354	-1.741396
75	8	0	-5.698173	0.954799	-0.301487
76	6	0	-6.937359	0.902393	-0.798646
77	8	0	-7.163776	0.772744	-1.986147
78	6	0	-7.992814	0.980991	0.298784
79	6	0	-7.687924	2.157335	1.239455
80	1	0	-7.667437	3.106469	0.693541
81	1	0	-8.468071	2.222279	2.004539
82	1	0	-6.726841	2.029479	1.744089
83	6	0	-9.371107	1.157516	-0.341352
84	1	0	-9.603279	0.334955	-1.023436
85	1	0	-10.137199	1.180118	0.439775
86	1	0	-9.430877	2.093789	-0.905060
87	6	0	-7.938852	-0.345060	1.082084
88	1	0	-8.704009	-0.335046	1.864827
89	1	0	-8.135933	-1.199672	0.426192
90	1	0	-6.963429	-0.490227	1.555598
91	1	0	-1.462170	2.596491	-0.628639
92	1	0	-1.079805	2.632135	-1.298809
93	1	0	-3.209529	1.124997	0.369283
94	1	0	-1.067976	4.872224	2.923653
95	1	0	0.134597	6.928505	2.219384
96	1	0	1.948504	6.784997	0.534090
97	1	0	5.926006	2.795147	-1.979296
98	1	0	5.193613	2.274779	-4.290662

99	1	0	2.831943	1.659704	-4.737740
100	1	0	-2.172710	-2.699174	-4.428197
101	1	0	-3.087477	-4.747390	-3.362080
102	1	0	-2.531223	-5.263262	-0.998772
103	1	0	-0.107658	-0.888974	4.477317
104	1	0	0.996436	-3.072354	4.891622
105	1	0	1.767194	-4.456376	2.979557

TS2b(S)_{reg}

RwB97XD SCF energy	-3305.848518 a.u.
RwB97XD SCF enthalpy	-3304.957271 a.u.
RwB97XD SCF free energy	-3305.101713 a.u.
Three lowest frequencies (cm ⁻¹)	-1096, -104.2, 17.1
Imaginary frequency (cm ⁻¹)	-1096

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.922746	-0.366406	1.062592
2	6	0	3.398780	-0.985277	2.195791
3	6	0	3.342086	-0.401049	3.457963
4	6	0	2.832417	0.859868	3.650814
5	6	0	2.352742	1.522623	2.511642
6	6	0	2.386558	0.937858	1.248169
7	1	0	2.793846	1.318214	4.631607
8	1	0	1.940941	2.517119	2.637334
9	6	0	3.006782	-1.071607	-0.245059
10	6	0	1.895327	-1.562145	-0.985345
11	6	0	4.244744	-1.277514	-0.811918
12	6	0	2.084281	-2.193205	-2.212481
13	6	0	4.419953	-1.884612	-2.051188
14	6	0	3.357024	-2.363528	-2.777293
15	1	0	1.230496	-2.570326	-2.762961
16	1	0	3.490989	-2.846387	-3.737885
17	8	0	3.845292	-1.258764	4.379334
18	8	0	3.944824	-2.224906	2.287231
19	8	0	5.448530	-0.896696	-0.311995
20	8	0	5.738773	-1.897448	-2.369557
21	6	0	4.224449	-2.444740	3.672474
22	1	0	3.632092	-3.289061	4.034665
23	1	0	5.295342	-2.617415	3.804216
24	6	0	6.433160	-1.318565	-1.260155
25	1	0	7.077989	-2.073118	-0.800947
26	1	0	7.004792	-0.452736	-1.601966
27	15	0	0.204979	-1.214274	-0.392639
28	15	0	1.625987	1.793438	-0.165448
29	46	0	-0.396963	0.979999	-0.845573
30	6	0	0.189166	-1.703068	1.354169
31	6	0	0.750998	-2.920251	1.759772
32	6	0	-0.327668	-0.821795	2.305077
33	6	0	0.787462	-3.248615	3.110079
34	1	0	1.176837	-3.600124	1.027368
35	6	0	-0.273455	-1.148381	3.657200
36	1	0	-0.755061	0.125648	1.989403
37	6	0	0.285656	-2.358349	4.059298
38	6	0	-0.909276	-2.321160	-1.309365
39	6	0	-1.427176	-3.491197	-0.746681
40	6	0	-1.281911	-1.952910	-2.608273
41	6	0	-2.302782	-4.285446	-1.480790
42	1	0	-1.170403	-3.779428	0.266434
43	6	0	-2.155872	-2.751532	-3.338050
44	1	0	-0.893329	-1.039033	-3.047092
45	6	0	-2.669364	-3.917194	-2.773365
46	6	0	1.386152	3.518972	0.369049
47	6	0	2.353506	4.503134	0.149731
48	6	0	0.207122	3.844953	1.051900
49	6	0	2.141021	5.799647	0.611715
50	1	0	3.269926	4.272357	-0.382735
51	6	0	0.005109	5.138725	1.518941
52	1	0	-0.554759	3.087319	1.216309
53	6	0	0.972151	6.117858	1.297728
54	6	0	2.869910	1.757075	-1.487960
55	6	0	2.482413	1.441711	-2.793510
56	6	0	4.220446	1.979247	-1.193497
57	6	0	3.442999	1.339061	-3.795570
58	1	0	1.435664	1.254402	-0.3019253
59	6	0	5.172872	1.890387	-2.202262
60	1	0	4.532070	2.195325	-0.175743
61	6	0	4.786205	1.561112	-3.500551
62	8	0	-2.358314	0.817402	-1.708638

63	6	0	-3.460352	1.010563	-0.849673	25	1	0	7.138145	-1.799937	-0.714658
64	6	0	-3.562665	-0.013370	0.238513	26	1	0	6.984230	-0.240201	-1.616474
65	6	0	-3.803952	-1.351600	0.244958	27	15	0	0.230704	-1.316751	-0.324790
66	8	0	-3.430335	0.435173	1.521750	28	15	0	1.550549	1.898677	-0.223085
67	6	0	-3.813668	-1.758629	1.617573	29	46	0	-0.373066	0.949451	-0.896098
68	1	0	-3.965760	-1.969430	-0.626684	30	6	0	0.261825	-1.832424	1.420784
69	6	0	-3.588123	-0.633922	2.343298	31	6	0	0.838410	-3.045658	1.814371
70	1	0	-3.970613	-2.754013	2.007886	32	6	0	-0.230664	-0.953281	2.388510
71	1	0	-3.510955	-0.434263	3.401070	33	6	0	0.909171	-3.376491	3.163599
72	6	0	-4.703919	0.985774	-1.743754	34	1	0	1.244025	-3.724792	1.069572
73	1	0	-4.781619	0.030808	-2.266446	35	6	0	-0.146237	-1.281225	3.738829
74	1	0	-4.661734	1.799476	-2.470254	36	1	0	-0.660598	-0.003349	2.085906
75	8	0	-5.857657	1.204327	-0.926391	37	6	0	0.424518	-2.491392	4.126282
76	6	0	-6.733552	0.200981	-0.757081	38	6	0	-0.833061	-2.500931	-1.220487
77	8	0	-6.96527	-0.832039	-1.394264	39	6	0	-1.426491	-3.610513	-0.616891
78	6	0	-7.740225	0.522478	0.340831	40	6	0	-1.126527	-2.213514	-2.564056
79	6	0	-6.966191	0.581402	1.671965	41	6	0	-2.299493	-4.418326	-1.344438
80	1	0	-6.209369	1.370135	1.659563	42	1	0	-1.230010	-3.842665	0.423944
81	1	0	-7.665085	0.786899	2.489317	43	6	0	-1.995138	-3.023614	-3.287016
82	1	0	-6.469347	-0.372033	1.879777	44	1	0	-0.665145	-1.353853	-3.047872
83	6	0	-8.403538	1.879121	0.055498	45	6	0	-2.876062	-4.127606	-2.674030
84	1	0	-8.925717	1.870026	-0.907029	46	6	0	1.354681	3.628135	0.334784
85	1	0	-9.138052	2.097296	0.837251	47	6	0	2.358364	4.587001	0.178885
86	1	0	-7.668543	2.687762	0.041658	48	6	0	0.164928	3.975455	0.986794
87	6	0	-8.794635	-0.584084	0.397818	49	6	0	2.171236	5.877128	0.670390
88	1	0	-9.516138	-0.361910	1.190138	50	1	0	3.284335	4.344912	-0.330997
89	1	0	-9.340034	-0.665186	-0.547475	51	6	0	-0.010785	5.259406	1.490326
90	1	0	-8.339700	-1.555403	0.612114	52	1	0	-0.624343	3.236597	1.101049
91	1	0	-0.912080	2.576076	-1.398363	53	6	0	0.992659	6.213507	1.330199
92	1	0	-1.609060	2.029682	-1.654278	54	6	0	2.826065	1.853697	-1.521561
93	1	0	-3.407829	1.993194	-0.355082	55	6	0	2.469830	1.499689	-2.826681
94	1	0	-0.910092	5.382221	2.049196	56	6	0	4.169544	2.094922	-1.210775
95	1	0	0.812040	7.129536	1.657367	57	6	0	3.449248	1.378888	-3.808061
96	1	0	2.893952	6.560816	0.433701	58	1	0	1.428788	1.298260	-3.066143
97	1	0	6.219013	2.064365	-1.971612	59	6	0	5.141577	1.993550	-2.199912
98	1	0	5.534588	1.475054	-4.282233	60	1	0	4.462843	2.333490	-0.192556
99	1	0	3.142285	1.078753	-4.805454	61	6	0	4.784452	1.624996	-3.495663
100	1	0	-2.705059	-5.190374	-1.036525	62	8	0	-2.377428	0.531445	-1.723650
101	1	0	-3.356039	-4.537664	-3.340907	63	6	0	-3.496337	0.716002	-0.834486
102	1	0	-2.439055	-2.459581	-4.344387	64	6	0	-3.746656	-0.483418	0.009160
103	1	0	1.221819	-4.192752	3.423036	65	6	0	-4.429632	-1.643699	-0.187541
104	1	0	0.334810	-2.608071	5.114693	66	8	0	-3.171761	-0.486981	1.243792
105	1	0	-0.660416	-0.452350	4.394673	67	6	0	-4.266540	-2.413010	1.008294
						68	1	0	-4.988505	-1.914269	-1.071741
						69	6	0	-3.495686	-1.663012	1.836156
						70	1	0	-4.669987	-3.393367	1.215911
						71	1	0	-3.105467	-1.814442	2.831145
						72	6	0	-4.713311	1.104601	-1.669394
						73	1	0	-5.023154	0.294673	-2.333104
						74	1	0	-4.490772	1.995842	-2.258451
						75	8	0	-5.754869	1.437437	-0.752006
						76	6	0	-6.858427	0.670761	-0.711761
						77	8	0	-7.108829	-0.173524	-1.546785
						78	6	0	-7.701165	0.968399	0.521818
						79	6	0	-7.854877	2.483340	0.718984
						80	1	0	-8.336265	2.948816	-0.147428
						81	1	0	-8.481277	2.671725	1.596549
						82	1	0	-6.889799	2.970478	0.878738
						83	6	0	-9.075021	0.314342	0.359765
						84	1	0	-8.989811	-0.767326	0.225809
						85	1	0	-9.676670	0.502906	1.254145
						86	1	0	-9.608923	0.724481	-0.503116
						87	6	0	-6.958103	0.350135	1.724261
						88	1	0	-7.541783	0.516381	2.635309
						89	1	0	-6.824743	-0.728667	1.594621
						90	1	0	-5.972280	0.804690	1.862045
						91	1	0	-6.004440	2.424739	-1.361638
						92	1	0	-2.447084	-0.343568	-2.135782
						93	1	0	-3.219264	1.554428	-0.191396
						94	1	0	3.169335	1.088701	-4.815921
						95	1	0	5.548022	1.527500	-4.261247
						96	1	0	6.181216	2.185425	-1.954183
						97	1	0	2.952146	6.619181	0.536554
						98	1	0	0.853246	7.218548	1.716356
						99	1	0	-0.934303	5.515781	1.999877
						100	1	0	-2.760741	-5.274762	-0.862557
						101	1	0	-3.270271	-4.758069	-3.234471
						102	1	0	-2.210311	-2.792011	-4.325411
						103	1	0	1.354817	-4.319328	3.464827
						104	1	0	0.497915	-2.743693	5.179743
						105	1	0	-0.515633	-0.586035	4.486245

6a(S)_{avg}#2b

RwB97XD SCF energy -3304.999750 a.u.
 RwB97XD SCF enthalpy -3304.999750 a.u.
 RwB97XD SCF free energy -3305.145827 a.u.
 Three lowest frequencies (cm⁻¹) 14.2, 16.8, 25.7
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.888956	-0.247728	1.047267
2	6	0	3.373571	-0.835853	2.194760
3	6	0	3.289632	-0.241991	3.449142
4	6	0	2.736486	1.002877	3.620867
5	6	0	2.251804	1.637223	2.467301
6	6	0	2.315114	1.045631	1.206963
7	1	0	2.670835	1.472286	4.595087
8	1	0	1.811055	2.620338	2.581703
9	6	0	3.014505	-0.997507	-0.233993
10	6	0	1.937761	-1.618841	-0.925520
11	6	0	4.265389	-1.163105	-0.787411
12	6	0	2.172462	-2.320708	-2.104887
13	6	0	4.482689	-1.840305	-1.981532
14	6	0	3.454229	-2.439517	-2.665877
15	1	0	1.349588	-2.800952	-2.621081
16	1	0	3.619737	-2.979023	-3.591021
17	8	0	3.814333	-1.073225	4.384839
18	8	0	3.961745	-2.056663	2.303628
19	8	0	5.444352	-0.685851	-0.308111
20	8	0	5.804081	-1.795615	-2.298141
21	6	0	4.248331	-2.247392	3.691280
22	1	0	3.694599	-3.114143	4.061946
23	1	0	5.325713	-2.371914	3.826840
24	6	0	6.456484	-1.112561	-1.223888

2.9. Catalytic cycle 2b-1a (R)

3a(R)_{avg}

RwB97XD SCF energy -3304.688615 a.u.
 RwB97XD SCF enthalpy -3303.814381 a.u.
 RwB97XD SCF free energy -3303.956798 a.u.
 Three lowest frequencies (cm⁻¹) 23.9, 27.1 28.8

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z (Angstroms)
1	6	0	2.393057	1.317000	-0.424487
2	6	0	2.519935	2.592357	-0.929098
3	6	0	2.576952	2.873371	-2.289289
4	6	0	2.543169	1.875046	-3.231237
5	6	0	2.430830	0.562261	-2.748382
6	6	0	2.353467	0.268727	-1.387872
7	1	0	2.598162	2.084991	-4.292779
8	1	0	2.405365	-0.239387	-3.476865
9	6	0	2.335651	1.154016	1.055367
10	6	0	1.169987	0.824182	1.800265
11	6	0	3.478075	1.387985	1.788713
12	6	0	1.228018	0.729810	3.188251
13	6	0	3.532229	1.254629	3.170808
14	6	0	2.417768	0.933943	3.905627
15	1	0	0.334223	0.490622	3.751622
16	1	0	2.451053	0.842147	4.984895
17	8	0	2.672552	4.214670	-2.475441
18	8	0	2.588473	3.749420	-0.218505
19	8	0	4.702965	1.733921	1.311380
20	8	0	4.799761	1.488008	3.603269
21	6	0	2.624531	4.811189	-1.174774
22	1	0	1.716271	5.414100	-1.084449
23	1	0	3.524682	5.409479	-1.017098
24	6	0	5.565797	1.838342	2.446923
25	1	0	5.917240	2.869870	2.540810
26	1	0	6.398233	1.139163	2.337283
27	15	0	-0.343298	0.367172	0.869409
28	15	0	2.073112	-1.463526	-0.855896
29	46	0	-0.041853	-1.793781	-0.161338
30	6	0	-0.667032	1.809575	-0.194268
31	6	0	-0.674373	3.107924	0.327911
32	6	0	-0.817440	1.616255	-1.570156
33	6	0	-0.841187	4.198192	-0.520056
34	1	0	-0.535323	3.267756	1.393558
35	6	0	-0.962897	2.709724	-2.418490
36	1	0	-0.778027	0.612948	-1.983728
37	6	0	-0.974576	4.000112	-1.893987
38	6	0	-1.684754	0.282029	2.105661
39	6	0	-2.738911	1.195940	2.159423
40	6	0	-1.676176	-0.804753	2.992688
41	6	0	-3.756489	1.038523	3.099905
42	1	0	-2.775521	2.035974	1.474957
43	6	0	-2.682085	-0.947816	3.940814
44	1	0	-0.880266	-1.543629	2.940727
45	6	0	-3.727458	-0.026130	3.994111
46	6	0	2.542958	-2.478098	-2.302991
47	6	0	3.824081	-3.009796	-2.464011
48	6	0	1.573836	-2.705528	-3.288604
49	6	0	4.130116	-3.759573	-3.598258
50	1	0	4.587235	-2.859405	-1.708575
51	6	0	1.888535	-3.438881	-4.426707
52	1	0	0.570376	-2.306938	-3.163701
53	6	0	3.168076	-3.970322	-4.581269
54	6	0	3.303259	-1.754416	0.453645
55	6	0	2.910826	-2.373457	1.644280
56	6	0	4.618591	-1.298671	0.307642
57	6	0	3.825088	-2.526706	2.682877
58	1	0	1.885677	-2.714717	1.764541
59	6	0	5.532765	-1.470930	1.340971
60	1	0	4.924419	-0.787028	-0.600226
61	6	0	5.134174	-2.074868	2.532302
62	8	0	-2.042352	-2.446771	0.401301
63	6	0	-3.120350	-1.998289	-0.020138
64	1	0	0.263531	-3.221542	-0.724236
65	6	0	-4.327823	-2.249962	0.712371
66	6	0	-4.555347	-2.861154	1.921364
67	8	0	-5.512086	-1.821919	1.810552
68	6	0	-5.951269	-2.795427	2.142158
69	1	0	-3.803033	-3.296044	2.562723

70	6	0	-6.473538	-2.155993	1.053187
71	1	0	-6.502421	-3.171015	2.991277
72	1	0	-7.482393	-1.886826	0.776828
73	6	0	-3.196527	-1.207569	-1.307188
74	1	0	-3.785746	-1.767812	-2.039979
75	1	0	-2.188325	-1.054169	-1.697983
76	8	0	-3.797611	0.052625	-1.037323
77	6	0	-4.819508	0.445762	-1.828605
78	8	0	-5.180799	-0.195095	-2.790798
79	6	0	-5.436010	1.749840	-1.342081
80	6	0	-6.066609	1.492504	0.038293
81	1	0	-5.321284	1.149946	0.760496
82	1	0	-6.507581	2.422025	0.412259
83	1	0	-6.859096	0.740102	-0.024077
84	6	0	-4.342532	2.824402	-1.232889
85	1	0	-3.875290	3.007941	-2.204963
86	1	0	-4.790884	3.761348	-0.887741
87	1	0	-3.561189	2.536835	-0.525744
88	6	0	-6.509820	2.194406	-2.337263
89	1	0	-6.967114	3.124401	-1.986063
90	1	0	-6.082807	2.375914	-3.328239
91	1	0	-7.298160	1.442823	-2.437347
92	1	0	1.131834	-3.603265	-5.187388
93	1	0	3.411602	-4.552156	-5.464960
94	1	0	5.124675	-4.180059	-3.709351
95	1	0	6.552069	-1.117690	1.221124
96	1	0	5.845613	-2.190011	3.344232
97	1	0	3.511619	-2.993561	3.611225
98	1	0	-1.061533	2.553271	-3.487942
99	1	0	-1.085329	4.853162	-2.556322
100	1	0	-0.850892	5.203061	-0.109768
101	1	0	-4.568975	1.757905	3.130666
102	1	0	-4.519033	-0.143200	4.727797
103	1	0	-2.657229	-1.785205	4.631113

TS1a(R)_{avg}

RwB97XD SCF energy -3304.668411 a.u.
 RwB97XD SCF enthalpy -3303.796755 a.u.
 RwB97XD SCF free energy -3303.939552 a.u.
 Three lowest frequencies (cm⁻¹) -590.9, 13.7, 24.2
 Imaginary frequency (cm⁻¹) -500.9

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z (Angstroms)
1	6	0	2.717518	-0.537071	0.496526
2	6	0	3.650791	-1.447198	0.939117
3	6	0	3.891023	-1.697200	2.286462
4	6	0	3.225199	-1.018152	3.277447
5	6	0	2.277882	-0.072136	2.858912
6	6	0	2.019793	0.173849	1.512340
7	1	0	3.411424	-1.208395	4.327629
8	1	0	1.733290	0.473102	3.621339
9	6	0	2.530092	-0.366696	-0.972960
10	6	0	1.417542	-0.838698	-1.727226
11	6	0	3.524769	0.256070	-1.694593
12	6	0	1.363985	-0.642696	-3.104565
13	6	0	3.444493	0.477011	-3.065101
14	6	0	2.378176	0.029417	-3.805401
15	1	0	0.518630	-1.015790	-3.670820
16	1	0	2.318644	0.184751	-4.876118
17	8	0	4.826972	-2.671573	2.409408
18	8	0	4.433624	-2.252727	0.175563
19	8	0	4.684354	0.773495	-1.212371
20	8	0	4.542310	1.161385	-3.480947
21	6	0	5.201495	-3.050444	1.080984
22	1	0	4.969401	-4.106837	0.923886
23	1	0	6.264736	-2.846280	0.930156
24	6	0	5.391945	1.299567	-2.338480
25	1	0	6.308364	0.721985	-2.491588
26	1	0	5.605252	2.357720	-2.171721
27	15	0	-0.036494	-1.482325	-0.820528
28	15	0	0.684767	1.322039	1.050809
29	46	0	-1.134379	0.408699	0.043071
30	6	0	0.621668	-2.737085	0.318842
31	6	0	1.504506	-3.716757	-0.151328
32	6	0	0.276041	-2.703141	1.671233
33	6	0	2.029456	-4.657071	0.727954
34	1	0	1.789253	-3.737761	-1.199539
35	6	0	0.810272	-3.642031	2.549676

36	1	0	-0.386960	-1.927399	2.042431	3	6	0	3.920204	-2.272177	-2.173053
37	6	0	1.687291	-4.616267	2.079320	4	6	0	2.771285	-2.913071	-2.568637
38	6	0	-1.121208	-2.377057	-1.984140	5	6	0	1.621331	-2.671080	-1.801438
39	6	0	-1.347424	-3.752806	-1.875124	6	6	0	1.636615	-1.819791	-0.700124
40	6	0	-1.841964	-1.637258	-2.932360	7	1	0	2.750393	-3.569776	-3.430220
41	6	0	-2.268999	-4.377995	-2.711439	8	1	0	0.701334	-3.166697	-2.090028
42	1	0	-0.819160	-4.344337	-1.135778	9	6	0	2.945387	-0.237019	0.857677
43	6	0	-2.751912	-2.268325	-3.772921	10	6	0	2.393983	1.074279	0.922257
44	1	0	-1.702518	-0.563401	-3.003990	11	6	0	3.630420	-0.654727	1.975807
45	6	0	-2.970078	-3.640258	-3.660779	12	6	0	2.550127	1.854239	2.066008
46	6	0	0.255248	2.219918	2.577802	13	6	0	3.762432	0.124183	3.121389
47	6	0	1.069358	3.241306	3.077363	14	6	0	3.238765	1.391724	3.197220
48	6	0	-0.901249	1.852365	3.274666	15	1	0	2.130164	2.852232	2.102763
49	6	0	0.722919	3.891505	4.257448	16	1	0	3.347164	2.003661	4.084604
50	1	0	1.971589	3.537000	2.552763	17	8	0	5.150176	-2.309475	-2.744162
51	6	0	-1.239614	2.501017	4.458792	18	8	0	5.199827	-0.940159	-0.889019
52	1	0	-1.540084	1.062404	2.887538	19	8	0	4.235947	-1.854878	2.163742
53	6	0	-0.429197	3.522306	4.948849	20	8	0	4.454666	-0.563821	4.062306
54	6	0	1.446339	2.506749	-0.107310	21	6	0	6.008295	-1.510983	-1.922184
55	6	0	0.716082	2.942356	-1.218210	22	1	0	6.447636	-0.712359	-2.524065
56	6	0	2.762962	2.945236	0.070894	23	1	0	6.775306	-2.147093	-1.471528
57	6	0	1.298922	3.799840	-2.145736	24	6	0	4.756236	-1.843652	3.496366
58	1	0	-0.302469	2.596505	-1.371058	25	1	0	5.839633	-1.981139	3.462855
59	6	0	3.337545	3.812183	-0.853220	26	1	0	4.268048	-2.625286	4.084224
60	1	0	3.351120	2.591624	0.912471	27	15	0	1.343417	1.667261	-0.441572
61	6	0	2.611153	4.231599	-1.966161	28	15	0	0.089634	-1.377056	0.147088
62	8	0	-3.029251	0.401481	-0.969098	29	46	0	-0.700965	0.684381	-0.441409
63	6	0	-3.189183	1.529341	-0.375677	30	6	0	2.285814	1.385153	-1.964477
64	1	0	-1.843147	1.760595	0.546812	31	6	0	3.651111	1.690951	-2.013072
65	6	0	-3.006029	2.758105	-1.164693	32	6	0	1.656895	0.804331	-3.068776
66	6	0	-2.793391	2.953438	-2.495517	33	6	0	4.380015	1.409641	-3.163171
67	8	0	-2.965848	3.941470	-0.496346	34	1	0	4.147364	2.128115	-1.151506
68	6	0	-2.612900	4.360408	-2.660297	35	6	0	2.395561	0.513599	-4.211782
69	1	0	-2.773217	2.188441	-3.258115	36	1	0	0.597449	0.564628	-3.025525
70	6	0	-2.721435	4.903864	-1.419275	37	6	0	3.755854	0.811284	-4.256802
71	1	0	-2.428950	4.893688	-3.581513	38	6	0	1.117082	3.456943	-0.216560
72	1	0	-2.660553	5.913318	-1.041737	39	6	0	1.803793	4.388384	-0.999472
73	6	0	-4.159948	1.578857	0.812690	40	6	0	0.210605	3.899629	0.756953
74	1	0	-5.142256	1.869841	0.429462	41	6	0	1.592872	5.750683	-0.799811
75	1	0	-3.842489	2.283762	1.579023	42	1	0	2.499812	4.063486	-1.765233
76	8	0	-4.197297	0.290137	1.397354	43	6	0	0.011777	5.260223	0.956325
77	6	0	-4.945155	-0.629431	0.742918	44	1	0	-0.343330	3.181685	1.355636
78	8	0	-5.812441	-0.314922	-0.044003	45	6	0	0.701892	6.187130	0.176195
79	6	0	-4.622379	-2.069485	1.121026	46	6	0	-1.183951	-2.559421	-0.400138
80	6	0	-4.659465	-2.895267	-0.175604	47	6	0	-1.564710	-3.659299	0.372827
81	1	0	-3.906184	-2.539638	-0.886467	48	6	0	-1.801333	-2.333152	-1.638891
82	1	0	-4.449018	-3.944793	0.051744	49	6	0	-2.544853	-4.530392	-0.096979
83	1	0	-5.638998	-2.834952	-0.656448	50	1	0	-1.106209	-3.839956	1.339479
84	6	0	-3.242513	-2.200630	1.769114	51	6	0	-2.769117	-3.214039	-2.107847
85	1	0	-3.176348	-1.659568	2.717039	52	1	0	-1.521061	-1.469227	-2.238051
86	1	0	-3.031536	-3.256995	1.964412	53	6	0	-3.142311	-4.313391	-1.335760
87	1	0	-2.466579	-1.817664	1.098351	54	6	0	0.383732	-1.623844	1.918638
88	6	0	-5.722046	-2.547186	2.086907	55	6	0	-0.051946	-0.651204	2.823253
89	1	0	-5.556581	-3.600445	2.334301	56	6	0	1.084962	-2.745065	2.375929
90	1	0	-5.711931	-1.970565	3.017730	57	6	0	0.226071	-0.793547	4.179577
91	1	0	-6.712309	-2.451896	1.631375	58	1	0	-0.587700	0.224222	2.464022
92	1	0	-2.139322	2.211651	4.992661	59	6	0	1.346386	-2.888630	3.734109
93	1	0	-0.696252	4.032987	5.868892	60	1	0	1.441640	-3.491991	1.672817
94	1	0	1.355408	4.687962	4.636475	61	6	0	0.926453	-1.909195	4.633389
95	1	0	4.359653	4.148159	-0.709611	62	8	0	-1.892670	2.238296	-1.044037
96	1	0	3.068574	4.895721	-2.693026	63	6	0	-2.926555	1.445788	-0.634172
97	1	0	0.727959	4.124015	-3.010305	64	6	0	-3.543798	1.911776	0.651367
98	1	0	0.551927	-3.602285	3.603168	65	6	0	-3.701913	3.143274	1.201213
99	1	0	2.107352	-5.343806	2.767077	66	8	0	-4.088828	0.961985	1.457063
100	1	0	2.713530	-5.415570	0.360606	67	6	0	-4.409968	2.939298	2.431608
101	1	0	-2.440309	-5.445340	-2.613317	68	1	0	-3.362693	4.078313	0.779228
102	1	0	-3.690014	-4.130864	-4.308539	69	6	0	-4.620665	1.603552	2.532171
103	1	0	-3.301233	-1.684284	-4.504582	70	1	0	-4.719090	3.692197	3.142377
						71	1	0	-5.097512	0.975077	3.268767
						72	6	0	-3.928362	1.142947	-1.762642
						73	1	0	-3.370064	0.940792	-2.677456
						74	1	0	-4.609270	1.983464	-1.909905
						75	8	0	-4.647740	-0.053215	-1.463137
						76	6	0	-5.833785	0.035275	-0.833010
						77	8	0	-6.382311	1.093055	-0.605894
						78	6	0	-6.364423	-1.344471	-0.460113
						79	6	0	-5.379881	-1.996722	0.528436
						80	1	0	-5.325598	-1.431206	1.463420
						81	1	0	-5.722224	-3.010111	0.761824
						82	1	0	-4.373974	-2.067683	0.105852
						83	6	0	-7.739773	-1.192077	0.190914
						84	1	0	-8.458136	-0.734696	-0.496027

4a(R)_{avg}

RwB97XD SCF energy -3304.677468 a.u.

RwB97XD SCF enthalpy -3303.802430 a.u.

RwB97XD SCF free energy -3303.947994 a.u.

Three lowest frequencies (cm⁻¹) 11.7, 20.4 25.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.833441	-1.163488	-0.302064
2	6	0	3.949618	-1.440596	-1.057604

85	1	0	-8.121127	-2.177901	0.474873
86	1	0	-7.687705	-0.574705	1.092587
87	6	0	-6.469622	-2.200344	-1.733812
88	1	0	-6.873568	-3.184585	-1.476445
89	1	0	-7.140434	-1.739143	-2.466417
90	1	0	-5.492752	-2.344207	-2.201663
91	1	0	-2.559193	0.353122	-0.387157
92	1	0	2.128139	6.469421	-1.412103
93	1	0	0.539355	7.249802	0.327093
94	1	0	-0.690552	5.595464	1.712750
95	1	0	1.910331	0.047585	-5.063382
96	1	0	4.331604	0.575989	-5.146625
97	1	0	5.439031	1.644398	-3.200033
98	1	0	-3.237031	-3.037457	-3.070993
99	1	0	-3.905338	-4.995725	-1.697169
100	1	0	-2.840010	-5.380893	0.509420
101	1	0	-0.099144	-0.031104	4.880097
102	1	0	1.145788	-2.017324	5.691079
103	1	0	1.887384	-3.759798	4.089531

5a(R)_{aq}

RwB97XD SCF energy -3305.859031 a.u.
 RwB97XD SCF enthalpy -3304.964062 a.u.
 RwB97XD SCF free energy -3305.107794 a.u.
 Three lowest frequencies (cm⁻¹) 15.8, 19.7, 28.6

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.801525	0.264045	1.268372
2	6	0	3.175909	0.149238	2.587817
3	6	0	2.913737	1.131813	3.536949
4	6	0	2.294306	2.311271	3.202629
5	6	0	1.918825	2.465676	1.859561
6	6	0	2.151605	1.476030	0.907572
7	1	0	2.101743	3.084249	3.936847
8	1	0	1.433881	3.391437	1.574015
9	6	0	3.119705	-0.841432	0.325595
10	6	0	2.168954	-1.712606	-0.274999
11	6	0	4.435643	-1.061082	-0.012640
12	6	0	2.583567	-2.715804	-1.148877
13	6	0	4.835194	-2.046309	-0.909720
14	6	0	3.930997	-2.902496	-1.489162
15	1	0	1.856197	-3.386750	-1.588078
16	1	0	4.238398	-3.679721	-2.178347
17	8	0	3.361253	0.723814	4.750202
18	8	0	3.805142	-0.901127	3.174347
19	8	0	5.518220	-0.363019	0.415793
20	8	0	6.179143	-1.992532	-1.077262
21	6	0	3.934864	-0.574243	4.561109
22	1	0	3.387073	-1.304203	5.162549
23	1	0	4.994378	-0.545282	4.827713
24	6	0	6.653815	-0.928375	-0.245163
25	1	0	7.345901	-1.329651	0.499575
26	1	0	7.128393	-0.166230	-0.868299
27	15	0	0.390817	-1.429269	0.007952
28	15	0	1.487368	1.639456	-0.782753
29	46	0	-0.444845	0.393156	-1.109759
30	6	0	0.197709	-1.284519	1.805978
31	6	0	0.835241	-2.199565	2.652405
32	6	0	-0.534380	-0.225253	2.346871
33	6	0	0.734874	-2.051189	4.030985
34	1	0	1.421123	-3.015047	2.238609
35	6	0	-0.617681	-0.072805	3.727406
36	1	0	-1.018612	0.489452	1.688498
37	6	0	0.018641	-0.982584	4.568628
38	6	0	-0.467568	-2.933648	-0.544677
39	6	0	-1.011642	-3.842363	0.364908
40	6	0	-0.598456	-3.165420	-1.920528
41	6	0	-1.659832	-4.985671	-0.099133
42	1	0	-0.940109	-3.669070	1.432922
43	6	0	-1.241714	-4.308638	-2.376675
44	1	0	-0.208396	-2.445954	-2.634793
45	6	0	-1.771959	-5.221895	-1.465698
46	6	0	1.079202	3.402489	-1.010590
47	6	0	1.874175	4.251650	-1.783981
48	6	0	-0.084171	3.903077	-0.409022
49	6	0	1.514492	5.588414	-1.942237
50	1	0	2.770040	3.882012	-2.270718
51	6	0	-0.432893	5.239647	-0.562481

52	1	0	-0.718386	3.248458	0.183194
53	6	0	0.366979	6.084225	-1.331376
54	6	0	2.862417	1.251136	-1.901545
55	6	0	2.641187	0.404017	-2.990004
56	6	0	4.142917	1.762208	-1.658812
57	6	0	3.700356	0.057069	-3.824330
58	1	0	1.649048	-0.002445	-3.168532
59	6	0	5.193380	1.424366	-2.504710
60	1	0	4.322857	2.408646	-0.804768
61	6	0	4.974315	0.564569	-3.580694
62	8	0	-2.146067	-0.690108	-1.329721
63	6	0	-3.366116	-0.031632	-1.203310
64	6	0	-4.454509	-1.052417	-1.372649
65	6	0	-4.502199	-2.392761	-1.156624
66	8	0	-5.685049	-0.592862	-1.731935
67	6	0	-5.861338	-2.787716	-1.390008
68	1	0	-3.674753	-3.019714	-0.855596
69	6	0	-6.531730	-1.659133	-1.729184
70	1	0	-6.278824	-3.781860	-1.314401
71	1	0	-7.554815	-1.452435	-2.004534
72	6	0	-3.468181	0.649786	0.175368
73	1	0	-2.695454	1.420223	0.254211
74	1	0	-3.340754	-0.088686	0.970008
75	8	0	-4.714678	1.338672	0.323067
76	6	0	-5.721499	0.709856	0.950397
77	8	0	-5.602056	-0.382315	1.468097
78	6	0	-6.992527	1.551778	0.979445
79	6	0	-7.233423	2.225191	-0.379169
80	1	0	-7.301415	1.844468	-1.181512
81	1	0	-8.177611	2.778092	-0.345070
82	1	0	-6.436753	2.929924	-0.629581
83	6	0	-8.173915	0.644502	1.333893
84	1	0	-8.033071	0.164244	2.305912
85	1	0	-9.093876	1.236142	1.374472
86	1	0	-8.305608	-0.141048	0.582223
87	6	0	-6.800143	2.622966	2.070718
88	1	0	-7.706166	3.232822	2.146039
89	1	0	-6.616345	2.163070	3.047283
90	1	0	-5.960972	3.284414	1.834765
91	1	0	-3.512899	0.754323	-1.967201
92	1	0	-1.444467	1.823986	-1.844280
93	1	0	-0.967168	1.616265	-2.426210
94	1	0	2.136166	6.240082	-2.547927
95	1	0	0.092242	7.126832	-1.457485
96	1	0	-1.331852	5.619751	-0.087748
97	1	0	3.530706	-0.616123	-4.658583
98	1	0	5.799780	0.288836	-4.229651
99	1	0	6.184797	1.824929	-2.318599
100	1	0	-1.340368	-4.481258	-3.443587
101	1	0	-2.278424	-6.112752	-1.823958
102	1	0	-2.077268	-5.689424	0.613939
103	1	0	-1.172187	0.761567	4.144684
104	1	0	-0.042828	-0.858315	5.645236
105	1	0	1.227568	-2.763189	4.685356

TS2a(R)_{aq}

RwB97XD SCF energy -3305.849237 a.u.
 RwB97XD SCF enthalpy -3304.956108 a.u.
 RwB97XD SCF free energy -3305.099631 a.u.
 Three lowest frequencies (cm⁻¹) -1057, 16.3, 21.1
 Imaginary frequency (cm⁻¹) -1057

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.258682	0.444388	1.475925
2	6	0	2.367301	0.409970	2.847148
3	6	0	1.816372	1.382735	3.675492
4	6	0	1.160974	2.477747	3.167041
5	6	0	1.054661	2.553036	1.770669
6	6	0	1.577367	1.568877	0.934278
7	1	0	0.740237	3.241572	3.809948
8	1	0	0.545191	3.410251	1.347017
9	6	0	2.842265	-0.662491	0.672939
10	6	0	2.088284	-1.620488	-0.058629
11	6	0	4.210976	-0.794889	0.609321
12	6	0	2.730664	-2.613793	-0.794521
13	6	0	4.842329	-1.775586	-0.148577
14	6	0	4.128855	-2.709900	-0.858750
15	1	0	2.147024	-3.341087	-1.346335

16	1	0	4.617651	-3.479931	-1.443575
17	8	0	2.032326	1.051811	4.972026
18	8	0	2.956036	-0.554845	3.599039
19	8	0	5.140114	-0.002251	1.202882
20	8	0	6.187476	-1.623516	-0.060061
21	6	0	2.787874	-0.164422	4.964935
22	1	0	2.233574	-0.939481	5.499585
23	1	0	3.768102	0.013705	5.415512
24	6	0	6.418286	-0.522795	0.825228
25	1	0	6.942185	-0.877647	1.716932
26	1	0	6.986813	0.250460	0.303252
27	15	0	0.271736	-1.451379	-0.146571
28	15	0	1.274179	1.643077	-0.859142
29	46	0	-0.377181	0.249315	-1.588545
30	6	0	-0.279640	-1.266755	1.573494
31	6	0	0.227671	-2.094129	2.581958
32	6	0	-1.165510	-0.237142	1.898834
33	6	0	-0.170397	-1.901310	3.900524
34	1	0	0.950882	-2.868784	2.345236
35	6	0	-1.554411	-0.041577	3.220161
36	1	0	-1.535804	0.424143	1.121863
37	6	0	-1.057182	-0.874124	4.220373
38	6	0	-0.314314	-3.043484	-0.804428
39	6	0	-0.657703	-4.115278	0.023971
40	6	0	-0.328698	-3.211392	-2.195429
41	6	0	-0.993111	-5.345324	-0.534584
42	1	0	-0.672007	-3.999418	1.101668
43	6	0	-0.672111	-4.440451	-2.747542
44	1	0	-0.063443	-2.383637	-2.846510
45	6	0	-0.999044	-5.510344	-1.916682
46	6	0	0.738720	3.349323	-1.214036
47	6	0	1.622215	4.312387	-1.706004
48	6	0	-0.601042	3.689807	-0.979736
49	6	0	1.168452	5.605679	-1.956942
50	1	0	2.659901	4.066118	-1.902858
51	6	0	-1.044543	4.984113	-1.223067
52	1	0	-1.300409	2.946696	-0.605026
53	6	0	-0.159629	5.943084	-1.714312
54	6	0	2.875804	1.357288	-1.659727
55	6	0	2.957288	0.461633	-2.729403
56	6	0	4.032869	1.976301	-1.172063
57	6	0	4.193778	0.180369	-3.303168
58	1	0	2.059110	-0.029162	-3.096541
59	6	0	5.262868	1.700482	-1.758602
60	1	0	3.978482	2.655721	-0.326302
61	6	0	5.344655	0.796353	-2.816837
62	8	0	-2.113895	-0.487096	-2.665156
63	6	0	-3.378724	-0.392343	-2.040900
64	6	0	-3.601950	-1.524488	-1.088676
65	6	0	-3.723077	-1.642729	0.262062
66	8	0	-3.747412	-2.750899	-1.667707
67	6	0	-3.960814	-3.028842	0.532464
68	1	0	-3.664761	-0.844836	0.986957
69	6	0	-3.960569	-3.648680	-0.673420
70	1	0	-4.104731	-3.494205	1.496885
71	1	0	-4.090423	-4.674727	-0.981828
72	6	0	-3.543160	0.964108	-1.352164
73	1	0	-3.416392	1.765926	-2.084377
74	1	0	-2.799267	1.081935	-0.560241
75	8	0	-4.858775	1.070870	-0.806564
76	6	0	-4.990735	1.493904	0.458266
77	8	0	-4.049974	1.861983	1.136412
78	6	0	-6.440831	1.435007	0.922401
79	6	0	-6.909396	-0.030702	0.869262
80	1	0	-6.299961	-0.665855	1.520268
81	1	0	-7.947218	-0.090577	1.212301
82	1	0	-6.858940	-0.433247	-0.145891
83	6	0	-6.529720	1.961955	2.355990
84	1	0	-6.197799	3.002374	2.422139
85	1	0	-7.567462	1.912139	2.699791
86	1	0	-5.915711	1.364297	3.036235
87	6	0	-7.302150	2.295797	-0.017350
88	1	0	-8.340892	2.279736	0.327478
89	1	0	-6.962509	3.336913	-0.023951
90	1	0	-7.276643	1.917277	-1.042655
91	1	0	-4.141178	-0.467177	-2.830453
92	1	0	-0.838794	1.426757	-2.810747
93	1	0	-1.483385	0.780260	-2.913683
94	1	0	1.859460	6.348295	-2.343023
95	1	0	-0.507907	6.952459	-1.910265
96	1	0	-2.082466	5.239753	-1.035053
97	1	0	4.257908	-0.529261	-4.121833
98	1	0	6.308508	0.571215	-3.262518
99	1	0	6.158879	2.181493	-1.379630
100	1	0	-0.681517	-4.562331	-3.825950
101	1	0	-1.263252	-6.470746	-2.348373
102	1	0	-1.258481	-6.172852	0.115726
103	1	0	-2.240192	0.763224	3.464945
104	1	0	-1.353891	-0.718124	5.252917
105	1	0	0.221475	-2.547385	4.679614

6a (R) _{avg} *2b				
RwB97XD SCF energy			-3305.895695 a.u.	
RwB97XD SCF enthalpy			-3304.997650 a.u.	
RwB97XD SCF free energy			-3305.145719 a.u.	
Three lowest frequencies (cm ⁻¹)	11.9,	18.8	20.2	
Cartesian coordinates:Å				
Center Number	Atomic Number	Atomic Type	Coordinates X Y Z	(Angstroms)
1	6	0	-3.269583 -0.078333 -0.061975	
2	6	0	-4.424523 -0.644133 -0.556792	
3	6	0	-5.043490 -0.217753 -1.726116	
4	6	0	-4.554835 0.838951 -2.454367	
5	6	0	-3.395925 1.455935 -1.960303	
6	6	0	-2.754798 1.025932 -0.799096	
7	1	0	-5.036377 1.181828 -3.362365	
8	1	0	-2.996598 2.296572 -2.515759	
9	6	0	-2.687523 -0.647589 1.185792	
10	6	0	-1.507213 -1.437537 1.252506	
11	6	0	-3.346235 -0.441109 2.377438	
12	6	0	-1.061110 -1.931170 2.476164	
13	6	0	-2.873628 -0.911931 3.596854	
14	6	0	-1.730804 -1.667869 3.681654	
15	1	0	-0.167161 -2.541796 2.519783	
16	1	0	-1.361595 -2.045471 4.627922	
17	8	0	-6.131691 -0.989595 -1.975343	
18	8	0	-5.113315 -1.690618 -0.028951	
19	8	0	-4.480686 0.283571 2.574196	
20	8	0	-3.691598 -0.481716 4.596280	
21	6	0	-6.198162 -1.955960 -0.921301	
22	1	0	-6.089431 -2.959146 -1.342394	
23	1	0	-7.144097 -1.844000 -0.385590	
24	6	0	-4.824766 0.102605 3.949890	
25	1	0	-5.678189 -0.580954 4.022363	
26	1	0	-5.042817 1.070563 4.402317	
27	15	0	-0.517313 -1.646619 -0.277985	
28	15	0	-1.153961 1.793465 -0.345338	
29	46	0	0.542303 0.435375 -0.904717	
30	6	0	-1.686785 -2.365731 -1.474791	
31	6	0	-2.551739 -3.407633 -1.121864	
32	6	0	-1.761666 -1.805314 -2.753236	
33	6	0	-3.479443 -3.882901 -2.042554	
34	1	0	-2.509724 -3.838267 -0.125297	
35	6	0	-2.702083 -2.273186 -3.667511	
36	1	0	-1.099694 -0.985524 -3.022443	
37	6	0	-3.562930 -3.308639 -3.310866	
38	6	0	0.712824 -2.939796 0.108166	
39	6	0	0.652270 -4.236338 -0.407794	
40	6	0	1.795159 -2.576297 0.920996	
41	6	0	1.652936 -5.157443 -0.101999	
42	1	0	-0.167412 -4.536541 -1.051978	
43	6	0	2.783283 -3.501556 1.237803	
44	1	0	1.864812 -1.562193 1.305122	
45	6	0	2.714372 -4.795205 0.722181	
46	6	0	-1.176251 3.423104 -1.179947	
47	6	0	-1.779944 4.540690 -0.596330	
48	6	0	-0.617594 3.536301 -2.458726	
49	6	0	-1.817290 5.752686 -1.280559	
50	1	0	-2.214943 4.482767 0.394759	
51	6	0	-0.669245 4.745246 -3.144929	
52	1	0	-0.140387 2.675966 -2.919261	
53	6	0	-1.266440 5.856961 -2.554756	
54	6	0	-1.232870 2.100211 1.448439	
55	6	0	-0.115522 1.805156 2.235418	
56	6	0	-2.402791 2.572127 2.054467	
57	6	0	-0.168584 1.980462 3.615311	
58	1	0	0.788596 1.422516 1.768945	
59	6	0	-2.447532 2.755916 3.432284	
60	1	0	-3.291399 2.764127 1.460371	
61	6	0	-1.333223 2.455449 4.213677	
62	8	0	2.340785 -0.600017 -1.666126	

63	6	0	3.684969	-0.100416	-1.505700
64	6	0	3.704283	0.925907	-0.430995
65	6	0	3.610034	0.869291	0.926180
66	8	0	3.788500	2.223090	-0.835787
67	6	0	3.622519	2.223767	1.387069
68	1	0	3.557308	-0.028032	1.524850
69	6	0	3.733771	2.996655	0.275367
70	1	0	3.564535	2.570538	2.408722
71	1	0	3.799877	4.061884	0.113595
72	6	0	4.581656	-1.295625	-1.185451
73	1	0	4.583341	-2.003704	-2.016456
74	1	0	4.243744	-1.799810	-0.279857
75	8	0	5.913507	-0.808551	-1.028605
76	6	0	6.465062	-0.827272	0.198258
77	8	0	5.978892	-1.424975	1.136187
78	6	0	7.735856	0.010953	0.247025
79	6	0	7.324865	1.481889	0.037961
80	1	0	6.630105	1.813425	0.817047
81	1	0	8.215483	2.116856	0.084490
82	1	0	6.848472	1.630016	-0.935137
83	6	0	8.397449	-0.160938	1.615448
84	1	0	8.665651	-1.205696	1.799558
85	1	0	9.311981	0.438742	1.659175
86	1	0	7.734963	0.167864	2.421194
87	6	0	8.693559	-0.434775	-0.869706
88	1	0	9.614854	0.153822	-0.816109
89	1	0	8.959899	-1.491466	-0.763051
90	1	0	8.252818	-0.288588	-1.859177
91	1	0	4.007157	0.372569	-2.437766
92	1	0	2.237798	-0.995082	-2.542079
93	1	0	1.183270	1.822730	-1.185093
94	1	0	-2.278462	6.616836	-0.812824
95	1	0	-1.298292	6.803718	-3.085074
96	1	0	-0.233327	4.819985	-4.136235
97	1	0	0.699205	1.739115	4.221450
98	1	0	-1.376257	2.586944	5.290469
99	1	0	-3.358535	3.120210	3.896383
100	1	0	-4.147938	-4.692173	-1.765540
101	1	0	-4.300765	-3.669022	-4.021174
102	1	0	-2.769866	-1.821230	-4.652107
103	1	0	1.597763	-6.161424	-0.511311
104	1	0	3.490247	-5.516537	0.959106
105	1	0	3.617270	-3.204830	1.866368

2.10. Catalytic cycle 2b-1b (S)

3b(S)_{avg}

RwB97XD SCF energy	-3378.446298 a.u.
RwB97XD SCF enthalpy	-3377.604319 a.u.
RwB97XD SCF free energy	-3377.748936 a.u.
Three lowest frequencies (cm ⁻¹)	14.1, 18.8 29.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.326292	1.110622	0.917311
2	6	0	3.416487	1.125727	1.760510
3	6	0	3.306924	1.203143	3.146442
4	6	0	2.085897	1.290291	3.769271
5	6	0	0.956919	1.294554	2.936941
6	6	0	1.053547	1.212813	1.548509
7	1	0	1.994001	1.357657	4.846761
8	1	0	-0.017116	1.367904	3.406237
9	6	0	2.566156	1.008340	-0.550552
10	6	0	2.348593	-0.161126	-1.332262
11	6	0	3.086694	2.095368	-1.218485
12	6	0	2.635235	-0.160058	-2.694811
13	6	0	3.349555	2.090578	-2.584900
14	6	0	3.138770	0.972839	-3.354327
15	1	0	2.468225	-1.056527	-3.280679
16	1	0	3.350516	0.960690	-4.417078
17	8	0	4.541300	1.195821	3.703462
18	8	0	4.726115	1.064637	1.410175
19	8	0	3.386303	3.312720	-0.698729
20	8	0	3.817600	3.305746	-2.964590
21	6	0	5.467479	1.007238	2.629254
22	1	0	5.941807	0.025583	2.726593
23	1	0	6.208762	1.809407	2.641891
24	6	0	3.910246	4.093056	-1.774726
25	1	0	4.960756	4.327727	-1.574448
26	1	0	3.315861	5.002704	-1.891578
27	15	0	1.513615	-1.595841	-0.552481
28	15	0	-0.483215	1.087480	0.565000
29	46	0	-0.779948	-1.014324	-0.146272
30	6	0	2.548248	-2.018571	0.884795
31	6	0	3.944805	-2.052775	0.803849
32	6	0	1.918972	-2.260248	2.109473
33	6	0	4.700070	-2.340543	1.935923
34	1	0	4.441630	-1.842643	-0.138874
35	6	0	2.678755	-2.529059	3.244956
36	1	0	0.834888	-2.217804	2.176910
37	6	0	4.068510	-2.569557	3.157974
38	6	0	1.668854	-2.963413	-1.752548
39	6	0	2.631206	-3.971029	-1.649603
40	6	0	0.751765	-2.995537	-2.812327
41	6	0	2.682547	-4.988648	-2.599795
42	6	0	0.814267	-4.005587	-3.766258
43	1	0	-0.011901	-2.226040	-2.891542
44	6	0	1.780010	-5.005241	-3.659696
45	6	0	-1.796980	1.688296	1.688967
46	6	0	-2.042326	3.051222	1.874075
47	6	0	-2.530125	0.753080	2.429093
48	6	0	-3.007352	3.469879	2.786608
49	1	0	-1.496021	3.795449	1.306066
50	6	0	-3.485389	1.174224	3.347575
51	1	0	-2.355054	-0.309102	2.285061
52	6	0	-3.725189	2.534841	3.527875
53	6	0	-0.307099	2.274124	-0.801347
54	6	0	-0.669483	1.881561	-2.093196
55	6	0	0.235506	3.546321	-0.587991
56	6	0	-0.493383	2.756725	-3.161213
57	1	0	-1.087397	0.892667	-2.263094
58	6	0	0.392876	4.422849	-1.655739
59	1	0	0.565841	3.844064	0.402266
60	6	0	0.034554	4.027016	-2.943356
61	8	0	-1.598657	-3.079509	-0.532968
62	6	0	-2.817122	-2.944964	-0.323612
63	1	0	-2.224116	-0.455812	0.016730
64	6	0	-3.377650	-2.990635	1.002594
65	6	0	-4.662073	-2.851365	1.470530
66	8	0	-2.515413	-3.107300	2.052056
67	6	0	-4.576578	-2.882868	2.884037
68	1	0	-5.552938	-2.735779	0.869741
69	6	0	-3.250084	-3.037896	3.171969

70	1	0	-5.383453	-2.805411	3.597340
71	1	0	-2.709086	-3.121724	4.103074
72	6	0	-3.778297	-2.729727	-1.489416
73	1	0	-4.570610	-3.480732	-1.474520
74	1	0	-3.220689	-2.785395	-2.423761
75	8	0	-4.399470	-1.454051	-1.334242
76	6	0	-3.871382	-0.420656	-2.027082
77	8	0	-3.115976	-0.565180	-2.964654
78	1	0	-4.045633	0.436917	3.914125
79	1	0	-4.475145	2.865617	4.239541
80	1	0	-3.196956	4.530699	2.915710
81	1	0	-0.768449	2.443845	-4.163619
82	1	0	0.173084	4.708566	-3.776937
83	1	0	0.813584	5.408523	-1.484457
84	1	0	5.782944	-2.374679	1.866139
85	1	0	4.660828	-2.777795	4.043756
86	1	0	2.185686	-2.700231	4.196689
87	1	0	3.342938	-3.973621	-0.831079
88	1	0	3.433385	-5.767595	-2.510485
89	1	0	1.824568	-5.797741	-4.400421
90	1	0	0.101758	-4.016911	-4.585217
91	6	0	-4.313246	0.891787	-1.493538
92	6	0	-4.962928	1.002179	-0.259504
93	6	0	-3.984336	2.040866	-2.217802
94	6	0	-5.276544	2.259377	0.244017
95	1	0	-5.204153	0.110811	0.308753
96	6	0	-4.293728	3.295550	-1.706936
97	1	0	-3.476820	1.940073	-3.170624
98	6	0	-4.936814	3.404754	-0.474674
99	1	0	-5.770692	2.347374	1.205718
100	1	0	-4.027600	4.187362	-2.265324
101	1	0	-5.169805	4.384864	-0.069851

TS1b(S)_{reg}

RwB97XD SCF energy -3378.434628 a.u.
 RwB97XD SCF enthalpy -3377.596079 a.u.
 RwB97XD SCF free energy -3377.739016 a.u.
 Three lowest frequencies (cm⁻¹) -550.3, 15.2, 16.5
 Imaginary frequency (cm⁻¹) -550.3
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.148778	1.152829	1.147393
2	6	0	3.183413	1.166512	2.056117
3	6	0	3.000593	0.964030	3.419689
4	6	0	1.751450	0.778911	3.959736
5	6	0	0.672467	0.792819	3.063069
6	6	0	0.846887	0.970880	1.692331
7	1	0	1.603539	0.627300	5.022338
8	1	0	-0.323897	0.656476	3.467331
9	6	0	2.468752	1.324499	-0.297153
10	6	0	2.416487	0.287636	-1.269061
11	6	0	2.877535	2.557688	-0.752785
12	6	0	2.744274	0.544754	-2.597618
13	6	0	3.176405	2.810609	-2.087156
14	6	0	3.127584	1.821134	-3.038301
15	1	0	2.702259	-0.254601	-3.328665
16	1	0	3.368530	2.013596	-4.077051
17	8	0	4.203470	0.976980	4.047942
18	8	0	4.505721	1.323565	1.787877
19	8	0	3.010689	3.698246	-0.026764
20	8	0	3.492512	4.122357	-2.242471
21	6	0	5.185912	1.252504	3.043906
22	1	0	5.915621	0.439692	3.018370
23	1	0	5.661156	2.215018	3.253890
24	6	0	3.435569	4.713384	-0.940515
25	1	0	4.431918	5.062927	-0.655342
26	1	0	2.708425	5.529138	-0.943783
27	15	0	1.740308	-1.337420	-0.780444
28	15	0	-0.588689	0.804080	0.572481
29	46	0	-0.581264	-1.253230	-0.398609
30	6	0	2.719802	-1.865006	0.656954
31	6	0	4.107084	-1.687615	0.698144
32	6	0	2.051434	-2.397036	1.763884
33	6	0	4.817044	-2.040427	1.840882
34	1	0	4.629491	-1.254749	-0.150188
35	6	0	2.765179	-2.736210	2.909858
36	1	0	0.972042	-2.526615	1.734068
37	6	0	4.145821	-2.553983	2.949777

38	6	0	2.100606	-2.474083	-2.158172
39	6	0	3.191224	-3.347504	-2.154357
40	6	0	1.226164	-2.463729	-3.253387
41	6	0	3.407135	-4.194815	-3.238489
42	6	0	1.452635	-3.303833	-4.338171
43	1	0	0.366996	-1.796890	-3.257535
44	6	0	2.543280	-4.171640	-4.330320
45	6	0	-2.061391	1.041464	1.630043
46	6	0	-2.656380	2.290910	1.820229
47	6	0	-2.575909	-0.074757	2.302711
48	6	0	-3.742175	2.420157	2.682561
49	1	0	-2.294631	3.166166	1.293219
50	6	0	-3.658926	0.059880	3.163990
51	1	0	-2.121139	-1.051014	2.160972
52	6	0	-4.241887	1.310332	3.357466
53	6	0	-0.474636	2.206990	-0.575800
54	6	0	-0.587791	1.976034	-1.948537
55	6	0	-0.206759	3.498152	-0.105612
56	6	0	-0.440533	3.029517	-2.846344
57	1	0	-0.780293	0.971993	-2.312883
58	6	0	-0.079467	4.550411	-1.005501
59	1	0	-0.072601	3.680915	0.956615
60	6	0	-0.189532	4.316091	-2.375493
61	8	0	-1.173062	-3.219774	-0.985936
62	6	0	-2.343205	-2.809358	-0.643248
63	1	0	-2.166098	-1.195382	-0.206452
64	6	0	-2.910254	-3.223699	0.649850
65	6	0	-4.183118	-3.245137	1.137931
66	8	0	-2.029746	-3.604464	1.613255
67	6	0	-4.079401	-3.680115	2.492933
68	1	0	-5.081430	-2.984420	0.596951
69	6	0	-2.753950	-3.875971	2.724515
70	1	0	-4.883907	-3.828168	3.198296
71	1	0	-2.191968	-4.206127	3.585103
72	6	0	-3.341181	-2.482188	-1.757418
73	1	0	-4.019789	-3.329813	-1.877262
74	1	0	-2.788149	-2.311314	-2.679929
75	8	0	-4.138888	-1.354004	-1.416231
76	6	0	-3.778629	-0.168636	-1.950251
77	8	0	-2.966794	-0.068573	-2.849525
78	1	0	-4.045079	-0.814189	3.678918
79	1	0	-5.090736	1.417145	4.025780
80	1	0	-4.203555	3.393323	2.816488
81	1	0	-0.517785	2.841930	-3.912629
82	1	0	-0.072306	5.136950	-3.076254
83	1	0	0.122164	5.551219	-0.636996
84	1	0	5.893186	-1.901332	1.870365
85	1	0	4.700743	-2.811315	3.846742
86	1	0	2.241731	-3.134353	3.773430
87	1	0	3.871365	-3.377848	-1.309557
88	1	0	4.254183	-4.873610	-3.227396
89	1	0	2.716063	-4.833683	-5.173237
90	1	0	0.772867	-3.286436	-5.184267
91	6	0	-4.470982	0.977347	-1.315180
92	6	0	-5.407702	0.800279	-0.291361
93	6	0	-4.145752	2.264589	-1.754704
94	6	0	-6.027635	1.909252	0.272111
95	1	0	-5.649619	-0.196107	0.060743
96	6	0	-4.758239	3.369687	-1.176506
97	1	0	-3.413965	2.390956	-2.545131
98	6	0	-5.704662	3.191548	-0.168864
99	1	0	-6.756403	1.773710	1.064609
100	1	0	-4.500170	4.368328	-1.514209
101	1	0	-6.186607	4.054701	0.280192

4b(S)_{reg}

RwB97XD SCF energy -3378.441735 a.u.
 RwB97XD SCF enthalpy -3377.598761 a.u.
 RwB97XD SCF free energy -3377.740933 a.u.
 Three lowest frequencies (cm⁻¹) 15.0, 20.3, 26.5
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.371055	0.969334	-1.183820
2	6	0	-3.419898	0.843752	-2.066416
3	6	0	-3.239856	0.594278	-3.423800
4	6	0	-1.989427	0.498279	-3.983987
5	6	0	-0.898628	0.650582	-3.113994
6	6	0	-1.069658	0.876783	-1.751482

7	1	0	-1.849044	0.315212	-5.042555
8	1	0	0.099933	0.582732	-3.530943
9	6	0	-2.650347	1.204685	0.259815
10	6	0	-2.417023	0.266140	1.304453
11	6	0	-3.163956	2.420071	0.651672
12	6	0	-2.89670	0.593558	2.630607
13	6	0	-3.405706	2.747964	1.982730
14	6	0	-3.187797	1.851350	3.000113
15	1	0	-2.513485	-0.134061	3.414373
16	1	0	-3.383365	2.100474	4.036126
17	8	0	-4.448780	0.484062	-4.029990
18	8	0	-4.745927	0.910269	-1.782702
19	8	0	-3.456403	3.480645	-0.143646
20	8	0	-3.846816	4.027422	2.062531
21	6	0	-5.436284	0.632994	-3.004836
22	1	0	-5.996940	-0.299980	-2.902509
23	1	0	-6.091089	1.472373	-3.249662
24	6	0	-3.954018	4.508188	0.718474
25	1	0	-5.005208	4.700570	0.485610
26	1	0	-3.344059	5.406981	0.605143
27	15	0	-1.617659	-1.322100	0.918732
28	15	0	0.366211	0.876514	-0.633182
29	46	0	0.592375	-1.138446	0.424055
30	6	0	-2.578230	-2.049916	-0.436433
31	6	0	-3.976626	-1.991090	-0.419430
32	6	0	-1.912476	-2.611361	-1.529917
33	6	0	-4.700834	-2.490412	-1.496252
34	1	0	-4.497090	-1.539647	0.420194
35	6	0	-2.643404	-3.092976	-2.611764
36	1	0	-0.826117	-2.654341	-1.540622
37	6	0	-4.035115	-3.028153	-2.596862
38	6	0	-1.771282	-2.376596	2.391062
39	6	0	-2.760454	-3.357199	2.502518
40	6	0	-0.851411	-2.192251	3.432576
41	6	0	-2.831714	-4.139698	3.652428
42	6	0	-0.934952	-2.970281	4.581190
43	1	0	-0.069224	-1.442495	3.343610
44	6	0	-1.924136	-3.946334	4.690381
45	6	0	1.867445	1.064447	-1.654785
46	6	0	2.529263	2.288517	-1.783302
47	6	0	2.388352	-0.073553	-2.288493
48	6	0	3.695634	2.369827	-2.539572
49	1	0	2.151066	3.177695	-1.290824
50	6	0	3.554958	0.013089	-3.038837
51	1	0	1.883138	-1.031384	-2.190231
52	6	0	4.210938	1.236547	-3.162529
53	6	0	0.202454	2.359221	0.398141
54	6	0	0.406665	2.262663	1.776570
55	6	0	-0.178500	3.580052	-0.171126
56	6	0	0.225626	3.382824	2.583722
57	1	0	0.691975	1.313253	2.218264
58	6	0	-0.349318	4.697030	0.639336
59	1	0	-0.360032	3.655159	-1.239446
60	6	0	-0.154960	4.596751	2.016544
61	8	0	1.348695	-2.957590	1.047639
62	6	0	2.536719	-2.472516	0.596987
63	6	0	3.080558	-3.125587	-0.637371
64	6	0	4.338807	-3.345273	-1.101810
65	8	0	2.165991	-3.472625	-1.581178
66	6	0	4.189276	-3.877630	-2.424286
67	1	0	5.261649	-3.147400	-0.575123
68	6	0	2.854768	-3.929056	-2.660548
69	1	0	4.973822	-4.183507	-3.101328
70	1	0	2.256972	-4.264030	-3.494587
71	6	0	3.597680	-2.251795	1.691223
72	1	0	4.278146	-3.100732	1.761774
73	1	0	3.091284	-2.096275	2.643548
74	8	0	4.405761	-1.118052	1.354669
75	6	0	3.923279	0.086026	1.704884
76	8	0	2.957772	0.224803	2.434416
77	1	0	3.952305	-0.876730	-3.516993
78	1	0	5.129449	1.304830	-3.737138
79	1	0	4.208588	3.321806	-2.628698
80	1	0	0.373547	3.301700	3.655838
81	1	0	-0.304290	5.466980	2.648118
82	1	0	-0.645675	5.642493	0.196523
83	1	0	-5.785231	-2.445291	-1.481815
84	1	0	-4.602961	-3.397781	-3.445039
85	1	0	-2.126022	-3.513371	-3.468139
86	1	0	-3.473901	-3.519348	1.701521
87	1	0	-3.599318	-4.902811	3.732703
88	1	0	-1.983533	-4.559786	5.584127

89	1	0	-0.220128	-2.822259	5.384324
90	6	0	4.671578	1.212743	1.097681
91	6	0	5.754739	1.002556	0.238571
92	6	0	4.246043	2.513629	1.386950
93	6	0	6.416274	2.093385	-0.314544
94	1	0	6.075466	-0.006226	0.003815
95	6	0	4.908082	3.599008	0.826979
96	1	0	3.398276	2.665857	2.047021
97	6	0	5.995675	3.389058	-0.020015
98	1	0	7.256191	1.931755	-0.982533
99	1	0	4.576894	4.608233	1.049860
100	1	0	6.511636	4.238158	-0.457874
101	1	0	2.398030	-1.349883	0.223531

5b(S)_{avg}

RwB97XD SCF energy -3379.614481 a.u.

RwB97XD SCF enthalpy -3378.751486 a.u.

RwB97XD SCF free energy -3378.898419 a.u.

Three lowest frequencies (cm⁻¹) 8.5, 9.9, 16.3

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.357550	-0.373357	-0.325881
2	6	0	4.548500	0.113737	-0.815809
3	6	0	4.942337	-0.041151	-2.141116
4	6	0	4.178327	-0.738242	-3.044826
5	6	0	2.969801	-1.267222	-2.568254
6	6	0	2.553475	-1.093295	-1.250568
7	1	0	4.487909	-0.871851	-4.074459
8	1	0	2.353674	-1.826683	-3.261675
9	6	0	3.018991	-0.145493	1.104996
10	6	0	1.995203	0.717409	1.587664
11	6	0	3.753828	-0.803583	2.065074
12	6	0	1.791054	0.869717	2.957666
13	6	0	3.516335	-0.671015	3.429105
14	6	0	2.547323	0.173791	3.911537
15	1	0	1.030305	1.548434	3.320843
16	1	0	2.371079	0.298583	4.973145
17	8	0	6.129609	0.583552	-2.339206
18	8	0	5.482804	0.829688	-0.139115
19	8	0	4.769599	-1.681129	1.859189
20	8	0	4.370936	-1.463956	4.120206
21	6	0	6.526216	1.121345	-1.073439
22	1	0	6.646532	2.203582	-1.161426
23	1	0	7.450302	0.636717	-0.746766
24	6	0	5.165618	-2.154549	3.149490
25	1	0	6.220658	-1.923460	3.313767
26	1	0	4.972538	-3.228372	3.220457
27	15	0	0.880316	1.533049	0.395949
28	15	0	0.893108	-1.635268	-0.732905
29	46	0	-0.622043	0.120312	-0.635757
30	6	0	1.977763	2.335648	-0.807213
31	6	0	3.089778	3.057755	-0.358232
32	6	0	1.748825	2.181723	-2.176399
33	6	0	3.971314	3.611656	-1.279380
34	1	0	3.276922	3.172688	0.705453
35	6	0	2.642635	2.727307	-3.093400
36	1	0	0.886178	1.618107	-2.521183
37	6	0	3.755390	3.435570	-2.645622
38	6	0	-0.006324	2.837603	1.302787
39	6	0	0.208994	4.188687	1.027589
40	6	0	-0.966092	2.468471	2.253761
41	6	0	-0.521234	5.161397	1.708710
42	6	0	-1.682718	3.441711	2.937448
43	1	0	-1.163963	1.419495	2.452654
44	6	0	-1.462895	4.791538	2.663047
45	6	0	0.326369	-2.830507	-1.990000
46	6	0	0.328168	-4.207996	-1.760380
47	6	0	-0.145486	-2.334863	-3.213945
48	6	0	-0.130799	-5.078634	-2.746819
49	1	0	0.678109	-4.613103	-0.817381
50	6	0	-0.594240	-3.208354	-4.197280
51	1	0	-0.162241	-1.263834	-3.401322
52	6	0	-0.588913	-4.582786	-3.963433
53	6	0	1.112985	-2.534819	0.827799
54	6	0	0.261107	-2.256691	1.899760
55	6	0	2.149272	-3.463452	0.979948
56	6	0	0.453386	-2.892207	3.123064
57	1	0	-0.535476	-1.526093	1.784453

58	6	0	2.326396	-4.107211	2.199495
59	1	0	2.826645	-3.670450	0.156457
60	6	0	1.485728	-3.815069	3.273120
61	8	0	-1.888732	1.707779	-0.722460
62	6	0	-3.253531	1.425052	-0.561568
63	6	0	-4.032747	2.676114	-0.822780
64	6	0	-4.481226	3.700402	-0.047118
65	8	0	-4.308708	2.938046	-2.132547
66	6	0	-5.074817	4.654920	-0.936605
67	1	0	-4.395229	3.777884	1.027620
68	6	0	-4.939833	4.139726	-2.183907
69	1	0	-5.542489	5.593914	-0.676638
70	1	0	-5.231594	4.480893	-3.165931
71	6	0	-3.550496	0.865622	0.837201
72	1	0	-3.604983	1.648320	1.593726
73	1	0	-2.771929	0.152448	1.116031
74	8	0	-4.830142	0.216497	0.867200
75	6	0	-4.866663	-1.070409	0.513366
76	8	0	-3.875717	-1.710365	0.199520
77	1	0	-0.955329	-2.814211	-5.141874
78	1	0	-0.946738	-5.265501	-4.727801
79	1	0	-0.130106	-6.147517	-2.558206
80	1	0	-0.199263	-2.660631	3.958789
81	1	0	1.637765	-4.307396	4.228620
82	1	0	3.127331	-4.830692	2.314112
83	1	0	4.834583	4.168855	-0.929753
84	1	0	4.457155	3.850929	-3.362296
85	1	0	2.473366	2.589735	-4.156516
86	1	0	0.935008	4.494072	0.282129
87	1	0	-0.350082	6.210167	1.488061
88	1	0	-2.029809	5.552197	3.190860
89	1	0	-2.421963	3.145899	3.675007
90	6	0	-6.237705	-1.641584	0.555463
91	6	0	-7.350757	-0.861798	0.886533
92	6	0	-6.398348	-2.996590	0.251154
93	6	0	-8.614856	-1.440270	0.914556
94	1	0	-7.227219	0.190380	1.116875
95	6	0	-7.663641	-3.570185	0.282551
96	1	0	-5.529240	-3.592502	-0.007381
97	6	0	-8.772027	-2.792512	0.614849
98	1	0	-9.478947	-0.835441	1.170971
99	1	0	-7.787133	-4.622992	0.049491
100	1	0	-9.760126	-3.241783	0.639990
101	1	0	-3.598337	0.671559	-1.290520
102	1	0	-2.044205	-1.040307	-0.994402
103	1	0	-1.788121	-0.842338	-1.709687

TS2b(S)₉₀

RwB97XD SCF energy -3379.590743 a.u.
 RwB97XD SCF enthalpy -3378.729511 a.u.
 RwB97XD SCF free energy -3378.876537 a.u.
 Three lowest frequencies (cm⁻¹) -1058, 8.5, 12.2
 Imaginary frequency (cm⁻¹) -1058

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		Z
			X	Y	
1	6	0	3.366652	-0.431277	-0.126704
2	6	0	4.629383	0.020032	-0.439740
3	6	0	5.182410	-0.088116	-1.711687
4	6	0	4.508328	-0.695179	-2.742622
5	6	0	3.223366	-1.176734	-2.452890
6	6	0	2.650558	-1.050034	-1.189383
7	1	0	4.942570	-0.795933	-3.730003
8	1	0	2.673897	-1.659578	-3.252047
9	6	0	2.886621	-0.256447	1.272833
10	6	0	1.879493	0.655557	1.696143
11	6	0	3.490956	-0.987860	2.269970
12	6	0	1.567404	0.788660	3.046418
13	6	0	3.145875	-0.873827	3.612636
14	6	0	2.195931	0.021401	4.038773
15	1	0	0.822968	1.507705	3.363755
16	1	0	1.942319	0.132957	5.086164
17	8	0	6.416918	0.472341	-1.721161
18	8	0	5.504575	0.643518	0.389995
19	8	0	4.465135	-1.921928	2.123385
20	8	0	3.887217	-1.738769	4.348773
21	6	0	6.656815	0.959236	-0.396336
22	1	0	6.793389	2.043252	-0.427704
23	1	0	7.530732	0.454578	0.022937

24	6	0	4.744465	-2.427538	3.432359
25	1	0	5.788074	-2.220663	3.682938
26	1	0	4.526364	-3.497915	3.464748
27	15	0	0.934167	1.534713	0.412205
28	15	0	0.913237	-1.526353	-0.928131
29	46	0	-0.505748	0.252055	-0.884216
30	6	0	2.189722	2.362094	-0.608198
31	6	0	3.250729	3.038541	0.004369
32	6	0	2.129403	2.269171	-2.000914
33	6	0	4.251033	3.606100	-0.776872
34	1	0	3.304419	3.108830	1.087039
35	6	0	3.140557	2.828238	-2.777169
36	1	0	1.305871	1.741435	-2.475054
37	6	0	4.420352	3.489419	-2.165735
38	6	0	-0.059693	2.833222	1.207112
39	6	0	0.104599	4.180326	0.871051
40	6	0	-1.073181	2.462609	2.100343
41	6	0	-0.726814	5.144013	1.436795
42	6	0	-1.886955	3.430908	2.675884
43	1	0	-1.234579	1.415741	2.340786
44	6	0	-1.717553	4.773232	2.341068
45	6	0	0.454625	-2.644990	-2.293736
46	6	0	0.370895	-4.027913	-2.115990
47	6	0	0.167046	-2.088601	-3.547533
48	6	0	0.010639	-4.844535	-3.186224
49	1	0	0.571284	-4.478511	-1.150150
50	6	0	-0.177771	-2.909532	-4.614127
51	1	0	0.210266	-1.012263	-3.690208
52	6	0	-0.258649	-4.289774	-4.433344
53	6	0	0.893087	-2.485044	0.612385
54	6	0	-0.068672	-2.210691	1.587738
55	6	0	1.878166	-3.450682	0.849674
56	6	0	-0.033931	-2.888079	2.803147
57	1	0	-0.826644	-1.453283	1.403607
58	6	0	1.897919	-4.135076	2.059546
59	1	0	2.640872	-3.652408	0.103359
60	6	0	0.949778	-3.846008	3.039846
61	8	0	-2.125146	1.638942	-1.301775
62	6	0	-3.445203	1.429087	-0.823204
63	6	0	-4.160124	2.739728	-0.839685
64	6	0	-4.595844	3.605256	0.115775
65	8	0	-4.426044	3.248311	-2.076504
66	6	0	-5.167723	4.721301	-0.578146
67	1	0	-4.527018	3.473445	1.185885
68	6	0	-5.033641	4.449698	-1.899782
69	1	0	-5.617346	5.602834	-0.144112
70	1	0	-5.307784	4.978440	-2.800392
71	6	0	-3.484779	0.781665	0.566523
72	1	0	-3.430253	1.514909	1.368366
73	1	0	-2.652674	0.079257	0.661358
74	8	0	-4.725827	0.094711	0.765380
75	6	0	-4.792209	-1.168912	0.329234
76	8	0	-3.853180	-1.747365	-0.189320
77	1	0	-0.391550	-2.469733	-5.582959
78	1	0	-0.538908	-4.930531	-5.263680
79	1	0	-0.062194	-5.917150	-3.037766
80	1	0	-0.770975	-2.661616	3.566845
81	1	0	0.979308	-4.367223	3.991566
82	1	0	2.662181	-4.883801	2.241733
83	1	0	5.075223	4.127865	-0.300894
84	1	0	4.995932	3.916789	-2.772057
85	1	0	3.101426	2.737935	-3.858054
86	1	0	0.873132	4.484836	0.168643
87	1	0	-0.594227	6.187621	1.169907
88	1	0	-2.363142	5.527506	2.779956
89	1	0	-2.662502	3.134189	3.374906
90	6	0	-6.124345	-1.786386	0.554415
91	6	0	-7.198140	-1.055113	1.072731
92	6	0	-6.287957	-3.196331	0.229851
93	6	0	-8.427387	-1.676261	1.263948
94	1	0	-7.073064	-0.006476	1.318270
95	6	0	-7.517542	-3.753063	0.426517
96	1	0	-5.448558	-3.693323	-0.173141
97	6	0	-8.587314	-3.023484	0.943541
98	1	0	-9.261860	-1.109105	1.663838
99	1	0	-7.643370	-4.802165	0.178544
100	1	0	-9.548137	-3.505863	1.095642
101	1	0	-3.973149	0.744288	-1.507772
102	1	0	-1.632586	-0.504973	-1.981646
103	1	0	-1.941225	0.378059	-1.914110

6b(S)_{25g}#2b

RwB97XD SCF energy -3379.646893 a.u.

RwB97XD SCF enthalpy -3378.780903 a.u.

RwB97XD SCF free energy -3378.931033 a.u.

Three lowest frequencies (cm⁻¹) 5.5, 11.2 13.6

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.368483	-0.450337	-0.233866
2	6	0	4.598474	-0.027606	-0.689071
3	6	0	5.032575	-0.208499	-1.997363
4	6	0	4.263257	-0.866637	-2.924945
5	6	0	3.017443	-1.337398	-2.484028
6	6	0	2.562534	-1.145208	-1.180295
7	1	0	4.596850	-1.016219	-3.944915
8	1	0	2.397731	-1.866696	-3.198407
9	6	0	3.008420	-0.150816	1.181256
10	6	0	2.069082	0.835335	1.592857
11	6	0	3.662685	-0.821473	2.190770
12	6	0	1.835143	1.062377	2.946252
13	6	0	3.399205	-0.606392	3.538431
14	6	0	2.492223	0.337182	3.953238
15	1	0	1.125148	1.821495	3.252099
16	1	0	2.293966	0.517615	5.003195
17	8	0	6.256902	0.355455	-2.155356
18	8	0	5.544140	0.645078	0.018740
19	8	0	4.606205	-1.790626	2.055236
20	8	0	4.158231	-1.445699	4.291671
21	6	0	6.630725	0.884658	-0.878945
22	1	0	6.801448	1.960262	-0.968442
23	1	0	7.521608	0.364069	-0.516985
24	6	0	4.978236	-2.181844	3.379396
25	1	0	6.029337	-1.931528	3.549881
26	1	0	4.795689	-3.250965	3.510567
27	15	0	1.068924	1.666004	0.301742
28	15	0	0.855583	-1.656815	-0.753130
29	46	0	-0.505591	0.126955	-0.683354
30	6	0	2.293784	2.421362	-0.813174
31	6	0	3.416381	3.098638	-0.323966
32	6	0	2.130079	2.254766	-2.191287
33	6	0	4.365792	3.599076	-1.208893
34	1	0	3.557134	3.221029	0.746200
35	6	0	3.087408	2.748340	-3.073804
36	1	0	1.264670	1.716724	-2.570929
37	6	0	4.207257	3.415197	-2.582316
38	6	0	0.190458	3.032740	1.133797
39	6	0	0.492239	4.378389	0.913470
40	6	0	-0.895929	2.698843	1.954634
41	6	0	-0.277041	5.374015	1.514184
42	6	0	-1.651692	3.693360	2.563868
43	1	0	-1.151448	1.654776	2.115885
44	6	0	-1.345248	5.035252	2.339466
45	6	0	0.414529	-2.908741	-2.011905
46	6	0	0.659396	-4.271699	-1.828388
47	6	0	-0.159656	-2.469346	-3.211409
48	6	0	0.330770	-5.181267	-2.831210
49	1	0	1.092197	-4.640356	-0.905461
50	6	0	-0.471139	-3.378519	-4.216260
51	1	0	-0.363882	-1.412155	-3.358235
52	6	0	-0.229565	-4.737780	-4.025409
53	6	0	0.989810	-2.507946	0.849973
54	6	0	0.065755	-2.216466	1.857784
55	6	0	2.035049	-3.403594	1.104416
56	6	0	0.192445	-2.807065	3.111886
57	1	0	-0.739820	-1.512728	1.663988
58	6	0	2.146271	-4.005365	2.353101
59	1	0	2.778934	-3.610697	0.340863
60	6	0	1.231792	-3.700753	3.359923
61	8	0	-2.043798	1.684903	-0.839957
62	6	0	-3.433760	1.308468	-0.718093
63	6	0	-4.324384	2.472368	-0.966013
64	6	0	-4.818259	3.467581	-0.180504
65	8	0	-4.732908	2.651499	-2.254813
66	6	0	-5.586287	4.314822	-1.040382
67	1	0	-4.657148	3.586616	0.881678
68	6	0	-5.496917	3.770962	-2.280981
69	1	0	-6.132643	5.205963	-0.766926
70	1	0	-5.905275	4.043273	-3.242571
71	6	0	-3.590398	0.748347	0.691842
72	1	0	-3.527525	1.537943	1.441192

73	1	0	-2.816685	0.000101	0.881253
74	8	0	-4.888080	0.173634	0.835403
75	6	0	-5.040873	-1.106498	0.464589
76	8	0	-4.125687	-1.797212	0.057282
77	1	0	-0.912208	-3.024847	-5.142859
78	1	0	-0.484481	-5.450004	-4.803994
79	1	0	0.513318	-6.239494	-2.673036
80	1	0	-0.519184	-2.564898	3.894819
81	1	0	1.332712	-4.158581	4.339062
82	1	0	2.956649	-4.701757	2.543901
83	1	0	5.236872	4.121455	-0.825777
84	1	0	4.958470	3.791744	-3.269831
85	1	0	2.963200	2.601365	-4.142057
86	1	0	1.320207	4.660067	0.271075
87	1	0	-0.038309	6.417531	1.333657
88	1	0	-1.940800	5.814212	2.805518
89	1	0	-2.484695	3.421438	3.205066
90	6	0	-6.441020	-1.577542	0.613303
91	6	0	-7.472487	-0.714209	0.997015
92	6	0	-6.713667	-2.923159	0.350988
93	6	0	-8.768989	-1.201859	1.118636
94	1	0	-7.262693	0.331389	1.192717
95	6	0	-8.010688	-3.405745	0.477313
96	1	0	-5.906275	-3.583294	0.051921
97	6	0	-9.038209	-2.545182	0.861249
98	1	0	-9.570401	-0.532396	1.414519
99	1	0	-8.220303	-4.451585	0.277089
100	1	0	-10.051421	-2.922948	0.960280
101	1	0	-3.647747	0.522660	-1.449985
102	1	0	-1.506690	-0.948391	-1.207633
103	1	0	-1.915900	2.154979	-1.675734

2.11. Catalytic cycle 2b-1b (R)

3b(R)_{reg}

RwB97XD SCF energy -3378.442921 a.u.
 RwB97XD SCF enthalpy -3377.600762 a.u.
 RwB97XD SCF free energy -3377.743934 a.u.
 Three lowest frequencies (cm⁻¹) 17.9, 20.2 26.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.340480	1.478451	-0.306494
2	6	0	2.312675	2.798951	-0.698242
3	6	0	2.316248	3.200770	-2.029268
4	6	0	2.374062	2.289507	-3.054594
5	6	0	2.420233	0.936035	-2.688201
6	6	0	2.404477	0.520177	-1.357846
7	1	0	2.382456	2.595134	-4.094048
8	1	0	2.469312	0.200518	-3.482412
9	6	0	2.321486	1.185035	1.154506
10	6	0	1.209704	0.661448	1.871229
11	6	0	3.434658	1.493096	1.904948
12	6	0	1.289211	0.467128	3.247485
13	6	0	3.514642	1.261127	3.272890
14	6	0	2.452095	0.755088	3.979885
15	1	0	0.433657	0.082167	3.789086
16	1	0	2.504835	0.586503	5.049056
17	8	0	2.255189	4.555010	-2.098153
18	8	0	2.255506	3.890222	0.110499
19	8	0	4.606681	2.016486	1.457725
20	8	0	4.748977	1.609448	3.723582
21	6	0	2.188445	5.030594	-0.749733
22	1	0	1.237917	5.548826	-0.595201
23	1	0	3.041244	5.684395	-0.551074
24	6	0	5.449944	2.157967	2.603692
25	1	0	5.643790	3.220227	2.780269
26	1	0	6.376938	1.601503	2.447797
27	15	0	-0.246850	0.111633	0.904379
28	15	0	2.337340	-1.272841	-0.984069
29	46	0	0.277321	-1.899752	-0.333971
30	6	0	-0.745220	1.596321	-0.028117
31	6	0	-0.898634	2.836684	0.604101
32	6	0	-0.912467	1.502447	-1.412380
33	6	0	-1.208037	3.966421	-0.143175
34	1	0	-0.741817	2.922011	1.676949
35	6	0	-1.220334	2.636122	-2.159310
36	1	0	-0.771377	0.548043	-1.910556
37	6	0	-1.367874	3.867505	-1.525518
38	6	0	-1.573270	-0.234305	2.111827
39	6	0	-2.756076	0.505705	2.163657
40	6	0	-1.433898	-1.357957	2.940239
41	6	0	-3.778625	0.138743	3.037178
42	1	0	-2.890451	1.372559	1.528495
43	6	0	-2.442344	-1.702508	3.832124
44	1	0	-0.535105	-1.967075	2.885735
45	6	0	-3.620572	-0.956967	3.878260
46	6	0	2.916954	-2.085107	-2.516933
47	6	0	4.263369	-2.374854	-2.751260
48	6	0	1.967387	-2.386044	-3.501383
49	6	0	4.652002	-2.958726	-3.955129
50	1	0	5.016519	-2.162995	-2.000940
51	6	0	2.361435	-2.954993	-4.707343
52	1	0	0.916245	-2.176666	-3.321642
53	6	0	3.705713	-3.244225	-4.934855
54	6	0	3.601051	-1.525029	0.301290
55	6	0	3.290748	-2.283747	1.433702
56	6	0	4.851168	-0.903116	0.202480
57	6	0	4.221011	-2.412524	2.461384
58	1	0	2.314247	-2.753438	1.519301
59	6	0	5.784141	-1.051245	1.222800
60	1	0	5.089407	-0.281179	-0.655368
61	6	0	5.466239	-1.796702	2.356631
62	8	0	-1.643366	-2.812580	0.157470
63	6	0	-2.768318	-2.423559	-0.196389
64	1	0	0.722599	-3.223762	-1.031616
65	6	0	-3.921194	-2.819840	0.558151
66	6	0	-4.054598	-3.604706	1.678190
67	8	0	-5.149113	-2.371544	0.160007
68	6	0	-5.435828	-3.630711	1.981822
69	1	0	-3.250492	-4.097936	2.204069

70	6	0	-6.043688	-2.862278	1.028881
71	1	0	-5.922298	-4.144659	2.797286
72	1	0	-7.074325	-2.591833	0.852077
73	6	0	-2.941687	-1.568354	-1.436358
74	1	0	-3.524071	-2.124945	-2.177021
75	1	0	-1.955527	-1.335221	-1.842594
76	8	0	-3.589477	-0.347087	-1.103608
77	6	0	-4.765258	-0.066827	-1.700679
78	8	0	-5.307172	-0.810290	-2.491102
79	1	0	1.617308	-3.180585	-5.464579
80	1	0	4.013338	-3.697925	-5.871909
81	1	0	5.699420	-3.188196	-4.123981
82	1	0	6.752665	-0.568807	1.138632
83	1	0	6.189725	-1.893785	3.160239
84	1	0	3.969486	-2.987952	3.346775
85	1	0	-1.339075	2.566772	-3.235211
86	1	0	-1.606385	4.752805	-2.106987
87	1	0	-1.322758	4.925811	0.351619
88	1	0	-4.696952	0.717438	3.057712
89	1	0	-4.415473	-1.240475	4.560991
90	1	0	-2.316686	-2.565844	4.477892
91	6	0	-5.307317	1.245384	-1.269786
92	6	0	-4.503833	2.203795	-0.645819
93	6	0	-6.655430	1.515742	-1.520604
94	6	0	-5.051587	3.423605	-0.265880
95	1	0	-3.453325	2.002425	-0.476961
96	6	0	-7.201413	2.732221	-1.128330
97	1	0	-7.268270	0.767893	-2.013195
98	6	0	-6.400315	3.685631	-0.500688
99	1	0	-4.422717	4.169385	0.210278
100	1	0	-8.250933	2.937666	-1.313035
101	1	0	-6.828346	4.636322	-0.197502

TS1b(R)_{reg}

RwB97XD SCF energy -3378.427681 a.u.
 RwB97XD SCF enthalpy -3377.588170 a.u.
 RwB97XD SCF free energy -3377.729826 a.u.
 Three lowest frequencies (cm⁻¹) -535.1, 15.6, 22.6
 Imaginary frequency (cm⁻¹) -535.1

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.529956	0.409723	-0.709475
2	6	0	3.343598	1.389596	-1.234928
3	6	0	3.299666	1.784141	-2.567691
4	6	0	2.452103	1.188054	-3.469143
5	6	0	1.626293	0.169957	-2.970878
6	6	0	1.652158	-0.223040	-1.633810
7	1	0	2.415484	1.490111	-4.508921
8	1	0	0.944934	-0.315864	-3.660404
9	6	0	2.656845	0.100430	0.743161
10	6	0	1.694209	0.408034	1.745497
11	6	0	3.819883	-0.487641	1.189053
12	6	0	1.939736	0.096961	3.080414
13	6	0	4.043804	-0.818568	2.520649
14	6	0	3.122285	-0.533629	3.497892
15	1	0	1.207134	0.349193	3.837741
16	1	0	3.296609	-0.777142	4.539249
17	8	0	4.181053	2.795040	-2.773851
18	8	0	4.262073	2.134138	-0.565559
19	8	0	4.878002	-0.885607	0.434047
20	8	0	5.244947	-1.444903	2.637268
21	6	0	4.820561	3.043354	-1.517216
22	1	0	4.618416	4.070975	-1.204461
23	1	0	5.893043	2.854599	-1.612728
24	6	0	5.870323	-1.346663	1.355300
25	1	0	6.683648	-0.612416	1.402562
26	1	0	6.229897	-2.327366	1.047023
27	15	0	0.079494	1.087101	1.218514
28	15	0	0.425114	-1.442805	-1.061297
29	46	0	-1.244473	-0.578135	0.216497
30	6	0	0.507785	2.521382	0.187805
31	6	0	1.451484	3.454325	0.634182
32	6	0	-0.058726	2.655539	-1.080670
33	6	0	1.817414	4.515884	-0.185329
34	1	0	1.909843	3.343293	1.612953
35	6	0	0.321149	3.712628	-1.903265
36	1	0	-0.777847	1.922694	-1.434409
37	6	0	1.258336	4.640747	-1.457089

38	6	0	-0.762002	1.729748	2.702564	7	1	0	-1.413387	4.753150	0.945002
39	6	0	-0.980520	3.095399	2.905571	8	1	0	-0.353128	2.827033	2.103335
40	6	0	-1.274715	0.806200	3.623974	9	6	0	-2.886663	-0.317599	-0.341058
41	6	0	-1.688552	3.528853	4.024235	10	6	0	-2.095239	-1.262489	-1.055632
42	1	0	-0.611393	3.825740	2.194171	11	6	0	-4.145054	-0.741911	0.018662
43	6	0	-1.967323	1.244849	4.746695	12	6	0	-2.596106	-2.529318	-1.349767
44	1	0	-1.133190	-0.258145	3.460750	13	6	0	-4.623917	-2.020021	-0.253872
45	6	0	-2.177533	2.608049	4.946677	14	6	0	-3.875664	-2.938403	-0.948829
46	6	0	-0.111233	-2.333774	-2.562307	15	1	0	-1.993113	-3.235416	-1.907256
47	6	0	0.755927	-3.223350	-3.208844	16	1	0	-4.249304	-3.930697	-1.171020
48	6	0	-1.384173	-2.106442	-3.091489	17	8	0	-3.374731	4.319302	-0.999016
49	6	0	0.345964	-3.882605	-4.361890	18	8	0	-3.996799	2.153674	-1.491867
50	1	0	1.750503	-3.408965	-2.817809	19	8	0	-5.072690	-0.045191	0.723242
51	6	0	-1.788109	-2.765034	-4.250676	20	8	0	-5.862869	-2.164239	0.274001
52	1	0	-2.063380	-1.411466	-2.607900	21	6	0	-4.241311	3.525490	-1.815763
53	6	0	-0.926353	-3.655081	-4.884473	22	1	0	-4.008664	3.699719	-2.869433
54	6	0	1.344689	-2.650427	-0.047792	23	1	0	-5.282379	3.768276	-1.587492
55	6	0	0.725092	-3.215861	1.071933	24	6	0	-6.201392	-0.910180	0.877007
56	6	0	2.664147	-2.997691	-0.357095	25	1	0	-7.062427	-0.479275	0.359261
57	6	0	1.423562	-4.111012	1.877360	26	1	0	-6.402579	-1.062604	1.939724
58	1	0	-0.299772	-2.950492	1.322668	27	15	0	-0.384062	-0.839504	-1.505263
59	6	0	3.357254	-3.893796	0.449420	28	15	0	-0.527277	-0.066691	1.742139
60	1	0	3.166626	-2.543483	-1.205630	29	46	0	1.059625	-0.771923	0.224686
61	6	0	2.740320	-4.445910	1.570165	30	6	0	-0.505501	0.766016	-2.341222
62	8	0	-2.977774	-0.517972	1.437873	31	6	0	-1.509861	0.961100	-3.297610
63	6	0	-3.429682	-1.410835	0.629234	32	6	0	0.333303	1.822751	-1.978709
64	1	0	-2.215974	-1.702323	-0.424821	33	6	0	-1.670133	2.099905	-3.886371
65	6	0	-3.483802	-2.808639	1.089264	34	1	0	-2.176060	0.147880	-3.570620
66	6	0	-3.103262	-3.400807	2.254687	35	6	0	0.150158	3.075806	-2.555318
67	8	0	-3.951427	-3.736052	0.212127	36	1	0	1.108005	1.673822	-1.230946
68	6	0	-3.359386	-4.795499	2.084525	37	6	0	-0.850055	3.270192	-3.504829
69	1	0	-2.694906	-2.903567	3.122518	38	6	0	0.188739	-2.090187	-2.689710
70	6	0	-3.869340	-4.938526	0.832875	39	6	0	0.318481	-1.807299	-4.050718
71	1	0	-3.192113	-5.584072	2.803550	40	6	0	0.525504	-3.361756	-2.206185
72	1	0	-4.215232	-5.788467	0.264370	41	6	0	0.763939	-2.797563	-4.924004
73	6	0	-4.492878	-0.972463	-0.388928	42	1	0	0.081142	-0.822924	-4.439081
74	1	0	-5.470122	-1.230418	0.026794	43	6	0	0.955759	-4.348146	-3.084497
75	1	0	-4.372509	-1.452939	-1.360014	44	1	0	0.456507	-3.577963	-1.143669
76	8	0	-4.456966	0.440716	-0.486037	45	6	0	1.077211	-4.085667	-4.444917
77	6	0	-3.791286	1.010106	-1.502231	46	6	0	0.359424	0.553425	3.206392
78	8	0	-3.446732	0.410753	-2.502824	47	6	0	-0.164108	0.458306	4.499721
79	1	0	-2.778944	-2.581130	-4.654156	48	6	0	1.619006	1.132105	3.011410
80	1	0	-1.243673	-4.172011	-5.784868	49	6	0	0.563838	0.949254	5.579362
81	1	0	1.022058	-4.575681	-4.852479	50	1	0	-1.130826	-0.001602	4.672997
82	1	0	4.384276	-4.149546	0.208818	51	6	0	2.343817	1.620084	4.093955
83	1	0	3.288157	-5.134259	2.206270	52	1	0	2.039201	1.203761	2.011991
84	1	0	0.939587	-4.540117	2.749161	53	6	0	1.814336	1.530620	5.379079
85	1	0	-0.112619	3.805520	-2.893491	54	6	0	-1.744097	-1.279046	2.329440
86	1	0	1.557099	5.461625	-2.101840	55	6	0	-1.521755	-2.637268	2.090070
87	1	0	2.547292	5.239601	0.163593	56	6	0	-2.905164	-0.866205	2.993680
88	1	0	-1.855629	4.591128	4.172973	57	6	0	-2.460777	-3.577589	2.505611
89	1	0	-2.726065	2.950957	5.818573	58	1	0	-0.625723	-2.956716	1.563996
90	1	0	-2.350539	0.521030	5.459121	59	6	0	-3.834667	-1.810473	3.414889
91	6	0	-3.535895	2.450655	-1.258590	60	1	0	-3.094576	0.189973	3.162350
92	6	0	-3.442929	2.955493	0.042490	61	6	0	-3.616221	-3.164699	3.164756
93	6	0	-3.310777	3.284304	-2.357051	62	8	0	2.582667	-1.288604	-0.991422
94	6	0	-3.122399	4.294906	0.237834	63	6	0	3.629622	-1.289113	-0.083270
95	1	0	-3.601546	2.299824	0.892195	64	6	0	4.145173	-2.677978	0.162687
96	6	0	-3.012210	4.626005	-2.154724	65	6	0	3.963875	-3.858807	-0.484089
97	1	0	-3.376932	2.876282	-3.360596	66	8	0	4.967756	-2.851322	1.234201
98	6	0	-2.911745	5.129667	-0.857976	67	6	0	4.729347	-4.832670	0.240724
99	1	0	-3.035749	4.686307	1.246347	68	1	0	3.364805	-4.015186	-1.369694
100	1	0	-2.846536	5.277945	-3.006369	69	6	0	5.314115	-4.167980	1.266927
101	1	0	-2.667002	6.175721	-0.701331	70	1	0	4.827866	-5.886563	0.021392
						71	1	0	5.971968	-4.463215	2.070291
						72	6	0	4.766293	-0.370786	-0.554718
						73	1	0	5.141191	-0.724538	-1.516554
						74	1	0	5.578726	-0.336393	0.174389
						75	8	0	4.274890	0.951521	-0.809779
						76	6	0	4.112457	1.760848	0.240299
						77	8	0	4.372140	1.432399	1.384319
						78	1	0	3.321262	2.061921	3.928573
						79	1	0	2.378089	1.908456	6.226387
						80	1	0	0.151781	0.872207	6.580560
						81	1	0	-4.733932	-1.487946	3.929962
						82	1	0	-4.349750	-3.898678	3.483292
						83	1	0	-2.291898	-4.631330	2.307784
						84	1	0	0.784800	3.901631	-2.253829
						85	1	0	-0.991809	4.250736	-3.948723
						86	1	0	-2.446958	2.357667	-4.629746
						87	1	0	0.866908	-2.572584	-5.980676
						88	1	0	1.423007	-4.833624	-5.129787

4b(R) _{avg}					
Center	Atomic	Atomic	Coordinates		(Angstroms)
Number	Number	Type	X	Y	Z
1	6	0	-2.452263	1.050011	0.055685
2	6	0	-3.033503	2.148656	-0.536122
3	6	0	-2.660678	3.455001	-0.233711
4	6	0	-1.701497	3.735604	0.709113
5	6	0	-1.111125	2.635910	1.351407
6	6	0	-1.468599	1.326044	1.044167

RwB97XD SCF energy	-3378.439960 a.u.
RwB97XD SCF enthalpy	-3377.595368 a.u.
RwB97XD SCF free energy	-3377.738241 a.u.
Three lowest frequencies (cm ⁻¹)	13.9, 23.7, 25.8
Cartesian coordinates:	

89	1	0	1.208002	-5.332960	-2.704364
90	6	0	3.577451	3.094522	-0.140278
91	6	0	3.678139	3.578079	-1.448494
92	6	0	2.982571	3.878375	0.852996
93	6	0	3.200405	4.848865	-1.751767
94	1	0	4.140548	2.970634	-2.218818
95	6	0	2.476898	5.133765	0.536450
96	1	0	2.912827	3.499265	1.866985
97	6	0	2.593692	5.623260	-0.763620
98	1	0	3.293508	5.232241	-2.762845
99	1	0	2.002165	5.734660	1.305617
100	1	0	2.210701	6.609423	-1.007553
101	1	0	3.298685	-0.895095	0.913530

5b(R)_{reg}

RwB97XD SCF energy -3379.622481 a.u.

RwB97XD SCF enthalpy -3378.759462 a.u.

RwB97XD SCF free energy -3378.903359 a.u.

Three lowest frequencies (cm⁻¹) 12.1, 23.4 26.5

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.478601	0.485476	0.753092
2	6	0	2.987655	0.944309	1.947749
3	6	0	2.742053	2.223358	2.436134
4	6	0	2.000586	3.135928	1.725600
5	6	0	1.501089	2.710613	0.485421
6	6	0	1.726788	1.425432	-0.005158
7	1	0	1.810305	4.134926	2.099287
8	1	0	0.919600	3.419674	-0.092313
9	6	0	2.746631	-0.918778	0.345982
10	6	0	1.761794	-1.940532	0.249805
11	6	0	4.029952	-1.285761	0.015788
12	6	0	2.111278	-3.222783	-0.168319
13	6	0	4.362834	-2.561552	-0.428889
14	6	0	3.424678	-3.559181	-0.526883
15	1	0	1.360039	-4.000440	-0.222343
16	1	0	3.680174	-4.555077	-0.868516
17	8	0	3.327327	2.366752	3.651432
18	8	0	3.750176	0.252650	2.832039
19	8	0	5.127299	-0.486247	-0.023402
20	8	0	5.678269	-2.597809	-0.757460
21	6	0	4.004285	1.135767	3.927997
22	1	0	3.604491	0.699414	4.846543
23	1	0	5.078966	1.321242	4.003197
24	6	0	6.226526	-1.337129	-0.359562
25	1	0	6.859503	-1.478701	0.522265
26	1	0	6.781716	-0.902680	-1.191636
27	15	0	0.028681	-1.542089	0.650026
28	15	0	0.847913	0.871917	-1.506731
29	46	0	-1.110686	-0.134688	-0.780375
30	6	0	0.120779	-0.854941	2.328490
31	6	0	0.942364	-1.465292	3.284099
32	6	0	-0.545284	0.333315	2.634602
33	6	0	1.094022	-0.883641	4.537828
34	1	0	1.476205	-2.380674	3.045690
35	6	0	-0.375878	0.918718	3.885709
36	1	0	-1.174320	0.806450	1.886475
37	6	0	0.445965	0.314442	4.834031
38	6	0	-0.844577	-3.136159	0.690966
39	6	0	-1.208528	-3.744515	1.892458
40	6	0	-1.137570	-3.763896	-0.527056
41	6	0	-1.844017	-4.985442	1.874708
42	1	0	-1.005247	-3.261044	2.842038
43	6	0	-1.762337	-5.004348	-0.537299
44	1	0	-0.877649	-3.281439	-1.465713
45	6	0	-2.113615	-5.617976	0.664986
46	6	0	0.511104	2.354153	-2.522515
47	6	0	1.259267	2.634481	-3.670722
48	6	0	-0.530009	3.216245	-2.157183
49	6	0	0.973857	3.765188	-4.431928
50	1	0	2.060446	1.976288	-3.985939
51	6	0	-0.804585	4.348425	-2.914844
52	1	0	-1.129137	3.006630	-1.276379
53	6	0	-0.053841	4.624029	-4.055557
54	6	0	1.984972	-0.138992	-2.496749
55	6	0	1.494463	-1.284117	-3.126566
56	6	0	3.328067	0.224272	-2.649964
57	6	0	2.345086	-2.069911	-3.899583

58	1	0	0.452773	-1.567577	-3.001580
59	6	0	4.172427	-0.562182	-3.425276
60	1	0	3.717390	1.107514	-2.151898
61	6	0	3.682205	-1.710880	-4.045987
62	8	0	-2.754594	-0.922982	0.122874
63	6	0	-4.039822	-0.620146	-0.323647
64	6	0	-4.825906	-1.888052	-0.514846
65	6	0	-4.741905	-3.115466	0.061346
66	8	0	-5.854598	-1.861805	-1.408440
67	6	0	-5.786055	-3.907069	-0.522309
68	1	0	-4.019549	-3.420436	0.804794
69	6	0	-6.427339	-3.097610	-1.400926
70	1	0	-6.018524	-4.942014	-0.314480
71	1	0	-7.261524	-3.235784	-2.072157
72	6	0	-4.777746	0.249890	0.708013
73	1	0	-4.914064	-0.310618	1.634627
74	1	0	-5.750221	0.574135	0.325771
75	8	0	-4.004221	1.392979	1.105221
76	6	0	-3.872594	2.404735	0.249648
77	8	0	-4.403200	2.435818	-0.847418
78	1	0	-1.609346	5.012975	-2.619410
79	1	0	-0.274423	5.504328	-4.651340
80	1	0	1.657832	3.969294	-5.323838
81	1	0	5.214991	-0.283024	-3.539831
82	1	0	4.345538	-2.328209	-4.643787
83	1	0	1.962815	-2.965251	-4.379385
84	1	0	-0.876830	1.852626	4.119494
85	1	0	0.583387	0.779001	5.805566
86	1	0	1.733047	-1.356845	5.276444
87	1	0	-2.125691	-5.455570	2.811506
88	1	0	-2.606906	-6.584821	0.656091
89	1	0	-1.982861	-5.488480	-1.483217
90	6	0	-2.986616	3.479195	0.776591
91	6	0	-2.350844	3.361410	2.015824
92	6	0	-2.763351	4.607950	-0.015812
93	6	0	-1.461576	4.343837	2.436032
94	1	0	-2.558803	2.505660	2.646817
95	6	0	-1.877011	5.591456	0.408349
96	1	0	-3.274189	4.698121	-0.968956
97	6	0	-1.216674	5.454044	1.628923
98	1	0	-0.960302	4.243494	3.393487
99	1	0	-1.696764	6.462286	-0.213716
100	1	0	-0.517297	6.217533	1.955726
101	1	0	-4.046623	-0.087219	-1.282718
102	1	0	-1.958599	0.528496	-2.284304
103	1	0	-2.219519	1.017302	-1.728883

TS2b(R)_{reg}

RwB97XD SCF energy -3379.605276 a.u.

RwB97XD SCF enthalpy -3378.745744 a.u.

RwB97XD SCF free energy -3378.889828 a.u.

Three lowest frequencies (cm⁻¹) -1094, 16.1, 21.3

Imaginary frequency (cm⁻¹) -1094

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.419553	0.498405	0.981311
2	6	0	2.818332	0.833530	2.255665
3	6	0	2.450475	2.023023	2.877650
4	6	0	1.683845	2.967344	2.238757
5	6	0	1.279430	2.663900	0.930260
6	6	0	1.625275	1.467102	0.306735
7	1	0	1.406851	3.899135	2.717381
8	1	0	0.676542	3.392494	0.400517
9	6	0	2.850301	-0.803053	0.403503
10	6	0	1.986926	-1.893371	0.104829
11	6	0	4.182407	-0.994484	0.116660
12	6	0	2.491445	-3.063175	-0.457572
13	6	0	4.671240	-2.154670	-0.475547
14	6	0	3.850457	-3.215282	-0.770966
15	1	0	1.829805	-3.895126	-0.664473
16	1	0	4.229371	-4.123167	-1.224718
17	8	0	2.968122	2.060419	4.129990
18	8	0	3.585264	0.093565	3.096890
19	8	0	5.192996	-0.100324	0.275238
20	8	0	6.001196	-2.016224	-0.710781
21	6	0	3.661024	0.822760	4.324912
22	1	0	3.171447	0.253832	5.120361
23	1	0	4.708236	1.026846	4.559195

24	6	0	6.392282	-0.798732	-0.070378
25	1	0	6.952038	-1.030821	0.842105
26	1	0	6.979742	-0.194382	-0.762273
27	15	0	0.198461	-1.677986	0.391927
28	15	0	0.916807	1.082851	-1.325703
29	46	0	-0.862850	-0.332974	-1.172921
30	6	0	0.085858	-1.143406	2.122738
31	6	0	0.827316	-1.794358	3.115945
32	6	0	-0.681298	-0.023755	2.444806
33	6	0	0.792356	-1.320037	4.422569
34	1	0	1.439658	-2.657044	2.869077
35	6	0	-0.703126	0.455133	3.750894
36	1	0	-1.242034	0.482155	1.666943
37	6	0	0.036908	-0.190521	4.738542
38	6	0	-0.571298	-3.319897	0.253933
39	6	0	-1.121345	-3.972630	1.360440
40	6	0	-0.632915	-3.925590	-1.009199
41	6	0	-1.692915	-5.233949	1.209229
42	1	0	-1.104149	-3.507576	2.340303
43	6	0	-1.185623	-5.193542	-1.149414
44	1	0	-0.242999	-3.409938	-1.882670
45	6	0	-1.713472	-5.850585	-0.038322
46	6	0	0.369739	2.679129	-2.019003
47	6	0	1.254138	3.519014	-2.704269
48	6	0	-0.950944	3.089829	-1.811465
49	6	0	0.814764	4.753266	-3.173819
50	1	0	2.281055	3.218277	-2.881760
51	6	0	-1.382843	4.328288	-2.274060
52	1	0	-1.644493	2.441947	-1.286032
53	6	0	-0.500030	5.160503	-2.957298
54	6	0	2.284591	0.472224	-2.353028
55	6	0	2.068669	-0.601191	-3.221375
56	6	0	3.558317	1.043643	-2.250962
57	6	0	3.125117	-1.106822	-3.974032
58	1	0	1.082380	-1.051851	-3.296758
59	6	0	4.607350	0.539630	-3.011516
60	1	0	3.741258	1.857904	-1.556139
61	6	0	4.392798	-0.539621	-3.866930
62	8	0	-2.743287	-1.344761	-1.453093
63	6	0	-3.930724	-0.990460	-0.787281
64	6	0	-4.784700	-2.221449	-0.692953
65	6	0	-4.511665	-3.548999	-0.766090
66	8	0	-6.107991	-2.027600	-0.436953
67	6	0	-5.756882	-4.226656	-0.541913
68	1	0	-3.546474	-3.991727	-0.960507
69	6	0	-6.684583	-3.258026	-0.347811
70	1	0	-5.930128	-5.293491	-0.530815
71	1	0	-7.745969	-3.268602	-0.150448
72	6	0	-3.726060	-0.447752	0.629926
73	1	0	-2.985358	-1.057144	1.154389
74	1	0	-4.668804	-0.457487	1.181055
75	8	0	-3.197935	0.890279	0.644347
76	6	0	-4.077873	1.892800	0.503260
77	8	0	-5.251177	1.712187	0.240088
78	1	0	-2.409017	4.636067	-2.100627
79	1	0	-0.837569	6.124090	-3.326526
80	1	0	1.503104	5.396195	-3.713071
81	1	0	5.594358	0.982413	-2.924305
82	1	0	5.217035	-0.942265	-4.447399
83	1	0	2.957656	-1.948382	-4.638657
84	1	0	-1.288385	1.337273	3.991968
85	1	0	0.028023	0.186650	5.756523
86	1	0	1.365853	-1.824761	5.193551
87	1	0	-2.118945	-5.733955	2.073147
88	1	0	-2.154660	-6.836075	-0.150233
89	1	0	-1.217881	-5.661478	-2.127900
90	6	0	-3.470782	3.235253	0.705255
91	6	0	-2.224219	3.406414	1.314826
92	6	0	-4.194660	4.351351	0.274882
93	6	0	-1.706412	4.685064	1.486504
94	1	0	-1.656583	2.548318	1.654256
95	6	0	-3.667869	5.627600	0.438661
96	1	0	-5.163445	4.209980	-0.192860
97	6	0	-2.423033	5.795065	1.043376
98	1	0	-0.739516	4.813117	1.963262
99	1	0	-4.227084	6.491469	0.093881
100	1	0	-2.011235	6.791486	1.171172
101	1	0	-4.484431	-0.228609	-1.357661
102	1	0	-2.319645	-0.211591	-2.215048
103	1	0	-1.754925	0.469773	-2.468192

6b(R)_{avg}*2b

RwB97XD SCF energy	-3379.661183 a.u.
RwB97XD SCF enthalpy	-3378.794609 a.u.
RwB97XD SCF free energy	-3378.935756 a.u.
Three lowest frequencies (cm ⁻¹)	21.4, 26.5, 32.9

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X	Coordinates Y	Coordinates Z (Angstroms)
1	6	0	2.400428	-0.599394	0.927591
2	6	0	2.895687	-0.824629	2.194587
3	6	0	2.968850	0.159940	3.171989
4	6	0	2.581887	1.453247	2.918410
5	6	0	2.118355	1.721679	1.623554
6	6	0	2.031798	0.741891	0.634928
7	1	0	2.626540	2.225768	3.676873
8	1	0	1.824218	2.736728	1.392955
9	6	0	2.240480	-1.774625	0.028111
10	6	0	0.989663	-2.391541	-0.255261
11	6	0	3.354426	-2.378927	-0.508342
12	6	0	0.939246	-3.539450	-1.041346
13	6	0	3.287280	-3.510186	-1.312988
14	6	0	2.091429	-4.124082	-1.592029
15	1	0	-0.013410	-0.014195	-1.244186
16	1	0	2.036160	-5.016804	-2.203873
17	8	0	3.427760	-0.377351	4.330664
18	8	0	3.318277	-2.011225	2.706441
19	8	0	4.649831	-1.989826	-0.367324
20	8	0	4.538051	-3.860894	-1.713009
21	6	0	3.703590	-1.755231	4.059334
22	1	0	3.112948	-2.383025	4.730594
23	1	0	4.775331	-1.939843	4.174607
24	6	0	5.432187	-2.896283	-1.149530
25	1	0	6.152146	-3.403167	-0.502039
26	1	0	5.932157	-2.350610	-1.954651
27	15	0	-0.545174	-1.546226	0.298010
28	15	0	1.254806	1.175652	-0.964942
29	46	0	-0.887603	0.504833	-0.962061
30	6	0	-0.377169	-1.438886	2.109998
31	6	0	0.129861	-2.505341	2.861678
32	6	0	-0.731295	-0.248491	2.749658
33	6	0	0.283028	-2.375555	4.237861
34	1	0	0.416191	-3.430754	2.370112
35	6	0	-0.565423	-0.117384	4.126465
36	1	0	-1.124487	0.581009	2.169430
37	6	0	-0.053145	-1.178014	4.869327
38	6	0	-1.891887	-2.741704	-0.009749
39	6	0	-2.533719	-3.444641	1.012610
40	6	0	-2.319506	-2.917148	-1.333380
41	6	0	-3.572489	-4.324114	0.712744
42	1	0	-2.232045	-3.312243	2.046213
43	6	0	-3.350096	-3.801278	-1.630243
44	1	0	-1.841077	-2.362634	-2.135845
45	6	0	-3.976977	-4.508829	-0.605591
46	6	0	1.641082	2.951870	-1.219038
47	6	0	2.903988	3.457223	-0.873402
48	6	0	0.713957	3.808861	-1.816851
49	6	0	3.221645	4.787785	-1.119347
50	1	0	3.640638	2.822612	-0.392111
51	6	0	1.038995	5.138811	-2.072022
52	1	0	-0.273465	3.444391	-2.078512
53	6	0	2.290764	5.632429	-1.720745
54	6	0	2.210838	0.295555	-2.254028
55	6	0	1.542442	-0.545139	-3.148984
56	6	0	3.602010	0.418891	-2.332527
57	6	0	2.258658	-1.273528	-4.094538
58	1	0	0.462035	-0.647465	-3.089085
59	6	0	4.312862	-0.300345	-3.287158
60	1	0	4.142395	1.055698	-1.640498
61	6	0	3.644429	-1.155199	-4.162040
62	8	0	-3.003406	0.039692	-1.358451
63	6	0	-4.169867	0.421568	-0.607061
64	6	0	-5.166930	-0.688772	-0.613719
65	6	0	-5.767300	-1.432496	0.352291
66	8	0	-5.639815	-1.045838	-1.839942
67	6	0	-6.677270	-2.308974	-0.324185
68	1	0	-5.591714	-1.368524	1.416799
69	6	0	-6.550484	-2.035517	-1.645763
70	1	0	-7.327366	-3.048756	0.120012
71	1	0	-7.009391	-2.436379	-2.536769
72	6	0	-3.772666	0.760599	0.820762

73	1	0	-3.311139	-0.101519	1.306509
74	1	0	-4.660799	1.065767	1.378279
75	8	0	-2.779842	1.788523	0.888858
76	6	0	-3.158933	3.041653	0.592927
77	8	0	-4.284964	3.321136	0.229526
78	1	0	0.302585	5.790095	-2.531695
79	1	0	2.538969	6.672459	-1.908671
80	1	0	4.200053	5.164515	-0.837979
81	1	0	5.392177	-0.198494	-3.341349
82	1	0	4.204290	-1.726760	-4.895863
83	1	0	1.732052	-1.936394	-4.773905
84	1	0	-0.826282	0.816556	4.614735
85	1	0	0.085201	-1.073022	5.940991
86	1	0	0.674961	-3.206159	4.816736
87	1	0	-4.065264	-4.863352	1.515866
88	1	0	-4.787355	-5.193450	-0.835879
89	1	0	-3.669278	-3.931455	-2.659602
90	6	0	-2.070036	4.037119	0.765087
91	6	0	-0.913924	3.759652	1.501155
92	6	0	-2.252362	5.303464	0.199958
93	6	0	0.040417	4.756053	1.683895
94	1	0	-0.765724	2.780632	1.944238
95	6	0	-1.283094	6.284846	0.363877
96	1	0	-3.156613	5.510158	-0.362977
97	6	0	-0.138251	6.013068	1.111423
98	1	0	0.926061	4.554679	2.278201
99	1	0	-1.421886	7.262209	-0.086973
100	1	0	0.616288	6.781715	1.247181
101	1	0	-4.600952	1.305293	-1.084441
102	1	0	-3.173190	0.204066	-2.293398
103	1	0	-1.028580	1.730173	-1.907440

2.12. Catalytic cycle 2b-1c(S)

3c(S)_{seg}	
RwB97XD SCF energy	-3186.757722 a.u.
RwB97XD SCF enthalpy	-3185.973717 a.u.
RwB97XD SCF free energy	-3186.114192 a.u.
Three lowest frequencies (cm ⁻¹)	11.5, 14.8 29.8

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates		Z (Angstroms)
			X	Y	
1	6	0	-2.317207	-0.789135	0.713928
2	6	0	-3.316728	-0.725265	1.660516
3	6	0	-3.208289	-1.305354	2.921709
4	6	0	-2.094415	-2.016488	3.296092
5	6	0	-1.069956	-2.123153	2.343821
6	6	0	-1.160401	-1.535113	1.083418
7	1	0	-2.008234	-2.475787	4.273572
8	1	0	-0.183021	-2.684216	2.614633
9	6	0	-2.523454	-0.095979	-0.589485
10	6	0	-1.878645	1.113775	-0.970055
11	6	0	-3.418464	-0.616561	-1.498658
12	6	0	-2.136254	1.691605	-2.210009
13	6	0	-3.650136	-0.042279	-2.745241
14	6	0	-3.025920	1.118193	-3.132470
15	1	0	-1.637788	2.612947	-2.488455
16	1	0	-3.207296	1.572347	-4.099503
17	8	0	-4.330642	-1.057218	3.636954
18	8	0	-4.515081	-0.099640	1.547230
19	8	0	-4.154943	-1.749370	-1.372043
20	8	0	-4.532536	-0.802810	-3.440419
21	6	0	-5.168527	-0.245429	2.808877
22	1	0	-5.295787	0.737469	3.272473
23	1	0	-6.130267	-0.744504	2.664195
24	6	0	-4.943729	-1.850066	-2.558541
25	1	0	-6.001125	-1.718247	-2.305680
26	1	0	-4.767673	-2.817711	-3.034243
27	15	0	-0.570904	1.792164	0.118105
28	15	0	0.295472	-1.600320	-0.024008
29	46	0	1.359211	0.370517	0.029800
30	6	0	-1.373020	2.030796	1.734581
31	6	0	-2.664707	2.556377	1.850682
32	6	0	-0.686814	1.618590	2.881200
33	6	0	-3.256300	2.677471	3.103704
34	1	0	-3.213750	2.854586	0.962228
35	6	0	-1.288242	1.726753	4.132191
36	1	0	0.309594	1.193095	2.790154
37	6	0	-2.572311	2.255549	4.243414
38	6	0	-0.187313	3.443532	-0.558377
39	6	0	-0.756246	4.623987	-0.073577
40	6	0	0.736097	3.505724	-1.611443
41	6	0	-0.413659	5.849327	-0.641330
42	6	0	1.064674	4.730125	-2.183853
43	1	0	1.203707	2.597992	-1.985839
44	6	0	0.491654	5.904219	-1.697921
45	6	0	1.312869	-2.990808	0.596212
46	6	0	1.125559	-4.305302	0.161868
47	6	0	2.299617	-2.718402	1.552580
48	6	0	1.921467	-5.328561	0.672869
49	1	0	0.376249	-4.542801	-0.584520
50	6	0	3.082713	-3.743500	2.070027
51	1	0	2.459220	-1.697326	1.887405
52	6	0	2.896779	-5.051945	1.626749
53	6	0	-0.341460	-2.058805	-1.663840
54	6	0	0.096186	-1.352797	-2.788083
55	6	0	-1.305324	-3.064210	-1.803821
56	6	0	-0.426400	-1.651883	-4.043207
57	1	0	0.828860	-0.557257	-2.681349
58	6	0	-1.812984	-3.367910	-3.062262
59	1	0	-1.685559	-3.587266	-0.931549
60	6	0	-1.379507	-2.658406	-4.181121
61	8	0	2.772297	2.051328	0.454081
62	6	0	3.869380	1.518629	0.208031
63	1	0	2.528830	-0.634870	-0.215184
64	6	0	4.586807	0.751368	1.194186
65	6	0	5.792800	0.095364	1.156722
66	8	0	3.974246	0.523381	2.390046
67	6	0	5.920999	-0.573024	2.399252
68	1	0	6.495675	0.093225	0.335606
69	6	0	4.786327	-0.275751	3.099087

70	1	0	6.740577	-1.190615	2.734905
71	1	0	4.441271	-0.550069	4.085353
72	6	0	4.518161	1.709107	-1.160068
73	1	0	5.541895	2.070170	-1.044687
74	1	0	3.924266	2.425298	-1.727633
75	8	0	4.598550	0.455653	-1.840789
76	6	0	3.594847	0.150360	-2.690569
77	8	0	2.705340	0.924051	-2.974360
78	1	0	3.844884	-3.515662	2.808660
79	1	0	3.516257	-5.852453	2.019065
80	1	0	1.777707	-6.344208	0.318081
81	1	0	-0.093150	-1.091383	-4.910997
82	1	0	-1.792944	-2.884411	-5.159081
83	1	0	-2.561658	-4.147008	-3.164951
84	1	0	-4.255976	3.091880	3.190462
85	1	0	-3.043274	2.337698	5.218103
86	1	0	-0.757312	1.392022	5.017793
87	1	0	-1.464256	4.597953	0.748005
88	1	0	-0.857951	6.761295	-0.254881
89	1	0	0.753446	6.860554	-2.140193
90	1	0	1.778230	4.766557	-3.001408
91	6	0	3.723992	-1.251888	-3.196174
92	1	0	3.327873	-1.927088	-2.428768
93	1	0	3.141690	-1.371910	-4.109285
94	1	0	4.769628	-1.511761	-3.370007

TS1c(S)_{neg}

RwB97XD SCF energy -3186.752423 a.u.
RwB97XD SCF enthalpy -3185.969864 a.u.
RwB97XD SCF free energy -3186.105342 a.u.
Three lowest frequencies (cm⁻¹) -488.3, 17.6, 26.3
Imaginary frequency (cm⁻¹) -488.3

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.048332	-0.818546	1.115404
2	6	0	-2.933237	-0.624588	2.153038
3	6	0	-2.576532	-0.746709	3.491707
4	6	0	-1.307058	-1.110242	3.868464
5	6	0	-0.387158	-1.338252	2.834006
6	6	0	-0.728471	-1.199011	1.490428
7	1	0	-1.027687	-1.218248	4.909751
8	1	0	0.620099	-1.629628	3.108082
9	6	0	-2.544726	-0.631447	-0.277973
10	6	0	-2.222632	0.468322	-1.120830
11	6	0	-3.421075	-1.554455	-0.803572
12	6	0	-2.767958	0.567338	-2.397998
13	6	0	-3.943167	-1.457644	-2.089193
14	6	0	-3.642927	-0.401395	-2.913563
15	1	0	-2.515356	1.411758	-3.029386
16	1	0	-4.057842	-0.317716	-3.911026
17	8	0	-3.647462	-0.467668	4.277157
18	8	0	-4.242491	-0.273044	2.057613
19	8	0	-3.887018	-2.679623	-0.201244
20	8	0	-4.744143	-2.525913	-2.337028
21	6	0	-4.721403	-0.121316	3.396613
22	1	0	-5.008930	0.919648	3.567277
23	1	0	-5.558991	-0.803315	3.560286
24	6	0	-4.716409	-3.340626	-1.161383
25	1	0	-5.728219	-3.436631	-0.759367
26	1	0	-4.286410	-4.315924	-1.404034
27	15	0	-0.957098	1.658835	-0.563899
28	15	0	0.566762	-1.332002	0.208734
29	46	0	1.205838	0.733989	-0.474096
30	6	0	-1.536104	2.272028	1.046893
31	6	0	-2.884131	2.568758	1.275567
32	6	0	-0.611799	2.382368	2.090313
33	6	0	-3.299527	2.972947	2.540102
34	1	0	-3.611385	2.465375	0.475241
35	6	0	-1.035372	2.772615	3.357415
36	1	0	0.435503	2.149514	1.913953
37	6	0	-2.378718	3.063613	3.583186
38	6	0	-1.001531	3.044587	-1.744062
39	6	0	-1.703664	4.226838	-1.496202
40	6	0	-0.287567	2.901123	-2.941231
41	6	0	-1.700484	5.248202	-2.443003
42	6	0	-0.299187	3.918388	-3.889178
43	1	0	0.273330	1.989786	-3.134449
44	6	0	-1.005371	5.093890	-3.639675

45	6	0	1.964655	-2.231670	0.971692
46	6	0	2.204258	-3.587998	0.741127
47	6	0	2.834275	-1.510272	1.801982
48	6	0	3.295091	-4.214396	1.342120
49	1	0	1.557827	-4.164367	0.088689
50	6	0	3.914662	-2.141057	2.406646
51	1	0	2.664333	-0.451745	1.981133
52	6	0	4.147233	-3.496682	2.176021
53	6	0	-0.136762	-2.387232	-1.089574
54	6	0	-0.065906	-1.975136	-2.422500
55	6	0	-0.804898	-3.571630	-0.757631
56	6	0	-0.668070	-2.739033	-3.417888
57	1	0	0.437557	-1.046324	-2.675157
58	6	0	-1.389001	-4.340110	-1.758398
59	1	0	-0.889372	-3.882584	0.279680
60	6	0	-1.329452	-3.919408	-3.086405
61	8	0	2.407947	2.453075	-0.891429
62	6	0	3.375826	1.650087	-0.611714
63	1	0	2.690234	0.138239	-0.414414
64	6	0	3.926212	1.711133	0.725179
65	6	0	5.181612	1.279086	1.234438
66	8	0	3.219933	2.231665	1.717131
67	6	0	5.140632	1.562741	2.632571
68	1	0	5.982762	0.810145	0.682546
69	6	0	3.928033	2.131992	2.865129
70	1	0	5.911145	1.368348	3.364096
71	1	0	3.446903	2.518895	3.750758
72	6	0	4.246487	1.169505	-1.770002
73	1	0	5.050777	1.896089	-1.910855
74	1	0	3.634958	1.113223	-2.670416
75	8	0	4.868274	-0.078596	-1.484556
76	6	0	4.286760	-1.200344	-1.962472
77	8	0	3.314587	-1.187579	-2.688097
78	1	0	4.576638	-1.570018	3.049879
79	1	0	4.996460	-3.988282	2.640210
80	1	0	3.477663	-5.267038	1.150805
81	1	0	-0.625928	-2.407686	-4.450563
82	1	0	-1.803501	-4.511144	-3.863353
83	1	0	-1.903686	-5.259961	-1.499431
84	1	0	-4.345868	3.203209	2.714540
85	1	0	-2.710317	3.361595	4.573185
86	1	0	-0.315971	2.842886	4.167302
87	1	0	-2.247001	4.360983	-0.566661
88	1	0	-2.243117	6.166718	-2.242358
89	1	0	-1.008508	5.890606	-4.377139
90	1	0	0.247644	3.795128	-4.818716
91	6	0	4.993416	-2.419806	-1.465383
92	1	0	4.888122	-2.471859	-0.377144
93	1	0	4.563651	-3.310275	-1.921627
94	1	0	6.060399	-2.353286	-1.693034

4c(S)_{neg}

RwB97XD SCF energy -3186.758619 a.u.
RwB97XD SCF enthalpy -3185.970683 a.u.
RwB97XD SCF free energy -3186.105921 a.u.
Three lowest frequencies (cm⁻¹) 22.5, 27.8, 31.2

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.289771	-0.104305	-1.285182
2	6	0	-2.635437	-0.548223	-2.540626
3	6	0	-2.396477	0.192300	-3.695216
4	6	0	-1.826123	1.441451	-3.651554
5	6	0	-1.476285	1.928394	-2.382525
6	6	0	-1.692528	1.184196	-1.227017
7	1	0	-1.650335	2.020007	-4.550548
8	1	0	-1.021828	2.910478	-2.315904
9	6	0	-2.580126	-0.950155	-0.094287
10	6	0	-1.609848	-1.600322	0.721961
11	6	0	-3.892191	-1.127053	0.281680
12	6	0	-2.002113	-2.363015	1.820189
13	6	0	-4.272195	-1.874483	1.392992
14	6	0	-3.348644	-2.517691	2.180338
15	1	0	-1.255842	-2.860548	2.427873
16	1	0	-3.640507	-3.110370	3.038993
17	8	0	-2.818681	-0.507593	-4.778141
18	8	0	-3.220955	-1.729170	-2.864446
19	8	0	-4.993530	-0.613416	-0.323403
20	8	0	-5.621492	-1.848734	1.518042

21	6	0	-3.282579	-1.772002	-4.293091
22	1	0	-2.627637	-2.565447	-4.663995
23	1	0	-4.317704	-1.924269	-4.605540
24	6	0	-6.108467	-0.968729	0.498765
25	1	0	-6.852892	-1.489961	-0.105900
26	1	0	-6.522126	-0.068700	0.963127
27	15	0	0.160867	-1.322461	0.407663
28	15	0	-1.067807	1.748053	0.381060
29	46	0	0.855927	0.712904	1.044525
30	6	0	0.392391	-1.599669	-1.369757
31	6	0	-0.172576	-2.731332	-1.969942
32	6	0	1.079223	-0.663180	-2.145691
33	6	0	-0.036126	-2.925769	-3.339856
34	1	0	-0.729022	-3.449580	-1.374799
35	6	0	1.196331	-0.854837	-3.518508
36	1	0	1.506665	0.219219	-1.678072
37	6	0	0.639451	-1.984101	-4.114776
38	6	0	1.092696	-2.579832	1.329727
39	6	0	1.669573	-3.680180	0.693030
40	6	0	1.263205	-2.402258	2.709575
41	6	0	2.400215	-4.604108	1.437368
42	6	0	1.984322	-3.332250	3.445824
43	1	0	0.841661	-1.530202	3.201372
44	6	0	2.556899	-4.433162	2.808579
45	6	0	-0.504319	3.466097	0.210664
46	6	0	-1.215637	4.549894	0.733423
47	6	0	0.738536	3.678636	-0.405542
48	6	0	-0.690647	5.834881	0.626590
49	1	0	-2.172316	4.397744	1.222726
50	6	0	1.255695	4.965103	-0.509863
51	1	0	1.298474	2.838776	-0.811619
52	6	0	0.540508	6.043177	0.008012
53	6	0	-2.479726	1.696547	1.515247
54	6	0	-2.316103	1.130050	2.782070
55	6	0	-3.737676	2.153580	1.105571
56	6	0	-3.411451	1.007240	3.631954
57	1	0	-1.340891	0.762681	3.091602
58	6	0	-4.824733	2.040925	1.965286
59	1	0	-3.871485	2.581853	0.116271
60	6	0	-4.664210	1.458098	3.222114
61	8	0	2.681007	0.155187	1.646562
62	6	0	3.689577	0.283281	0.678868
63	6	0	4.308335	-1.038905	0.330678
64	6	0	5.165259	-1.882203	0.968226
65	8	0	3.933019	-1.585861	-0.860387
66	6	0	5.329305	-3.020576	0.113580
67	1	0	5.630306	-1.713558	1.929366
68	6	0	4.557312	-2.785797	-0.977060
69	1	0	5.937537	-3.895479	0.294274
70	1	0	4.352828	-3.338861	-1.881403
71	6	0	4.724851	1.271164	1.224984
72	1	0	5.263844	0.844280	2.072868
73	1	0	4.216008	2.184097	1.540517
74	8	0	5.728149	1.586310	0.247965
75	6	0	5.405250	2.499294	-0.678690
76	8	0	4.321255	3.049723	-0.725624
77	1	0	2.217661	5.119756	-0.987569
78	1	0	0.945589	7.047437	-0.068602
79	1	0	-1.244800	6.675617	1.031633
80	1	0	-3.287402	0.549827	4.608314
81	1	0	-5.518811	1.355804	3.883760
82	1	0	-5.799936	2.397927	1.649592
83	1	0	-0.470118	-3.805755	-3.803627
84	1	0	0.730921	-2.131037	-5.186429
85	1	0	1.718625	-0.119281	-4.121884
86	1	0	1.567318	-3.820729	-0.377032
87	1	0	2.854906	-5.452970	0.937077
88	1	0	3.132413	-5.152342	3.383118
89	1	0	2.113963	-3.189784	4.513826
90	6	0	6.540093	2.748619	-1.624704
91	1	0	6.805451	1.817590	-2.133454
92	1	0	6.251651	3.502390	-2.356363
93	1	0	7.418991	3.084943	-1.067933
94	1	0	3.301892	0.706642	-0.259642

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.443072	0.054114	1.050549
2	6	0	2.971876	-0.299082	2.271412
3	6	0	2.787515	0.457362	3.424035
4	6	0	2.088712	1.639748	3.405647
5	6	0	1.553680	2.035540	2.170050
6	6	0	1.710921	1.272318	1.015826
7	1	0	1.953490	2.237448	4.299105
8	1	0	1.004769	2.968598	2.132775
9	6	0	2.688613	-0.824727	-0.123400
10	6	0	1.703366	-1.616193	-0.776077
11	6	0	3.963242	-0.905526	-0.635758
12	6	0	2.045824	-2.411801	-1.867875
13	6	0	4.289000	-1.684100	-1.741631
14	6	0	3.351318	-2.460243	-2.377885
15	1	0	1.294176	-3.022799	-2.351581
16	1	0	3.602938	-3.077336	-3.232141
17	8	0	3.394690	-0.153831	4.472071
18	8	0	3.705875	-1.404523	2.558897
19	8	0	5.066232	-0.247173	-0.196113
20	8	0	5.604260	-1.535090	-2.032327
21	6	0	3.959205	-1.368616	3.966021
22	1	0	3.474774	-2.226009	4.447200
23	1	0	5.037849	-1.366846	4.139274
24	6	0	6.135717	-0.615166	-1.072132
25	1	0	6.924232	-1.106151	-0.496490
26	1	0	6.506481	0.273821	-1.588735
27	15	0	-0.034392	-1.493935	-0.240365
28	15	0	0.847067	1.729824	-0.526138
29	46	0	-1.072212	0.458711	-0.818320
30	6	0	-0.012987	-1.752032	1.553518
31	6	0	0.741212	-2.796224	2.101666
32	6	0	-0.698559	-0.868358	2.389447
33	6	0	0.802211	-2.951338	3.481721
34	1	0	1.292489	-3.473448	1.455796
35	6	0	-0.620043	-0.119223	3.770417
36	1	0	-1.272166	-0.051863	1.961279
37	6	0	0.131069	-2.057544	4.315960
38	6	0	-0.911503	-2.878989	-1.024968
39	6	0	-1.318313	-3.997762	-0.296569
40	6	0	-1.195666	-2.799200	-2.394505
41	6	0	-1.989299	-5.036586	-0.938936
42	6	0	-1.857314	-3.841894	-3.030717
43	1	0	-0.908213	-1.918189	-2.962039
44	6	0	-2.254938	-4.962868	-2.302717
45	6	0	0.354888	3.475882	-0.339790
46	6	0	1.015111	4.511221	-1.005765
47	6	0	-0.737671	3.772111	0.487266
48	6	0	0.592494	5.827901	-0.834124
49	1	0	1.852901	4.303088	-1.662281
50	6	0	-1.149028	5.087840	0.661568
51	1	0	-1.268578	2.971573	0.994824
52	6	0	-0.483243	6.118533	-0.000457
53	6	0	2.097400	1.647646	-1.837362
54	6	0	1.792656	1.005413	-3.039761
55	6	0	3.374778	2.181724	-1.630422
56	6	0	2.767303	0.885441	-4.026684
57	1	0	0.804707	0.578460	-3.191402
58	6	0	4.339503	2.070542	-2.624996
59	1	0	3.618967	2.669387	-0.691039
60	6	0	4.038890	1.414715	-3.818538
61	8	0	-2.776517	-0.650114	-0.901112
62	6	0	-3.948605	-0.034980	-0.438257
63	6	0	-3.898471	0.327371	1.017944
64	6	0	-4.284458	-0.287331	2.168043
65	8	0	-3.290680	1.513362	1.318727
66	6	0	-3.887206	0.569828	3.246438
67	1	0	-4.799833	-1.234397	2.243689
68	6	0	-3.285097	1.641295	2.673676
69	1	0	-4.036595	0.406142	4.304122
70	1	0	-2.837268	2.542707	3.064274
71	6	0	-5.074752	-1.035267	-0.715011
72	1	0	-4.924864	-1.947459	-0.134410
73	1	0	-5.078222	-1.281771	-1.778285
74	8	0	-6.359410	-0.533995	-0.320944
75	6	0	-6.979066	0.305085	-1.163778
76	8	0	-6.512498	0.643412	-2.233516
77	1	0	-1.992683	5.306679	1.308616
78	1	0	-0.806750	7.146435	0.130840

5c(S)_{iso}
RwB97XD SCF energy -3187.942587 a.u.
RwB97XD SCF enthalpy -3187.137230 a.u.
RwB97XD SCF free energy -3187.274935 a.u.
Three lowest frequencies (cm⁻¹) 12.2, 17.2, 30.9
Cartesian coordinates:

79	1	0	1.108662	6.627396	-1.356190
80	1	0	2.535434	0.371878	-4.954322
81	1	0	4.799093	1.316377	-4.587325
82	1	0	5.328207	2.488789	-2.465211
83	1	0	1.383928	-3.763159	3.906573
84	1	0	0.196893	-2.172174	5.393440
85	1	0	-1.143437	-0.321219	4.415862
86	1	0	-1.124576	-4.068288	0.768141
87	1	0	-2.303224	-5.904350	-0.367442
88	1	0	-2.776170	-5.775576	-2.799188
89	1	0	-2.070721	-3.773998	-4.092727
90	6	0	-8.299316	0.753454	-0.613586
91	1	0	-8.145126	1.263531	0.341472
92	1	0	-8.784918	1.426262	-1.319567
93	1	0	-8.936415	-0.115384	-0.426438
94	1	0	-4.167009	0.891102	-0.996024
95	1	0	-2.179782	1.964131	-1.180570
96	1	0	-1.811663	1.847582	-1.856104

TS2c(S)_{eq}

RwB97XD SCF energy -3187.925627 a.u.
 RwB97XD SCF enthalpy -3187.122451 a.u.
 RwB97XD SCF free energy -3187.259043 a.u.
 Three lowest frequencies (cm⁻¹) -1059, 17.9, 24.5
 Imaginary frequency (cm⁻¹) -1059

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.538644	-0.293770	0.947479
2	6	0	3.110916	-0.735875	2.118612
3	6	0	3.199200	0.049597	3.263975
4	6	0	2.749911	1.347482	3.287208
5	6	0	2.173866	1.832178	2.103780
6	6	0	2.058735	1.045275	0.960377
7	1	0	2.827004	1.963867	4.174789
8	1	0	1.809142	2.852527	2.098910
9	6	0	2.477039	-1.219488	-0.216913
10	6	0	1.290215	-1.803546	-0.742515
11	6	0	3.651148	-1.577390	-0.840577
12	6	0	1.351577	-2.676333	-1.825786
13	6	0	3.679942	-2.426353	-1.941228
14	6	0	2.562690	-3.004955	-2.453630
15	1	0	0.445876	-3.128989	-2.210466
16	1	0	2.595591	-3.682183	-3.298812
17	8	0	3.773995	-0.665267	4.262263
18	8	0	3.634597	-1.964583	2.362265
19	8	0	4.904609	-1.161718	-0.526232
20	8	0	4.981723	-2.560065	-2.358901
21	6	0	4.027984	-1.973287	3.737220
22	1	0	3.429756	-2.706725	4.284790
23	1	0	5.096365	-2.190046	3.807648
24	6	0	5.783081	-1.756671	-1.486120
25	1	0	6.506230	-2.392538	-0.969531
26	1	0	6.276935	-0.971431	-2.064310
27	15	0	-0.316558	-1.262205	-0.066948
28	15	0	1.178863	1.679743	-0.499720
29	46	0	-0.907529	0.828986	-0.858104
30	6	0	-0.164860	-1.449312	1.730263
31	6	0	0.358788	-2.630708	2.269371
32	6	0	-0.520386	-0.393090	2.569410
33	6	0	0.522457	-2.747579	3.644499
34	1	0	0.649498	-3.449243	1.617056
35	6	0	-0.346458	-0.512380	3.945289
36	1	0	-0.913560	0.526464	2.147368
37	6	0	0.178014	-1.685642	4.481330
38	6	0	-1.583882	-2.433324	-0.637968
39	6	0	-2.250828	-3.288322	0.244847
40	6	0	-1.941413	-2.422342	-1.993406
41	6	0	-3.242450	-4.142485	-0.231682
42	6	0	-2.920740	-3.288934	-2.465167
43	1	0	-1.459252	-1.731817	-2.679381
44	6	0	-3.572189	-4.150138	-1.584611
45	6	0	1.023133	3.479264	-0.271058
46	6	0	1.881912	4.384998	-0.897497
47	6	0	-0.003214	3.952446	0.557611
48	6	0	1.715895	5.752850	-0.690518
49	1	0	2.673730	4.038635	-1.552809
50	6	0	-0.156575	5.317249	0.768230
51	1	0	-0.682590	3.253481	1.038503

52	6	0	0.703068	6.219253	0.142244
53	6	0	2.282336	1.359916	-1.905720
54	6	0	1.764745	0.798975	-3.076714
55	6	0	3.656172	1.602723	-1.792445
56	6	0	2.620169	0.467853	-4.123315
57	1	0	0.699230	0.598497	-3.156708
58	6	0	4.503206	1.284209	-2.848030
59	1	0	4.066627	2.019147	-0.877146
60	6	0	3.987826	0.706424	-4.007417
61	8	0	-2.912030	0.537762	-1.569608
62	6	0	-4.055361	0.644230	-0.741287
63	6	0	-3.764140	0.963603	0.690574
64	6	0	-3.853774	0.270814	1.858013
65	8	0	-3.355426	2.241152	0.946520
66	6	0	-3.476654	1.178069	2.901198
67	1	0	-4.164373	-0.758328	1.969179
68	6	0	-3.177648	2.350774	2.290232
69	1	0	-3.429241	0.975707	3.961564
70	1	0	-2.850723	3.315391	2.648616
71	6	0	-4.808599	-0.681133	-0.867907
72	1	0	-4.243761	-1.489532	-0.402328
73	1	0	-4.962830	-0.902342	-1.925041
74	8	0	-0.609201	-0.658938	-0.183751
75	6	0	-7.104476	-0.081167	-0.811217
76	8	0	-7.019431	0.424051	-1.912541
77	1	0	-0.950758	5.675903	1.415313
78	1	0	0.577320	7.285824	0.300343
79	1	0	2.382543	6.452679	-1.184272
80	1	0	2.218225	0.015639	-5.024279
81	1	0	4.655204	0.439597	-4.821000
82	1	0	5.568087	1.473442	-2.758253
83	1	0	0.929332	-3.662564	4.062937
84	1	0	0.322296	-1.775247	5.553528
85	1	0	-0.611624	0.315492	4.595352
86	1	0	-2.008758	-3.292938	1.301940
87	1	0	-3.756238	-4.803498	0.458996
88	1	0	-4.342336	-4.821454	-1.951494
89	1	0	-3.183640	-3.279482	-3.518047
90	6	0	-8.351000	-0.156041	0.017247
91	1	0	-8.182850	0.327864	0.983336
92	1	0	-9.173798	0.331493	-0.504746
93	1	0	-8.599855	-1.203566	0.209525
94	1	0	-4.698066	1.447663	-1.130761
95	1	0	-1.469588	2.340691	-1.581705
96	1	0	-2.200237	1.788818	-1.663624

6c(S)_{eq}#2a

RwB97XD SCF energy -3187.977658 a.u.
 RwB97XD SCF enthalpy -3187.168643 a.u.
 RwB97XD SCF free energy -3187.307734 a.u.
 Three lowest frequencies (cm⁻¹) 14.5, 21.9, 30.0
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.240622	-0.342825	1.177531
2	6	0	2.580220	-0.798667	2.432246
3	6	0	2.435418	-0.036684	3.585865
4	6	0	1.969389	1.254276	3.539960
5	6	0	1.644739	1.759098	2.271915
6	6	0	1.769779	0.998872	1.109750
7	1	0	1.856704	1.854431	4.434935
8	1	0	1.283968	2.779362	2.213926
9	6	0	2.401511	-1.272348	0.024693
10	6	0	1.331410	-1.894675	-0.674388
11	6	0	3.671412	-1.604860	-0.391863
12	6	0	1.591403	-2.757570	-1.736121
13	6	0	3.918621	-2.443094	-1.472655
14	6	0	2.896987	-3.043506	-2.166706
15	1	0	0.768785	-3.232047	-2.258875
16	1	0	3.085861	-3.706217	-3.003046
17	8	0	2.807614	-0.768130	4.667069
18	8	0	3.056820	-2.030294	2.752708
19	8	0	4.847609	-1.149129	0.115328
20	8	0	5.259555	-2.521353	-1.689326
21	6	0	3.238101	-2.040113	4.171103
22	1	0	2.622998	-2.828208	4.612231
23	1	0	4.298256	-2.181402	4.398321
24	6	0	5.880019	-1.831663	-0.600998
25	1	0	6.361951	-2.556769	0.063291

26	1	0	6.595200	-1.104857	-0.990057
27	15	0	-0.383423	-1.397014	-0.261542
28	15	0	1.186765	1.695649	-0.481670
29	46	0	-0.802074	0.837006	-1.079403
30	6	0	-0.530878	-1.689992	1.529748
31	6	0	-0.036285	-2.851712	2.133182
32	6	0	-1.105027	-0.690480	2.319888
33	6	0	-0.124384	-3.009736	3.512429
34	1	0	0.431765	-3.623947	1.529201
35	6	0	-1.183395	-0.846995	3.701054
36	1	0	-1.471001	0.220284	1.853454
37	6	0	-0.690815	-2.005446	4.297273
38	6	0	-1.471955	-2.608447	-1.085067
39	6	0	-2.145136	-3.623375	-0.400605
40	6	0	-1.705862	-2.433070	-2.455668
41	6	0	-3.036536	-4.451456	-1.079370
42	6	0	-2.585856	-3.269566	-3.133120
43	1	0	-1.205113	-1.631150	-2.992443
44	6	0	-3.257437	-4.277538	-2.443081
45	6	0	1.151814	3.502948	-0.210859
46	6	0	2.238295	4.333173	-0.494359
47	6	0	-0.016528	4.055957	0.326675
48	6	0	2.150707	5.701694	-0.245587
49	1	0	3.149086	3.929855	-0.922789
50	6	0	-0.094127	5.418351	0.588994
51	1	0	-0.871094	3.418907	0.538431
52	6	0	0.990461	6.244919	0.298612
53	6	0	2.503367	1.327799	-1.682243
54	6	0	2.160276	0.795873	-2.928971
55	6	0	3.851611	1.498485	-1.347235
56	6	0	3.157024	0.430100	-3.828606
57	1	0	1.113167	0.648068	-3.181692
58	6	0	4.843589	1.148328	-2.257086
59	1	0	4.130373	1.875000	-0.367380
60	6	0	4.497753	0.605400	-3.493200
61	8	0	-2.841333	0.423971	-1.829330
62	6	0	-3.984478	0.639837	-0.974914
63	6	0	-3.792399	1.825074	-0.092955
64	6	0	-3.624454	1.996614	1.246394
65	8	0	-3.781436	3.035444	-0.719773
66	6	0	-3.497643	3.407774	1.459617
67	1	0	-3.616791	1.217870	1.995851
68	6	0	-3.594669	3.982880	0.234599
69	1	0	-3.355334	3.918501	2.401012
70	1	0	-3.559524	5.003513	-0.114864
71	6	0	-4.178390	-0.657687	-0.196810
72	1	0	-3.345516	-0.832426	0.485806
73	1	0	-4.258203	-1.487994	-0.900891
74	8	0	-5.337943	-0.592024	0.634153
75	6	0	-6.526970	-0.832883	0.051311
76	8	0	-6.644931	-1.082185	-1.130182
77	1	0	-1.004686	5.833368	1.010294
78	1	0	0.927485	7.311681	0.490257
79	1	0	2.994295	6.342611	-0.482325
80	1	0	2.886116	0.000143	-4.787674
81	1	0	5.274068	0.313049	-4.193376
82	1	0	5.887709	1.283625	-1.993306
83	1	0	0.260897	-3.912128	3.976799
84	1	0	-0.746216	-2.127386	5.374663
85	1	0	-1.618958	-0.060609	4.309780
86	1	0	-1.992858	-3.766097	0.663802
87	1	0	-3.559499	-5.233872	-0.538092
88	1	0	-3.954164	-4.923751	-2.968108
89	1	0	-2.757144	-3.125596	-4.195309
90	6	0	-7.641313	-0.761126	1.048742
91	1	0	-7.612444	0.199878	1.568752
92	1	0	-8.598656	-0.885426	0.543927
93	1	0	-7.513327	-1.548594	1.797240
94	1	0	-4.847223	0.801533	-1.627579
95	1	0	-0.906035	2.253567	-1.725928
96	1	0	-2.957226	0.939578	-2.637408

2.13. Catalytic cycle 2b-1c(R)

3c(R)_{avg}

RwB97XD SCF energy	-3186.767217 a.u.
RwB97XD SCF enthalpy	-3185.983013 a.u.
RwB97XD SCF free energy	-3186.118672 a.u.
Three lowest frequencies (cm ⁻¹)	22.8, 25.3 28.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates X	Coordinates Y	(Angstroms) Z
1	6	0	2.237346	-0.954570	0.665718
2	6	0	2.575067	-1.943836	1.563307
3	6	0	2.794373	-1.706250	2.915259
4	6	0	2.712362	-0.442658	3.445857
5	6	0	2.385358	0.589947	2.554207
6	6	0	2.149051	0.362708	1.199485
7	1	0	2.887856	-0.249824	4.497459
8	1	0	2.315665	1.594442	2.953976
9	6	0	2.017122	-1.350098	-0.754435
10	6	0	0.750323	-1.423743	-1.398130
11	6	0	3.101075	-1.749569	-1.505066
12	6	0	0.655893	-1.862401	-2.715896
13	6	0	2.997432	-2.158066	-2.830091
14	6	0	1.783431	-2.231313	-3.466090
15	1	0	-0.313038	-1.930464	-3.195650
16	1	0	1.694983	-2.566621	-4.493370
17	8	0	3.084048	-2.873834	3.543985
18	8	0	2.727826	-3.269337	1.300364
19	8	0	4.401374	-1.792049	-1.111290
20	8	0	4.232886	-2.447723	-3.316278
21	6	0	3.003643	-3.902628	2.552125
22	1	0	2.188863	-4.587473	2.803860
23	1	0	3.962222	-4.422891	2.489899
24	6	0	5.152852	-2.251188	-2.238304
25	1	0	5.631909	-3.202459	-1.990454
26	1	0	5.887670	-1.493562	-2.521153
27	15	0	-0.709367	-0.776166	-0.498020
28	15	0	1.602383	1.753941	0.139079
29	46	0	-0.591720	1.631562	-0.345931
30	6	0	-0.735095	-1.735549	1.050268
31	6	0	-0.614966	-3.129871	1.045108
32	6	0	-0.794032	-1.051154	2.266189
33	6	0	-0.561511	-3.827485	2.247621
34	1	0	-0.548310	-3.667955	0.103521
35	6	0	-0.730687	-1.750198	3.468328
36	1	0	-0.868137	0.032411	2.273490
37	6	0	-0.610819	-3.137717	3.459112
38	6	0	-2.178635	-1.271709	-1.463272
39	6	0	-3.128654	-2.175439	-0.983101
40	6	0	-2.405990	-0.625853	-2.687485
41	6	0	-4.280948	-2.440757	-1.721065
42	1	0	-2.983071	-2.670952	-0.029764
43	6	0	-3.545032	-0.910174	-3.431582
44	1	0	-1.692796	0.106446	-3.057272
45	6	0	-4.487947	-1.816021	-2.946437
46	6	0	2.072143	3.257955	1.067602
47	6	0	3.302998	3.894514	0.894329
48	6	0	1.163000	3.760577	2.007325
49	6	0	3.618058	5.020618	1.652301
50	1	0	4.018738	3.532420	0.164968
51	6	0	1.487904	4.874728	2.772710
52	1	0	0.198243	3.277715	2.139577
53	6	0	2.716376	5.508624	2.593272
54	6	0	2.655641	1.647102	-1.341319
55	6	0	2.071318	1.740235	-2.607950
56	6	0	4.026977	1.390854	-1.226011
57	6	0	2.850140	1.568863	-3.748871
58	1	0	1.003392	1.921993	-2.698577
59	6	0	4.804421	1.241186	-2.369341
60	1	0	4.485520	1.279164	-0.247822
61	6	0	4.215524	1.319092	-3.630088
62	8	0	-2.692483	1.889612	-0.867192
63	6	0	-3.674502	1.539207	-0.193817
64	1	0	-0.415989	3.185093	-0.358776
65	6	0	-4.956771	1.415064	-0.820605
66	6	0	-5.359979	1.584471	-2.123473
67	8	0	-6.023614	1.045186	-0.049940
68	6	0	-6.745277	1.300351	-2.149452
69	1	0	-4.726092	1.875921	-2.948205

70	6	0	-7.085632	0.979650	-0.864860
71	1	0	-7.409490	1.326210	-3.000448
72	1	0	-8.019844	0.694742	-0.403554
73	6	0	-3.549838	1.241982	1.285708
74	1	0	-4.247869	1.865074	1.853892
75	1	0	-2.526236	1.453171	1.608040
76	8	0	-3.861524	-0.139636	1.447648
77	6	0	-3.875121	-0.599444	2.712573
78	8	0	-3.660501	0.119029	3.665161
79	1	0	0.777447	5.252440	3.501361
80	1	0	2.966509	6.385927	3.182038
81	1	0	4.572602	5.515528	1.503212
82	1	0	5.867733	1.045755	-2.273204
83	1	0	4.820297	1.179945	-4.520812
84	1	0	2.388001	1.625971	-4.729223
85	1	0	-0.771107	-1.210393	4.408878
86	1	0	-0.554566	-3.683079	4.396150
87	1	0	-0.467985	-4.909015	2.239418
88	1	0	-5.014829	-3.140947	-1.333978
89	1	0	-5.386749	-2.024028	-3.518801
90	1	0	-3.703810	-0.412196	-4.382948
91	6	0	-4.170552	-2.065946	2.752287
92	1	0	-3.338850	-2.611300	2.295288
93	1	0	-4.292335	-2.389318	3.785504
94	1	0	-5.073810	-2.283972	2.177069

TS1c(R)_{avg}

RwB97XD SCF energy	-3186.746891 a.u.
RwB97XD SCF enthalpy	-3185.964823 a.u.
RwB97XD SCF free energy	-3186.101631 a.u.
Three lowest frequencies (cm ⁻¹)	-500.0, 17.6, 26.3
Imaginary frequency (cm ⁻¹)	-500.0

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.378523	0.415124	-0.727370
2	6	0	-3.388104	-0.057260	-1.537432
3	6	0	-3.359799	0.039049	-2.924330
4	6	0	-2.328827	0.663008	-3.583357
5	6	0	-1.301653	1.186515	-2.784568
6	6	0	-1.308399	1.074900	-1.395296
7	1	0	-2.305526	0.746628	-4.663364
8	1	0	-0.476726	1.686343	-3.280263
9	6	0	-2.493953	0.205812	0.743347
10	6	0	-1.703483	-0.697404	1.505945
11	6	0	-3.445994	0.910083	1.445025
12	6	0	-1.891975	-0.819176	2.880084
13	6	0	-3.608349	0.801764	2.822004
14	6	0	-2.848446	-0.061056	3.572906
15	1	0	-1.287100	-1.515566	3.449235
16	1	0	-2.977471	-0.153761	4.644671
17	8	0	-4.458675	-0.562751	-3.446146
18	8	0	-4.514313	-0.708061	-1.144842
19	8	0	-4.301578	1.844950	0.953945
20	8	0	-4.565237	1.673791	3.235920
21	6	0	-5.232611	-1.033011	-2.337730
22	1	0	-5.350118	-2.116956	-2.411407
23	1	0	-6.199374	-0.522982	-2.327750
24	6	0	-5.131425	2.238496	2.050049
25	1	0	-6.140191	1.838975	1.901891
26	1	0	-5.136728	3.326398	2.131912
27	15	0	-0.349103	-1.590343	0.668527
28	15	0	0.181077	1.597129	-0.476233
29	46	0	1.456309	-0.213058	0.025902
30	6	0	-1.148306	-2.453257	-0.717943
31	6	0	-2.374846	-3.107408	-0.556651
32	6	0	-0.552853	-2.389703	-1.980316
33	6	0	-2.993906	-3.697631	-1.653495
34	1	0	-2.854268	-3.140468	0.417468
35	6	0	-1.181757	-2.971498	-3.077363
36	1	0	0.387786	-1.861946	-2.107516
37	6	0	-2.403180	-3.621095	-2.914540
38	6	0	0.247299	-2.844585	1.848162
39	6	0	-0.101074	-4.194612	1.760950
40	6	0	1.119725	-2.420291	2.859922
41	6	0	0.411080	-5.106157	2.681852
42	1	0	-0.766308	-4.544049	0.978302
43	6	0	1.617815	-3.331461	3.784109
44	1	0	1.409006	-1.374520	2.925127

45	6	0	1.265727	-4.677268	3.693551
46	6	0	1.008024	2.844438	-1.529649
47	6	0	0.637963	4.193049	-1.490521
48	6	0	2.012406	2.432917	-2.413675
49	6	0	1.267674	5.114819	-2.321939
50	1	0	-0.130147	4.539205	-0.808349
51	6	0	2.630198	3.357353	-3.250819
52	1	0	2.305917	1.388612	-2.463269
53	6	0	2.262063	4.699544	-3.204120
54	6	0	-0.396830	2.471338	1.011332
55	6	0	0.250491	2.241383	2.228511
56	6	0	-1.491925	3.341202	0.959659
57	6	0	-0.198118	2.872680	3.385544
58	1	0	1.091510	1.553064	2.272514
59	6	0	-1.930227	3.978828	-2.115903
60	1	0	-2.022851	3.498313	0.025516
61	6	0	-1.287493	3.738753	3.329690
62	8	0	3.073426	-1.540006	0.415741
63	6	0	3.802774	-0.547363	0.054299
64	1	0	2.743087	0.669043	-0.363350
65	6	0	4.448497	0.253987	1.109195
66	6	0	4.433412	0.148141	2.466520
67	8	0	5.185943	1.327255	0.720765
68	6	0	5.224213	1.234875	2.950258
69	1	0	3.928188	-0.614248	3.042126
70	6	0	5.650374	1.913184	1.852356
71	1	0	5.449256	1.472734	3.979645
72	1	0	6.265252	2.789030	1.711358
73	6	0	4.540343	-0.627384	-1.294725
74	1	0	5.606237	-0.733635	-1.081535
75	1	0	4.382497	0.262644	-1.905078
76	8	0	4.171252	-1.810387	-1.985278
77	6	0	3.103184	-1.777786	-2.797321
78	8	0	2.478675	-0.762842	-3.035381
79	1	0	3.403223	3.025332	-3.936905
80	1	0	2.750536	5.421114	-3.851808
81	1	0	0.980510	6.160600	-2.275431
82	1	0	-2.781208	4.649180	2.071171
83	1	0	-1.641348	4.224254	4.233879
84	1	0	0.300134	2.682584	4.330953
85	1	0	-0.723593	-2.904811	-4.059073
86	1	0	-2.897455	-4.068211	-3.771571
87	1	0	-3.945341	-4.204484	-1.526416
88	1	0	0.140276	-6.154506	2.604545
89	1	0	1.660806	-5.391682	4.409316
90	1	0	2.289320	-2.992359	4.566720
91	6	0	2.784676	-3.135911	-3.335732
92	1	0	2.314575	-3.719783	-2.537146
93	1	0	2.091455	-3.049298	-4.171732
94	1	0	3.695124	-3.655028	-3.641781

4c(R)_{avg}

RwB97XD SCF energy	-3186.760305 a.u.
RwB97XD SCF enthalpy	-3185.972019 a.u.
RwB97XD SCF free energy	-3186.107243 a.u.
Three lowest frequencies (cm ⁻¹)	16.6, 25.7, 31.1

Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.506430	0.453067	0.676842
2	6	0	3.276366	0.497809	1.816899
3	6	0	3.178164	1.522425	2.753663
4	6	0	2.330564	2.588891	2.574948
5	6	0	1.557074	2.588289	1.403436
6	6	0	1.630666	1.554215	0.474504
7	1	0	2.259972	3.389189	3.301988
8	1	0	0.882834	3.420495	1.233012
9	6	0	2.636384	-0.699033	-0.256365
10	6	0	1.645977	-1.699503	-0.471966
11	6	0	3.786796	-0.824711	-1.000260
12	6	0	1.858126	-2.720216	-1.397506
13	6	0	3.977234	-1.832503	-1.941298
14	6	0	3.032327	-2.805566	-2.158387
15	1	0	1.102264	-3.481499	-1.547700
16	1	0	3.179608	-3.595392	-2.885058
17	8	0	4.010615	1.266231	3.794349
18	8	0	4.179174	-0.424655	2.234957
19	8	0	4.860872	0.004649	-0.991907
20	8	0	5.173462	-1.663482	-2.553499

21	6	0	4.712939	0.062555	3.469864
22	1	0	4.549053	-0.678324	4.255356
23	1	0	5.776094	0.284126	3.339898
24	6	0	5.788194	-0.521788	-1.945465
25	1	0	6.700901	-0.833051	-1.430258
26	1	0	5.991822	0.230640	-2.710528
27	15	0	0.043745	-1.578117	0.377467
28	15	0	0.452550	1.479008	-0.911615
29	46	0	-1.289542	0.068932	-0.387028
30	6	0	0.421472	-1.333568	2.135282
31	6	0	1.446047	-2.065606	2.746442
32	6	0	-0.273170	-0.362030	2.859896
33	6	0	1.769442	-1.818333	4.076389
34	1	0	2.002852	-2.809720	2.184747
35	6	0	0.068190	-0.106533	4.183511
36	1	0	-1.068606	0.200290	2.381211
37	6	0	1.091576	-0.831272	4.790234
38	6	0	-0.801943	-3.169844	0.162010
39	6	0	-0.835887	-4.121604	1.183382
40	6	0	-1.432585	-3.435047	-1.060911
41	6	0	-1.482652	-5.337725	0.974430
42	1	0	-0.365810	-3.925651	2.141149
43	6	0	-2.068268	-4.653417	-1.265023
44	1	0	-1.432323	-2.687171	-1.848829
45	6	0	-2.094198	-5.605565	-0.246464
46	6	0	-0.282128	3.134201	-1.091686
47	6	0	0.190520	4.074777	-2.011764
48	6	0	-1.375203	3.453027	-0.275824
49	6	0	-0.422176	5.321251	-2.102371
50	1	0	1.027478	3.842160	-2.661617
51	6	0	-1.982047	4.700587	-0.367039
52	1	0	-1.750654	2.722759	0.435213
53	6	0	-1.503847	5.635903	-1.282093
54	6	0	1.427681	1.140041	-2.402937
55	6	0	0.959178	0.198690	-3.322788
56	6	0	2.655748	1.776977	-2.615283
57	6	0	1.722332	-0.113555	-4.444518
58	1	0	0.010129	-0.303150	-3.152251
59	6	0	3.408915	1.468246	-3.742700
60	1	0	3.032109	2.495573	-1.892965
61	6	0	2.946840	0.517368	-4.651857
62	8	0	-2.904627	-0.983816	0.193848
63	6	0	-3.961157	-0.086429	0.087333
64	6	0	-4.981629	-0.603099	-0.887094
65	6	0	-5.104913	-1.785065	-1.545374
66	8	0	-6.016023	0.222533	-1.208787
67	6	0	-6.301188	-1.682482	-2.331516
68	1	0	-4.429117	-2.625347	-1.477196
69	6	0	-6.810116	-0.450238	-2.087741
70	1	0	-6.719892	-2.430726	-2.989514
71	1	0	-7.682479	0.080424	-2.438210
72	6	0	-4.608490	0.165690	1.454880
73	1	0	-4.881875	-0.789287	1.906870
74	1	0	-5.489044	0.806085	1.370241
75	8	0	-3.666747	0.755985	2.365352
76	6	0	-3.516314	2.086389	2.319280
77	8	0	-4.139396	2.799664	1.555784
78	1	0	-2.827335	4.932924	0.272527
79	1	0	-1.978436	6.609002	-1.361031
80	1	0	-0.053312	6.048215	-2.819028
81	1	0	4.361812	1.962083	-3.904959
82	1	0	3.543852	0.267098	-5.523451
83	1	0	1.363888	-0.854991	-5.151464
84	1	0	-0.460547	0.663696	4.736217
85	1	0	1.361271	-0.628289	5.821959
86	1	0	2.564036	-2.385903	4.550047
87	1	0	-1.506544	-6.075058	1.770384
88	1	0	-2.597313	-6.554506	-0.404286
89	1	0	-2.552382	-4.854243	-2.215449
90	6	0	-2.481073	2.570906	3.289093
91	1	0	-2.509231	1.996387	4.216637
92	1	0	-1.489830	2.443303	2.838896
93	1	0	-2.637403	3.631219	3.488485
94	1	0	-3.619143	0.906111	-0.292832

Center Number	Atomic Number	Atomic Type	Coordinates X Y Z			(Angstroms)
1	6	0	2.371137	-0.333012	1.079099	
2	6	0	2.794805	-0.663947	2.346551	
3	6	0	2.875858	0.261085	3.382312	
4	6	0	2.585113	1.589021	3.187821	
5	6	0	2.181343	1.961744	1.896826	
6	6	0	2.064042	1.038621	0.860460	
7	1	0	2.660106	2.315663	3.988026	
8	1	0	1.957148	3.006703	1.721342	
9	6	0	2.272601	-1.397723	0.045957	
10	6	0	1.053863	-1.906106	-0.480404	
11	6	0	3.425812	-1.948835	-0.462856	
12	6	0	1.063547	-2.896056	-1.461554	
13	6	0	3.425104	-2.920536	-1.458560	
14	6	0	2.256554	-3.423859	-1.976103	
15	1	0	0.129991	-3.281821	-1.853226	
16	1	0	2.253228	-4.185871	-2.746253	
17	8	0	3.263137	-0.364309	4.521764	
18	8	0	3.146372	-1.894698	2.799915	
19	8	0	4.703199	-1.624730	-0.137121	
20	8	0	4.701593	-3.234061	-1.789185	
21	6	0	3.488974	-1.735583	4.179657	
22	1	0	2.847209	-2.373043	4.792273	
23	1	0	4.546872	-1.973297	4.321188	
24	6	0	5.549976	-2.430895	-0.961546	
25	1	0	6.160294	-3.080005	-0.328238	
26	1	0	6.167757	-1.786931	-1.592454	
27	15	0	-0.524539	-1.170005	0.045762	
28	15	0	1.324873	1.541225	-0.734389	
29	46	0	-0.917239	0.955024	-0.696220	
30	6	0	-0.521839	-1.216032	1.862319	
31	6	0	-0.056740	-2.351410	2.535478	
32	6	0	-0.913319	-0.085709	2.588199	
33	6	0	0.010933	-2.354373	3.924813	
34	1	0	0.275326	-3.223629	1.979954	
35	6	0	-0.829160	-0.090931	3.976997	
36	1	0	-1.264831	0.803573	2.072692	
37	6	0	-0.364483	-1.222074	4.645047	
38	6	0	-1.818158	-2.279958	-0.590831	
39	6	0	-2.358601	-3.300347	0.192101	
40	6	0	-2.265964	-2.098873	-1.904862	
41	6	0	-3.338775	-4.136490	-0.339014	
42	1	0	-2.034491	-3.445231	1.217084	
43	6	0	-3.241492	-2.937294	-2.429940	
44	1	0	-1.861241	-1.292537	-2.511021	
45	6	0	-3.780455	-3.956908	-1.645926	
46	6	0	1.468312	3.358727	-0.821123	
47	6	0	2.413867	3.989973	-1.633493	
48	6	0	0.587612	4.136302	-0.055533	
49	6	0	2.484835	5.380885	-1.667931	
50	1	0	3.093901	3.408236	-2.245885	
51	6	0	0.669864	5.523503	-0.086509	
52	1	0	-0.165572	3.659567	0.566009	
53	6	0	1.619893	6.147916	-0.893262	
54	6	0	2.388791	0.855627	-2.033704	
55	6	0	1.808748	0.211051	-3.128535	
56	6	0	3.782113	0.944703	-1.929228	
57	6	0	2.620031	-0.352703	-4.109880	
58	1	0	0.727409	0.130832	-3.202972	
59	6	0	4.586415	0.390523	-2.918234	
60	1	0	4.237405	1.430292	-1.070837	
61	6	0	4.005856	-0.265119	-4.003549	
62	8	0	-2.811889	0.471916	-0.185056	
63	6	0	-3.879382	0.789406	-1.015030	
64	6	0	-4.944386	-0.259488	-0.841258	
65	6	0	-5.280382	-1.081023	0.187179	
66	8	0	-5.792314	-0.453518	-1.889190	
67	6	0	-6.412085	-1.841994	-0.259142	
68	1	0	-4.777145	-1.147442	-1.140578	
69	6	0	-6.676655	-1.422393	-1.520594	
70	1	0	-6.947009	-2.605717	0.287733	
71	1	0	-7.414859	-1.695040	-2.259332	
72	6	0	-4.426357	2.189302	-0.678799	
73	1	0	-5.397225	2.362398	-1.147923	
74	1	0	-3.729641	2.969400	-0.989744	
75	8	0	-4.640892	2.263046	0.736191	
76	6	0	-3.641244	2.712562	1.502425	
77	8	0	-2.664656	3.303782	1.076452	
78	1	0	-0.011412	6.115612	0.516302	

5c(R)_{avg}
 Rwb97XD SCF energy -3187.943043 a.u.
 Rwb97XD SCF enthalpy -3187.137164 a.u.
 Rwb97XD SCF free energy -3187.272132 a.u.
 Three lowest frequencies (cm⁻¹) 20.0, 28.5, 29.2
 Cartesian coordinates:

79	1	0	1.681393	7.231444	-0.921747
80	1	0	3.220703	5.862523	-2.304078
81	1	0	5.666154	0.463079	-2.836142
82	1	0	4.637067	-0.709319	-4.766951
83	1	0	2.167997	-0.864656	-4.953386
84	1	0	-1.118778	0.794135	4.534816
85	1	0	-0.291136	-1.220693	5.728181
86	1	0	0.371973	-3.237475	4.442166
87	1	0	-3.761022	-4.923901	0.277158
88	1	0	-4.550147	-4.605195	-2.052920
89	1	0	-3.590836	-2.786491	-3.446388
90	6	0	-3.883350	2.403981	2.948721
91	1	0	-3.684000	1.338993	3.109763
92	1	0	-3.216941	2.996169	3.575743
93	1	0	-4.925798	2.591843	3.215154
94	1	0	-3.615706	0.807331	-2.085884
95	1	0	-1.275961	2.384765	-1.879490
96	1	0	-1.555659	2.675346	-1.213309

TS2c(R)_{eq}

RwB97XD SCF energy -3187.922202 a.u.
 RwB97XD SCF enthalpy -3187.120455 a.u.
 RwB97XD SCF free energy -3187.258904 a.u.
 Three lowest frequencies (cm⁻¹) -1098, 17.2, 19.1
 Imaginary frequency (cm⁻¹) -1098
 Cartesian coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.692449	-0.219321	0.822556
2	6	0	3.406975	-0.701582	1.895894
3	6	0	3.562159	0.005550	3.083806
4	6	0	3.036784	1.263961	3.248286
5	6	0	2.320408	1.791387	2.163864
6	6	0	2.139661	1.082055	0.978281
7	1	0	3.164782	1.822086	4.167985
8	1	0	1.899815	2.784124	2.271069
9	6	0	2.561460	-1.068338	-0.391984
10	6	0	1.359999	-1.696740	-0.818354
11	6	0	3.670283	-1.292335	-1.175557
12	6	0	1.340761	-2.483252	-1.967540
13	6	0	3.633186	-2.052006	-2.340132
14	6	0	2.482791	-2.674161	-2.759736
15	1	0	0.423664	-2.970367	-2.275858
16	1	0	2.454068	-3.277211	-3.659375
17	8	0	4.278847	-0.735224	3.964641
18	8	0	4.028048	-1.905053	1.992639
19	8	0	4.918641	-0.798030	-0.992352
20	8	0	4.855413	-2.041785	-2.928884
21	6	0	4.578285	-1.973718	3.311427
22	1	0	4.110273	-2.795299	3.860002
23	1	0	5.662005	-2.097323	3.245681
24	6	0	5.720372	-1.299986	-2.062360
25	1	0	6.486724	-1.966312	-1.655836
26	1	0	6.161228	-0.467662	-2.615174
27	15	0	-0.180074	-1.333214	0.085729
28	15	0	1.042592	1.751152	-0.315904
29	46	0	-1.030927	0.806887	-0.213550
30	6	0	0.174515	-1.711626	1.825387
31	6	0	0.882738	-2.867608	2.172786
32	6	0	-0.208259	-0.800918	2.814106
33	6	0	1.207299	-3.104892	3.503863
34	1	0	1.196205	-3.569910	1.405765
35	6	0	0.131750	-1.037274	4.143011
36	1	0	-0.750653	0.100487	2.540144
37	6	0	0.842450	-2.185187	4.486478
38	6	0	-1.426949	-2.507570	-0.519102
39	6	0	-1.858428	-3.598253	0.240126
40	6	0	-1.980575	-2.279010	-1.785251
41	6	0	-2.827536	-4.456757	-0.271076
42	1	0	-1.448560	-3.780739	1.227824
43	6	0	-2.946551	-3.141655	-2.291014
44	1	0	-1.655749	-1.426345	-2.376557
45	6	0	-3.371085	-4.230960	-1.533105
46	6	0	0.906750	3.542856	0.005633
47	6	0	1.674606	4.477854	-0.693040
48	6	0	0.011204	3.980194	0.990924
49	6	0	1.547673	5.835024	-0.405238
50	1	0	2.365132	4.162889	-1.467512
51	6	0	-0.102772	5.334504	1.281135

52	1	0	-0.599410	3.261192	1.530642
53	6	0	0.664445	6.264221	0.580740
54	6	0	1.913168	1.528287	-1.892066
55	6	0	1.220852	1.020150	-2.993833
56	6	0	3.279942	1.813675	-1.993280
57	6	0	1.895603	0.787313	-4.188840
58	1	0	0.162728	0.786616	-2.908186
59	6	0	3.945169	1.591702	-3.193695
60	1	0	3.828782	2.184920	-1.132636
61	6	0	3.255860	1.070640	-4.287755
62	8	0	-3.133770	0.552503	0.124914
63	6	0	-4.026003	0.201047	-0.901425
64	6	0	-4.827650	-0.978039	-0.433283
65	6	0	-4.912875	-1.632469	0.753281
66	8	0	-5.698035	-1.516572	-1.329976
67	6	0	-5.906386	-2.653585	0.575983
68	1	0	-4.339696	-1.418001	1.643136
69	6	0	-6.343963	-2.537642	-0.701029
70	1	0	-6.240578	-3.377848	1.305207
71	1	0	-7.070748	-3.072826	-1.293121
72	6	0	-4.930560	1.383657	-1.261823
73	1	0	-5.677279	1.083824	-1.999494
74	1	0	-4.337284	2.209986	-1.659013
75	8	0	-5.661018	1.813069	-0.106874
76	6	0	-5.158921	2.813260	0.628513
77	8	0	-4.176286	3.459021	0.316563
78	1	0	-0.797033	5.663332	2.047763
79	1	0	0.568642	7.322960	0.800890
80	1	0	2.141909	6.555961	-0.957706
81	1	0	5.004855	1.813343	-3.270206
82	1	0	3.781900	0.881603	-5.218386
83	1	0	1.360061	0.377034	-5.039023
84	1	0	-0.151063	-0.320696	4.907502
85	1	0	1.113674	-2.364366	5.522310
86	1	0	1.756497	-4.001771	3.772415
87	1	0	-3.162810	-5.300427	0.323764
88	1	0	-4.132614	-4.898973	-1.923066
89	1	0	-3.375062	-2.955951	-3.270553
90	6	0	-5.964805	3.024282	1.874159
91	1	0	-7.030986	3.056492	1.638119
92	1	0	-5.797012	2.178364	2.548345
93	1	0	-5.656469	3.947171	2.364547
94	1	0	-3.509421	-0.076239	-1.832493
95	1	0	-1.801513	2.332219	-0.497100
96	1	0	-2.516500	1.786334	-0.239590

6c(R)_{eq}#2b

RwB97XD SCF energy -3187.977536 a.u.
 RwB97XD SCF enthalpy -3187.169557 a.u.
 RwB97XD SCF free energy -3187.309597 a.u.
 Three lowest frequencies (cm⁻¹) 11.3, 17.5, 26.1
 Cartesian coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.694623	-0.293831	0.749394
2	6	0	3.409190	-0.818925	1.803771
3	6	0	3.638666	-0.130365	2.989167
4	6	0	3.191162	1.155104	3.170536
5	6	0	2.486461	1.730397	2.102309
6	6	0	2.232491	1.042831	0.916461
7	1	0	3.369904	1.699006	4.090488
8	1	0	2.131349	2.747137	2.223397
9	6	0	2.477518	-1.161500	-0.442672
10	6	0	1.244092	-1.784253	-0.780315
11	6	0	3.545780	-1.451794	-1.261796
12	6	0	1.157042	-2.613835	-1.895134
13	6	0	3.439034	-2.255701	-2.390746
14	6	0	2.255705	-2.861744	-2.733659
15	1	0	0.217104	-3.095309	-2.137629
16	1	0	2.171190	-3.500650	-3.604811
17	8	0	4.326734	-0.920566	3.852032
18	8	0	3.956929	-2.060308	1.881276
19	8	0	4.819222	-0.990119	-1.144809
20	8	0	4.638724	-2.307782	-3.028502
21	6	0	4.557154	-2.160460	3.175108
22	1	0	4.086341	-2.973761	3.733199
23	1	0	5.632869	-2.319771	3.063287
24	6	0	5.564951	-1.593723	-2.205072
25	1	0	6.292378	-2.294725	-1.783401

26	1	0	6.052255	-0.816420	-2.797206
27	15	0	-0.241971	-1.324662	0.187046
28	15	0	1.159632	1.818635	-0.352212
29	46	0	-0.911550	0.953080	-0.227299
30	6	0	0.175717	-1.745013	1.908444
31	6	0	0.833352	-2.935490	2.237667
32	6	0	-0.120866	-0.816023	2.909965
33	6	0	1.191044	-3.188946	3.557785
34	1	0	1.078627	-3.656322	1.462815
35	6	0	0.250485	-1.067221	4.228304
36	1	0	-0.624314	0.112994	2.653191
37	6	0	0.910247	-2.250772	4.551007
38	6	0	-1.564119	-2.472599	-0.329801
39	6	0	-2.077586	-3.460100	0.514080
40	6	0	-2.134479	-2.289724	-1.596958
41	6	0	-3.134544	-4.262631	0.089042
42	1	0	-1.661149	-3.607330	1.505113
43	6	0	-3.180337	-3.101049	-2.023125
44	1	0	-1.760206	-1.508111	-2.253782
45	6	0	-3.682738	-4.089737	-1.178552
46	6	0	1.242618	3.612928	-0.002046
47	6	0	2.179765	4.455179	-0.605115
48	6	0	0.344756	4.143071	0.933663
49	6	0	2.215250	5.808759	-0.276050
50	1	0	2.877639	4.073958	-1.341812
51	6	0	0.394139	5.490866	1.270999
52	1	0	-0.397447	3.498783	1.397327
53	6	0	1.328808	6.327199	0.663185
54	6	0	1.998951	1.517597	-1.938025
55	6	0	1.259742	1.031053	-3.020199
56	6	0	3.381506	1.696367	-2.065276
57	6	0	1.898549	0.721287	-4.217263
58	1	0	0.189769	0.872349	-2.913326
59	6	0	4.012103	1.403681	-3.269481
60	1	0	3.971886	2.034727	-1.218828
61	6	0	3.273474	0.908029	-4.342524
62	8	0	-2.993604	0.423328	0.106769
63	6	0	-3.943495	0.466721	-0.958012
64	6	0	-4.982130	-0.581171	-0.708497
65	6	0	-5.374880	-1.240708	0.410757
66	8	0	-5.735692	-0.956362	-1.773137
67	6	0	-6.452036	-2.097010	0.004597
68	1	0	-4.947707	-1.136753	1.397430
69	6	0	-6.624831	-1.885204	-1.322881
70	1	0	-7.015025	-2.780448	0.623905
71	1	0	-7.299766	-2.288809	-2.062226
72	6	0	-4.538635	1.863361	-1.147959
73	1	0	-4.975209	1.931082	-2.143945
74	1	0	-3.754498	2.619996	-1.044980
75	8	0	-5.637419	2.178019	-0.271845
76	6	0	-5.415521	2.353829	1.026008
77	8	0	-4.333854	2.143890	1.561871
78	1	0	-0.304771	5.888067	2.000482
79	1	0	1.361155	7.382523	0.915996
80	1	0	2.939481	6.457126	-0.759190
81	1	0	5.083586	1.547836	-3.364730
82	1	0	3.771612	0.663493	-5.275586
83	1	0	1.323269	0.328024	-5.049413
84	1	0	0.032055	-0.335302	4.999527
85	1	0	1.204323	-2.444740	5.577953
86	1	0	1.699744	-4.114294	3.809773
87	1	0	-3.528799	-5.023942	0.755081
88	1	0	-4.508574	-4.714462	-1.504229
89	1	0	-3.615766	-2.948536	-3.005532
90	6	0	-6.628421	2.843085	1.746466
91	1	0	-7.498245	2.247120	1.460620
92	1	0	-6.466855	2.789393	2.822202
93	1	0	-6.821671	3.880248	1.455734
94	1	0	-3.403543	0.236058	-1.880654
95	1	0	-1.313699	2.411228	-0.630707
96	1	0	-3.329772	1.035591	0.803125

2.14. Catalytic cycle for destructive hydrogenation with 2a

Acetone
 Rwb97XD SCF energy -193.109404 a.u.
 Rwb97XD SCF enthalpy -193.018624 a.u.
 Rwb97XD SCF free energy -193.051893 a.u.
 Three lowest frequencies (cm⁻¹) 161.5, 182.5, 384.0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.000002	0.183999	-0.000002
2	8	0	-0.000003	1.400929	0.000000
3	6	0	-1.281461	-0.613887	-0.002610
4	1	0	-2.139041	0.041420	-0.162865
5	1	0	-1.251023	-1.390083	-0.773814
6	1	0	-1.389983	-1.123754	0.961529
7	6	0	1.281462	-0.613883	0.002608
8	1	0	1.251042	-1.390057	0.773836
9	1	0	1.389991	-1.123765	-0.961519
10	1	0	2.139038	0.041434	0.162856

7
 Rwb97XD SCF energy -4485.238995 a.u.
 Rwb97XD SCF enthalpy -4483.434913 a.u.
 Rwb97XD SCF free energy -4483.660677 a.u.
 Three lowest frequencies (cm⁻¹) 11.4, 14.3, 18.1

Cartesian coordinates
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.170687	1.348651	2.045798
2	6	0	-0.591992	2.372736	2.868323
3	6	0	-0.002866	3.633909	2.875537
4	6	0	1.024917	3.955940	2.023990
5	6	0	1.466719	2.937515	1.165382
6	6	0	0.906956	1.661507	1.171402
7	1	0	1.487905	4.935547	2.027724
8	1	0	2.291366	3.158782	0.498243
9	6	0	-0.726216	-0.017098	2.269119
10	6	0	-1.474962	-0.826775	1.366879
11	6	0	-0.485120	-0.570398	3.510757
12	6	0	-1.886259	-2.102874	1.755158
13	6	0	-0.900824	-1.844397	3.881832
14	6	0	-1.600541	-2.646891	3.015746
15	1	0	-2.466739	-2.710094	1.072678
16	1	0	-1.930213	-3.641859	3.289966
17	8	0	-0.596436	4.405231	3.824825
18	8	0	-1.583877	2.334474	3.799184
19	8	0	0.206736	-0.008271	4.541310
20	8	0	-0.487486	-2.105832	5.150245
21	6	0	-1.394388	3.502497	4.592518
22	1	0	-2.358473	3.962484	4.809724
23	1	0	-0.858007	3.236240	5.512418
24	6	0	-0.056220	-0.844754	5.665451
25	1	0	-0.859878	-0.403597	6.268440
26	1	0	0.857892	-0.978123	6.244231
27	15	0	-1.859807	-0.241469	-0.334634
28	15	0	1.495445	0.383324	0.006439
29	46	0	-0.059298	-0.265182	-1.691790
30	6	0	-2.508930	1.435294	-0.116687
31	6	0	-3.511309	1.719397	0.802365
32	6	0	-1.946948	2.468408	-0.864845
33	6	0	-3.956670	3.027407	1.021324
34	1	0	-3.959074	0.903819	1.361439
35	6	0	-2.286674	3.798464	-0.640689
36	1	0	-1.201292	2.212242	-1.607654
37	6	0	-3.241230	4.056526	0.372462
38	6	0	-3.185134	-1.343171	-0.929443
39	6	0	-4.511274	-0.949606	-1.081725
40	6	0	-2.802286	-2.617877	-1.332854
41	6	0	-5.476479	-1.842213	-1.555018
42	1	0	-4.789690	0.068593	-0.842811
43	6	0	-3.716919	-3.566454	-1.792168
44	1	0	-1.749642	-2.877233	-1.284785
45	6	0	-5.072779	-3.176439	-1.799362

46	6	0	2.998945	1.037340	-0.782086	128	1	0	2.377521	4.772335	-2.231036
47	6	0	4.235692	0.422920	-0.611954	129	1	0	4.060883	5.316152	-2.306610
48	6	0	2.867413	2.041937	-1.731750	130	1	0	2.964066	5.636973	-3.660683
49	6	0	5.363221	0.850450	-1.308595	131	6	0	4.762395	3.825151	-4.578411
50	1	0	4.315636	-0.408824	0.073289	132	1	0	4.358539	4.441536	-5.388925
51	6	0	3.953893	2.523860	-2.465550	133	1	0	5.612209	4.362083	-4.157852
52	1	0	1.879399	2.449624	-1.918382	134	1	0	5.129272	2.892611	-5.015537
53	6	0	5.216718	1.971191	-2.161215	135	6	0	2.435763	3.057461	-4.394176
54	6	0	2.085790	-1.013657	0.996976	136	1	0	2.206085	3.781762	-5.182665
55	6	0	1.969422	-2.276289	0.436959	137	1	0	2.671837	2.100123	-4.870801
56	6	0	2.724168	-0.861434	2.226758	138	1	0	1.526484	2.924915	-3.803760
57	6	0	2.551468	-3.407466	1.018666	139	6	0	-6.901873	-1.350577	-1.890461
58	1	0	1.413323	-2.375823	-0.490149	140	6	0	-1.879613	-4.654923	-3.121855
59	6	0	3.340306	-1.941011	2.852940	141	1	0	-2.106501	-3.990963	-3.962775
60	1	0	2.743327	0.120469	2.683544	142	1	0	-1.062738	-4.213154	-2.546750
61	6	0	3.329115	-3.185853	2.170997	143	1	0	-1.507624	-5.601930	-3.525846
62	6	0	2.259737	-4.767285	0.341951	144	6	0	-7.176111	-1.616552	-3.384348
63	6	0	3.035938	-4.864397	-0.985112	145	1	0	-8.177540	-1.257280	-3.647060
64	1	0	2.769854	-5.788286	-1.510779	146	1	0	-6.451856	-1.085425	-4.011612
65	1	0	2.800793	-4.021684	-1.643459	147	1	0	-7.123199	-2.681876	-3.617081
66	1	0	4.117833	-4.870602	-0.821827	148	6	0	-7.987580	-2.033435	-1.036910
67	6	0	2.568561	-6.001744	1.207332	149	1	0	-7.743590	-1.984482	0.029835
68	1	0	2.098447	-5.927892	2.191923	150	1	0	-8.942535	-1.516970	-1.184107
69	1	0	2.162392	-6.886024	0.704463	151	1	0	-8.133385	-3.076498	-1.316853
70	1	0	3.635012	-6.172019	1.351429	152	6	0	-7.039056	0.162231	-1.658957
71	6	0	0.745997	-4.841669	0.026974	153	1	0	-8.036656	0.481187	-1.976444
72	1	0	0.149955	-4.704116	0.935544	154	1	0	-6.933891	0.419667	-0.601560
73	1	0	0.422958	-4.097758	-0.706705	155	6	0	-2.848745	5.746884	1.927705
74	1	0	0.508484	-5.824474	-0.392454	156	1	0	-3.137071	6.782430	2.118065
75	6	0	3.928313	-1.790105	4.271165	157	1	0	-3.175737	5.119898	2.763387
76	6	0	3.206259	-2.784839	5.201993	158	1	0	-1.760038	5.679400	1.848914
77	1	0	3.407659	-3.817347	4.909176	159	6	0	-5.215296	3.200089	1.907895
78	1	0	3.546618	-2.647551	6.234611	160	6	0	-4.894137	2.848372	3.370160
79	1	0	2.123101	-2.628303	5.172853	161	1	0	-5.810962	2.877195	3.969512
80	6	0	5.446464	-2.044355	4.323576	162	1	0	-4.457229	1.849713	3.462311
81	1	0	5.975237	-1.446175	3.573458	163	1	0	-4.189646	3.564547	3.801747
82	1	0	5.828577	-1.755266	5.308887	164	6	0	-5.872178	4.591729	1.860258
83	1	0	5.691739	-3.095383	4.171990	165	1	0	-6.840446	4.527552	2.368648
84	6	0	3.691077	-0.373783	4.821588	166	1	0	-5.292559	5.362460	2.367927
85	1	0	4.242788	0.383851	4.254035	167	1	0	-6.052538	4.918931	0.833064
86	1	0	2.631817	-0.101035	4.819121	168	6	0	-6.290654	2.219586	1.387825
87	1	0	4.047725	-0.331454	5.855533	169	1	0	-6.536639	2.439843	0.344091
88	8	0	4.097959	-4.197016	2.690487	170	1	0	-5.981767	1.172973	1.453659
89	8	0	6.355106	2.499895	-2.718530	171	1	0	-7.204701	2.326682	1.981026
90	8	0	-3.475348	5.365331	0.706789	172	6	0	-1.685342	4.912330	-1.523392
91	8	0	-6.053520	-4.091744	-2.088352	173	6	0	-0.709995	4.333141	-2.562390
92	6	0	-6.412104	-4.904999	-0.976195	174	1	0	-0.330297	5.145700	-3.189482
93	1	0	-7.273980	-5.498461	-1.286993	175	1	0	0.153047	3.858530	-2.082221
94	1	0	-5.599123	-5.578266	-0.687145	176	1	0	-1.185309	3.602004	-3.224630
95	1	0	-6.684187	-4.294402	-0.108450	177	6	0	-0.896190	5.955925	-0.710147
96	6	0	-3.141641	-4.922442	-2.268075	178	1	0	-0.179563	5.472200	-0.037916
97	6	0	-4.084457	-5.749314	-3.160492	179	1	0	-0.332627	6.599124	-1.395014
98	1	0	-3.517583	-6.590873	-3.572948	180	1	0	-1.552745	6.597308	-0.122396
99	1	0	-4.936165	-6.164356	-2.623166	181	6	0	-2.829133	5.610004	-2.284389
100	1	0	-4.464975	-5.157304	-3.997637	182	1	0	-3.365500	4.896773	-2.919661
101	6	0	-2.722964	-5.758634	-1.044310	183	1	0	-3.542809	6.064885	-1.593653
102	1	0	-2.240952	-6.687485	-1.369592	184	1	0	-2.423778	6.398849	-2.928107
103	1	0	-2.011657	-5.209698	-0.418456	185	8	0	1.532255	-0.372469	-3.128043
104	1	0	-3.581414	-6.026837	-0.421200	186	6	0	1.946736	-1.368597	-3.726942
105	6	0	5.330793	-4.370656	1.999354	187	6	0	1.205810	-2.666902	-3.678522
106	1	0	5.891237	-5.132189	2.544968	188	1	0	0.957684	-2.907629	-2.641116
107	1	0	5.174594	-4.707857	0.969776	189	1	0	0.258802	-2.529929	-4.214242
108	1	0	5.908563	-3.439950	1.976572	190	1	0	1.764324	-3.485758	-4.133209
109	6	0	6.810192	3.671744	-2.050176	191	6	0	3.205086	-1.272787	-4.521514
110	1	0	7.740675	3.969111	-2.537470	192	1	0	3.920020	-2.005587	-4.130685
111	1	0	6.085819	4.489137	-2.127050	193	1	0	3.002262	-1.553291	-5.560964
112	1	0	7.000401	3.475633	-0.989332	194	1	0	3.628463	-0.269224	-4.470058
113	6	0	6.676978	0.046250	-1.204941	195	1	0	-1.119907	-0.630542	-2.791921
114	6	0	6.507797	-1.189771	-0.300934	196	1	0	-6.309409	0.742111	-2.233747
115	1	0	6.292259	-0.914116	0.737398						
116	1	0	5.714741	-1.859156	-0.651995						
117	1	0	7.442572	-1.759095	-0.302508						
118	6	0	7.055328	-0.457880	-2.611736						
119	1	0	7.212912	0.373845	-3.301620						
120	1	0	7.979926	-1.044144	-2.563500						
121	1	0	6.267569	-1.102275	-3.017791						
122	6	0	7.839592	0.874043	-0.626492						
123	1	0	8.183864	1.635290	-1.326777						
124	1	0	7.552282	1.360896	0.311602						
125	1	0	8.687748	0.213839	-0.414192						
126	6	0	3.635327	3.569550	-3.562062						
127	6	0	3.237780	4.900498	-2.896822						

TS3			
RwB97XD SCF energy			-4485.225774 a.u.
RwB97XD' SCF enthalpy			-4483.423888 a.u.
RwB97XD SCF free energy			-4483.647177 a.u.
Three lowest frequencies (cm ⁻¹)			490.3, 9.5, 13.5
Imaginary frequency (cm ⁻¹)			490.3
Standard orientation:			
Center	Atomic	Atomic	Coordinates (Angstroms)
Number	Number	Type	X Y Z

1	6	0	-0.273192	-0.904615	2.181984	82	1	0	-6.214929	3.230000	4.110069
2	6	0	-0.057214	-1.837214	3.175004	83	1	0	-5.716475	4.385817	2.875938
3	6	0	-0.715200	-3.062936	3.225366	84	6	0	-4.237709	1.546979	4.141135
4	6	0	-1.616226	-3.436335	2.258583	85	1	0	-4.796775	0.793841	3.574598
5	6	0	-1.861738	-2.503949	1.239319	86	1	0	-3.236740	1.154150	4.343711
6	6	0	-1.229249	-1.262110	1.192807	87	1	0	-4.747852	1.679318	5.100425
7	1	0	-2.131061	-4.389286	2.289155	88	8	0	-3.738116	5.102494	1.602683
8	1	0	-2.589844	-2.765063	0.480717	89	8	0	-6.461700	-2.585694	-2.524172
9	6	0	0.392827	0.420664	2.303742	90	8	0	2.536626	-5.506693	1.473527
10	6	0	1.336522	0.999702	1.408758	91	8	0	6.668502	3.083803	-1.919893
11	6	0	0.085166	1.170154	3.420334	92	6	0	7.084110	3.970590	-0.885222
12	6	0	1.866180	2.262928	1.674401	93	1	0	8.090960	4.303900	-1.144246
13	6	0	0.621002	2.428825	3.672312	94	1	0	6.429434	4.844217	-0.812094
14	6	0	1.514627	3.011258	2.807555	95	1	0	7.106387	3.466246	0.086442
15	1	0	2.590163	2.696596	0.996322	96	6	0	3.956517	4.329073	-2.455017
16	1	0	1.940057	3.990879	2.990318	97	6	0	5.078182	4.876679	-3.356391
17	8	0	-0.315276	-3.744416	4.331432	98	1	0	4.688581	5.742195	-3.903029
18	8	0	0.782714	-1.734530	4.240396	99	1	0	5.955872	5.210799	-2.805177
19	8	0	-0.784413	0.845622	4.416515	100	1	0	5.399577	4.132575	-4.090970
20	8	0	0.106804	2.915404	4.832776	101	6	0	3.627509	5.351222	-1.350672
21	6	0	0.377182	-2.776751	5.123523	102	1	0	3.346378	6.312003	-1.796637
22	1	0	1.251585	-3.235030	5.582825	103	1	0	2.791172	5.005156	-0.735167
23	1	0	-0.308036	-2.368282	5.877369	104	1	0	4.480388	5.523673	-0.687859
24	6	0	-0.530542	1.794045	5.450253	105	6	0	-4.811026	5.373031	0.704874
25	1	0	0.148115	1.353429	6.191356	106	1	0	-5.312968	6.267866	1.077621
26	1	0	-1.472419	2.106554	5.900594	107	1	0	-4.452674	5.558181	-0.312900
27	15	0	1.798980	0.143758	-0.146204	108	1	0	-5.523106	4.540637	0.676388
28	15	0	-1.582973	-0.109905	-0.183605	109	6	0	-6.793167	-3.724896	-1.736246
29	46	0	0.161952	0.142428	-1.726904	110	1	0	-7.768896	-4.071821	-2.081882
30	6	0	2.207555	-1.563292	0.301019	111	1	0	-6.062750	-4.530660	-1.858715
31	6	0	3.022765	-1.890945	1.377621	112	1	0	-6.853375	-3.469175	-0.672969
32	6	0	1.661703	-2.579217	-0.481761	113	6	0	-6.842110	-0.058806	-1.158785
33	6	0	3.270290	-3.223897	1.727666	114	6	0	-6.694109	1.242888	-0.349058
34	1	0	3.477662	-1.093439	1.957250	115	1	0	-6.368513	1.050789	0.679537
35	6	0	1.806218	-3.919858	-0.145472	116	1	0	-5.989552	1.942828	-0.810483
36	1	0	1.079747	-2.296984	-1.351067	117	1	0	-7.667395	1.740894	-0.298342
37	6	0	2.539746	-4.210162	1.029039	118	6	0	-7.375851	0.319798	-2.554209
38	6	0	3.307529	0.973893	-0.741556	119	1	0	-7.528982	-0.566546	-3.173620
39	6	0	4.564036	0.376563	-0.699461	120	1	0	-8.334761	0.841759	-2.458117
40	6	0	3.165528	2.223380	-1.336177	121	1	0	-6.676990	0.988282	-3.069018
41	6	0	5.695104	1.043206	-1.173876	122	6	0	-7.884753	-0.924891	-0.427161
42	1	0	4.656718	-0.626173	-0.303284	123	1	0	-8.234595	-1.752237	-1.044489
43	6	0	4.258573	2.959959	-1.799497	124	1	0	-7.481152	-1.327787	0.508046
44	1	0	2.168576	2.641793	-1.428159	125	1	0	-8.756365	-0.310016	-0.176853
45	6	0	5.531477	2.376947	-1.620474	126	6	0	-3.750883	-3.574612	-3.476680
46	6	0	-3.078492	-0.768173	-0.979687	127	6	0	-3.295095	-4.831793	-2.711484
47	6	0	-4.337759	-0.217590	-0.759020	128	1	0	-2.417217	-4.619335	-2.092362
48	6	0	-2.947706	-1.836165	-1.857432	129	1	0	-4.083140	-5.215170	-2.055994
49	6	0	-5.482424	-0.771851	-1.326003	130	1	0	-3.025572	-5.626304	-3.416665
50	1	0	-4.420955	0.655773	-0.128296	131	6	0	-4.913809	-3.936188	-4.417943
51	6	0	-4.051712	-2.441698	-2.464972	132	1	0	-4.529934	-4.605653	-5.195496
52	1	0	-1.953211	-2.212626	-2.068187	133	1	0	-5.731339	-4.456590	-3.920314
53	6	0	-5.322567	-1.946241	-2.102668	134	1	0	-5.321997	-3.048761	-4.909624
54	6	0	-2.075062	1.475462	0.541217	135	6	0	-2.593263	-3.122781	-4.397934
55	6	0	-1.681365	2.631566	-0.115039	136	1	0	-2.394902	-3.904079	-5.138973
56	6	0	-2.875000	1.569604	1.680910	137	1	0	-2.852580	-2.203224	-4.932896
57	6	0	-2.128857	3.898276	0.275281	138	1	0	-1.660681	-2.947939	-3.857830
58	1	0	-1.005525	2.543738	-0.960771	139	6	0	7.045512	0.302020	-1.286138
59	6	0	-3.387502	2.794249	2.098643	140	6	0	2.718515	4.193092	-3.370755
60	1	0	-3.109162	0.664756	2.228186	141	1	0	2.884950	3.437343	-4.145113
61	6	0	-3.080517	3.934246	1.310741	142	1	0	1.806273	3.934259	-2.828176
62	6	0	-1.504935	5.108247	-0.457167	143	1	0	2.530697	5.150672	-3.866878
63	6	0	-1.990276	5.139861	-1.918231	144	6	0	7.492464	0.309950	-2.761605
64	1	0	-1.521914	5.975303	-2.450622	145	1	0	8.441349	-0.228661	-2.864204
65	1	0	-1.728244	4.215989	-2.445427	146	1	0	6.750730	-0.190486	-3.394034
66	1	0	-3.075769	5.265713	-1.979392	147	1	0	7.635048	1.327424	-3.130692
67	6	0	-1.763757	6.476902	0.196045	148	6	0	8.146886	0.926563	-0.408559
68	1	0	-1.506972	6.470393	1.258729	149	1	0	7.801669	1.067084	0.621424
69	1	0	-1.128671	7.218647	-0.300654	150	1	0	9.012462	0.255494	-0.381373
70	1	0	-2.794974	6.815198	0.095914	151	1	0	8.488649	1.884961	-0.798506
71	6	0	0.030679	4.927100	-0.456223	152	6	0	6.911504	-1.166547	-0.853268
72	1	0	0.419415	4.885482	0.567011	153	1	0	7.868642	-0.167264	-1.013059
73	1	0	0.351824	4.021440	-0.977779	154	1	0	6.667571	-1.253346	0.209271
74	1	0	0.496935	5.776797	-0.965337	155	6	0	1.682311	-5.705723	2.596558
75	6	0	-4.191123	2.899685	3.410858	156	1	0	1.771342	-5.675531	2.874716
76	6	0	-3.488631	3.910706	4.338728	157	1	0	1.973956	-5.079303	3.444551
77	1	0	-3.516238	4.918016	3.919155	158	1	0	0.641146	-5.482094	2.342211
78	1	0	-3.984057	3.930761	5.315947	159	6	0	4.360759	-3.481525	2.797147
79	1	0	-2.439985	3.636449	4.490418	160	6	0	3.888602	-3.001316	4.178989
80	6	0	-5.648558	3.340787	3.178617	161	1	0	4.710855	-3.075642	4.899457
81	1	0	-6.134385	2.721767	2.416235	162	1	0	3.544672	-1.963473	4.156100
						163	1	0	3.067787	-3.623142	4.546469

164	6	0	4.834106	-4.941489	2.914885
165	1	0	5.719728	-4.960308	3.559628
166	1	0	4.091940	-5.600642	3.365176
167	1	0	5.116934	-5.355432	1.943348
168	6	0	5.612978	-2.672698	2.388908
169	1	0	5.974240	-2.997602	1.407904
170	1	0	5.432784	-1.595279	2.348844
171	1	0	6.413000	-2.842314	3.117046
172	6	0	1.218642	-5.013674	-1.060427
173	6	0	0.610629	-4.401192	-2.334498
174	1	0	0.237380	-5.205907	-2.975511
175	1	0	-0.235869	-3.743052	-2.111117
176	1	0	1.348822	-3.833210	-2.910914
177	6	0	0.102489	-5.811714	-0.361553
178	1	0	-0.645798	-5.142055	0.076087
179	1	0	-0.403183	-6.452103	-1.092863
180	1	0	0.496084	-6.457216	0.424419
181	6	0	2.344322	-5.969117	-1.500865
182	1	0	3.124227	-5.425036	-2.045083
183	1	0	2.802025	-6.466904	-0.643976
184	1	0	1.939388	-6.737091	-2.169525
185	8	0	-0.968126	0.184579	-3.490696
186	6	0	0.168176	0.206423	-4.096801
187	6	0	0.609592	1.498119	-4.748044
188	1	0	0.318616	2.356846	-4.140784
189	1	0	1.686117	1.512019	-4.926811
190	1	0	0.098317	1.560121	-5.716424
191	6	0	0.674069	-1.078934	-4.716565
192	1	0	0.158982	-1.199464	-5.677301
193	1	0	1.749093	-1.039776	-4.903434
194	1	0	0.436558	-1.935153	-4.082962
195	1	0	1.310562	0.269709	-2.855274
196	1	0	6.153073	-1.705971	-1.430385

8

RwB97XD SCF energy -4485.232658 a.u.

RwB97XD SCF enthalpy -4483.426630 a.u.

RwB97XD SCF free energy -4483.850204 a.u.

Three lowest frequencies (cm⁻¹) 11.5, 16.1, 20.3

Cartesian coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.250414	-0.974313	2.185833
2	6	0	0.007018	-1.940103	3.136114
3	6	0	-0.572952	-3.206020	3.113310
4	6	0	-1.429229	-3.588458	2.110402
5	6	0	-1.703310	-2.630266	1.124000
6	6	0	-1.148236	-1.350998	1.147547
7	1	0	-1.886162	-4.570545	2.087545
8	1	0	-2.393084	-2.903810	0.335400
9	6	0	0.336523	0.378320	2.384908
10	6	0	1.258723	1.038264	1.526477
11	6	0	-0.010644	1.061004	3.531480
12	6	0	1.737451	2.307116	1.847577
13	6	0	0.469698	2.330222	3.839670
14	6	0	1.345582	2.987630	3.010599
15	1	0	2.450047	2.795175	1.193907
16	1	0	1.727960	3.974352	3.243346
17	8	0	-0.153715	-3.915769	4.190368
18	8	0	0.825305	-1.840403	4.217216
19	8	0	-0.868033	0.655163	4.506861
20	8	0	-0.073883	2.744821	5.014727
21	6	0	0.504392	-2.965016	5.032271
22	1	0	1.416568	-3.403351	5.435185
23	1	0	-0.180513	-2.654293	5.831062
24	6	0	-0.670263	1.574473	5.579465
25	1	0	0.015777	1.135113	6.314401
26	1	0	-1.631677	1.829149	6.025221
27	15	0	1.736487	0.239587	-0.046076
28	15	0	-1.550773	-0.177567	-0.193602
29	46	0	0.126530	0.228264	-1.673899
30	6	0	2.278730	-1.432764	0.380492
31	6	0	3.162040	-1.680484	1.422819
32	6	0	1.792785	-2.493971	-0.379921
33	6	0	3.542250	-2.982458	1.765706
34	1	0	3.568012	-0.840483	1.978216

35	6	0	2.077446	-3.814813	-0.052656
36	1	0	1.149618	-2.270027	-1.222061
37	6	0	2.885833	-4.033696	1.088872
38	6	0	3.168419	1.145512	-0.706084
39	6	0	4.420209	0.550104	-0.845474
40	6	0	2.963349	2.427211	-1.207282
41	6	0	5.495588	1.250563	-1.390277
42	1	0	4.549788	-0.476138	-0.528313
43	6	0	4.002610	3.193527	-1.741888
44	1	0	1.963973	2.848148	-1.168165
45	6	0	5.287146	2.610641	-1.726842
46	6	0	-2.978033	-0.881669	-1.062564
47	6	0	-4.255234	-0.352029	-0.905843
48	6	0	-2.782615	-1.954136	-1.923638
49	6	0	-5.360791	-0.936256	-1.518023
50	1	0	-4.384773	0.526999	-0.291025
51	6	0	-3.846240	-2.594564	-2.564918
52	1	0	-1.770782	-2.304406	-2.091998
53	6	0	-5.142612	-2.119513	-2.265987
54	6	0	-2.129751	1.352238	0.579703
55	6	0	-1.803551	2.562384	-0.012079
56	6	0	-2.947421	1.334493	1.711670
57	6	0	-2.334351	3.775352	0.438748
58	1	0	-1.117058	2.561020	-0.852712
59	6	0	-3.545199	2.499949	2.180687
60	1	0	-3.128914	0.390219	2.210332
61	6	0	-3.303580	3.695085	1.455034
62	6	0	-1.773116	5.061572	-0.209379
63	6	0	-2.218443	5.141346	-1.681140
64	1	0	-1.793336	6.034102	-2.153266
65	1	0	-1.881434	4.267928	-2.249991
66	1	0	-3.308248	5.199124	-1.767991
67	6	0	-2.140757	6.373855	0.504961
68	1	0	-1.913187	6.328333	1.573250
69	1	0	-1.541994	7.179628	0.066369
70	1	0	-3.188550	6.650847	0.389408
71	6	0	-0.229799	4.979766	-0.164256
72	1	0	0.128644	4.918911	0.869807
73	1	0	0.165808	4.119585	-0.710210
74	1	0	0.196419	5.878214	-0.622242
75	6	0	-4.370942	2.489024	3.483058
76	6	0	-3.748855	3.499826	4.467039
77	1	0	-3.837103	4.521817	4.093698
78	1	0	-4.257009	3.441437	5.436088
79	1	0	-2.686611	3.286927	4.622761
80	6	0	-5.851368	2.842804	3.247391
81	1	0	-6.286368	2.223600	2.455093
82	1	0	-6.419725	2.658126	4.165803
83	1	0	-5.984433	3.892306	2.984138
84	6	0	-4.334886	1.103547	4.149134
85	1	0	-4.833271	0.341904	3.539072
86	1	0	-3.311972	0.771740	4.351375
87	1	0	-4.866573	1.155861	5.104392
88	8	0	-4.046118	4.798866	1.786566
89	8	0	-6.250246	-2.785007	-2.726853
90	8	0	3.032030	-5.325430	1.523854
91	8	0	6.387301	3.350674	-2.076799
92	6	0	6.876603	4.170036	-1.018645
93	1	0	7.815770	4.603019	-1.368050
94	1	0	6.179000	4.977015	-0.773643
95	1	0	7.060984	3.581656	-0.113507
96	6	0	3.626652	4.587884	-2.297674
97	6	0	4.676178	5.227962	-3.224155
98	1	0	4.227516	6.111821	-3.690427
99	1	0	5.572822	5.558633	-2.701444
100	1	0	4.978018	4.543751	-4.022095
101	6	0	3.332518	5.535818	-1.120196
102	1	0	2.994832	6.508965	-1.494095
103	1	0	2.547841	5.130294	-0.473559
104	1	0	4.221983	5.701092	-0.504599
105	6	0	-5.109450	5.041321	0.868686
106	1	0	-5.673633	5.889645	1.260366
107	1	0	-4.734476	5.286470	-0.130322
108	1	0	-5.768906	4.169614	0.788752
109	6	0	-6.605160	-3.915409	-1.936062
110	1	0	-7.576577	-4.257971	-2.297685
111	1	0	-5.879222	-4.727551	-2.039488
112	1	0	-6.683873	-3.650410	-0.876357
113	6	0	-6.739911	-0.247717	-1.423644
114	6	0	-6.650351	1.075852	-0.641162
115	1	0	-6.366776	0.916362	0.405356
116	1	0	-5.939386	1.777297	-1.090350

117	1	0	-7.633809	1.556052	-0.645167
118	6	0	-7.224055	0.087298	-2.847981
119	1	0	-7.333752	-0.816004	-3.451749
120	1	0	-8.196272	0.591137	-2.802493
121	1	0	-6.518439	0.758575	-3.349727
122	6	0	-7.792708	-1.118869	-0.712953
123	1	0	-8.100317	-1.968130	-1.322990
124	1	0	-7.418462	-1.490744	0.246971
125	1	0	-8.686269	-0.517435	-0.512413
126	6	0	-3.482668	-3.744815	-3.536208
127	6	0	-3.076551	-4.989792	-2.724018
128	1	0	-2.238140	-4.767750	-2.055221
129	1	0	-3.902872	-5.364737	-2.112693
130	1	0	-2.764236	-5.794361	-3.399466
131	6	0	-4.589106	-4.118696	-4.539261
132	1	0	-4.164030	-4.803860	-5.280659
133	1	0	-5.438139	-4.624957	-4.081860
134	1	0	-4.961487	-3.237854	-5.070071
135	6	0	-2.268839	-3.314896	-4.393678
136	1	0	-2.050046	-4.098153	-5.126561
137	1	0	-2.479153	-2.388450	-4.937848
138	1	0	-1.359463	-3.168457	-3.805902
139	6	0	6.825911	0.525362	-1.687199
140	6	0	2.346015	4.453043	-3.153285
141	1	0	2.505612	3.758979	-3.984653
142	1	0	1.478653	4.111059	-2.583780
143	1	0	2.085694	5.430090	-3.573010
144	6	0	7.139042	0.660268	-3.190918
145	1	0	8.071287	0.133496	-3.423930
146	1	0	6.340575	0.214588	-3.794631
147	1	0	7.254217	1.705763	-3.483053
148	6	0	8.002246	1.079632	-0.861865
149	1	0	7.753900	1.121110	0.204208
150	1	0	8.869439	0.420117	-0.977164
151	1	0	8.301264	2.074489	-1.192222
152	6	0	6.723103	-0.976409	-1.373672
153	1	0	7.660350	-1.463335	-1.660432
154	1	0	6.570781	-1.161713	-0.306038
155	6	0	2.232893	-5.615802	2.667432
156	1	0	2.436591	-6.654046	2.936235
157	1	0	2.484452	-4.966466	3.511794
158	1	0	1.167964	-5.498307	2.443961
159	6	0	4.676239	-3.125200	2.810581
160	6	0	4.185785	-2.665342	4.194089
161	1	0	5.018869	-2.674176	4.905859
162	1	0	3.772771	-1.652889	4.165132
163	1	0	3.411939	-3.335516	4.578616
164	6	0	5.283918	-4.533419	2.939782
165	1	0	6.183575	-4.459444	3.560606
166	1	0	4.617846	-5.249166	3.421755
167	1	0	5.578494	-4.938050	1.968037
168	6	0	5.841789	-2.211863	2.365152
169	1	0	6.223254	-2.528241	1.388838
170	1	0	5.560344	-1.157883	2.298262
171	1	0	6.661392	-2.285758	3.087522
172	6	0	1.571051	-4.959406	-0.954602
173	6	0	0.803185	-4.409107	-2.169652
174	1	0	0.486632	-5.244949	-2.801173
175	1	0	-0.099361	-3.865219	-1.869329
176	1	0	1.420346	-3.746649	-2.786116
177	6	0	0.615720	-5.914550	-0.215490
178	1	0	-0.182951	-5.361011	0.289415
179	1	0	0.149443	-6.594297	-0.937290
180	1	0	1.139133	-6.525202	0.520475
181	6	0	2.783137	-5.748945	-1.485050
182	1	0	3.447578	-5.098348	-2.064422
183	1	0	3.356143	-6.190710	-0.666946
184	1	0	2.443366	-6.557109	-2.142582
185	8	0	-0.939543	0.298734	-3.384832
186	6	0	0.256586	0.441481	-4.026808
187	6	0	0.389891	1.764587	-4.776341
188	1	0	0.141859	2.600694	-4.117753
189	1	0	1.402271	1.902636	-5.166397
190	1	0	-0.310479	1.762036	-5.618440
191	6	0	0.654397	-0.776951	-4.858732
192	1	0	-0.038498	-0.874149	-5.701118
193	1	0	1.670154	-0.674698	-5.252633
194	1	0	0.597833	-1.685954	-4.253632
195	1	0	1.137167	0.509945	-3.206050
196	1	0	5.914837	-1.463387	-1.929547

9a(DTBM-Segphos)

RwB97XD SCF energy -5213.551305 a.u.
 RwB97XD SCF enthalpy -5211.485047 a.u.
 RwB97XD SCF free energy -5211.736837 a.u.
 Three lowest frequencies (cm⁻¹) 13.4, 17.8, 21.3
 Cartesian coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates X	Coordinates Y	Coordinates Z (Angstroms)
1	6	0	-0.836715	-0.501342	2.725579
2	6	0	-0.512047	-1.207236	3.864585
3	6	0	-0.807576	-2.555575	4.033682
4	6	0	-1.429735	-3.282961	3.049300
5	6	0	-1.728504	-2.601741	1.860532
6	6	0	-1.445344	-1.248579	1.679036
7	1	0	-1.681772	-4.328665	3.178767
8	1	0	-2.221037	-3.160063	1.075309
9	6	0	-0.639787	0.972207	2.747011
10	6	0	0.241158	1.722637	1.924304
11	6	0	-1.346777	1.690278	3.687403
12	6	0	0.355940	3.101631	2.088133
13	6	0	-1.231188	3.068742	3.838503
14	6	0	-0.381655	3.807653	3.051634
15	1	0	1.041197	3.663577	1.464893
16	1	0	-0.275898	4.879450	3.169384
17	8	0	-0.398141	-2.961486	5.262089
18	8	0	0.109435	-0.735859	4.977298
19	8	0	-2.255452	1.213807	4.581868
20	8	0	-2.064173	3.484025	4.829896
21	6	0	0.000888	-1.771426	5.951272
22	1	0	0.971212	-1.931860	6.423662
23	1	0	-0.766976	-1.505008	6.686729
24	6	0	-2.459760	2.285033	5.500800
25	1	0	-1.823860	2.135242	6.382544
26	1	0	-3.513951	2.342938	5.769301
27	15	0	1.186301	0.843468	0.630618
28	15	0	-1.825774	-0.436152	0.080925
29	46	0	-0.006835	0.040650	-1.180351
30	6	0	2.081785	-0.454380	1.523204
31	6	0	2.904112	-0.167206	2.603675
32	6	0	1.886202	-1.780429	1.139738
33	6	0	3.539571	-1.177709	3.334337
34	1	0	3.052100	0.870044	2.886094
35	6	0	2.439107	-2.837941	1.854631
36	1	0	1.269735	-1.971583	0.270137
37	6	0	3.209398	-2.508944	2.998110
38	6	0	2.324829	2.068823	-0.076631
39	6	0	3.706330	2.028448	0.041874
40	6	0	1.737331	3.011585	-0.916444
41	6	0	4.521334	2.948224	-0.630398
42	1	0	4.155628	1.257364	0.654782
43	6	0	2.481338	3.945778	-1.630050
44	1	0	0.659971	2.991566	-1.036030
45	6	0	3.884569	3.924715	-1.434448
46	6	0	-2.870207	-1.596909	-0.836941
47	6	0	-4.167427	-1.277228	-1.200930
48	6	0	-2.308618	-2.783443	-1.295952
49	6	0	-4.951463	-2.144029	-1.967548
50	1	0	-4.585595	-0.328291	-0.890209
51	6	0	-3.042340	-3.717322	-2.020862
52	1	0	-1.267265	-2.984735	-1.073569
53	6	0	-4.394960	-3.399272	-2.293643
54	6	0	-2.895677	0.962299	0.509660
55	6	0	-2.758317	2.198324	-0.102355
56	6	0	-3.921826	0.761620	1.436892
57	6	0	-3.689861	3.227016	0.098773
58	1	0	-1.907511	2.364835	-0.755509
59	6	0	-4.896500	1.728038	1.652542
60	1	0	-3.960926	-0.177450	1.975290
61	6	0	-4.820944	2.908467	0.871800
62	6	0	-3.358945	4.610265	-0.507666
63	6	0	-3.366142	4.526503	-2.043900
64	1	0	-3.106129	5.499919	-2.474524
65	1	0	-2.640799	3.796633	-2.412043
66	1	0	-4.352676	4.240506	-2.423347
67	6	0	-4.273362	5.769398	-0.073609

Three lowest frequencies (cm⁻¹) -1004, 11.7, 11.9
 Imaginary frequency (cm⁻¹) -1004
 Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.252674	-0.899454	2.716742
2	6	0	1.127758	-0.845612	4.088420
3	6	0	1.462720	0.280148	4.836787
4	6	0	1.910201	1.434982	4.243459
5	6	0	2.024047	1.417032	2.845922
6	6	0	1.716217	0.288362	2.087018
7	1	0	2.178767	2.311405	4.821070
8	1	0	2.392847	2.311089	2.359907
9	6	0	1.020680	-2.196179	2.029534
10	6	0	0.040415	-2.467181	1.035810
11	6	0	1.825742	-3.256065	2.388609
12	6	0	-0.059043	-3.741167	0.478071
13	6	0	1.723793	-4.520692	1.816758
14	6	0	0.786421	-4.796925	0.851653
15	1	0	-0.820824	-3.946907	-0.263193
16	1	0	0.692640	-5.779302	0.404423
17	8	0	1.280226	0.020584	6.153965
18	8	0	0.699506	-1.830033	4.920081
19	8	0	2.840248	-3.252300	3.294834
20	8	0	2.668203	-5.336169	2.354653
21	6	0	1.006146	-1.381431	6.238829
22	1	0	0.148909	-1.545082	6.893072
23	1	0	1.897922	-1.903306	6.605612
24	6	0	3.163083	-4.627450	3.493983
25	1	0	2.658572	-4.993382	4.396920
26	1	0	4.244569	-4.743433	3.559193
27	15	0	-1.032336	-1.111699	0.434753
28	15	0	1.907849	0.338738	0.275294
29	46	0	0.035777	0.300715	-1.011435
30	6	0	-1.719105	-0.338487	1.915939
31	6	0	-2.290723	-1.122601	2.909310
32	6	0	-1.677716	1.046468	2.061309
33	6	0	-2.787504	-0.563505	4.089666
34	1	0	-2.355922	-2.195800	2.758587
35	6	0	-2.090309	1.659984	3.241954
36	1	0	-1.288629	1.638515	1.241704
37	6	0	-2.558101	0.815798	4.278998
38	6	0	-2.387973	-1.872663	-0.500080
39	6	0	-3.718851	-1.722476	-0.119991
40	6	0	-2.089099	-2.451428	-1.728062
41	6	0	-4.754038	-2.223174	-0.909373
42	1	0	-3.945201	-1.198994	0.799163
43	6	0	-3.073596	-2.964730	-2.571120
44	1	0	-1.055112	-2.474548	-2.053885
45	6	0	-4.399603	-2.915292	-2.092946
46	6	0	2.777004	1.880722	-0.110377
47	6	0	4.038936	1.853388	-0.690299
48	6	0	2.108559	3.090919	0.023838
49	6	0	4.691208	3.027133	-1.058439
50	1	0	4.512946	0.898206	-0.864975
51	6	0	2.699674	4.306781	-0.325805
52	1	0	1.091642	3.085857	0.401621
53	6	0	4.037737	4.251415	-0.777694
54	6	0	3.003532	-1.017548	-0.199196
55	6	0	2.750282	-1.689899	-1.384734
56	6	0	4.120004	-1.358895	0.566106
57	6	0	3.630332	-2.648919	-1.894845

58	1	0	1.842944	-1.456899	-1.932768
59	6	0	5.053362	-2.276759	0.095350
60	1	0	4.257762	-0.883933	1.529811
61	6	0	4.838664	-2.822256	-1.197097
62	6	0	3.155110	-3.426014	-3.143368
63	6	0	3.057142	-2.466293	-4.343287
64	1	0	2.696711	-3.004834	-5.226851
65	1	0	2.359582	-1.646218	-4.143472
66	1	0	4.031579	-2.029286	-4.585356
67	6	0	4.012750	-4.640656	-3.536725
68	1	0	4.177637	-5.310775	-2.689224
69	1	0	3.475418	-5.199819	-4.310601
70	1	0	4.983106	-4.367004	-3.951671
71	6	0	1.746785	-3.986884	-2.837527
72	1	0	1.783495	-4.696583	-2.004141
73	1	0	1.026967	-3.205607	-2.580053
74	1	0	1.362168	-4.511542	-3.718362
75	6	0	6.223269	-2.735445	0.988515
76	6	0	6.167142	-4.270712	1.120351
77	1	0	6.351131	-4.758987	0.161589
78	1	0	6.925157	-4.613864	1.833234
79	1	0	5.185202	-4.592825	1.481973
80	6	0	7.593232	-2.312723	0.426805
81	1	0	7.620211	-1.237853	0.216398
82	1	0	8.372573	-2.527926	1.166422
83	1	0	7.846231	-2.854524	-0.484950
84	6	0	6.104332	-2.142382	2.402210
85	1	0	6.217992	-1.052784	2.402553
86	1	0	5.147054	-2.391497	2.870767
87	1	0	6.902779	-2.554080	3.027463
88	8	0	5.857263	-3.548083	-1.758362
89	8	0	4.745812	5.407602	-0.989268
90	8	0	-2.806137	1.385695	5.500773
91	8	0	-5.410383	-3.512867	-2.803193
92	6	0	-5.498666	-4.917603	-2.587561
93	1	0	-6.391506	-5.260077	-3.116257
94	1	0	-4.625572	-5.445604	-2.980362
95	1	0	-5.596953	-5.150838	-1.521894
96	6	0	-2.601966	-3.481356	-3.952439
97	6	0	-3.710268	-3.612465	-5.012106
98	1	0	-3.238165	-3.817945	-5.978975
99	1	0	-4.409241	-4.424173	-4.814814
100	1	0	-4.280692	-2.684192	-5.108063
101	6	0	-1.890723	-4.835800	-3.776774
102	1	0	-1.479377	-5.173057	-4.735110
103	1	0	-1.063316	-4.755567	-3.063661
104	1	0	-2.573574	-5.609750	-3.413089
105	6	0	6.584247	-2.802089	-2.731680
106	1	0	7.398055	-3.443590	-3.074498
107	1	0	5.954133	-2.528598	-3.584637
108	1	0	6.999256	-1.885054	-2.297578
109	6	0	5.282494	5.967397	0.205487
110	1	0	5.922847	6.797911	-0.097850
111	1	0	4.495905	6.344830	0.866384
112	1	0	5.877340	5.231401	0.756986
113	6	0	6.028163	2.949462	-1.826840
114	6	0	6.434230	1.488195	-2.096094
115	1	0	6.631433	0.937267	-1.169436
116	1	0	5.674462	0.943758	-2.667219
117	1	0	7.356464	1.480584	-2.685368
118	6	0	5.851003	3.638627	-3.194176
119	1	0	5.586382	4.691443	-3.076420
120	1	0	6.784339	3.580347	-3.765657
121	1	0	5.065583	3.145450	-3.777601
122	6	0	7.193008	3.608275	-1.064774

123	1	0	7.098476	4.693750	-1.033782	188	6	0	-1.449521	2.738793	-2.559617
124	1	0	7.260559	3.230679	-0.038763	189	1	0	-1.785721	3.634319	-3.071654
125	1	0	8.136959	3.374481	-1.569569	190	1	0	-0.718336	2.808556	-1.762827
126	6	0	1.814390	5.572753	-0.207840	191	8	0	-2.823290	2.969651	-1.139229
127	6	0	1.630140	5.929714	1.279196	192	6	0	-3.734784	3.838223	-1.434246
128	1	0	1.188559	5.095838	1.834594	193	8	0	-3.626880	4.694806	-2.318055
129	1	0	2.582091	6.183454	1.755649	194	6	0	-5.026972	3.750729	-0.593773
130	1	0	0.961477	6.792104	1.379421	195	6	0	-5.044061	4.960399	0.354221
131	6	0	2.333060	6.803841	-0.972550	196	1	0	-5.031446	5.895787	-0.213672
132	1	0	1.547653	7.567419	-0.964704	197	1	0	-5.947473	4.945360	0.974500
133	1	0	3.221956	7.249927	-0.528016	198	1	0	-4.176167	4.954255	1.021515
134	1	0	2.556398	6.562121	-2.015588	199	6	0	-6.223967	3.825303	-1.552016
135	6	0	0.422173	5.270661	-0.810650	200	1	0	-6.234367	2.968143	-2.235519
136	1	0	-0.202292	6.167840	-0.748480	201	1	0	-7.162335	3.817205	-0.986098
137	1	0	0.504281	4.990941	-1.866269	202	1	0	-6.184305	4.737368	-2.152556
138	1	0	-0.114470	4.476744	-0.287458	203	6	0	-5.087849	2.441819	0.197670
139	6	0	-6.222896	-1.907941	-0.549184	204	1	0	-6.020536	2.392368	0.771764
140	6	0	-1.587092	-2.471606	-4.538648	205	1	0	-5.056601	1.581073	-0.478381
141	1	0	-2.023841	-1.470036	-4.584968	206	1	0	-4.248844	2.343353	0.891533
142	1	0	-0.659370	-2.415494	-3.963885	207	8	0	1.140705	1.403171	-2.400119
143	1	0	-1.312450	-2.778761	-5.553111	208	6	0	0.725628	1.802728	-3.586303
144	6	0	-6.807143	-1.017444	-1.664211	209	1	0	-0.400097	2.390222	-3.450158
145	1	0	-7.848145	-0.763039	-1.430412	210	6	0	1.549310	2.960545	-4.133774
146	1	0	-6.241884	-0.083022	-1.752496	211	1	0	1.090876	3.396259	-5.025720
147	1	0	-6.785852	-1.530633	-2.628627	212	1	0	1.671757	3.730380	-3.368052
148	6	0	-7.097196	-3.166069	-0.386013	213	1	0	2.542284	2.580455	-4.400044
149	1	0	-6.628794	-3.890892	0.288583	214	6	0	0.393412	0.725829	-4.609185
150	1	0	-8.060821	-2.881263	0.050531	215	1	0	1.336680	0.305065	-4.976082
151	1	0	-7.300735	-3.652254	-1.339435	216	1	0	-0.186356	-0.078863	-4.153743
152	6	0	-6.322123	-1.134286	0.775599	217	1	0	-0.157897	1.133192	-5.461704
153	1	0	-5.766742	-0.192956	0.758874	218	6	0	-3.293515	1.361806	-3.616229
154	1	0	-7.371828	-0.890136	0.966572	219	6	0	-3.999103	2.294049	-4.337086
155	1	0	-5.962731	-1.734200	1.617582	220	8	0	-3.870925	0.135315	-3.755180
156	6	0	-1.780957	1.117700	6.453274	221	6	0	-5.067747	1.592338	-4.949084
157	1	0	-2.099198	1.572489	7.393264	222	1	0	-3.791418	3.353160	-4.380252
158	1	0	-1.639242	0.042293	6.601322	223	6	0	-4.934198	0.290898	-4.554751
159	1	0	-0.828383	1.554970	6.140163	224	1	0	-5.836189	1.994393	-5.592272
160	6	0	-3.577008	-1.510275	5.026016	225	1	0	-5.505883	-0.600648	-4.766280
161	6	0	-2.638667	-2.580373	5.610374						
162	1	0	-3.214893	-3.289741	6.214958						
163	1	0	-2.124907	-3.144100	4.826102						
164	1	0	-1.877924	-2.130830	6.254720						
165	6	0	-4.336050	-0.829728	6.178839						
166	1	0	-4.989820	-1.577369	6.641460						
167	1	0	-3.680761	-0.448392	6.962047						
168	1	0	-4.963084	-0.008517	5.823161						
169	6	0	-4.662013	-2.206690	4.171927						
170	1	0	-5.353140	-1.466054	3.756435						
171	1	0	-4.249014	-2.790276	3.344943						
172	1	0	-5.239544	-2.893051	4.800079						
173	6	0	-2.086714	3.198568	3.364025						
174	6	0	-1.611454	3.850704	2.055336						
175	1	0	-1.662994	4.939558	2.157245						
176	1	0	-0.567459	3.594155	1.840802						
177	1	0	-2.217160	3.566976	1.188892						
178	6	0	-1.149748	3.700841	4.478299						
179	1	0	-0.152602	3.258491	4.385608						
180	1	0	-1.042700	4.788370	4.397902						
181	1	0	-1.540995	3.481617	5.471884						
182	6	0	-3.520553	3.684114	3.651754						
183	1	0	-4.206760	3.377168	2.856912						
184	1	0	-3.888051	3.286668	4.600217						
185	1	0	-3.538040	4.778526	3.708458						
186	8	0	-1.705068	0.395683	-2.238369						
187	6	0	-2.140178	1.437856	-2.757843						

TS5a(DTBM-Segphos)

RwB97XD SCF energy -5213.443785 a.u.
RwB97XD SCF enthalpy -5211.384672 a.u.
RwB97XD SCF free energy -5211.640436 a.u.
Three lowest frequencies (cm⁻¹) -674.9, 8.2, 9.6 a.u.
Imaginary frequency (cm⁻¹) -674.9

Cartesian coordinates:

Standard		orientation:				
Center Number	Atomic Number	Atomic Type	Coordinates X	Y	Z (Angstroms)	
1	6	0	1.282538	2.517062	1.315915	
2	6	0	2.035490	3.063184	2.333145	
3	6	0	1.582768	3.157934	3.645567	
4	6	0	0.342449	2.699104	4.014930	
5	6	0	-0.438402	2.121569	3.002710	
6	6	0	0.003233	2.016823	1.684238	
7	1	0	-0.025697	2.787931	5.030192	
8	1	0	-1.425135	1.768032	3.272287	
9	6	0	1.813916	2.596938	-0.070061	
10	6	0	2.168925	1.503532	-0.907301	
11	6	0	2.041997	3.854682	-0.586056	
12	6	0	2.700304	1.738900	-2.174273	
13	6	0	2.569963	4.075753	-1.854416	
14	6	0	2.904604	3.031901	-2.681336	
15	1	0	2.996649	0.906694	-2.799201	
16	1	0	3.326227	3.189317	-3.667037	
17	8	0	2.531849	3.753945	4.410801	
18	8	0	3.287327	3.582679	2.245867	
19	8	0	1.800534	5.053022	0.014572	
20	8	0	2.671497	5.414927	-2.071384	
21	6	0	3.522873	4.230334	3.493924	

22	1	0	4.515406	3.969864	3.862184	104	1	0	3.872435	-0.751540	-5.874194
23	1	0	3.409070	5.313798	3.371190	105	6	0	-3.753106	4.860361	-4.213937
24	6	0	2.512811	6.000893	-0.777254	106	1	0	-4.022485	5.687689	-4.873445
25	1	0	3.501754	6.173999	-0.332970	107	1	0	-3.917921	3.915618	-4.740593
26	1	0	1.937780	6.922671	-0.855239	108	1	0	-4.393443	4.878261	-3.324774
27	15	0	1.916192	-0.202743	-0.273420	109	6	0	-6.301331	0.697784	4.266823
28	15	0	-1.020947	1.177434	0.425957	110	1	0	-7.285631	0.487321	4.688816
29	46	0	-0.264865	-0.801930	-0.403734	111	1	0	-5.538322	0.539190	5.034925
30	6	0	2.785475	-0.187720	1.314359	112	1	0	-6.256211	1.745413	3.951936
31	6	0	4.113196	0.218470	1.347031	113	6	0	-6.345154	1.175757	0.598188
32	6	0	2.159819	-0.600863	2.485472	114	6	0	-6.091983	1.841443	-0.766856
33	6	0	4.853625	0.233793	2.531319	115	1	0	-5.594134	2.812505	-0.670426
34	1	0	4.590801	0.516434	0.419570	116	1	0	-5.494621	1.208377	-1.431320
35	6	0	2.819015	-0.549120	3.711316	117	1	0	-7.054989	2.015986	-1.256635
36	1	0	1.135996	-0.944647	2.427488	118	6	0	-7.161098	-0.104833	0.337156
37	6	0	4.147715	-0.056687	3.717861	119	1	0	-7.444784	-0.588331	1.272796
38	6	0	2.838343	-1.311749	-1.374244	120	1	0	-8.077101	0.143123	-0.210934
39	6	0	3.814673	-2.178863	-0.892375	121	1	0	-6.589648	-0.818120	-0.266277
40	6	0	2.442789	-1.407267	-2.703165	122	6	0	-7.191943	2.157024	1.429119
41	6	0	4.491955	-3.049927	-1.744500	123	1	0	-7.627434	1.679957	2.307702
42	1	0	4.048621	-2.173799	0.163720	124	1	0	-6.600776	3.020224	1.753139
43	6	0	3.098536	-2.234575	-3.617029	125	1	0	-8.020205	2.530421	0.816842
44	1	0	1.594790	-0.819283	-3.039197	126	6	0	-3.570433	-1.514791	4.142551
45	6	0	4.200148	-2.966401	-3.126840	127	6	0	-2.918568	-0.759042	5.318408
46	6	0	-2.590521	0.750927	1.232226	128	1	0	-1.966188	-0.304506	5.028101
47	6	0	-3.806409	1.180026	0.711861	129	1	0	-3.568931	0.037448	5.693911
48	6	0	-2.580218	-0.141937	2.297160	130	1	0	-2.723266	-1.450600	6.145820
49	6	0	-5.015539	0.800097	1.291495	131	6	0	-4.849470	-2.204538	4.646920
50	1	0	-3.802088	1.810982	-0.166939	132	1	0	-4.556225	-2.963275	5.380467
51	6	0	-3.750108	-0.531350	2.956569	133	1	0	-5.543270	-1.952813	5.144279
52	1	0	-1.628652	-0.532869	2.642705	134	1	0	-5.380898	-2.711144	3.839081
53	6	0	-4.956802	0.026047	2.478936	135	6	0	-2.624231	-2.659766	3.709969
54	6	0	-1.354153	2.390240	-0.875691	136	1	0	-2.490557	-3.354741	4.545430
55	6	0	-1.372117	1.961181	-2.196365	137	1	0	-3.043585	-3.220371	2.869002
56	6	0	-1.520377	3.743781	-0.584981	138	1	0	-1.631164	-2.310438	3.423151
57	6	0	-1.605896	2.841298	-3.257664	139	6	0	5.468963	-4.095131	-1.166498
58	1	0	-1.201972	0.910503	-2.399278	140	6	0	0.993935	-2.476469	-4.963819
59	6	0	-1.801877	4.663414	-1.590615	141	1	0	0.753020	-3.405796	-4.437643
60	1	0	-1.420092	4.072982	0.442027	142	1	0	0.483767	1.655271	-4.455832
61	6	0	-1.939253	4.166020	-2.912078	143	1	0	0.572431	-2.539376	-5.972679
62	6	0	-1.429056	2.281494	-4.690421	144	6	0	5.072787	-5.498477	-1.666678
63	6	0	-2.624284	1.388254	-5.063855	145	1	0	5.742329	-6.248955	-1.231796
64	1	0	-2.467767	0.940187	-6.051648	146	1	0	4.048415	-5.743077	-1.364235
65	1	0	-2.742263	0.575920	-4.342621	147	1	0	5.137687	-5.571161	-2.753246
66	1	0	-3.563912	1.947745	-5.092747	148	6	0	6.929661	-3.796723	-1.551014
67	6	0	-1.229131	3.357900	-5.772369	149	1	0	7.195843	-2.759929	-1.316462
68	1	0	-0.439856	4.062828	-5.494892	150	1	0	7.600452	-4.450805	-0.982862
69	1	0	-0.927198	2.862244	-6.701326	151	1	0	7.115522	-3.975322	-2.611165
70	1	0	-2.133653	3.927525	-5.984836	152	6	0	5.395142	-4.130011	0.370095
71	6	0	-0.151127	1.407476	-4.721919	153	1	0	6.037681	-4.936237	0.738033
72	1	0	0.729143	1.988089	-4.426828	154	1	0	5.749042	-3.199751	0.825037
73	1	0	-0.215859	0.531018	-4.070912	155	6	0	4.802676	1.452185	5.381453
74	1	0	0.009286	1.037071	-5.739642	156	1	0	5.247605	1.437427	6.378255
75	6	0	-1.862768	6.171986	-1.274552	157	1	0	5.422390	2.073336	4.726788
76	6	0	-0.860663	6.913298	-2.182703	158	1	0	3.801459	1.889763	5.435213
77	1	0	-1.163071	6.871455	-3.230009	159	6	0	6.367299	0.529888	2.398240
78	1	0	-0.789480	7.965249	-1.884737	160	6	0	6.574727	2.011325	2.035382
79	1	0	0.134583	6.465752	-2.102924	161	1	0	7.641228	2.215052	1.887225
80	6	0	-3.273792	6.754202	-1.474667	162	1	0	6.048982	2.273629	1.111921
81	1	0	-4.022233	6.177317	-0.920420	163	1	0	6.211926	2.674601	2.826790
82	1	0	-3.301384	7.783740	-1.100451	164	6	0	7.218361	0.180056	3.632715
83	1	0	-3.559628	6.778891	-2.526438	165	1	0	8.274538	0.256078	3.352029
84	6	0	-1.454780	6.449025	0.182855	166	1	0	7.061173	0.851489	4.476097
85	1	0	-2.167440	6.026384	0.899858	167	1	0	7.033476	-0.843136	3.970928
86	1	0	-0.457831	6.056981	0.407784	168	6	0	6.934641	-0.345355	1.254837
87	1	0	-1.434655	7.531261	0.345351	169	1	0	6.820071	-1.407735	1.492950
88	8	0	-2.383638	5.041971	-3.869090	170	1	0	6.461105	-0.160978	0.287593
89	8	0	-6.130810	-0.184862	3.161079	171	1	0	8.003826	-0.141697	1.135663
90	8	0	4.756543	0.100459	4.936429	172	6	0	2.142629	-1.113892	4.977843
91	8	0	5.019392	-3.648486	-3.992185	173	6	0	0.732994	-1.634536	4.656841
92	6	0	5.979809	-2.810377	-4.626196	174	1	0	0.280084	-2.038363	5.567524
93	1	0	6.614541	-3.461063	-5.230869	175	1	0	0.079381	-0.834983	4.289596
94	1	0	5.505375	-2.067982	-5.277015	176	1	0	0.750809	-2.438158	3.913876
95	1	0	6.596581	-2.281666	-3.890032	177	6	0	1.993898	-0.067816	6.098230
96	6	0	2.524158	-2.275805	-5.053947	178	1	0	1.550410	0.858041	5.718468
97	6	0	3.042069	-3.423533	-5.937948	179	1	0	1.329957	-0.461053	6.876093
98	1	0	2.457623	-3.433002	-6.864659	180	1	0	2.948638	0.166092	6.569162
99	1	0	4.090055	-3.318665	-6.215822	181	6	0	2.975282	-2.305819	5.489123
100	1	0	2.914121	-4.393773	-5.450075	182	1	0	3.033052	-3.092267	4.728519
101	6	0	2.799553	-0.929356	-5.748752	183	1	0	3.990664	-1.998427	5.748850
102	1	0	2.337288	-0.915599	-6.742148	184	1	0	2.507224	-2.734762	6.382595
103	1	0	2.384607	-0.093750	-5.175043	185	8	0	0.211820	-2.685270	-1.070921

186	6	0	0.105757	-3.731402	-0.227585	31	6	0	2.312655	3.180363	-0.503351
187	6	0	0.439162	-3.456533	1.239164	32	6	0	1.379215	2.145588	1.469659
188	1	0	-0.178508	-2.636795	1.622145	33	6	0	2.710018	4.295812	0.229491
189	1	0	0.258870	-4.343535	1.855880	34	1	0	2.542718	3.110750	-1.559526
190	1	0	1.493995	-3.172889	1.333286	35	6	0	1.716631	3.250556	2.252197
191	6	0	0.836296	-4.954492	-0.771079	36	1	0	0.893380	1.286716	1.919370
192	1	0	1.916603	-4.771320	-0.733381	37	6	0	2.287864	4.354509	1.581388
193	1	0	0.620047	-5.854932	-0.186065	38	6	0	2.571678	-0.129667	-1.531890
194	1	0	0.558663	-5.135310	-1.814295	39	6	0	3.854177	0.388865	-1.255429
195	1	0	-1.025646	-4.028420	-0.171579	40	6	0	2.409706	-1.289017	-2.292276
196	8	0	-2.174379	-1.047096	-1.271789	41	6	0	4.981831	-0.280673	-1.786129
197	8	0	-2.739265	-3.022781	-0.455449	42	1	0	3.968875	1.214497	-0.632718
198	6	0	-2.746853	-2.174310	-1.385346	43	6	0	3.494902	-1.956792	-2.863791
199	6	0	-3.492765	-2.374339	-2.713451	44	1	0	1.408932	-1.675160	-2.446804
200	6	0	-4.504004	-1.221927	-2.847949	45	6	0	4.779764	-1.403654	-2.630553
201	1	0	-5.009883	-1.279199	-3.817703	46	6	0	-2.818495	-0.358726	1.625111
202	1	0	-5.266283	-1.283229	-2.063375	47	6	0	-4.030603	-0.985609	1.367111
203	1	0	-4.009558	-0.251479	-2.767232	48	6	0	-2.331389	-0.323864	2.929846
204	6	0	-4.238894	-3.704711	-2.794185	49	6	0	-4.810775	-1.531921	2.385148
205	1	0	-4.978938	-3.800118	-1.995475	50	1	0	-4.393370	-1.046916	0.350433
206	1	0	-4.771256	-3.762907	-3.749513	51	6	0	-3.080713	-0.806747	4.002728
207	1	0	-3.558455	-4.559768	-2.754012	52	1	0	-1.359065	0.120178	3.115886
208	6	0	-2.445659	-2.299234	-3.837199	53	6	0	-4.354173	-1.353931	3.708708
209	1	0	-1.725664	-3.120479	-3.754495	54	6	0	-2.856659	-0.073930	-1.219664
210	1	0	-2.934851	-2.371772	-4.814444	55	6	0	-2.729209	-1.312093	-1.827906
211	1	0	-1.892269	-1.358098	-3.792150	56	6	0	-3.908042	0.772226	-1.579147
212	6	0	-2.303489	-5.128869	-0.318455	57	6	0	-3.675345	-1.794427	-2.736441
213	1	0	-1.706295	-5.520807	0.503022	58	1	0	-1.881971	-1.932291	-1.565601
214	1	0	-1.935887	-5.327736	-1.318847	59	6	0	-4.892640	0.346744	-2.466615
215	6	0	-3.745724	-5.497127	-0.126132	60	1	0	-3.966595	1.758904	-1.136363
216	8	0	-3.865197	-6.652767	-0.510454	61	6	0	-4.809819	-0.987038	-2.947139
217	6	0	-4.823622	-4.781023	0.525090	62	6	0	-3.374783	-3.164227	-3.386755
218	6	0	-5.047596	-3.522644	1.029052	63	6	0	-3.540913	-4.272533	-2.329816
219	8	0	-5.950933	-5.540406	0.688265	64	1	0	-3.208132	-5.233585	-2.737759
220	6	0	-6.374625	-3.519334	1.526379	65	1	0	-2.939669	-4.054187	-1.441212
221	1	0	-4.348270	-2.702672	1.023795	66	1	0	-4.582425	-4.383338	-2.014786
222	6	0	-6.865880	-4.769912	1.289014	67	6	0	-4.216233	-3.504261	-4.628838
223	1	0	-6.890178	-2.698453	2.001638	68	1	0	-4.202260	-2.689462	-5.357291
224	1	0	-7.821527	-5.232931	1.487400	69	1	0	-3.780492	-4.390284	-5.102511
225	1	0	4.378563	-4.325446	0.728359	70	1	0	-5.255266	-3.738063	-4.397255

10a											
RwB97XD SCF energy			-5213.548817 a.u.								
RwB97XD SCF enthalpy			-5211.487545 a.u.								
RwB97XD SCF free energy			-5211.743333 a.u.								
Three lowest frequencies (cm ⁻¹)			-21.8, -16.0, 10.6								
Standard orientation:											

Center	Atomic	Atomic	Coordinates			(Angstroms)					
Number	Number	Type	X	Y	Z						

1	6	0	-1.227501	2.865454	-0.694013						
2	6	0	-1.148686	4.222599	-0.476600						
3	6	0	-1.564029	4.827623	0.709042						
4	6	0	-2.053427	4.093695	1.762202						
5	6	0	-2.121865	2.705200	1.580484						
6	6	0	-1.729704	2.090041	0.392378						
7	1	0	-2.386200	4.558763	2.682123						
8	1	0	-2.520663	2.112024	2.394163						
9	6	0	-0.868526	2.334490	-2.034295						
10	6	0	0.161962	1.392622	-2.304002						
11	6	0	-1.566621	2.789537	-3.131354						
12	6	0	0.402115	0.951426	-3.604053						
13	6	0	-1.332181	2.328934	-4.424807						
14	6	0	-0.354332	1.402224	-4.695387						
15	1	0	1.206234	0.253469	-3.800381						
16	1	0	-0.162223	1.047808	-5.700971						
17	8	0	-1.410171	6.167245	0.610724						
18	8	0	-0.686894	5.168661	-1.330544						
19	8	0	-2.584158	3.687487	-3.149182						
20	8	0	-2.200441	2.923538	-5.279158						
21	6	0	-1.043016	6.422988	-0.750015						
22	1	0	-0.185254	7.097040	-0.778322						
23	1	0	-1.904135	6.842643	-1.281550						
24	6	0	-2.812695	3.977295	-4.529613						
25	1	0	-2.334867	4.930353	-4.783901						
26	1	0	-3.884589	3.996094	-4.727381						
27	15	0	1.109370	0.727004	-0.903323						
28	15	0	-1.853239	0.285255	0.236830						
29	46	0	0.070482	-0.918751	0.215273						
30	6	0	1.625354	2.129480	0.101613						
31	6	0									
32	6	0									
33	6	0									
34	1	0									
35	6	0									
36	1	0									
37	6	0									
38	6	0									
39	6	0									
40	6	0									
41	6	0									
42	1	0									
43	6	0									
44	1	0									
45	6	0									
46	6	0									
47	6	0									
48	6	0									
49	6	0									
50	1	0									
51	6	0									
52	1	0									
53	6	0									
54	6	0									
55	6	0									
56	6	0									
57	6	0									
58	1	0									
59	6	0									
60	1	0									
61	6	0									
62	6	0									
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64	1	0									
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66	1	0									
67	6	0									
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69	1	0									
70	1	0									
71	6	0									
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78	1	0									
79	1	0									
80	6	0									
81	1	0									
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83	1	0									
84	6	0									
85	1	0									
86	1	0									
87	1	0									
88	8	0									
89	8	0									
90	8	0									
91	8	0									
92	6	0									
93	1	0									
94	1	0									
95	1	0									
96	6	0									
97	6	0									
98	1	0									
99	1	0									
100	1	0									
101	6	0									
102	1	0									
103	1	0									
104	1	0									
105	6	0									

113	6	0	-6.101873	-2.255361	1.927999	195	1	0	1.648935	-3.723470	2.758905
114	6	0	-5.734449	-3.246084	0.796314	196	8	0	2.759369	-3.395131	0.921785
115	1	0	-5.320241	-2.753531	-0.087494	197	8	0	2.522925	-5.263445	-0.307967
116	1	0	-5.008059	-3.988440	1.143546	198	6	0	3.184414	-4.460274	0.402521
117	1	0	-6.634738	-3.778801	0.471662	199	6	0	4.679329	-4.795237	0.694958
118	6	0	-6.818702	-3.084836	3.006891	200	6	0	4.857507	-4.871248	2.217362
119	1	0	-7.283264	-2.473841	3.780700	201	1	0	4.632806	-3.903935	2.670316
120	1	0	-7.615963	-3.658113	2.521175	202	1	0	4.190135	-5.618890	2.663636
121	1	0	-6.140923	-3.794303	3.489206	203	1	0	5.888576	-5.141781	2.476101
122	6	0	-7.088233	-1.212403	1.367584	204	6	0	5.543529	-3.646491	0.157851
123	1	0	-7.384816	-0.490086	2.135464	205	1	0	6.599656	-3.796163	0.415024
124	1	0	-6.650717	-0.653967	0.533023	206	1	0	5.475171	-3.564476	-0.932576
125	1	0	-7.993898	-1.710651	1.004245	207	1	0	5.209800	-2.699399	0.590980
126	6	0	-2.453684	-0.655167	5.410735	208	6	0	5.108459	-6.119129	0.061680
127	6	0	-2.449641	0.840439	5.781706	209	1	0	6.154200	-6.339105	0.311955
128	1	0	-1.887023	1.435753	5.055138	210	1	0	4.488413	-6.946717	0.419346
129	1	0	-3.469255	1.237778	5.828724	211	1	0	5.023453	-6.088828	-1.028167
130	1	0	-1.985409	0.982981	6.763854	212	6	0	1.499437	-3.275760	3.754458
131	6	0	-3.145703	-1.434077	6.543490	213	1	0	0.792339	-2.452527	3.627026
132	1	0	-2.514122	-1.365964	7.436235	214	1	0	1.083525	-4.009612	4.447563
133	1	0	-4.122286	-1.027015	6.806646	215	6	0	2.825670	-2.799717	4.280966
134	1	0	-3.268833	-2.491248	6.296995	216	8	0	3.422084	-3.366450	5.184422
135	6	0	-1.000746	-1.174433	5.368492	217	6	0	3.397133	-1.616648	3.625064
136	1	0	-0.539355	-1.058425	6.354728	218	6	0	2.934929	-0.814119	2.624716
137	1	0	-0.979489	-2.237513	5.109908	219	8	0	4.648273	-1.218614	3.992688
138	1	0	-0.370386	-0.631484	4.659961	220	6	0	3.955596	0.140536	2.362259
139	6	0	6.381486	0.288054	-1.460175	221	1	0	1.979352	-0.912520	2.135295
140	6	0	1.823949	-3.813720	-3.372500	222	6	0	4.969544	-0.163218	3.221201
141	1	0	1.762513	-4.082386	-2.314824	223	1	0	3.920320	0.951071	1.649339
142	1	0	0.999535	-3.148024	-3.641116	224	1	0	5.941266	0.275576	3.393124
143	1	0	1.688078	-4.730892	-3.954887	225	1	0	5.840510	1.152337	0.485460
144	6	0	7.282673	-0.782564	-0.818244	-----					
145	1	0	8.276853	-0.357559	-0.638449	11a					
146	1	0	6.872864	-1.097326	0.147311	RwB97XD SCF energy					
147	1	0	7.393398	-1.661282	-1.454084	-5213.607895 au					
148	6	0	7.038452	0.845540	-2.737635	RwB97XD SCF enthalpy					
149	1	0	6.357871	1.519660	-3.269164	-5211.544648 au					
150	1	0	7.935142	1.415961	-2.470778	RwB97XD SCF free energy					
151	1	0	7.349362	0.058646	-3.423022	-5211.803308 au					
152	6	0	6.302258	1.454793	-0.458341	Three lowest frequencies (cm ⁻¹)					
153	1	0	7.318308	1.793195	-0.233324	12.5, 15.2, 18.6					
154	1	0	5.756268	2.314729	-0.860809	-----					
155	6	0	1.385352	6.428065	2.153972	Standard orientation:					
156	1	0	1.684004	7.347352	2.660600	-----					
157	1	0	1.171565	6.641926	1.105682	Center Atomic Atomic Coordinates (Angstroms)					
158	1	0	0.479973	6.031646	2.617169	Number Number Type X Y Z					
159	6	0	3.694131	5.314263	-0.390447	1	6	0	0.357339	-1.348044	2.660210
160	6	0	4.092154	4.902036	-1.818282	2	6	0	0.062305	-1.320975	4.006172
161	1	0	4.842692	5.605161	-2.191615	3	6	0	0.574097	-0.360896	4.876169
162	1	0	4.534587	3.901524	-1.856496	4	6	0	1.386589	0.654143	4.434620
163	1	0	3.241675	4.931177	-2.508421	5	6	0	1.685664	0.664871	3.064269
164	6	0	3.148950	6.751001	-0.481478	6	6	0	1.199118	-0.302987	2.187675
165	1	0	3.823445	7.354218	-1.098647	7	1	0	1.794005	1.398225	5.108623
166	1	0	2.160225	6.773817	-0.952484	8	1	0	2.342937	1.443770	2.699068
167	1	0	3.087635	7.231656	0.494603	9	6	0	-0.086764	-2.512738	1.849866
168	6	0	4.972338	5.306480	0.472797	10	6	0	-0.919798	-2.485734	0.697123
169	1	0	4.757860	5.618764	1.497660	11	6	0	0.367030	-3.756898	2.235403
170	1	0	5.419290	4.306558	0.500197	12	6	0	-1.209021	-3.666564	0.012954
171	1	0	5.711649	5.997408	0.052759	13	6	0	0.071293	-4.927120	1.543643
172	6	0	1.599442	3.172956	3.791191	14	6	0	-0.710561	-4.914393	0.414727
173	6	0	0.978687	1.833841	4.219746	15	1	0	-1.857932	-3.644679	-0.853132
174	1	0	0.910503	1.797933	5.311055	16	1	0	-0.946113	-5.819429	-0.132607
175	1	0	-0.035349	1.720401	3.822292	17	8	0	0.152322	-0.622927	6.137947
176	1	0	1.578610	0.977168	3.902071	18	8	0	-0.716095	-2.190123	4.702188
177	6	0	0.735916	4.284334	4.416166	19	8	0	1.185854	-4.048527	3.281893
178	1	0	-0.230255	4.377352	3.910339	20	8	0	0.684500	-5.977528	2.147332
179	1	0	0.540554	4.038166	5.465244	21	6	0	-0.446650	-1.920486	6.075546
180	1	0	1.240077	5.250315	4.402304	22	1	0	-1.377508	-1.920557	6.642559
181	6	0	3.021263	3.254163	4.380878	23	1	0	0.262076	-2.663350	6.461686
182	1	0	3.646061	2.430502	4.019547	24	6	0	1.149253	-5.469352	3.400941
183	1	0	3.500230	4.199482	4.112842	25	1	0	0.443120	-5.751358	4.191145
184	1	0	2.974461	3.189980	5.473814	26	1	0	2.152468	-5.846368	3.599880
185	8	0	-0.761284	-2.572199	1.287489	27	15	0	-1.573371	-0.887119	0.085617
186	6	0	-0.773987	-3.752219	0.898709	28	15	0	1.618288	-0.221641	0.415164
187	6	0	-0.276750	-4.156507	-0.431661	29	46	0	-0.061218	0.388913	-1.020433
188	1	0	-0.182493	-3.292117	-1.096220	30	6	0	-2.235687	-0.052923	1.546403
189	1	0	0.739388	-4.592369	-0.294407	31	6	0	-3.103958	-0.707360	2.411126
190	1	0	-0.901639	-4.935906	-0.878921	32	6	0	-1.838819	1.254081	1.818406
191	6	0	-1.272285	-4.805986	1.828991	33	6	0	-3.584403	-0.091897	3.571386
192	1	0	-2.144754	-5.292485	1.378070	34	1	0	-3.420710	-1.718372	2.174839
193	1	0	-0.502793	-5.576968	1.944833	35	6	0	-2.209180	1.892346	2.997849
194	1	0	-1.538500	-4.383656	2.797898	36	1	0	-1.217566	1.761310	1.091808
						37	6	0	-3.033002	1.167207	3.894026
						38	6	0	-2.929132	-1.304438	-1.043673

39	6	0	-4.262988	-1.040456	-0.745430	121	1	0	7.278339	2.680868	-2.003064
40	6	0	-2.602868	-1.866660	-2.273458	122	6	0	7.177901	-0.044663	0.145973
41	6	0	-5.285874	-1.445185	-1.604340	123	1	0	7.434308	0.489774	1.066780
42	1	0	-4.504009	-0.511344	0.167396	124	1	0	6.478057	-0.846852	0.403596
43	6	0	-3.576486	-2.317438	-3.166034	125	1	0	8.091517	-0.508428	-0.242723
44	1	0	-1.555167	-1.968660	-2.537467	126	6	0	3.306636	4.762549	0.653688
45	6	0	-4.918540	-2.196496	-2.745513	127	6	0	3.027480	4.891767	2.163704
46	6	0	2.958351	0.990246	0.245871	128	1	0	2.243433	4.199606	2.488819
47	6	0	4.215475	0.591800	-0.183716	129	1	0	3.927605	4.684685	2.752281
48	6	0	2.706826	2.342845	0.454376	130	1	0	2.695990	5.909528	2.399190
49	6	0	5.260632	1.501408	-0.351800	131	6	0	4.325465	5.840783	0.246514
50	1	0	4.395687	-0.455301	-0.387822	132	1	0	3.849355	6.820317	0.366337
51	6	0	3.713616	3.301053	0.351205	133	1	0	5.223755	5.836940	0.864300
52	1	0	1.700381	2.651487	0.716643	134	1	0	4.628546	5.739411	-0.798719
53	6	0	5.009292	2.842029	0.008663	135	6	0	2.012470	5.091703	-0.121802
54	6	0	2.385715	-1.796926	-0.027196	136	1	0	1.725533	6.129511	0.074223
55	6	0	2.249087	-2.250547	-1.328325	137	1	0	2.170419	4.981271	-1.199774
56	6	0	3.218256	-2.478661	0.860593	138	1	0	1.163229	4.465833	0.161575
57	6	0	2.978828	-3.340255	-1.815091	139	6	0	-6.748094	-1.034201	-1.326024
58	1	0	1.562991	-1.729905	-1.988097	140	6	0	-2.003711	-1.929247	-5.088288
59	6	0	3.999405	-3.547535	0.432787	141	1	0	-2.397808	-0.913888	-5.202842
60	1	0	3.266532	-2.145704	1.890133	142	1	0	-1.104850	-1.882346	-4.468975
61	6	0	3.934123	-3.895048	-0.942263	143	1	0	-1.689924	-2.284892	-6.075276
62	6	0	2.639219	-3.814720	-3.246227	144	6	0	-7.365678	-0.384678	-2.580745
63	6	0	3.171361	-2.796653	-4.271516	145	1	0	-8.398650	-0.088439	-2.366335
64	1	0	2.866693	-3.085863	-5.283624	146	1	0	-6.811550	0.515443	-2.865592
65	1	0	2.777348	-1.794697	-4.075528	147	1	0	-7.375889	-1.070042	-3.428604
66	1	0	4.263645	-2.735754	-4.254994	148	6	0	-7.605221	-2.236744	-0.889463
67	6	0	3.152005	-5.220859	-3.603267	149	1	0	-7.133414	-2.777760	-0.061895
68	1	0	2.864198	-5.956343	-2.846954	150	1	0	-8.583066	-1.883535	-0.542912
69	1	0	2.698258	-5.520341	-4.554065	151	1	0	-7.780540	-2.935769	-1.708424
70	1	0	4.233321	-5.267775	-3.730958	152	6	0	-6.819685	0.013355	-0.203265
71	6	0	1.098841	-3.881150	-3.377122	153	1	0	-7.856061	0.377782	-0.092914
72	1	0	0.673760	-4.561609	-2.631097	154	1	0	-6.505446	-0.393177	0.761135
73	1	0	0.616186	-2.906221	-3.262220	155	6	0	-2.553392	1.197491	6.177084
74	1	0	0.832606	-4.256319	-4.370404	156	1	0	-2.901509	1.684204	7.089967
75	6	0	4.838066	-4.356098	1.443672	157	1	0	-2.696112	0.116056	6.266669
76	6	0	4.363140	-5.822250	1.406665	158	1	0	-1.486470	1.395256	6.043190
77	1	0	4.564023	-6.281106	0.436331	159	6	0	-4.698654	-0.842429	4.343964
78	1	0	4.882147	-6.404549	2.176318	160	6	0	-4.128155	-2.118170	4.987056
79	1	0	3.286962	-5.888780	1.595571	161	1	0	-4.936651	-2.690973	5.455041
80	6	0	6.349258	-4.296770	1.150973	162	1	0	-3.636059	-2.761402	4.251704
81	1	0	6.694597	-3.262596	1.041056	163	1	0	-3.398206	-1.874396	5.763475
82	1	0	6.896432	-4.742368	1.989039	164	6	0	-5.432081	-0.025281	5.423253
83	1	0	6.616813	-4.853160	0.252804	165	1	0	-6.302623	-0.603681	5.751937
84	6	0	4.638663	-3.831661	2.875529	166	1	0	-4.826657	0.172435	6.307653
85	1	0	5.021819	-2.812072	2.995199	167	1	0	-5.793277	0.929305	5.032203
86	1	0	3.588007	-3.844393	3.179398	168	6	0	-5.792017	-1.243028	3.327251
87	1	0	5.196045	-4.471824	3.566394	169	1	0	-6.240387	-0.349346	2.882040
88	8	0	4.832274	-4.822237	-1.403073	170	1	0	-5.420589	-1.880498	2.520756
89	8	0	6.051775	3.728306	0.025883	171	1	0	-6.585808	-1.796080	3.840358
90	8	0	-3.316332	1.742730	5.104983	172	6	0	-1.800226	3.362994	3.232074
91	8	0	-5.923806	-2.793916	-3.462096	173	6	0	-0.842983	3.851788	2.131089
92	6	0	-6.064714	-4.182781	-3.183099	174	1	0	-0.589083	4.900191	2.315666
93	1	0	-6.959535	-4.518203	-3.710550	175	1	0	0.091392	3.278046	2.136355
94	1	0	-5.203208	-4.757808	-3.536817	176	1	0	-1.279591	3.788103	1.130918
95	1	0	-6.185896	-4.362875	-2.109327	177	6	0	-1.080087	3.594063	4.574190
96	6	0	-3.080977	-2.881734	-4.518992	178	1	0	-0.264386	2.877434	4.714756
97	6	0	-4.161874	-2.994268	-5.608650	179	1	0	-0.643741	4.598894	4.579139
98	1	0	-3.670445	-3.240399	-6.556046	180	1	0	-1.761201	3.525295	5.422131
99	1	0	-4.896146	-3.774530	-5.410799	181	6	0	-3.074806	4.227529	3.182871
100	1	0	-4.695230	-2.048722	-5.742265	182	1	0	-3.566961	4.140913	2.207799
101	6	0	-2.435711	-4.261137	-4.291499	183	1	0	-3.785477	3.923409	3.956264
102	1	0	-2.002430	-4.635426	-5.225829	184	1	0	-2.822982	5.281513	3.347663
103	1	0	-1.636810	-4.205004	-3.545401	185	8	0	1.327917	1.557284	-2.177840
104	1	0	-3.166670	-4.997249	-3.943194	186	6	0	1.580590	1.406209	-3.377610
105	6	0	5.923784	-4.242255	-2.111940	187	6	0	0.933162	0.345941	-4.206902
106	1	0	6.598031	-5.059999	-2.372819	188	1	0	0.674868	-0.527099	-3.602937
107	1	0	5.593589	-3.744020	-3.027984	189	1	0	-0.000814	0.766580	-4.596559
108	1	0	6.459511	-3.514672	-1.492394	190	1	0	1.562856	0.062134	-5.052129
109	6	0	6.715524	3.772301	1.281228	191	6	0	2.553976	2.327065	-4.032634
110	1	0	7.508524	4.520005	1.198001	192	1	0	3.408548	1.736941	-4.382602
111	1	0	6.028468	4.060916	2.085774	193	1	0	2.095626	2.775364	-4.920411
112	1	0	7.160300	2.801430	1.533115	194	1	0	2.893551	3.098144	-3.340773
113	6	0	6.581682	0.912695	-0.904164	195	1	0	-0.184163	4.340320	-2.553051
114	6	0	6.255359	0.108312	-2.184874	196	8	0	-1.790034	2.851348	-1.194395
115	1	0	5.575990	-0.729599	-2.003189	197	8	0	-1.503663	0.981985	-2.381430
116	1	0	5.803028	0.754214	-2.945193	198	6	0	-2.040849	2.135101	-2.173574
117	1	0	7.177941	-0.308739	-2.602380	199	6	0	-3.060915	2.552808	-3.248505
118	6	0	7.660166	1.933998	-1.302532	200	6	0	-2.408496	2.439962	-4.634565
119	1	0	8.088803	2.455564	-0.446152	201	1	0	-1.494154	3.040321	-4.698620
120	1	0	8.474920	1.393192	-1.797207	202	1	0	-2.154117	1.400493	-4.858908

203	1	0	-3.101509	2.795976	-5.404857
204	6	0	-3.550295	3.981624	-3.007962
205	1	0	-4.305033	4.244007	-3.757513
206	1	0	-4.002639	4.084589	-2.017527
207	1	0	-2.736354	4.707674	-3.081435
208	6	0	-4.250667	1.583191	-3.166451
209	1	0	-4.997535	1.846116	-3.923922
210	1	0	-3.932900	0.551278	-3.337245
211	1	0	-4.732242	1.636416	-2.184076
212	6	0	0.112405	5.105370	-3.274113
213	1	0	1.056295	4.835060	-3.750685
214	1	0	-0.657734	5.154250	-4.052566
215	6	0	0.248907	6.477757	-2.659722
216	8	0	1.012229	7.315864	-3.114178
217	6	0	-0.602188	6.772421	-1.501941
218	6	0	-1.470611	6.010396	-0.767439
219	8	0	-0.527269	8.028248	-0.975922
220	6	0	-1.958916	6.854641	0.270366
221	1	0	-1.713809	4.967392	-0.939538
222	6	0	-1.348458	8.059061	0.088874
223	1	0	-2.663985	6.598884	1.048085
224	1	0	-1.404556	8.998622	0.619157
225	1	0	-6.207579	0.894614	-0.423946

2.15. Catalytic cycle for destructive hydrogenation with 2b

9b(Segphos)

RwB97XD SCF energy	-3497.815855 a.u.
RwB97XD SCF enthalpy	-3496.845004 a.u.
RwB97XD SCF free energy	-3497.000074 a.u.
Three lowest frequencies (cm ⁻¹)	18.9, 25.3, 27.0

Cartesian coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.256222	0.332914	1.544066
2	6	0	2.427552	0.209905	2.905242
3	6	0	1.797756	1.042281	3.826737
4	6	0	0.981503	2.072198	3.426914
5	6	0	0.804338	2.233387	2.044726
6	6	0	1.409282	1.392038	1.112597
7	1	0	0.496989	2.730761	4.137982
8	1	0	0.168179	3.043403	1.711111
9	6	0	2.949997	-0.622323	0.640079
10	6	0	2.296141	-1.653802	-0.087753
11	6	0	4.316772	-0.546868	0.491754
12	6	0	3.026357	-2.520129	-0.897290
13	6	0	5.034130	-1.403012	-0.339410
14	6	0	4.418129	-2.409893	-1.042422
15	1	0	2.519729	-3.309068	-1.440512
16	1	0	4.975935	-3.085802	-1.679543
17	8	0	2.137941	0.671931	5.083280
18	8	0	3.182504	-0.707363	3.559150
19	8	0	5.161553	0.338049	1.076809
20	8	0	6.348797	-1.079577	-0.301662
21	6	0	2.977094	-0.480008	4.954553
22	1	0	2.477512	-1.346265	5.398151
23	1	0	3.938809	-0.286487	5.436667
24	6	0	6.459618	0.069706	0.543093
25	1	0	7.151859	-0.146586	1.360647
26	1	0	6.796834	0.926320	-0.048295
27	15	0	0.470214	-1.718963	-0.059453
28	15	0	0.995333	1.553700	-0.661469
29	46	0	-0.504305	-0.016938	-1.303761
30	6	0	0.019630	-1.839068	1.696721
31	6	0	0.747732	-2.662381	2.562676
32	6	0	-1.021835	-1.051091	2.194900
33	6	0	0.433227	-2.695656	3.916739
34	1	0	1.569744	-3.262537	2.184049
35	6	0	-1.317623	-1.071304	3.555253
36	1	0	-1.586460	-0.405424	1.526973
37	6	0	-0.589776	-1.890561	4.415149
38	6	0	0.024083	-3.293109	-0.860993
39	6	0	-0.346038	-4.428562	-0.137612
40	6	0	0.043836	-3.341104	-2.261477
41	6	0	-0.683823	-5.601624	-0.809274
42	1	0	-0.381211	-4.406157	0.946413
43	6	0	-0.285621	-4.515850	-2.926810
44	1	0	0.316844	-2.457558	-2.833583
45	6	0	-0.651106	-5.648327	-2.200024
46	6	0	0.242213	3.199756	-0.841563
47	6	0	0.930745	4.286346	-1.381164
48	6	0	-1.084337	3.359781	-0.423149
49	6	0	0.299963	5.525695	-1.483589
50	1	0	1.951511	4.177189	-1.731389
51	6	0	-1.705932	4.597368	-0.514538
52	1	0	-1.629648	2.507554	-0.031853
53	6	0	-1.012203	5.683820	-1.047674
54	6	0	2.577726	1.536638	-1.549112
55	6	0	2.729874	0.709832	-2.664770
56	6	0	3.657366	2.301306	-1.092198
57	6	0	3.958013	0.640234	-3.315591
58	1	0	1.894489	0.107277	-3.007935
59	6	0	4.877502	2.240179	-1.756277
60	1	0	3.552049	2.926998	-0.211063
61	6	0	5.030930	1.403567	-2.861226
62	8	0	-2.282125	-1.289130	-1.508574
63	6	0	-3.393698	-0.937885	-1.082108
64	6	0	-3.775152	0.524530	-0.940517
65	1	0	-4.786349	0.693861	-1.319588
66	1	0	-3.057811	1.142754	-1.489079
67	8	0	-3.714634	0.802722	0.462686
68	6	0	-4.252296	1.978459	0.855059

69	8	0	-4.724569	2.762465	0.063819	24	6	0	6.516962	-0.607471	-1.397089
70	6	0	-4.167391	2.162041	2.366387	25	1	0	7.298350	-1.345836	-1.202722
71	6	0	-2.696744	2.432725	2.734815	26	1	0	6.918235	0.410688	-1.384268
72	1	0	-2.333830	3.348934	2.257902	27	15	0	0.282215	-1.153995	-0.898496
73	1	0	-2.612887	2.558721	3.818967	28	15	0	1.534299	1.536320	0.602535
74	1	0	-2.044040	1.608565	2.437576	29	46	0	-0.415441	0.982997	-0.443284
75	6	0	-5.029944	3.361115	2.767043	30	6	0	0.203148	-2.342328	0.469801
76	1	0	-6.082122	3.195332	2.517512	31	6	0	0.825206	-3.590783	0.349949
77	1	0	-4.955523	3.517268	3.847618	32	6	0	-0.443347	-1.991997	1.656890
78	1	0	-4.700002	4.274278	2.265025	33	6	0	0.801680	-4.479438	1.418388
79	6	0	-4.666466	0.889772	3.069377	34	1	0	1.339059	-3.860623	-0.567998
80	1	0	-4.604108	1.027482	4.153493	35	6	0	-0.446917	-2.879763	2.730068
81	1	0	-5.711531	0.682798	2.815099	36	1	0	-0.936183	-1.028015	1.745689
82	1	0	-4.070248	0.015482	2.797456	37	6	0	0.176150	-4.119593	2.611846
83	8	0	-1.237186	1.393675	-2.551910	38	6	0	-0.756459	-1.795238	-2.248372
84	6	0	-1.683151	0.915122	-3.793242	39	6	0	-1.403535	-3.028821	-2.153080
85	1	0	-2.439626	0.118829	-3.656914	40	6	0	-0.942418	-1.000464	-3.387905
86	6	0	-2.366356	2.078499	-4.510210	41	6	0	-2.208291	-3.473525	-3.200110
87	1	0	-2.778767	1.762029	-5.474711	42	1	0	-1.290465	-3.646235	-1.268736
88	1	0	-3.182493	2.475029	-3.897866	43	6	0	-1.732644	-1.456196	-4.435431
89	1	0	-1.647060	2.886586	-4.686213	44	1	0	-0.474959	-0.021519	-3.453152
90	6	0	-0.549228	0.332006	-4.638320	45	6	0	-2.366805	-2.694864	-4.342191
91	1	0	0.224424	1.089598	-4.810719	46	6	0	1.168584	2.879891	1.772211
92	1	0	-0.085434	-0.520159	-4.126936	47	6	0	1.915256	4.057444	1.796716
93	1	0	-0.916864	-0.018942	-5.609645	48	6	0	0.076605	2.729844	2.637360
94	6	0	-4.363678	-1.914453	-0.680666	49	6	0	1.579148	5.073328	2.690540
95	6	0	-5.634192	-1.786534	-0.167762	50	1	0	2.751177	4.197344	1.119808
96	8	0	-4.019655	-3.231614	-0.735865	51	6	0	-0.245992	3.738778	3.535003
97	6	0	-6.087197	-3.098610	0.101488	52	1	0	-0.523984	1.824451	2.603800
98	1	0	-6.166449	-0.860113	-0.003499	53	6	0	0.504815	4.915176	3.559687
99	6	0	-5.062667	-3.926683	-0.265731	54	6	0	2.837330	2.088503	-0.531523
100	1	0	-7.039894	-3.397666	0.511967	55	6	0	2.545365	2.269457	-1.885912
101	1	0	-4.946990	-5.000519	-0.245181	56	6	0	4.143077	2.274283	-0.063370
102	1	0	0.838572	6.367079	-1.907836	57	6	0	3.558729	2.622503	-2.772063
103	1	0	-1.499049	6.650548	-1.130976	58	1	0	1.533016	2.112055	-2.247964
104	1	0	-2.735387	4.705310	-0.187843	59	6	0	5.147739	2.641944	-0.951191
105	1	0	4.077434	-0.016195	-4.171510	60	1	0	4.376662	2.117578	0.985529
106	1	0	5.990333	1.343845	-3.365441	61	6	0	4.858531	2.805949	-2.305335
107	1	0	5.712733	2.836131	-1.402410	62	8	0	-2.365364	0.474872	-1.161757
108	1	0	-0.263043	-4.545292	-4.011683	63	6	0	-3.410560	0.870454	-0.611827
109	1	0	-0.912790	-6.565059	-2.719373	64	6	0	-3.374137	1.674760	0.635091
110	1	0	-0.971708	-6.480368	-0.240662	65	1	0	-4.290248	2.052601	1.075726
111	1	0	-2.108299	-0.437813	3.944073	66	1	0	-2.443881	1.726505	1.190035
112	1	0	-0.817475	-1.900262	5.476537	67	8	0	-3.634026	-0.120605	1.471889
113	1	0	0.999256	-3.337158	4.584655	68	6	0	-4.852687	-0.344798	1.855531
						69	8	0	-5.690526	0.535356	2.067003
						70	6	0	-5.214497	-1.841213	1.964384
						71	6	0	-6.567403	-2.009494	2.656587
						72	1	0	-7.356182	-1.480267	2.115369
						73	1	0	-6.833391	-3.071392	2.707745
						74	1	0	-6.541244	-1.615556	3.677702
						75	6	0	-5.289653	-2.388769	0.526494
						76	1	0	-4.332816	-2.266626	0.009542
						77	1	0	-5.534841	-3.456847	0.544811
						78	1	0	-6.063425	-1.875049	-0.055485
						79	6	0	-4.123044	-2.590282	2.739035
						80	1	0	-4.379386	-3.652008	2.828044
						81	1	0	-3.161906	-2.510408	2.227393
						82	1	0	-4.005696	-2.186085	3.751134
						83	8	0	-0.908810	2.998225	-0.239021
						84	6	0	-2.064966	3.542984	-0.569305
						85	1	0	-3.007112	2.842276	-0.073930
						86	6	0	-2.329697	4.849219	0.166757
						87	1	0	-3.345071	5.212907	-0.011713
						88	1	0	-2.172138	4.710809	1.239372
						89	1	0	-1.618289	5.601473	-0.191791
						90	6	0	-2.429936	3.558106	-2.047397
						91	1	0	-1.788065	4.295002	-2.543871
						92	1	0	-2.250276	2.584983	-2.511352
						93	1	0	-3.473378	3.845364	-2.203321
						94	6	0	-4.680568	0.635373	-1.245349
						95	6	0	-5.960687	1.040724	-0.954289
						96	8	0	-4.681542	-0.128180	-2.372695
						97	6	0	-6.788220	0.487310	-1.961892
						98	1	0	-6.263339	1.636008	-0.106544
						99	6	0	-5.953406	-0.213342	-2.785389
						100	1	0	-7.857623	0.591812	-2.067407
						101	1	0	-6.125208	-0.794720	-3.679509
						102	1	0	3.334509	2.748224	-3.826358
						103	1	0	5.648988	3.076830	-2.998187
						104	1	0	6.159695	2.787989	-0.587059
						105	1	0	2.160207	5.989963	2.702180

TS4b(Segphos)

RwB97XD SCF energy -3497.738313 a.u.

RwB97XD SCF enthalpy -3496.773588 a.u.

RwB97XD SCF free energy -3496.928626 a.u.

Three lowest frequencies (cm⁻¹) -987.6, 17.2, 19.3

Imaginary frequency (cm⁻¹) -987.6

Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.878753	-0.903934	0.912367
2	6	0	3.325673	-1.933536	1.709791
3	6	0	3.180344	-1.936025	3.094673
4	6	0	2.606882	-0.880644	3.761557
5	6	0	2.154341	0.188973	2.975385
6	6	0	2.270629	0.190256	1.586756
7	1	0	2.502357	-0.871933	4.839881
8	1	0	1.703749	1.032317	3.483183
9	6	0	3.060881	-0.998894	-0.560037
10	6	0	2.007416	-1.198864	-1.495216
11	6	0	4.330504	-0.914324	-1.086374
12	6	0	2.283325	-1.309823	-2.855924
13	6	0	4.590377	-0.999413	-2.451603
14	6	0	3.586974	-1.210643	-3.365247
15	1	0	1.480127	-1.479871	-3.561719
16	1	0	3.786129	-1.298084	-4.426607
17	8	0	3.683411	-3.083879	3.603671
18	8	0	3.923804	-3.082014	1.310027
19	8	0	5.491132	-0.731549	-0.410136
20	8	0	5.919848	-0.868580	-2.670963
21	6	0	4.142540	-3.857350	2.490304
22	1	0	3.569561	-4.786909	2.429688
23	1	0	5.211768	-4.054914	2.603433

106	1	0	0.246239	5.707858	4.254741
107	1	0	-1.088825	3.613554	4.207251
108	1	0	-1.865103	-0.839370	-5.318543
109	1	0	-2.992236	-3.046560	-5.156908
110	1	0	-2.709304	-4.432716	-3.117997
111	1	0	1.281853	-5.447981	1.322972
112	1	0	0.173884	-4.809725	3.449782
113	1	0	-0.939587	-2.601796	3.656205

67	8	0	3.402219	-0.702092	-0.477010
68	6	0	4.219830	-1.105967	-1.350857
69	8	0	4.542668	-0.499028	-2.401465
70	6	0	4.944014	-2.459978	-1.087322
71	6	0	4.953794	-3.291588	-2.374977
72	1	0	5.401445	-2.723622	-3.194213
73	1	0	5.519252	-4.221864	-2.238296
74	1	0	3.933017	-3.562658	-2.670847
75	6	0	6.387922	-2.117830	-0.682850
76	1	0	6.406783	-1.521587	0.237885
77	1	0	6.973245	-3.028912	-0.505527
78	1	0	6.880584	-1.538161	-1.469736
79	6	0	4.269938	-3.250846	0.033100
80	1	0	4.788464	-4.203911	0.200008
81	1	0	4.274926	-2.684385	0.967050
82	1	0	3.225728	-3.472456	-0.213553
83	8	0	0.337154	3.447685	-0.458544
84	6	0	0.384979	4.418192	0.305410
85	1	0	3.301499	3.057578	-1.694058
86	6	0	0.521477	5.783855	-0.281557
87	1	0	1.548301	6.126559	-0.106851
88	1	0	0.323063	5.765570	-1.353759
89	1	0	-0.144359	6.487094	0.225476
90	6	0	0.324784	4.286105	1.790212
91	1	0	-0.583029	4.785279	2.146441
92	1	0	0.321554	3.242882	2.110130
93	1	0	1.174809	4.812614	2.235865
94	6	0	4.579749	1.698503	0.439089
95	6	0	5.786462	1.799828	-0.197659
96	8	0	4.770796	1.505135	1.770297
97	6	0	6.779758	1.652549	0.809301
98	1	0	5.937500	1.931190	-1.258533
99	6	0	6.090075	1.474603	1.977380
100	1	0	7.852519	1.672011	0.684997
101	1	0	6.416825	1.326744	2.999074
102	1	0	0.136564	-5.481412	-0.470262
103	1	0	0.921272	-4.976145	-2.770912
104	1	0	1.419399	-2.636334	-3.426840
105	1	0	-3.646839	2.810657	3.417626
106	1	0	-6.007113	2.467344	2.736006
107	1	0	-6.533636	1.604162	0.470866
108	1	0	-3.311452	5.147265	-3.429948
109	1	0	-1.471892	4.978134	-5.085331
110	1	0	0.188630	3.138826	-4.910098
111	1	0	2.379826	0.961392	5.002358
112	1	0	3.695663	-1.106622	5.403718
113	1	0	3.493750	-3.022894	3.837598

11b(Segphos)

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1	6	0	-2.503999	-1.497396	-0.653404
2	6	0	-2.730685	-2.726759	-1.227466
3	6	0	-2.674252	-2.939753	-2.602772
4	6	0	-2.422139	-1.915462	-3.483772
5	6	0	-2.196987	-0.647947	-2.926903
6	6	0	-2.223901	-0.431589	-1.551149
7	1	0	-2.391660	-2.075902	-4.554728
8	1	0	-1.997969	0.173166	-3.604006
9	6	0	-2.585207	-1.345170	0.822156
10	6	0	-1.482075	-1.070286	1.677447
11	6	0	-3.814616	-1.455192	1.432517
12	6	0	-1.675831	-0.931047	3.050603
13	6	0	-3.998834	-1.290152	2.802591
14	6	0	-2.942843	-1.036718	3.644268
15	1	0	-0.831290	-0.731358	3.698351
16	1	0	-3.077497	-0.917817	4.712665
17	8	0	-2.911246	-4.244078	-2.870592
18	8	0	-3.006413	-3.891588	-0.593586
19	8	0	-5.006550	-1.701313	0.836458
20	8	0	-5.310304	-1.429812	3.105907
21	6	0	-3.079315	-4.896204	-1.607134
22	1	0	-2.273955	-5.622355	-1.462641
23	1	0	-4.060011	-5.377134	-1.572725
24	6	0	-5.996371	-1.615713	1.863204
25	1	0	-6.564890	-2.547988	1.898388
26	1	0	-6.646942	-0.756449	1.673109
27	15	0	0.166576	-0.754217	0.951384
28	15	0	-1.793582	1.190556	-0.855591
29	46	0	0.278036	1.360514	0.097691
30	6	0	0.454330	-2.108883	-0.216738
31	6	0	0.167574	-3.426844	0.154752
32	6	0	0.914524	-1.826920	-1.503915
33	6	0	0.352287	-4.458168	-0.760611
34	1	0	-0.215736	-3.648319	1.146438
35	6	0	1.073656	-2.858496	-2.422395
36	1	0	1.153840	-0.806062	-1.779154
37	6	0	0.795395	-4.173141	-2.051150
38	6	0	1.331580	-0.877455	2.341239
39	6	0	2.070311	-2.038899	2.569559
40	6	0	1.452952	0.205501	3.220368
41	6	0	2.919793	-2.117048	3.669834
42	1	0	2.000726	-2.879012	1.889339
43	6	0	2.294101	0.119037	4.323300
44	1	0	0.894936	1.120220	3.043513
45	6	0	3.031285	-1.042240	4.547440
46	6	0	-1.762017	2.375877	-2.231670
47	6	0	-2.693078	3.411412	-2.328782
48	6	0	-0.716797	2.286512	-3.161121
49	6	0	-2.584603	4.344584	-3.357702
50	1	0	-3.497592	3.500855	-1.606631
51	6	0	-0.619346	3.215136	-4.189622
52	1	0	0.025129	1.496705	-3.075956
53	6	0	-1.552768	4.247096	-4.286973
54	6	0	-3.143974	1.641232	0.268191
55	6	0	-2.848132	2.140073	1.539396
56	6	0	-4.475451	1.446538	-0.117452
57	6	0	-3.879113	2.437062	2.425571
58	1	0	-1.812940	2.268912	1.842778
59	6	0	-5.501089	1.754842	0.769130
60	1	0	-4.710158	1.042844	-1.097910
61	6	0	-5.203791	2.242165	2.041631
62	8	0	2.280681	1.623161	0.753021
63	6	0	3.219996	1.703433	-0.068362
64	6	0	3.035011	2.008532	-1.519035
65	1	0	3.674543	1.339046	-2.106914
66	1	0	1.994391	1.859169	-1.812859

13

RwB97XD SCF energy -4678.375067 a.u.

RwB97XD SCF enthalpy -4676.473232 a.u.

RwB97XD SCF free energy -4676.705155 a.u.

Three lowest frequencies (cm⁻¹) 18.5, 193, 21.3

Cartesian coordinates

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.195503	-1.118353	2.235454
2	6	0	0.210653	-2.118298	3.093572
3	6	0	-0.273301	-3.420829	3.026899
4	6	0	-1.195785	-3.797813	2.083258
5	6	0	-1.608178	-2.806926	1.181370
6	6	0	-1.128573	-1.498478	1.229847
7	1	0	-1.594503	-4.804061	2.035201
8	1	0	-2.340832	-3.087001	0.436569
9	6	0	0.292619	0.262555	2.495893
10	6	0	1.144922	1.030452	1.657694
11	6	0	-0.074450	0.852084	3.686301
12	6	0	1.547175	2.307541	2.044032
13	6	0	0.322270	2.132581	4.056877
14	6	0	1.134252	2.892991	3.251240
15	1	0	2.214268	2.880583	1.412615
16	1	0	1.454696	3.888968	3.533457
17	8	0	0.293676	-4.169658	4.004488
18	8	0	1.110129	-2.019489	4.106447
19	8	0	-0.871982	0.328386	4.656467
20	8	0	-0.220632	2.440845	5.265558

21	6	0	1.049077	-3.259147	4.809622	103	1	0	2.299406	5.193145	-0.002084
22	1	0	2.056705	-3.652595	4.949689	104	1	0	3.976552	5.752628	0.073746
23	1	0	0.538175	-3.112575	5.767941	105	6	0	-5.345555	4.745454	1.454512
24	6	0	-0.714963	1.199851	5.774718	106	1	0	-5.974001	5.457125	1.992930
25	1	0	0.019847	0.773376	6.469252	107	1	0	-5.012019	5.201861	0.517698
26	1	0	-1.680935	1.355856	6.254847	108	1	0	-5.929148	3.848987	1.216558
27	15	0	1.640103	0.301883	0.054609	109	6	0	-6.816323	-3.889215	-1.714310
28	15	0	-1.625084	-0.306399	-0.068667	110	1	0	-7.746290	-4.276126	-2.135308
29	46	0	-0.002510	0.202631	-1.574155	111	1	0	-6.088068	-4.703533	-1.644400
30	6	0	2.319229	-1.321000	0.487149	112	1	0	-7.004280	-3.505672	-0.705609
31	6	0	3.344810	-1.438671	1.414495	113	6	0	-6.741146	-0.174458	-1.533184
32	6	0	1.831492	-2.456584	-0.151070	114	6	0	-6.591880	1.208615	-0.871995
33	6	0	3.921073	-2.674465	1.723020	115	1	0	-6.385726	1.131597	0.201334
34	1	0	3.724936	-0.540474	1.889529	116	1	0	-5.800995	1.807841	-1.335578
35	6	0	2.296241	-3.727639	0.170398	117	1	0	-7.532008	1.757279	-0.987093
36	1	0	1.056897	-2.326504	-0.895673	118	6	0	-7.119731	0.058177	-3.009235
37	6	0	3.309650	-3.816201	1.158059	119	1	0	-7.259863	-0.888322	-3.535565
38	6	0	3.027260	1.283562	-0.591266	120	1	0	-8.054773	0.626694	-3.070297
39	6	0	4.246182	0.693366	-0.918581	121	1	0	-6.341089	0.631147	-3.524656
40	6	0	2.806128	2.611063	-0.941062	122	6	0	-7.895588	-0.896242	-0.813967
41	6	0	5.294636	1.439421	-1.455908	123	1	0	-8.219000	-1.785925	-1.354100
42	1	0	4.381700	-0.365224	-0.743761	124	1	0	-7.612554	-1.184010	0.204362
43	6	0	3.819532	3.421619	-1.457938	125	1	0	-8.757349	-0.223339	-0.742320
44	1	0	1.815245	3.030179	-0.801893	126	6	0	-3.631343	-4.020442	-3.203168
45	6	0	5.095572	2.833821	-1.586096	127	6	0	-3.252741	-5.204694	-2.293620
46	6	0	-3.061969	-1.035504	-0.897841	128	1	0	-2.402965	-4.954095	-1.649247
47	6	0	-4.305144	-0.414607	-0.850652	129	1	0	-4.085909	-5.501734	-1.648758
48	6	0	-2.896931	-2.170573	-1.680165	130	1	0	-2.969212	-6.072323	-2.900417
49	6	0	-5.416519	-0.966415	-1.483212	131	6	0	-4.741955	-4.457817	-4.174795
50	1	0	-4.404737	0.518211	-0.314840	132	1	0	-4.327000	-5.206703	-4.858479
51	6	0	-3.969348	-2.789279	-2.326075	133	1	0	-5.597736	-4.915556	-3.678805
52	1	0	-1.902776	-2.589153	-1.788066	134	1	0	-5.103276	-3.619326	-4.776044
53	6	0	-5.244080	-2.215502	-2.127359	135	6	0	-2.411181	-3.679122	-4.090233
54	6	0	-2.246597	1.163459	0.789853	136	1	0	-2.185747	-4.530484	-4.741012
55	6	0	-1.983349	2.425278	0.279282	137	1	0	-2.619838	-2.811947	-4.725294
56	6	0	-3.040845	1.031786	1.930278	138	1	0	-1.505274	-3.469029	-3.515395
57	6	0	-2.545510	3.581528	0.834543	139	6	0	6.596305	0.733321	-1.893551
58	1	0	-1.323730	2.509935	-0.577162	140	6	0	2.156831	4.796615	-2.734169
59	6	0	-3.671709	2.133433	2.497895	141	1	0	2.350729	4.234342	-3.654155
60	1	0	-3.175135	0.047290	2.361215	142	1	0	1.305582	4.334989	-2.228807
61	6	0	-3.486877	3.389386	1.864024	143	1	0	1.854316	5.811028	-3.014559
62	6	0	-2.057533	4.941791	0.281956	144	6	0	7.044860	1.220427	-3.285571
63	6	0	-2.637041	5.181286	-1.123413	145	1	0	7.948410	0.678913	-3.586524
64	1	0	-2.284931	6.142377	-1.515169	146	1	0	6.273375	1.024368	-4.037615
65	1	0	-2.317922	4.399296	-1.818048	147	1	0	7.265059	2.287490	-3.291745
66	1	0	-3.730888	5.199725	-1.117653	148	6	0	7.727204	0.972031	-0.876710
67	6	0	-2.369419	6.150953	1.181664	149	1	0	7.408082	0.714278	0.139084
68	1	0	-2.050564	5.976304	2.213130	150	1	0	8.589315	0.343779	-1.128208
69	1	0	-1.815694	7.015246	0.799191	151	1	0	8.065539	2.010333	-0.882078
70	1	0	-3.424839	6.421672	1.193228	152	6	0	6.379447	-0.786549	-2.009416
71	6	0	-0.517104	4.894133	0.162689	153	1	0	5.549727	-1.028985	-2.683511
72	1	0	-0.051280	4.713405	1.137042	154	1	0	7.285010	-1.244779	-2.418799
73	1	0	-0.171285	4.123076	-0.530513	155	1	0	6.187730	-1.262682	-1.043531
74	1	0	-0.151742	5.853858	-0.217286	156	6	0	3.201873	-5.493043	2.787768
75	6	0	-4.481090	1.984722	3.802958	157	1	0	3.556379	-6.513286	2.945355
76	6	0	-3.923098	2.963841	4.854828	158	1	0	3.562067	-4.862628	3.606491
77	1	0	-4.094773	4.001609	4.565693	159	1	0	2.107761	-5.481042	2.792684
78	1	0	-4.408099	2.791335	5.822165	160	6	0	5.192821	-2.644577	2.608537
79	1	0	-2.845332	2.822904	4.982786	161	6	0	4.815295	-2.306859	4.062258
80	6	0	-5.982460	2.251393	3.589027	162	1	0	5.722071	-2.209576	4.669721
81	1	0	-6.382008	1.635274	2.776011	163	1	0	4.265300	-1.362339	4.122278
82	1	0	-6.531831	1.995980	4.502256	164	1	0	4.195134	-3.087653	4.512317
83	1	0	-6.186077	3.298967	3.367239	165	6	0	6.038848	-3.931245	2.581148
84	6	0	-4.349544	0.563834	4.377195	166	1	0	6.994275	-3.724301	3.075188
85	1	0	-4.800279	-0.189116	3.721477	167	1	0	5.581135	-4.768011	3.107497
86	1	0	-3.305241	0.288956	4.553900	168	1	0	6.253113	-4.247958	1.556736
87	1	0	-4.877409	0.518097	5.334822	169	6	0	6.129608	-1.530938	2.080722
88	8	0	-4.250714	4.436531	2.311508	170	1	0	6.412851	-1.723415	1.041293
89	8	0	-6.370011	-2.855017	-2.585252	171	1	0	5.689219	-0.532686	2.136601
90	8	0	3.719384	-5.070012	1.530372	172	1	0	7.046189	-1.512250	2.679342
91	8	0	6.191181	3.614877	-1.852128	173	6	0	1.782461	-4.950713	-0.619547
92	6	0	6.697219	4.267783	-0.691907	174	6	0	0.644169	-4.556257	-1.579442
93	1	0	7.616681	4.772872	-0.993158	175	1	0	0.307406	-5.446585	-2.119323
94	1	0	5.989889	5.007671	-0.301689	176	1	0	-0.217904	-4.148239	-1.039222
95	1	0	6.918594	3.547635	0.103544	177	1	0	0.963389	-3.824694	-2.328309
96	6	0	3.425031	4.863870	-1.851966	178	6	0	1.233954	-6.071292	0.283499
97	6	0	4.468061	5.630831	-2.683734	179	1	0	0.522592	-5.679583	1.017373
98	1	0	4.004991	6.557414	-3.040280	180	1	0	0.705068	-6.805733	-0.333557
99	1	0	5.355803	5.910921	-2.116533	181	1	0	2.030189	-6.596772	0.810014
100	1	0	4.787698	5.058412	-3.558768	182	6	0	2.946489	-5.502111	-1.464819
101	6	0	3.101070	5.666511	-0.577904	183	1	0	3.310471	-4.746451	-2.170184
102	1	0	2.774691	6.679064	-0.840459	184	1	0	3.780176	-5.813765	-0.830543

185	1	0	2.613725	-6.371813	-2.042965	48	6	0	-2.608863	-2.436478	-1.424342
186	8	0	1.410565	0.847019	-3.076097	49	6	0	-5.182125	-1.329136	-1.435546
187	6	0	2.255594	0.151528	-3.646114	50	1	0	-4.286895	0.282709	-0.348784
188	6	0	2.321264	-1.325859	-3.439280	51	6	0	-3.625357	-3.147862	-2.066195
189	1	0	2.833304	-1.829367	-4.261281	52	1	0	-1.593522	-2.814348	-1.460204
190	1	0	1.317954	-1.735301	-3.299017	53	6	0	-4.929553	-2.612803	-1.976412
191	8	0	-1.407341	0.011335	-3.001150	54	6	0	-2.257466	1.122912	0.756063
192	6	0	-1.482374	0.959046	-4.026396	55	6	0	-2.114032	2.346478	0.120389
193	1	0	-0.552361	0.977260	-4.624583	56	6	0	-3.088617	1.014918	1.873528
194	6	0	-2.624079	0.536347	-4.951298	57	6	0	-2.852374	3.471123	0.512835
195	1	0	-2.736904	1.232699	-5.790199	58	1	0	-1.415107	2.423052	-0.706930
196	1	0	-2.439592	-0.463733	-5.356261	59	6	0	-3.879811	2.081166	2.284448
197	1	0	-3.567041	0.506937	-4.392489	60	1	0	-3.128732	0.071056	2.403238
198	6	0	-1.717076	2.371643	-3.489341	61	6	0	-3.826453	3.266180	1.507183
199	1	0	-2.642210	2.393760	-2.900663	62	6	0	-2.493714	4.820995	-0.150612
200	1	0	-0.889103	2.678011	-2.838808	63	6	0	-2.875156	4.798657	-1.641159
201	1	0	-1.800345	3.107622	-4.297953	64	1	0	-2.602090	5.749632	-2.112021
202	6	0	3.252322	0.796649	-4.547564	65	1	0	-2.352904	3.999500	-2.174559
203	1	0	2.892430	-1.498487	-2.517666	66	1	0	-3.950503	4.649473	-1.781300
204	1	0	4.228897	0.321929	-4.423434	67	6	0	-3.110566	6.067560	0.507908
205	1	0	3.314684	1.869974	-4.363495	68	1	0	-2.942998	6.081976	1.587851
206	1	0	2.939494	0.619444	-5.584184	69	1	0	-2.624837	6.951180	0.079493
						70	1	0	-4.180491	6.169459	0.324795
						71	6	0	-0.963567	5.001556	-0.037186
						72	1	0	-0.649782	5.041762	1.011181
						73	1	0	-0.410707	4.194843	-0.523862
						74	1	0	-0.668598	5.938233	-0.520942
						75	6	0	-4.717591	1.990553	3.575362
						76	6	0	-4.287506	3.134389	4.515707
						77	1	0	-4.530197	4.110037	4.090149
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						79	1	0	-3.208136	3.103287	4.696202
						80	6	0	-6.230745	2.083590	3.305102
						81	1	0	-6.543685	1.357950	2.546221
						82	1	0	-6.779401	1.859587	4.226826
						83	1	0	-6.527603	3.081125	2.980816
						84	6	0	-4.465638	0.661741	4.306491
						85	1	0	-4.826576	-0.198351	3.731677
						86	1	0	-3.404940	0.509440	4.527028
						87	1	0	-5.009139	0.670324	5.256511
						88	8	0	-4.757628	4.237171	1.768237
						89	8	0	-6.005322	-3.324754	-2.445785
						90	8	0	4.023504	-4.511495	2.186074
						91	8	0	5.598745	4.081707	-2.576918
						92	6	0	6.056929	5.115053	-1.710766
						93	1	0	6.836159	5.655276	-2.251715
						94	1	0	5.254958	5.811427	-1.447128
						95	1	0	6.476144	4.702126	-0.786873
						96	6	0	2.664881	4.860994	-2.612857
						97	6	0	3.493972	5.479073	-3.752740
						98	1	0	2.865424	6.204158	-4.280678
						99	1	0	4.378582	6.010690	-3.403538
						100	1	0	3.812752	4.722112	-4.474805
						101	6	0	2.346976	5.944554	-1.565625
						102	1	0	1.793983	6.768299	-2.030908
						103	1	0	1.734852	5.541206	-0.752984
						104	1	0	3.258203	6.360533	-1.125187
						105	6	0	-5.810890	4.259605	0.808512
						106	1	0	-6.499529	5.049027	1.114885
						107	1	0	-5.437401	4.474680	-0.197617
						108	1	0	-6.343661	3.302092	0.784336
						109	6	0	-6.466933	-4.313044	-1.530376
						110	1	0	-7.376118	-4.739191	-1.958712
						111	1	0	-5.731105	-5.110871	-1.387568
						112	1	0	-6.694847	-3.873338	-0.553524
						113	6	0	-6.534562	-0.600582	-1.592335
						114	6	0	-6.478403	0.816455	-0.990955
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						119	1	0	-6.919256	-1.432106	-3.579626
						120	1	0	-7.795324	0.069506	-3.232358
						121	1	0	-6.061493	0.122890	-3.598736
						122	6	0	-7.694930	-1.336958	-0.897877
						123	1	0	-7.953446	-2.263928	-1.409640
						124	1	0	-7.454425	-1.564322	0.146356
						125	1	0	-8.586247	-0.699439	-0.902450
						126	6	0	-3.202424	-4.431588	-2.822088
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14-acetone

RwB97XD SCF energy	-4679.539687 a.u.				
RwB97XD SCF enthalpy	-4677.621165 a.u.				
RwB97XD SCF free energy	-4677.858751 a.u.				
Three lowest frequencies (cm ⁻¹)	15.2, 17.3, 19.6				
Cartesian coordinates					
Standard	orientation:				

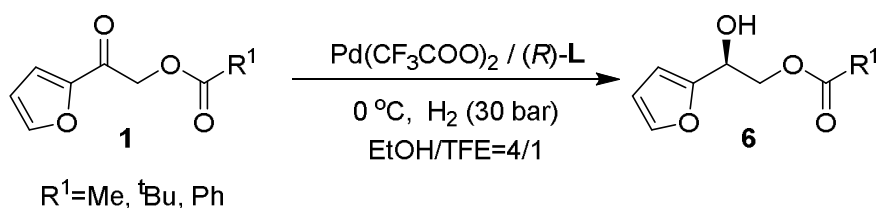
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Number	Number	Type	X	Y	Z
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2	6	O	0.344764	-1.702763	3.440679
3	6	O	-0.027232	-3.043614	3.482238
4	6	O	-0.852208	-3.592805	2.532292
5	6	O	-1.295951	-2.733083	1.517760
6	6	O	-0.935943	-1.387043	1.463964
7	1	C	-1.159830	-4.630993	2.568382
8	1	C	-1.963151	-3.144483	0.772047
9	6	O	0.263926	0.608881	2.601368
10	6	O	1.061201	1.372557	1.706126
11	6	O	-0.197630	1.277419	3.714490
12	6	O	1.317489	2.718721	1.958637
13	6	O	0.057302	2.624343	3.954266
14	6	O	0.810644	3.379338	3.088588
15	1	C	1.938892	3.287718	1.277564
16	1	C	1.016199	4.427533	3.270150
17	8	H	0.529483	-3.637863	4.565397
18	8	H	1.160176	-1.427135	4.491221
19	8	H	-0.977771	0.781534	4.712739
20	8	H	-0.554559	2.999895	5.108637
21	6	O	1.125603	-2.583225	5.326455
22	1	C	2.140768	-2.865274	5.607986
23	1	C	0.507068	-2.379731	6.208196
24	6	O	-0.944703	1.775708	5.735663
25	1	C	-0.196468	1.498161	6.488423
26	1	C	-1.937222	1.885440	6.172445
27	15	O	1.681340	0.564023	0.193712
28	15	O	-1.496809	-0.362357	0.057185
29	46	O	0.134430	0.116241	-1.468372
30	6	O	2.495841	-0.950261	0.752135
31	6	O	3.480220	-0.930784	1.729746
32	6	O	2.114412	-2.159407	0.176955
33	6	O	4.097167	-2.105955	2.170965
34	1	C	3.780705	0.022815	2.152375
35	6	O	2.634252	-3.371281	0.616798
36	1	C	1.371844	-2.138936	-0.609788
37	6	O	3.582535	-3.321293	1.668764
38	6	O	2.925523	1.648450	-0.564729
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42	1	C	4.545751	0.266857	-0.388790
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44	1	C	1.431431	3.086231	-1.060615
45	6	O	4.674258	3.253733	-1.993668
46	6	O	-2.855775	-1.250310	-0.746281
47	6	O	-4.124150	-0.683001	-0.803579

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133	1	0	-5.121175	-5.382667	-3.383463
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135	6	0	-1.921343	-4.132208	-3.634117
136	1	0	-1.648909	-5.016158	-4.220610
137	1	0	-2.078477	-3.298018	-4.325048
138	1	0	-1.062587	-3.893439	-3.002834
139	6	0	6.510427	1.426780	-1.907261
140	6	0	1.335577	4.400863	-3.258929
141	1	0	1.499854	3.568959	-3.952718
142	1	0	0.587682	4.094882	-2.524302
143	1	0	0.899119	5.231309	-3.823216
144	6	0	6.616536	1.379840	-3.444899
145	1	0	7.585109	0.959291	-3.737979
146	1	0	5.831634	0.741580	-3.865899
147	1	0	6.528162	2.375366	-3.884333
148	6	0	7.673470	2.253790	-1.328653
149	1	0	7.548970	2.412727	-0.252114
150	1	0	8.615099	1.714236	-1.478912
151	1	0	7.771731	3.222913	-1.817533
152	6	0	6.683227	-0.012079	-1.393038
153	1	0	5.908923	-0.687633	-1.771331
154	1	0	7.649394	-0.396477	-1.734727
155	1	0	6.680634	-0.058847	-0.299669
156	6	0	3.403227	-4.847149	3.424053
157	1	0	3.861299	-5.778515	3.762250
158	1	0	3.564579	-4.070607	4.178548
159	1	0	2.326540	-4.993492	3.300656
160	6	0	5.299892	-1.932833	3.132000
161	6	0	4.803617	-1.390354	4.484365
162	1	0	5.653376	-1.219268	5.154617
163	1	0	4.269966	-0.442131	4.368326
164	1	0	4.129282	-2.100781	4.971490
165	6	0	6.150039	-3.192104	3.380086
166	1	0	7.059380	-2.887803	3.909937
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168	1	0	6.450151	-3.671405	2.445276
169	6	0	6.268056	-0.902889	2.504476
170	1	0	6.663039	-1.278332	1.554895
171	1	0	5.804752	0.069923	2.322192
172	1	0	7.114129	-0.738532	3.179940
173	6	0	2.261520	-4.672700	-0.125431
174	6	0	1.154712	-4.424228	-1.167811
175	1	0	0.929809	-5.364042	-1.681123
176	1	0	0.230718	-4.069174	-0.696119
177	1	0	1.453249	-3.698839	-1.929760
178	6	0	1.751305	-5.791394	0.800894
179	1	0	0.950430	-5.432500	1.455041
180	1	0	1.344224	-6.605644	0.191689
181	1	0	2.549529	-6.206519	1.415305
182	6	0	3.520290	-5.161266	-0.867800
183	1	0	3.874845	-4.402969	-1.574154
184	1	0	4.327448	-5.382021	-0.163817
185	1	0	3.298159	-6.075611	-1.430284
186	8	0	2.819681	-1.497471	-3.336016
187	6	0	2.395588	-2.384844	-4.062992
188	6	0	1.006603	-2.337813	-4.642597
189	1	0	1.065989	-1.819608	-5.608245
190	1	0	0.321437	-1.783946	-3.991859
191	8	0	-1.151602	-0.389269	-2.931191
192	6	0	-1.247212	0.458919	-4.040128
193	1	0	-0.269858	0.545219	-4.558805
194	6	0	-2.238037	-0.171419	-5.016784
195	1	0	-2.370934	0.452740	-5.907607
196	1	0	-1.884526	-1.156450	-5.337907
197	1	0	-3.211581	-0.301082	-4.529863
198	6	0	-1.681681	1.868829	-3.641467
199	1	0	-2.650075	1.830458	-3.128462
200	1	0	-0.948971	2.305519	-2.952083
201	1	0	-1.768025	2.532693	-4.509341
202	6	0	3.246417	-3.569171	-4.432579
203	1	0	0.621100	-3.341800	-4.837403
204	1	0	2.813103	-4.469326	-3.981097
205	1	0	4.271287	-3.439575	-4.081875
206	1	0	3.231521	-3.719294	-5.517317
207	1	0	1.517042	0.075204	-2.780663
208	1	0	1.241928	0.813667	-2.789760

3. General Details

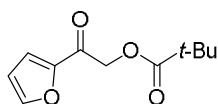
All reactions were performed in a glove box under an atmosphere of dry nitrogen, and the workup was carried out in air, unless otherwise noted. Acetone was dried and distilled before use by standard procedures. Commercially available reagents were used without further purification. (±)-DTBM-Segphos was purchased from Strem Chemicals Inc. and used without further purification. GC-MS was performed at the Analysis Center of Shanghai Jiao Tong University (7890A-5975C).

4. General Procedure for Asymmetric Hydrogenation of α -Acyloxy-1-arylethanone

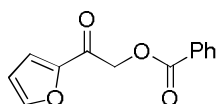


(*R*)-DTBM-SegPHOS (2.83 mg, 2.4 mol%) and Pd(OCOCF₃)₂ (0.66 mg, 2.0 mol%) were placed in a dried Schlenk tube under nitrogen atmosphere, and degassed anhydrous acetone was added. The mixture was stirred at room temperature for 10 min, then the solvent was removed under vacuum to give the dry catalyst. In a glovebox, substrate **1** (0.1 mmol) was stirred in a solvent (0.5 mL) at room temperature for 10 min. Subsequently, the above catalyst together with a mixed solvent (EtOH/TFE=4/1, 1.0 mL) was added to the reaction mixture. The hydrogenation was performed at 0 °C under H₂ (30 bar) in a stainless steel autoclave for 2 h. After carefully releasing the hydrogen, the conversion of the product **6** was determined by ¹H NMR spectroscopic analysis of the crude

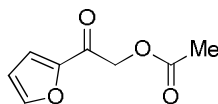
reaction mixture. The enantiomeric excess of the products was determined by HPLC with chiral columns.



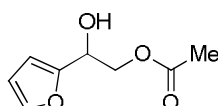
^1H NMR (400 MHz, CDCl_3): δ 7.60 (1H, dd, $J = 3.2, 0.8$ Hz), 7.26–7.24 (1H, m), 6.57 (1H, dd, $J = 7.2, 3.2$ Hz), 5.16 (2H, s), 1.29 (9H, s); ^{13}C NMR (100 MHz, CDCl_3): δ 182.2, 178.2, 150.9, 146.9, 117.8, 112.7, 65.4, 39.0, 27.4.



^1H NMR (400 MHz, CDCl_3): δ 8.11 (2H, d, $J = 7.2$ Hz), 7.61–7.55 (2H, m), 7.47–7.45 (2H, m), 7.30 (1H, s), 6.57 (1H, s), 5.40 (2H, s); ^{13}C NMR (100 MHz, CDCl_3): δ 181.6, 165.9, 150.6, 146.8, 133.4, 130.0, 128.4, 117.8, 112.5, 65.8; HRMS (ESI-MS) Calcd. For $\text{C}_{13}\text{H}_{10}\text{O}_4$ $[\text{M}+\text{H}]^+$ 231.0657, found: 231.0671.

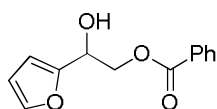


^1H NMR (400 MHz, CDCl_3): δ 7.55 (1H, s), 7.21 (1H, s), 6.51 (1H, s), 5.11 (2H, s), 2.14 (3H, s); ^{13}C NMR (100 MHz, CDCl_3): δ 181.7, 170.4, 150.4, 146.8, 117.8, 112.5, 65.3, 20.5; HRMS (ESI-MS) Calcd. For $\text{C}_8\text{H}_8\text{O}_4$ $[\text{M}+\text{Na}]^+$ 191.0320, found: 191.0314.

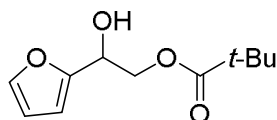


^1H NMR (400 MHz, CDCl_3): δ 7.38 (1H, s), 6.32 (2H, d, $J = 7.6$ Hz), 4.95 (1H, s), 4.35 (2H, d, $J = 5.6$ Hz), 2.52 (1H, s), 2.08 (3H, s); ^{13}C NMR (100 MHz, CDCl_3): δ 171.1, 152.6, 142.5, 110.3, 107.2, 66.5, 66.3, 20.8. The ee was determined by

HPLC on a Daicel Chiralcel IE-H column (hexane/2-propanol = 80/20, 210 nm, flow = 0.6 mL/min), t_{R1} = 21.3 min, t_{R2} = 31.5 min, ee = 64%. HRMS (ESI-MS) Calcd. For $C_8H_{10}O_4$ $[M+H]^+$ 171.0657, found: 171.0687.

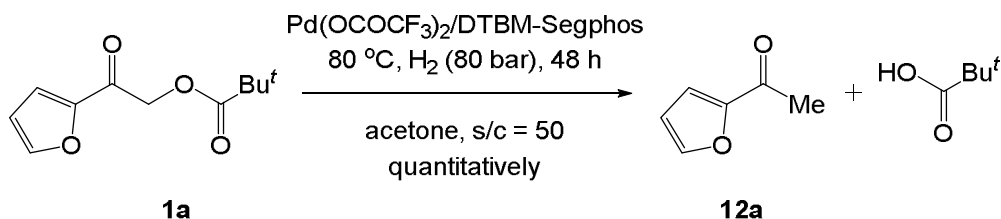


1H NMR (400 MHz, $CDCl_3$): δ 8.02 (2H, d, J = 7.6 Hz), 7.58–7.54 (1H, m), 7.45–7.41 (3H, m), 6.37–6.35 (2H, m) 5.10 (2H, s), 4.61 (2H, d, J = 4.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 152.7, 142.6, 133.3, 129.7, 128.4, 110.4, 107.4, 67.0, 66.5. The ee was determined by HPLC on a Daicel Chiralcel IE-H column (hexane/2-propanol = 90/10, 210 nm, flow = 0.8 mL/min), t_{R1} = 17.8 min, t_{R2} = 18.6 min, ee = 79%. HRMS (ESI-MS) Calcd. For $C_{13}H_{12}O_4$ $[M+Na]^+$ 255.0633, found: 255.0642.

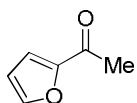


1H NMR (400 MHz, $CDCl_3$): δ 7.39 (3H, dd, J = 2.0, 0.4 Hz), 6.35–6.31 (2H, m), 4.96 (1H, dd, J = 6.0, 4.8 Hz), 4.38–4.36 (2H, m), 1.10 (9H, s); ^{13}C NMR (100 MHz, $CDCl_3$): δ 178.9, 153.2, 142.7, 110.5, 107.5, 66.7, 66.6, 39.1, 27.3; The ee was determined by HPLC on a Daicel Chiralcel IE-H column (hexane/2-propanol = 95/5, 210 nm, flow = 0.6 mL/min), t_{R1} = 20.1 min, t_{R2} = 21.1 min, ee = 97%.

5. Palladium-Catalyzed Chemo- and Enantioselective C–O Bond Cleavage of 2-(Furan-2-yl)-2-oxoethyl pivalate via Hydrogenolysis



(±)-DTBM-Segphos (2.2 mol%) and Pd(OCOCF₃)₂ (2.0 mol%) were placed in a dried Schlenk tube under a nitrogen atmosphere, and degassed anhydrous acetone (1.0 mL) was added. The mixture was stirred at room temperature for 10 min. In a glove box, substrate **1a** (45.9 mg, 0.3 mmol) was stirred in acetone (1.5 mL) at room temperature for 10 min. Subsequently, the above catalyst together with acetone was added to the reaction mixture. The hydrogenation was carried out at 80 °C under H₂ (80 bar) in a stainless steel autoclave for 48 h. After carefully releasing the hydrogen, the mixture was concentrated in vacuo to afford the corresponding crude product. The compound **1a** was completely transformed to **12a** and t-Butyl alcohol as determined by ¹H NMR analysis.



¹H NMR (400 MHz, CDCl₃): δ 7.56 (1H, s), 7.15 (1H, d, *J* = 2.8 Hz), 6.51–6.50 (1H, m), 2.45 (3H, s).

6. Mechanism Experiments. Relates to the Scheme 3.

Table S1 The results of mechanism experiments. Relates to Scheme 3.

entry	catalyst	solvent	substrate	isopropanol (GC-MS)
1	Pd(OCOCF ₃) ₂	acetone	no	No Detected
2	Pd(OCOCF ₃) ₂ - DTBM-Segphos	acetone	no	Detected
3	Pd(OCOCF ₃) ₂ - DTBM-Segphos	d6- acetone	no	Detected the d6- isopropanol
4	Pd(OCOCF ₃) ₂ - DTBM-Segphos	acetone	yes	Detected

DTBM-Segphos (2.60 mg), Pd(OCOCF₃)₂ (0.66 mg), H₂ (30 bar), RT, acetone (1.0 mL) 12 h. Substrate: 2-oxo-2-phenylethyl pivalate (s/c = 50).

As shown in Table S1, no isopropanol was detected in the absence of DTBM-Segphos and substrate according to GC-MS analysis (entry 1). A trace amount of isopropanol was detected in the reaction mixture when the reaction was carried out in the presence of Pd-DTBM-Segphos catalyst (entry 2). When d6-acetone was used, a trace amount of d6-isopropanol was detected (entry 3). A small amount of isopropanol was also detected if the substrate (2-oxo-2-phenylethyl pivalate) was added. Moreover, isopropanol was also detected when **1a** was used as the substrate (see the above experiment). These results suggest the possibility that acetone takes part in the hydride transfer during the catalytic reaction.

Figure S1. ESI mass-spectra of the reaction mixtures described in the Table S1: Acetone (standard sample and entry 1, peak, $m/z = 43$). Relates to the Scheme 3.



Figure S2. ESI mass-spectra of the reaction mixtures described in the Table S1: Acetone+H₂ (entry 2 and 4, peak, m/z = 45). Relates to the Scheme 3.

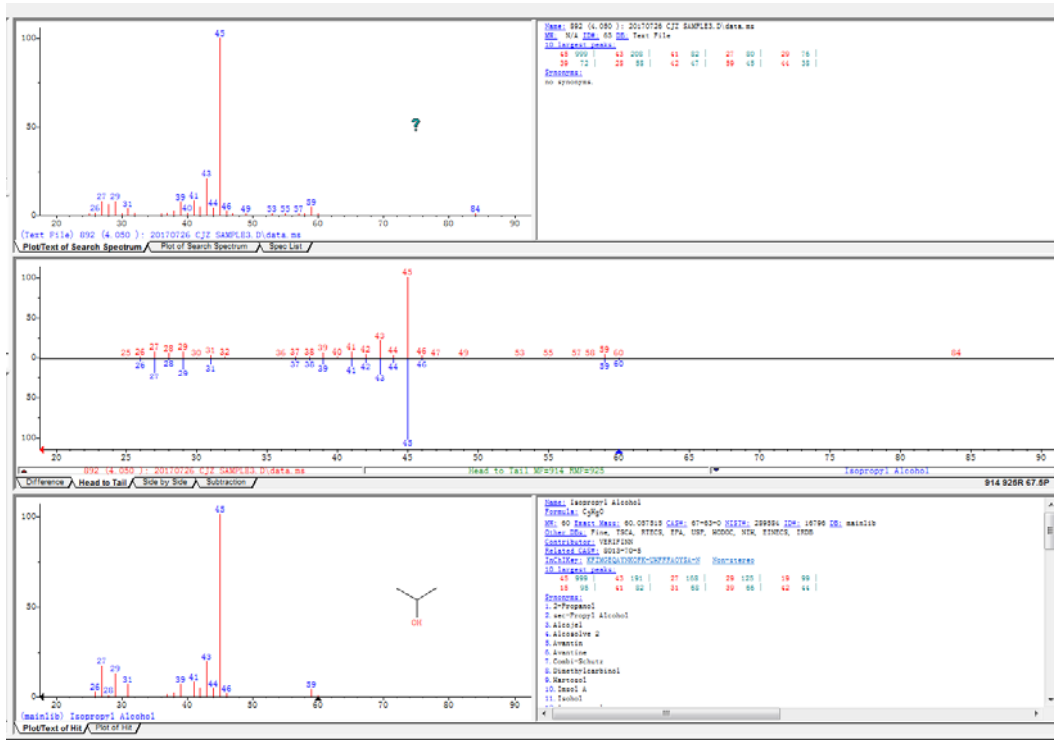


Figure S3. ESI mass-spectra of the reaction mixtures described in the Table

S1: d₆-Acetone (standard sample, peak, m/z = 46). Relates to the Scheme 3.

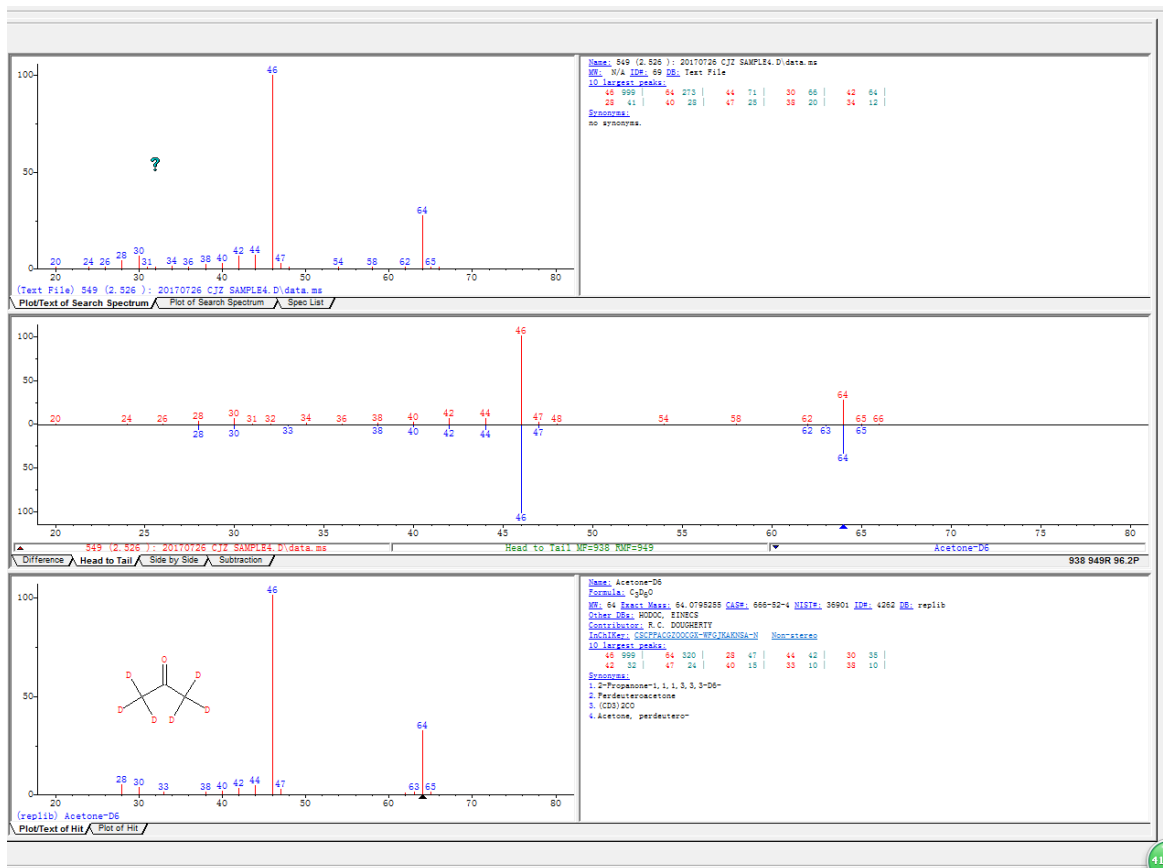


Figure S4. ESI mass-spectra of the reaction mixtures described in the Table

S1: d_6 -Acetone+H₂ (entry 3, peak, $m/z = 48$). Relates to the Scheme 3.

