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Data Article

Electronic structure data at ground and excited state of the structural and opto-electronic properties of organic photovoltaic materials

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A B S T R A C T

This work presents data coming from electronic structure calculations at the Density Functional Theory level, performed in a series of organic photovoltaic materials. The data represents the Cartesian coordinates of such molecular systems at the lowest energy geometry and at the first excited state. Data evidencing the nature of the photo-isomerization in the OPV systems was also obtained. Additionally, the highest probabilities of the molecular electronic transitions giving rise to the absorption spectra observed in excited state were also computed. These data may aid to estimate photovoltaic parameters, and to tailor materials intended to be implemented in solar cell devices. They may also be used as input to design a training set for machine learning analysis and artificial intelligence.

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Specifications Table

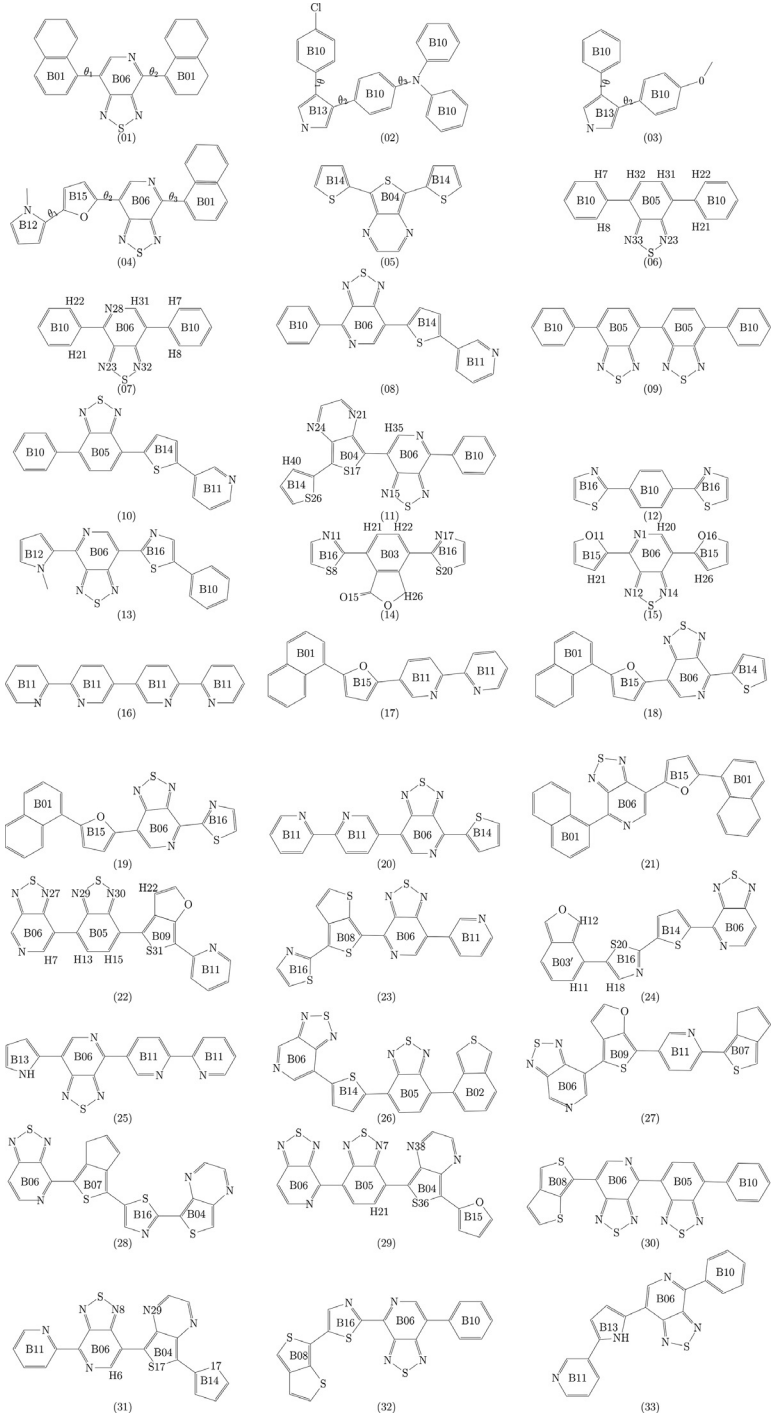
Subject	Organic Chemistry Physical and Theoretical Chemistry Renewable Energy, Sustainability and the Environment
Specific subject area	Computational Chemistry
Type of data	Table Graph Figure
How data were acquired	Data obtained with TURBOMOLE computational code at the DFT/PBE level. Data processing using gnuplot and molecular viewer TmoleX.
Data format	Raw data At Supplementary information
Parameters for data collection	Data was acquired from electronic structure properties coming from the computational evaluation of electron density at ground and excited states in a series of organic photovoltaic materials.
Description of data collection	The data collected corresponds to structural and optoelectronic parameters, which are presented in tables (raw data) and graphs (secondary data). Additionally, all Cartesian coordinates are given at an electronic data base located at: http://dx.doi.org/10.17632/k9fts9zjd6.1 They can also be accessed at the Supplementary information of this article.
Data source location	http://dx.doi.org/10.17632/k9fts9zjd6.1 Data collected at Instituto de Energías Renovables, Universidad Nacional Autónoma de México, Priv. Xochicalco s/n Col. Centro, Temixco, Morelos, Mexico.
Data accessibility	Dataset published on Mendeley Data: (http://dx.doi.org/10.17632/k9fts9zjd6.1)
Related research article	C. Delesma, C. Amador-Bedolla, M. Robles, J. Muñiz, Photoisomerization and its effect in the opto-electronic properties of organic photovoltaic materials: A quantum chemistry study, Journal of Photochemistry and Photobiology A: Chemistry (2021) 409, 113155 [1]

Value of the Data

- The electronic structure data of the organic photovoltaic (OPV) series in this study may aid to select descriptors to tailor heterojunctions for solar cell devices.
- The data may be used as a tool for organic chemists and materials scientists to identify potential OPV materials, acting as an active layer in a solar cell device.
- The data obtained at ground and excited states for this series of OPV materials may be implemented as training sets for machine-learning and artificial intelligence methodologies to search novel OPV materials with enhanced photovoltaic properties.
- The structural data could be directly related to understand the mechanisms behind photoisomerization.

1. Data Description

The data collected corresponds to structural and optoelectronic parameters, which are presented in tables (raw data) and graphs (secondary data). Additionally, all Cartesian coordinates are given at an electronic data base located at: http://dx.doi.org/10.17632/k9fts9zjd6.1. They can also be accessed at the Supplementary information of this article. The data show the electronic structure properties of a series of 33 OPV materials with potential to be implemented as a component in a solar cell device. The data was obtained considering ground state geometries (lowest energy geometries), and also excited states at the Density Functional Theory (DFT) level by using the PBE/def2-TZVP methodology. Scheme 1 presents the molecular representations of the OPV materials under study. Fig. 1 depicts the molecular building blocks forming the OPV systems. Fig. 2 presents the molecular orbital (MO) representations of the most likely excitations in the title molecules; while Fig. 3 shows the most likely transitions at the first-excited state for



Scheme 1. Organic photovoltaic materials under study.

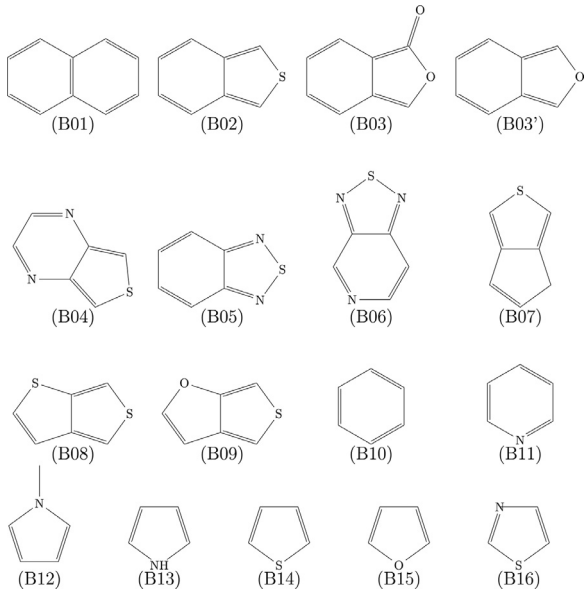


Fig. 1. Building blocks forming the OPV series.

Table 1
IUPAC nomenclature used for the building blocks.

Building Blocks	IUPAC Name
B01	Naphthalene
B02	Benzo(c)thiophene
B03	2-benzofuran-1(3H)-one
B03′	Benzo[c]furan
B04	Thieno[3,4-b]pyrazine
B05	Benzo[1,2,5]thiadiazole
B06	Thiadiazolo[3,4-c]pyridine
B08	Thieno[3,4-b]thiophen
B09	Thieno[3,4-b]furan
B10	Benzene
B11	Pyridine
B13	Pyrrole
B12	1-Methyl-1H-pyrrole
B14	Thiophene
B15	Furan
B16	Thiazole

selected OPV systems. Figs. 4 and 5 show the electron occupation with 2D plots of the frontier molecular orbitals in selected systems. Moreover, Table 1 presents the IUPAC nomenclature of the building blocks forming the OPV systems. Tables 2–34 show the Cartesian coordinates of the optimized molecular structure at ground and excited states. Table 35 shows the probabilities in the electronic transitions giving rise to the absorption spectra obtained via Time-Dependent DFT (TDDFT) calculations. Finally, in Table 36, the shifting in the absorption spectra maxima from the geometries at ground and excited state are presented. Additionally, the changes from ground to excited state in the average of dihedral angles, are also shown.

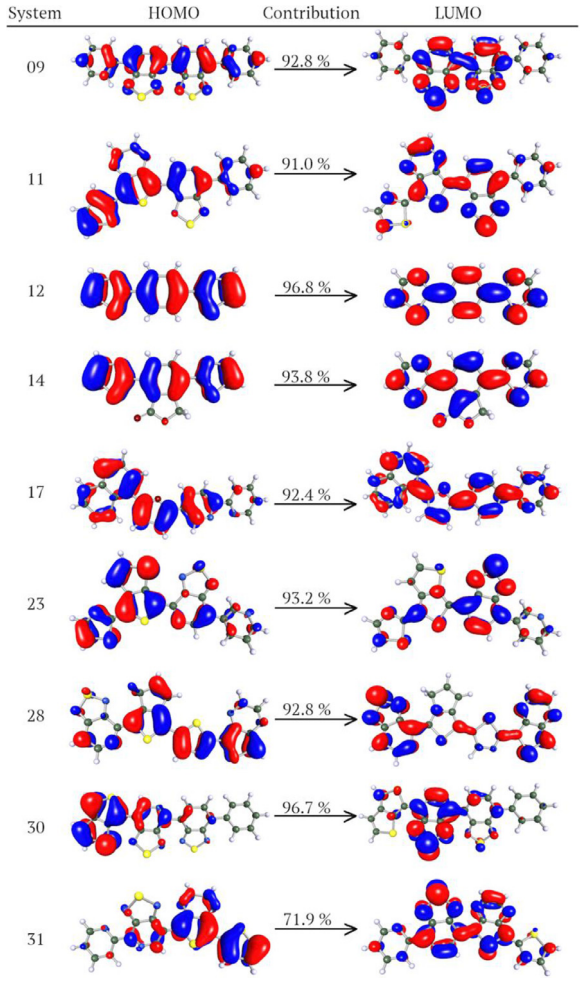


Fig. 2. Contributions with highest probability corresponding to one-electron HOMO-LUMO electronic transitions, in accordance to Table 35.

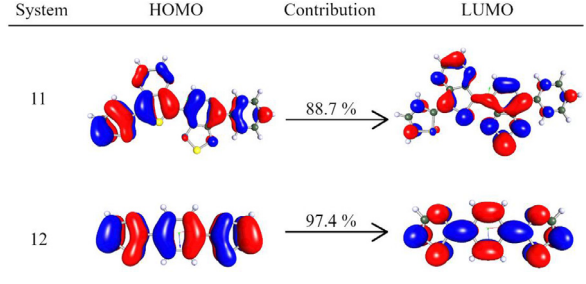


Fig. 3. Contributions with highest probability corresponding to one-electron HOMO-LUMO electronic transitions in excited state.

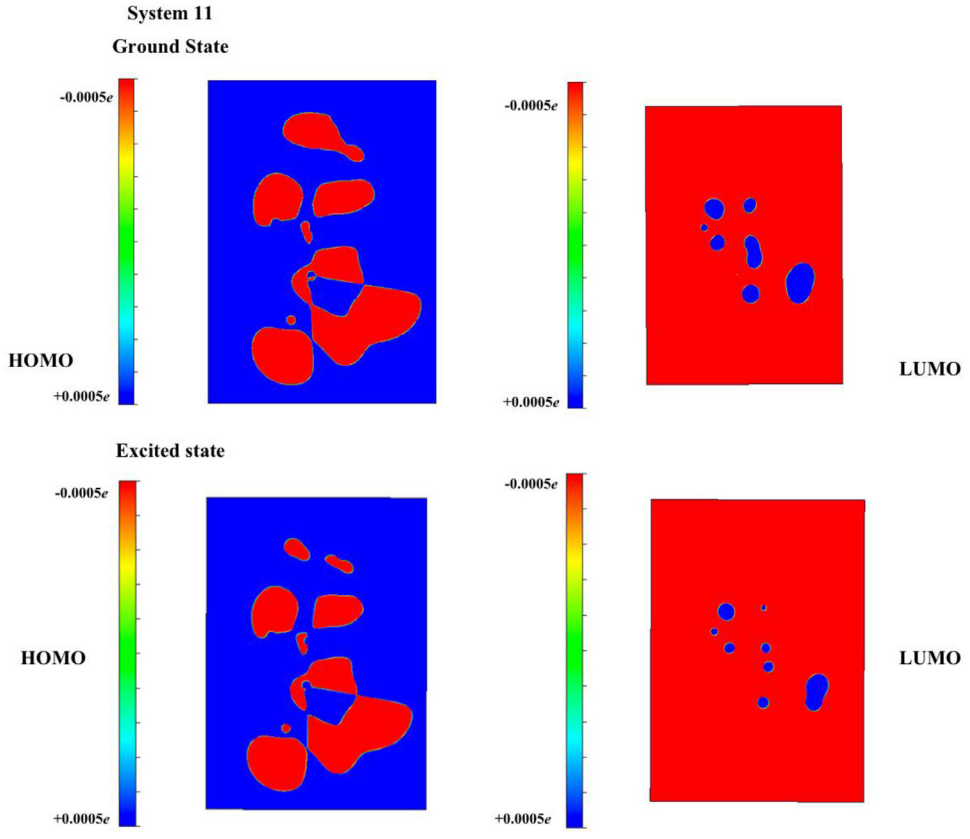


Fig. 4. 2D slices of the frontier molecular orbitals at the xy-plane of system 11. Note that both contributions (HOMO and LUMO) were evaluated at ground and excited state. The heat scale is given in electrons.

2. Experimental Design, Materials and Methods

All electronic structure data was found by implementing DFT calculations on a series of OPV systems. Such calculations were performed by considering ground and excited states of the molecular systems under study. The ground state geometries were disclosed at the Perdew-Becke-Ernzerhof (PBE) [2] functional level and using the basis set functions *def2*-TZVP [3,4]. Note that a benchmark study is a comparative process in which different functionals are tested. The theoretical results obtained with the functional that is in closer agreement with available experimental evidence, is used through the investigation. In this work, the comparative study was performed to compute the HOMO-LUMO gap with different functionals, such as B3LYP, PBE0, CAM-B3LYP, M06 and B97-3C. In this regard, the PBE functional appeared to show the smallest energy differences in band gap energy with respect to a set of OPV systems experimentally synthesized (see Table 1 in [1]).

The one-electron excitations were calculated using TDDFT with the same basis set *def2*-TZVP. Moreover, the geometries of the systems under study were also optimized at the first excited state. The electronic structure calculations were performed using the computational code TURBOMOLE version 7.3 [5]. The visualization of the molecular systems and isosurfaces mapping were performed using the TmoleX suite [6].

The analysis of dihedral angles at ground and excited states (θ_{Grd} and θ_{Exc}, respectively) was performed using a computational code developed in Python 2.7 programming language [7]. The

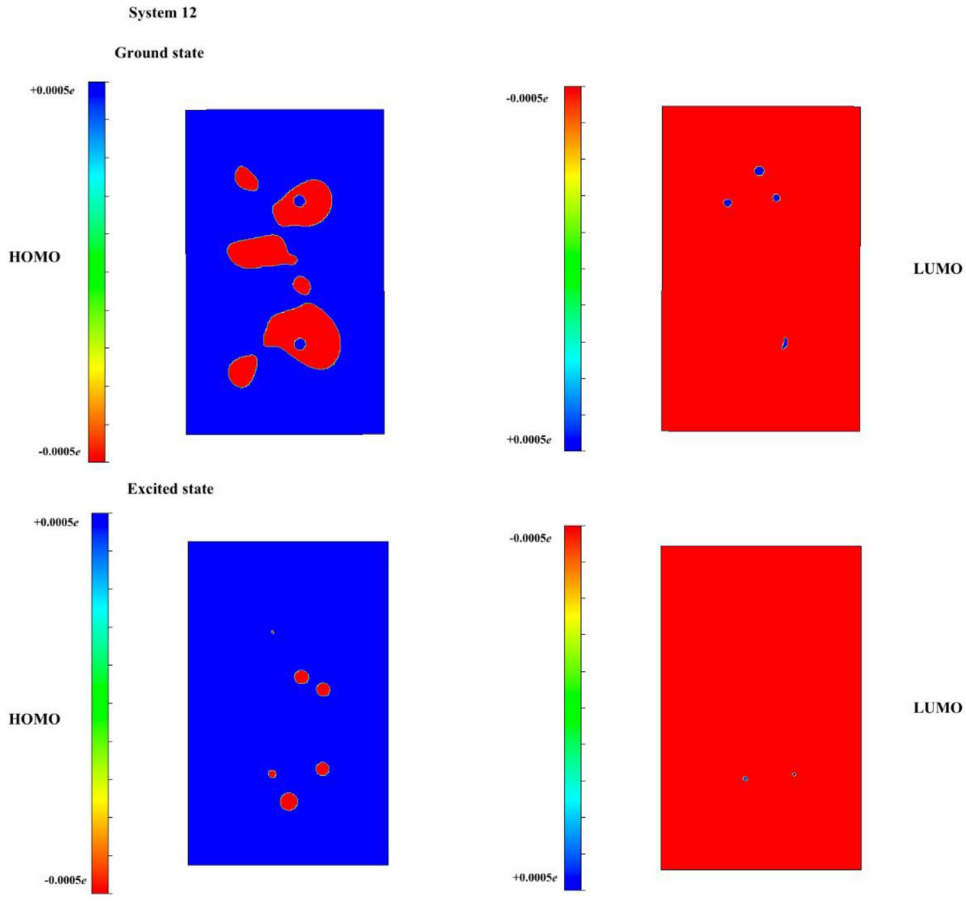


Fig. 5. 2D slices of the frontier molecular orbitals at the *xy*-plane of system 12. Note that both contributions (HOMO and LUMO) were evaluated at ground and excited state. The heat scale is given in electrons.

Table 2
Molecular system 01: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	0.560523	-1.074601	5.941410	C	0.343144	-0.933834	5.752700
2	C	0.674049	-1.433892	4.579097	C	0.555458	-1.339888	4.426087
3	C	1.302771	-0.024565	6.436102	C	1.112522	0.090120	6.288260
4	C	1.502624	-0.725297	3.733043	C	1.506338	-0.698717	3.636816
5	C	2.175214	0.718491	5.596492	C	2.097101	0.753349	5.512031
6	C	2.263880	0.381179	4.199771	C	2.270959	0.386615	4.133326
7	C	2.970433	1.772219	6.114722	C	2.933350	1.741182	6.082378
8	C	3.144285	1.146340	3.359171	C	3.245559	1.081377	3.334270
9	C	3.837649	2.463597	5.296955	C	3.936689	2.332251	5.322305
10	C	3.923847	2.147290	3.926273	C	4.096619	2.000737	3.973999
11	H	-0.103427	-1.637706	6.599511	H	-0.405502	-1.435544	6.367350
12	H	0.106252	-2.282668	4.193796	H	-0.014995	-2.172393	4.011963

(*continued on next page*)

Table 2 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
13	H	1.239763	0.250288	7.491707	H	0.976935	0.393806	7.328829
14	H	1.588238	-1.028589	2.689609	H	1.694196	-1.054195	2.624339
15	H	2.888913	2.018343	7.175944	H	2.798234	2.009620	7.132302
16	H	4.455332	3.267159	5.701396	H	4.599699	3.071023	5.775362
17	H	4.602897	2.714882	3.289418	H	4.884595	2.467821	3.385532
18	C	0.628152	2.772841	-3.740263	C	0.528129	2.686247	-3.612962
19	C	0.582741	2.406631	-5.103974	C	0.400082	2.275187	-4.953433
20	C	1.435204	2.091452	-2.851397	C	1.428885	2.062290	-2.763014
21	C	1.365145	1.367135	-5.556179	C	1.199304	1.253190	-5.430616
22	C	2.248327	1.006638	-3.277069	C	2.247881	0.991677	-3.208681
23	C	2.215445	0.651168	-4.671780	C	2.140951	0.602152	-4.589460
24	C	3.132371	0.277039	-2.404006	C	3.209342	0.323068	-2.369182
25	C	3.037838	-0.400282	-5.151537	C	2.988873	-0.407834	-5.104101
26	C	3.935418	-0.727287	-2.935901	C	4.053913	-0.630580	-2.945654
27	C	3.884603	-1.074478	-4.299744	C	3.939407	-1.003028	-4.293357
28	H	0.016184	3.603364	-3.383355	H	-0.084007	3.507849	-3.236645
29	H	-0.065348	2.949706	-5.794102	H	-0.315448	2.768428	-5.613459
30	H	1.439798	2.373306	-1.800994	H	1.511083	2.385627	-1.728163
31	H	1.351643	1.078374	-6.609846	H	1.127475	0.934822	-6.473372
32	H	2.989194	-0.661300	-6.211393	H	2.892555	-0.693529	-6.154225
33	H	4.605752	-1.276552	-2.275971	H	4.813517	-1.096941	-2.320554
34	H	4.516032	-1.882890	-4.671695	H	4.604453	-1.768494	-4.696812
35	C	2.098079	0.918306	1.079391	C	2.181251	0.876120	1.085523
36	N	2.079176	0.736927	-0.265267	N	2.151528	0.740010	-0.243811
37	C	3.201137	0.531155	-0.947780	C	3.314789	0.575291	-0.912793
38	C	4.450457	0.542762	-0.231621	C	4.565907	0.600072	-0.230766
39	N	5.690454	0.408078	-0.753672	N	5.805273	0.456368	-0.794995
40	S	6.716300	0.514138	0.499747	S	6.875353	0.634472	0.465828
41	N	5.694090	0.734654	1.742749	N	5.821639	0.866564	1.745565
42	C	4.453326	0.741246	1.203337	C	4.586951	0.804059	1.189058
43	C	3.220803	0.917974	1.899884	C	3.342355	0.887413	1.881501
44	H	1.116467	1.089052	1.530674	H	1.209687	1.037794	1.563381

Table 3
Molecular system 02: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-2.169082	2.759604	-1.029992	C	-2.175851	2.853616	-0.992660
2	C	-1.382239	3.916827	-1.178860	C	-1.375446	4.038301	-1.014651
3	C	-1.542983	4.769441	-2.269165	C	-1.624609	5.073853	-1.904365
4	C	-2.508038	4.475540	-3.234228	C	-2.689134	4.978461	-2.813986
5	C	-3.306256	3.337320	-3.116414	C	-3.513253	3.836354	-2.813717
6	C	-3.128234	2.489864	-2.023625	C	-3.259210	2.807753	-1.920810
7	H	-0.637970	4.159438	-0.419411	H	-0.573635	4.155083	-0.284652
8	H	-0.929627	5.665072	-2.369482	H	-1.009849	5.975246	-1.887181
9	Cl	-2.715012	5.538954	-4.602165	Cl	-2.993006	6.278881	-3.951898
10	H	-4.050670	3.112861	-3.880564	H	-4.337001	3.762241	-3.524876
11	H	-3.735168	1.585395	-1.947607	H	-3.889389	1.915733	-1.955777
12	C	5.004728	0.129040	-1.546211	C	5.003545	-0.020714	-1.289090
13	C	5.303960	1.500494	-1.462652	C	5.462893	1.319887	-1.273972
14	C	6.227013	2.049095	-2.370824	C	6.574922	1.679254	-2.080346
15	C	6.838091	1.241782	-3.328700	C	7.226500	0.714682	-2.835277
16	C	6.533690	-0.119769	-3.412632	C	6.794424	-0.616220	-2.808343
17	C	5.610477	-0.666700	-2.517275	C	5.678668	-0.972080	-2.035057
18	H	4.292308	-0.306800	-0.844661	H	4.128931	-0.282371	-0.696160
19	N	4.683463	2.316034	-0.482652	N	4.776788	2.269671	-0.524618

(*continued on next page*)

Table 3 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
20	H	6.460845	3.113214	-2.319454	H	6.872826	2.724664	-2.150132
21	H	7.548889	1.687480	-4.027246	H	8.062262	1.005980	-3.472314
22	H	7.009645	-0.746873	-4.167650	H	7.307635	-1.369561	-3.406665
23	H	5.366620	-1.729793	-2.564177	H	5.332390	-2.005857	-2.022311
24	C	0.573319	1.723740	0.487193	C	0.616651	1.650065	0.378692
25	C	1.529266	2.002110	1.482126	C	1.644601	1.421030	1.346269
26	C	2.874328	2.184127	1.172948	C	2.985604	1.620739	1.062681
27	C	3.315845	2.118213	-0.159081	C	3.364812	2.050992	-0.221218
28	C	2.368635	1.853277	-1.163454	C	2.392127	2.284849	-1.203584
29	C	1.030112	1.651317	-0.842437	C	1.049132	2.097188	-0.910169
30	H	1.206965	2.081102	2.522598	H	1.364014	1.117496	2.356259
31	H	3.592689	2.392435	1.967087	H	3.741909	1.457255	1.833886
32	H	2.692172	1.796219	-2.203704	H	2.689195	2.607617	-2.204321
33	H	0.319772	1.433130	-1.641142	H	0.308326	2.266797	-1.688887
34	C	4.845089	4.571769	0.466351	C	4.614029	4.594762	0.156857
35	C	5.576930	5.557205	1.126824	C	5.213427	5.747266	0.640104
36	C	6.903698	5.328368	1.501950	C	6.576985	5.760227	0.968592
37	C	7.488788	4.092462	1.212801	C	7.341174	4.599128	0.814109
38	C	6.760912	3.095307	0.565596	C	6.762433	3.440626	0.311917
39	C	5.428072	3.324541	0.179924	C	5.391501	3.431101	-0.044752
40	H	3.813572	4.761085	0.166702	H	3.553682	4.569988	-0.088930
41	H	5.107354	6.520140	1.336883	H	4.612964	6.648273	0.767637
42	H	7.475000	6.104106	2.013499	H	7.034979	6.667141	1.364606
43	H	8.521170	3.893743	1.507034	H	8.390827	4.590386	1.109959
44	H	7.220961	2.129424	0.353211	H	7.342764	2.520780	0.245294
45	N	-2.613128	0.634567	1.905102	N	-2.512184	0.245708	1.529829
46	C	-1.243965	0.709542	1.923417	C	-1.168819	0.432538	1.653181
47	C	-0.833289	1.475907	0.839471	C	-0.765964	1.369519	0.678816
48	C	-2.031579	1.879589	0.140368	C	-1.981357	1.794847	-0.020941
49	C	-3.105009	1.333851	0.834440	C	-3.025136	1.041326	0.534388
50	H	-0.656743	0.171953	2.660689	H	-0.578750	-0.183631	2.323057
51	H	-4.172020	1.448516	0.673725	H	-4.094421	1.103668	0.364375
52	H	-3.177024	0.138462	2.583405	H	-3.059564	-0.386809	2.099028

Table 4
Molecular system 03: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-5.094181	2.836552	3.841470	C	-5.372523	2.184640	3.734550
2	C	-4.375491	1.908137	4.609780	C	-4.319752	1.833706	4.635884
3	C	-3.399226	1.137982	3.945678	C	-2.985131	1.819854	4.120681
4	C	-3.149788	1.291196	2.587533	C	-2.715545	2.141042	2.812896
5	C	-3.882348	2.223348	1.836885	C	-3.777397	2.498768	1.943726
6	C	-4.861610	2.997842	2.473349	C	-5.106914	2.513813	2.421662
7	H	-5.849958	3.458100	4.323984	H	-6.399107	2.163934	4.101788
8	H	-2.838759	0.389360	4.509703	H	-2.154072	1.552138	4.772606
9	H	-2.396224	0.686546	2.080486	H	-1.699929	2.130917	2.416814
10	O	-3.571917	2.298086	0.505087	O	-3.413367	2.800413	0.686008
11	H	-5.442999	3.733839	1.919046	H	-5.933701	2.775978	1.763441
12	C	-9.894838	1.875509	5.390061	C	-9.892818	2.293565	5.357399
13	C	-9.520414	2.611354	6.516767	C	-9.236757	3.243228	6.231890
14	C	-8.196779	2.596015	6.958119	C	-7.923735	2.955640	6.656448
15	C	-7.216244	1.836668	6.291994	C	-7.243080	1.814165	6.248517

(*continued on next page*)

Table 4 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
16	C	-7.610455	1.099073	5.159713	C	-7.906234	0.855112	5.370758
17	C	-8.931663	1.121227	4.714086	C	-9.231009	1.141557	4.968200
18	H	-10.928543	1.890722	5.040207	H	-10.912017	2.478609	5.013222
19	H	-10.261265	3.210199	7.050523	H	-9.738928	4.151971	6.558770
20	H	-7.905524	3.195500	7.823430	H	-7.408970	3.665680	7.312841
21	H	-6.870127	0.494841	4.633747	H	-7.442507	-0.102540	5.136248
22	H	-9.213263	0.537185	3.835570	H	-9.750969	0.420245	4.329461
23	N	-4.138991	1.590636	8.243747	N	-4.156826	1.101877	8.158504
24	C	-3.574704	1.638795	6.994021	C	-3.572333	1.242327	6.960510
25	C	-4.593969	1.763236	6.058352	C	-4.592718	1.535503	6.007991
26	C	-5.834734	1.788868	6.797916	C	-5.865119	1.552429	6.729758
27	C	-5.502531	1.682719	8.143389	C	-5.543784	1.273296	8.032369
28	H	-2.498125	1.639688	6.858102	H	-2.498328	1.143582	6.843251
29	H	-6.142274	1.605787	9.016546	H	-6.195372	1.182644	8.894974
30	C	-4.304818	3.224433	-0.288514	C	-4.428355	3.174251	-0.262598
31	H	-3.913670	3.122489	-1.307410	H	-3.893360	3.372472	-1.196263
32	H	-4.155934	4.261616	0.056990	H	-4.954589	4.081002	0.067576
33	H	-5.383925	2.994808	-0.287016	H	-5.145331	2.354011	-0.408783
34	H	-3.625070	1.497436	9.110381	H	-3.669785	0.893965	9.022622

Table 5
Molecular system 04: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	N	-0.696245	2.212344	1.475705	N	-0.857081	0.159008	1.159561
2	N	-0.592818	2.285736	-1.037154	N	-0.928458	0.425566	-1.392946
3	C	-1.908008	2.101909	0.889521	C	-1.962162	0.762560	0.682870
4	C	-1.849438	2.136846	-0.560531	C	-2.022496	0.924901	-0.753014
5	C	-3.179485	1.976505	1.539047	C	-3.053961	1.249029	1.444146
6	C	-3.057190	2.049343	-1.335469	C	-3.147883	1.575662	-1.337967
7	C	-4.269196	1.933860	0.660074	C	-4.112280	1.864011	0.760127
8	S	0.375715	2.356498	0.263353	S	0.059296	-0.186480	-0.205508
9	N	-4.219078	1.968337	-0.684790	N	-4.167567	2.031827	-0.559018
10	H	-5.278426	1.857606	1.074951	H	-4.972727	2.240872	1.325320
11	O	-2.279886	1.978985	3.788963	O	-2.531866	2.080191	3.667221
12	C	-3.376312	1.901952	2.963338	C	-3.077132	1.093506	2.898457
13	C	-4.510693	1.753679	3.742548	C	-3.565781	0.089130	3.729730
14	C	-4.092089	1.740165	5.092580	C	-3.304756	0.468868	5.050623
15	C	-2.710189	1.880767	5.087039	C	-2.657378	1.711275	4.987157
16	H	-5.530987	1.660538	3.384399	H	-4.043694	-0.819673	3.382623
17	H	-4.735234	1.637487	5.958224	H	-3.550823	-0.088829	5.946991
18	C	-0.639504	1.959863	8.066942	C	-1.529825	3.572293	7.848264
19	C	0.346807	2.106092	7.103782	C	-1.137687	4.456715	6.828347
20	C	-0.291911	2.097222	5.846738	C	-1.505695	3.879640	5.622989
21	C	-1.665755	1.944876	6.068334	C	-2.130538	2.630579	5.915820
22	N	-1.858366	1.862320	7.441800	N	-2.125259	2.477250	7.298854
23	H	1.410269	2.207825	7.295809	H	-0.638399	5.407584	6.979259
24	H	0.165577	2.189246	4.866804	H	-1.361652	4.266131	4.620380
25	C	-3.118491	1.699075	8.139161	C	-2.646750	1.352232	8.060915
26	H	-0.575939	1.916837	9.149846	H	-1.419390	3.655404	8.925243
27	C	-5.895955	4.267047	-3.875577	C	-4.640121	5.236974	-3.296139
28	C	-5.856903	4.109600	-5.279011	C	-4.808010	5.271638	-4.699110
29	C	-5.006188	3.592508	-3.063672	C	-4.158970	4.104236	-2.671287

(*continued on next page*)

Table 5 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
30	C	-4.908148	3.287165	-5.845448	C	-4.469202	4.168347	-5.450960
31	C	-4.021203	2.725444	-3.608915	C	-3.811708	2.939169	-3.410062
32	C	-3.968826	2.587982	-5.041083	C	-3.957591	2.990332	-4.842039
33	C	-3.048899	2.018800	-2.813320	C	-3.280812	1.742505	-2.805229
34	C	-2.974248	1.769826	-5.635610	C	-3.573956	1.875280	-5.630841
35	C	-2.079644	1.252315	-3.454431	C	-2.892087	0.694974	-3.634333
36	C	-2.043670	1.119102	-4.855706	C	-3.042769	0.753456	-5.034265
37	H	-6.639020	4.928971	-3.426662	H	-4.893757	6.115941	-2.699569
38	H	-6.571047	4.643140	-5.908869	H	-5.196529	6.170414	-5.182478
39	H	-5.064497	3.709787	-1.984029	H	-4.053966	4.080822	-1.589019
40	H	-4.854903	3.164355	-6.929914	H	-4.579078	4.182379	-6.538502
41	H	-2.957765	1.671424	-6.723646	H	-3.696913	1.930630	-6.715351
42	H	-1.341777	0.721298	-2.854519	H	-2.462158	-0.197540	-3.182048
43	H	-1.278586	0.491177	-5.315253	H	-2.737739	-0.101925	-5.640531
44	H	-3.797046	2.540301	7.934599	H	-3.727167	1.241551	7.898086
45	H	-3.613761	0.760831	7.848902	H	-2.133601	0.423620	7.777878
46	H	-2.917947	1.667864	9.216145	H	-2.468829	1.542791	9.124351

Table 6
Molecular system 05: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	S	-2.454968	0.508086	3.565883	S	-2.373756	0.521205	3.611993
2	C	-1.158159	0.459270	2.395345	C	-1.115511	0.458601	2.382337
3	C	-1.680843	0.428806	1.105201	C	-1.689212	0.423529	1.098296
4	C	-3.092921	0.444171	1.069671	C	-3.089180	0.446824	1.117522
5	C	-3.648713	0.486424	2.329053	C	-3.594452	0.499535	2.409530
6	H	-1.052996	0.396748	0.214606	H	-1.087966	0.382499	0.190341
7	H	-3.679126	0.425133	0.152090	H	-3.714837	0.426218	0.226470
8	H	-4.701308	0.506812	2.598397	H	-4.640396	0.526545	2.706283
9	S	5.473524	0.396023	3.536967	S	5.392929	0.408205	3.583746
10	C	6.657046	0.338117	2.291417	C	6.603693	0.351336	2.372372
11	C	6.090984	0.309308	1.036198	C	6.087657	0.313611	1.084073
12	C	4.679292	0.334180	1.082072	C	4.687479	0.331038	1.075084
13	C	4.167203	0.382072	2.375964	C	4.124443	0.382432	2.363307
14	H	7.711782	0.328908	2.553027	H	7.652136	0.347858	2.661485
15	H	6.669648	0.271756	0.114385	H	6.705928	0.274974	0.188464
16	H	4.044201	0.318031	0.196159	H	4.078655	0.307761	0.171539
17	C	0.806204	0.570974	6.338334	C	0.823234	0.563387	6.291602
18	C	2.235247	0.550984	6.333222	C	2.217771	0.542912	6.286609
19	N	2.950092	0.501331	5.224973	N	2.983587	0.492977	5.161504
20	C	2.233801	0.469934	4.070173	C	2.212567	0.465152	4.031629
21	C	2.791232	0.416157	2.781249	C	2.758502	0.412522	2.716307
22	S	1.501202	0.392590	1.621882	S	1.500862	0.389024	1.509498
23	C	0.221169	0.453115	2.790468	C	0.253246	0.448967	2.725371
24	C	0.789189	0.490512	4.075356	C	0.809981	0.485572	4.036680
25	N	0.082407	0.541724	5.235207	N	0.048247	0.535903	5.172044
26	H	0.267614	0.612184	7.290452	H	0.292525	0.604223	7.246960
27	H	2.781616	0.577267	7.281434	H	2.756286	0.567810	7.238140

Table 7
Molecular system 06: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-1.174118	2.718694	-1.640288	C	-1.224941	2.595801	-1.586525
2	C	0.022774	2.396161	-0.972029	C	0.023663	2.403593	-0.928447
3	C	1.138020	2.030072	-1.748857	C	1.169024	2.197475	-1.747154
4	C	1.050269	1.974022	-3.139179	C	1.058565	2.162051	-3.130458
5	C	-0.145829	2.290895	-3.787408	C	-0.181756	2.351545	-3.753114
6	C	-1.257970	2.667425	-3.030549	C	-1.322484	2.577594	-2.968813
7	H	-2.040846	3.041320	-1.060183	H	-2.118726	2.801927	-0.998422
8	H	2.076909	1.783143	-1.255311	H	2.134590	2.073719	-1.261337
9	H	1.925309	1.678773	-3.721118	H	1.949828	1.988269	-3.735784
10	H	-0.209225	2.251354	-4.876183	H	-0.260652	2.330323	-4.841492
11	H	-2.193860	2.932798	-3.525703	H	-2.289195	2.745356	-3.446423
12	C	-1.230568	2.702608	6.991557	C	-1.296365	2.608930	6.930616
13	C	-0.115588	2.326978	7.744668	C	-0.151581	2.387434	7.710293
14	C	1.076145	2.002793	7.092007	C	1.085453	2.194050	7.082313
15	C	1.156735	2.050659	5.700947	C	1.188678	2.221068	5.698258
16	C	0.038449	2.415535	4.927985	C	0.039045	2.422242	4.884320
17	C	-1.153898	2.745671	5.600586	C	-1.206065	2.618680	5.547752
18	H	-2.163077	2.973458	7.490113	H	-2.260524	2.779843	7.412250
19	H	-0.173312	2.293987	8.833976	H	-0.224797	2.372724	8.799174
20	H	1.953290	1.708130	7.671061	H	1.979861	2.023863	7.684011
21	H	2.092167	1.797801	5.203824	H	2.151681	2.094307	5.208151
22	H	-2.022662	3.067496	5.023081	H	-2.102894	2.821334	4.963092
23	N	2.386288	3.312112	3.224868	N	2.536115	2.944381	3.251434
24	C	1.229062	2.847883	2.701676	C	1.325661	2.654704	2.688413
25	C	1.225205	2.843132	1.245103	C	1.321866	2.650057	1.259068
26	C	0.081880	2.429746	3.451566	C	0.112060	2.420414	3.428005
27	C	0.074129	2.419861	0.504015	C	0.104377	2.411001	0.527442
28	C	-1.009014	2.033118	2.688955	C	-1.064181	2.164461	2.671839
29	S	3.338223	3.686698	1.965195	S	3.575650	3.164020	1.966073
30	C	-1.012699	2.028331	1.275070	C	-1.067846	2.160011	1.291462
31	H	-1.900032	1.669203	3.203759	H	-1.985826	1.907773	3.192135
32	H	-1.906483	1.661093	0.767480	H	-1.992286	1.900175	0.777727
33	N	2.379621	3.304203	0.712912	N	2.529291	2.936028	0.687735

Table 8
Molecular system 07: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-1.110306	2.940628	-1.541458	C	-1.203742	2.768300	-1.471230
2	C	0.051110	2.417435	-0.939649	C	0.048513	2.418394	-0.885375
3	C	1.048039	1.878154	-1.775011	C	1.125045	2.110200	-1.765735
4	C	0.878207	1.849811	-3.158269	C	0.946274	2.134813	-3.140806
5	C	-0.282650	2.364742	-3.740372	C	-0.296268	2.477503	-3.692614
6	C	-1.275278	2.913836	-2.925034	C	-1.367914	2.802605	-2.845755
7	H	-1.878595	3.399435	-0.916434	H	-2.039543	3.049098	-0.831025
8	H	1.957791	1.474447	-1.332552	H	2.093558	1.869502	-1.331528
9	H	1.660141	1.420049	-3.786959	H	1.783037	1.890113	-3.796993
10	H	-0.410058	2.345061	-4.824024	H	-0.429646	2.498547	-4.775579
11	H	-2.179482	3.333848	-3.369246	H	-2.331533	3.088077	-3.270443
12	C	-1.339269	2.100764	6.841143	C	-1.371458	2.238161	6.787824
13	C	-0.258802	2.361302	7.690633	C	-0.289313	2.531819	7.628592
14	C	0.993202	2.640618	7.140641	C	0.984787	2.732848	7.079664
15	C	1.172496	2.661041	5.757352	C	1.186419	2.646652	5.707784
16	C	0.092518	2.400050	4.890770	C	0.101032	2.357420	4.842124
17	C	-1.167238	2.119557	5.461486	C	-1.182693	2.148654	5.416993

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Table 8 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
18	H	-2.323177	1.880133	7.259446	H	-2.362884	2.070552	7.212226
19	H	-0.393668	2.346103	8.773754	H	-0.436192	2.595170	8.708603
20	H	1.843251	2.846809	7.793590	H	1.828762	2.957233	7.734235
21	H	2.154793	2.881007	5.345431	H	2.174204	2.796305	5.274761
22	H	-2.002706	1.917993	4.791683	H	-2.007807	1.910060	4.747321
23	N	2.676214	2.815120	3.182922	N	2.727955	2.492382	3.231763
24	C	1.437804	2.609812	2.680545	C	1.478674	2.385639	2.673075
25	C	1.413842	2.611876	1.227898	C	1.467169	2.437000	1.246757
26	C	0.211998	2.411336	3.415099	C	0.241434	2.285412	3.385975
27	C	0.185323	2.418611	0.528080	C	0.206449	2.380491	0.558667
28	N	-0.903754	2.221890	2.714290	N	-0.930458	2.138268	2.707456
29	S	3.665623	2.993678	1.910456	S	3.767438	2.626767	1.939947
30	C	-0.910113	2.219463	1.363823	C	-0.937716	2.200682	1.387213
31	H	-1.886543	2.019661	0.912475	H	-1.909816	2.026923	0.918346
32	N	2.628800	2.827954	0.673890	N	2.685750	2.576634	0.664160

Table 9
Molecular system 08: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	1.371568	2.454372	-3.924816	C	1.370589	2.461491	-3.907493
2	C	-0.020247	2.471238	-4.131243	C	-0.030626	2.469425	-4.092932
3	C	-0.452951	2.481929	-5.476582	C	-0.487922	2.480732	-5.438744
4	N	0.360673	2.473785	-6.534105	N	0.308588	2.482243	-6.504514
5	C	1.682897	2.455814	-6.303313	C	1.635795	2.473310	-6.291838
6	C	2.229899	2.446900	-5.018512	C	2.206578	2.463911	-5.013644
7	H	1.777725	2.444651	-2.910797	H	1.791261	2.452074	-2.899833
8	H	-1.522403	2.498777	-5.705189	H	-1.560758	2.490779	-5.649160
9	H	2.328228	2.448672	-7.186426	H	2.266996	2.473486	-7.184727
10	H	3.311881	2.433231	-4.878767	H	3.290868	2.457363	-4.895250
11	C	-1.383859	2.519034	7.102656	C	-1.395338	2.512595	7.072919
12	C	-2.569567	2.494943	7.844775	C	-2.593830	2.507056	7.797766
13	C	-3.795189	2.471562	7.177048	C	-3.815540	2.494512	7.116517
14	C	-3.844695	2.471506	5.783207	C	-3.851269	2.487480	5.725552
15	C	-2.657394	2.495255	5.023298	C	-2.648997	2.492871	4.978387
16	C	-1.425673	2.518811	5.713035	C	-1.419753	2.505597	5.685175
17	H	-0.419267	2.537468	7.613373	H	-0.438806	2.522422	7.598643
18	H	-2.536614	2.494980	8.935815	H	-2.574405	2.512502	8.889443
19	H	-4.726881	2.452581	7.745455	H	-4.751881	2.490158	7.677366
20	H	-4.808372	2.452677	5.279420	H	-4.800454	2.477789	5.192772
21	H	-0.507191	2.536695	5.127200	H	-0.497217	2.509707	5.106330
22	N	-5.098550	2.460101	3.074617	N	-5.089824	2.467021	3.084697
23	C	-3.801627	2.476417	2.693528	C	-3.786820	2.473773	2.665572
24	C	-3.644080	2.474284	1.248861	C	-3.631283	2.467940	1.249301
25	C	-2.637889	2.494564	3.545383	C	-2.619141	2.485834	3.510076
26	C	-2.335241	2.489595	0.667806	C	-2.312568	2.474348	0.706311
27	N	-1.443604	2.511947	2.951657	N	-1.378800	2.491486	2.960390
28	S	-5.983055	2.442961	1.716623	S	-5.995414	2.454052	1.693009
29	C	-1.306828	2.509584	1.614945	C	-1.255321	2.485892	1.637384
30	H	-0.268826	2.524282	1.265140	H	-0.222628	2.491017	1.266193
31	N	-4.819073	2.454638	0.584394	N	-4.790645	2.456552	0.531573
32	C	-0.978947	2.476054	-3.032667	C	-0.961339	2.467845	-2.991093

(*continued on next page*)

Table 9 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
33	S	-0.449544	2.490854	-1.375476	S	-0.410242	2.478492	-1.335899
34	C	-2.082176	2.482754	-0.758115	C	-2.043817	2.469775	-0.711330
35	C	-2.983367	2.471112	-1.817220	C	-2.967540	2.458975	-1.772111
36	C	-2.365928	2.467205	-3.082458	C	-2.364364	2.458252	-3.029162
37	H	-4.058976	2.464087	-1.659381	H	-4.036998	2.451996	-1.570065
38	H	-2.927531	2.454688	-4.015124	H	-2.929811	2.449255	-3.959533

Table 10
Molecular system 09: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	1.119050	3.254786	16.711506	C	1.103203	3.032482	16.669131
2	C	2.256122	2.998577	17.481593	C	2.265553	2.863184	17.433841
3	C	3.491597	2.837736	16.849981	C	3.516006	2.850113	16.803105
4	C	3.594120	2.930110	15.462610	C	3.611967	3.006853	15.427216
5	C	2.455501	3.175840	14.672657	C	2.447539	3.168989	14.631747
6	C	1.218153	3.341574	15.324057	C	1.189985	3.175870	15.292522
7	H	0.150575	3.397689	17.194299	H	0.127645	3.059845	17.156457
8	H	2.180579	2.931394	18.568249	H	2.195796	2.742947	18.515982
9	H	4.386051	2.637259	17.442626	H	4.422513	2.710209	17.393609
10	H	4.563089	2.804830	14.981353	H	4.586320	2.990985	14.943949
11	H	0.328570	3.570216	14.734005	H	0.278800	3.339553	14.716767
12	N	4.706141	4.418693	13.053616	N	4.753004	4.386218	13.054925
13	C	3.635895	3.811920	12.491871	C	3.664658	3.831949	12.483686
14	C	3.667347	3.842288	11.038915	C	3.686293	3.898616	11.035108
15	C	2.529953	3.234134	13.198480	C	2.522480	3.305266	13.183707
16	C	2.603165	3.284737	10.264413	C	2.602775	3.398005	10.233408
17	C	1.509410	2.733527	12.400262	C	1.445117	2.920072	12.357140
18	S	5.617118	4.959339	11.823022	S	5.673382	4.941804	11.825708
19	C	1.541464	2.760227	10.985383	C	1.480782	2.961545	10.961813
20	H	0.710744	2.309803	10.438393	H	0.626823	2.575040	10.404656
21	N	4.746655	4.482333	10.540057	N	4.769971	4.530100	10.549193
22	H	0.654348	2.257998	12.883761	H	0.555315	2.499923	12.827629
23	S	5.652135	1.653152	7.250981	S	5.795595	1.831354	7.300712
24	C	3.683445	2.745472	8.022457	C	3.748352	2.857305	8.044526
25	H	0.660841	4.288889	6.158884	H	0.611966	4.230927	6.163556
26	H	2.226281	3.624425	0.483346	H	2.199297	3.500754	0.516325
27	C	3.659668	2.773432	6.569258	C	3.718089	2.851162	6.604159
28	C	3.527239	3.734306	2.208278	C	3.530605	3.491918	2.224839
29	C	2.550307	3.335964	5.855615	C	2.570116	3.340571	5.894363
30	N	4.741019	2.180065	6.014412	N	4.823572	2.299234	6.033610
31	C	1.250731	3.212051	3.723340	C	1.226984	3.332019	3.779077
32	C	3.623347	3.645895	3.596366	C	3.638325	3.433494	3.611682
33	C	1.543475	3.799906	8.062706	C	1.494773	3.783987	8.055380
34	N	4.768374	2.120585	8.528224	N	4.853739	2.289721	8.597713
35	H	0.360209	2.976147	4.309117	H	0.317192	3.234644	4.372747
36	H	4.588557	3.781392	4.082362	H	4.616565	3.435103	4.088042
37	C	2.483014	3.390824	4.380974	C	2.484995	3.363746	4.428365
38	C	1.519187	3.824773	6.647645	C	1.478083	3.804961	6.668280
39	C	1.158067	3.295209	2.335244	C	1.125515	3.375077	2.392989
40	C	2.296703	3.560440	1.570532	C	2.278194	3.463109	1.604421
41	H	0.193475	3.142400	1.847735	H	0.141642	3.332813	1.921604
42	H	4.422891	3.941977	1.619935	H	4.437131	3.556803	1.619814
43	C	2.607611	3.289669	8.790309	C	2.629834	3.349790	8.775482
44	H	0.703796	4.239914	8.604480	H	0.639528	4.183838	8.604319

Table 11
Molecular system 10: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	1.344245	2.465934	-4.080816	C	1.339113	2.635824	-4.025443
2	C	-0.053473	2.558262	-4.208464	C	-0.062018	2.516324	-4.167806
3	C	-0.552765	2.801812	-5.507396	C	-0.557536	2.468564	-5.498932
4	N	0.206136	2.922577	-6.598628	N	0.204210	2.524063	-6.588671
5	C	1.535951	2.822353	-6.445898	C	1.532657	2.634829	-6.416733
6	C	2.146184	2.605018	-5.208577	C	2.138875	2.696317	-5.156606
7	H	1.793016	2.268166	-3.104729	H	1.788173	2.676344	-3.030894
8	H	-1.630081	2.919868	-5.659047	H	-1.633121	2.385474	-5.676776
9	H	2.136119	2.922905	-7.354898	H	2.135079	2.675271	-7.328421
10	H	3.232449	2.534419	-5.133989	H	3.222520	2.787152	-5.071194
11	C	-1.693255	2.146677	7.271492	C	-1.627714	2.185484	7.220952
12	C	-2.798646	2.740761	7.885472	C	-2.785149	2.666957	7.843454
13	C	-3.832186	3.248807	7.094835	C	-3.869952	3.074789	7.060695
14	C	-3.765889	3.166790	5.704689	C	-3.808948	3.002847	5.672711
15	C	-2.653498	2.580789	5.070826	C	-2.639792	2.539667	5.022950
16	C	-1.621747	2.068811	5.882060	C	-1.552989	2.130172	5.834492
17	H	-0.886276	1.731719	7.878138	H	-0.783194	1.845330	7.822865
18	H	-2.856944	2.801393	8.973556	H	-2.842799	2.715220	8.932385
19	H	-4.699969	3.715775	7.564353	H	-4.776885	3.449068	7.538885
20	H	-4.578921	3.565655	5.099821	H	-4.661692	3.299736	5.065969
21	H	-0.767258	1.576018	5.414460	H	-0.655027	1.724595	5.367100
22	N	-4.925749	2.085026	3.121064	N	-4.955682	2.203220	3.109657
23	C	-3.647776	2.284671	2.728170	C	-3.666491	2.348952	2.688125
24	C	-3.482400	2.212287	1.282180	C	-3.498228	2.306239	1.270903
25	C	-2.535822	2.516200	3.601294	C	-2.529515	2.496774	3.562436
26	C	-2.192268	2.382633	0.669878	C	-2.194664	2.434772	0.698227
27	C	-1.310291	2.668856	2.962090	C	-1.258307	2.611318	2.957065
28	S	-5.791524	1.845679	1.771310	S	-5.852881	2.034866	1.720133
29	C	-1.145780	2.604263	1.564263	C	-1.101069	2.590134	1.579427
30	H	-0.137031	2.742122	1.168714	H	-0.096465	2.708818	1.166664
31	N	-4.640136	1.969244	0.632363	N	-4.655230	2.127470	0.559643
32	C	-0.960429	2.418871	-3.075560	C	-0.956178	2.449380	-3.038123
33	S	-0.413787	2.674871	-1.445782	S	-0.368019	2.571858	-1.402458
34	C	-1.986315	2.335015	-0.767030	C	-1.975704	2.409231	-0.726989
35	C	-2.883026	2.046626	-1.789605	C	-2.919142	2.264056	-1.762443
36	C	-2.308438	2.094030	-3.075598	C	-2.351843	2.288633	-3.034452
37	H	-3.923312	1.802724	-1.590636	H	-3.975420	2.148277	-1.526871
38	H	-2.861061	1.868000	-3.986667	H	-2.936440	2.188958	-3.947690
39	H	-0.427399	2.874552	3.569697	H	-0.381883	2.773198	3.583168

Table 12
Molecular system 11: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-6.279332	2.275816	-0.036380	C	-6.257582	2.255336	-0.071315
2	C	-7.235954	1.305518	-0.354061	C	-7.198067	1.261329	-0.368502
3	C	-6.821227	0.005139	-0.647397	C	-6.767474	-0.042578	-0.632384
4	C	-5.467824	-0.330669	-0.624771	C	-5.412631	-0.360614	-0.601850
5	C	-4.493449	0.637523	-0.306077	C	-4.450940	0.632396	-0.303559
6	C	-4.928368	1.948502	-0.012810	C	-4.903929	1.948109	-0.039011
7	C	-3.045680	0.348410	-0.265666	C	-3.007964	0.359736	-0.256878
8	N	-2.226454	1.364545	0.014037	N	-2.221981	1.417631	0.031202
9	C	-0.889314	1.232295	0.081866	C	-0.892333	1.280456	0.097187

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Table 12 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
10	C	-0.169008	0.042319	-0.124129	C	-0.191188	0.074294	-0.116129
11	C	-1.003951	-1.080915	-0.426378	C	-0.994028	-1.058008	-0.419343
12	C	-2.445311	-0.940111	-0.500404	C	-2.407411	-0.933876	-0.494001
13	N	-3.064885	-2.105544	-0.793944	N	-3.049787	-2.099597	-0.792516
14	S	-1.904782	-3.227989	-0.950920	S	-1.857419	-3.236813	-0.952865
15	N	-0.574723	-2.335675	-0.664229	N	-0.502510	-2.306570	-0.654175
16	C	1.269086	-0.038244	-0.037809	C	1.246082	-0.010407	-0.030627
17	S	2.125248	-1.532077	-0.282071	S	2.068769	-1.518854	-0.287915
18	C	3.698145	-0.870836	-0.031040	C	3.656429	-0.858631	-0.032433
19	C	3.585132	0.510459	0.243425	C	3.568304	0.525882	0.251202
20	C	2.216952	0.978375	0.239553	C	2.212370	1.009152	0.253317
21	N	1.926774	2.284623	0.485061	N	1.929732	2.306896	0.503604
22	C	2.960824	3.071810	0.720987	C	2.973119	3.091250	0.743499
23	C	4.305380	2.606523	0.724102	C	4.307906	2.612559	0.740827
24	N	4.626959	1.346784	0.490267	N	4.621324	1.348081	0.499651
25	C	4.880243	-1.682364	-0.110165	C	4.820731	-1.676466	-0.118708
26	S	4.797058	-3.390027	-0.472664	S	4.712618	-3.388858	-0.485044
27	C	6.503666	-3.562167	-0.378182	C	6.414706	-3.575635	-0.399321
28	C	7.119855	-2.366869	-0.081560	C	7.052905	-2.384665	-0.103350
29	C	6.206716	-1.298620	0.071462	C	6.160733	-1.308360	0.056475
30	H	-6.591392	3.295968	0.195306	H	-6.587171	3.275074	0.135981
31	H	-8.296614	1.562790	-0.372503	H	-8.262450	1.503325	-0.393878
32	H	-7.558430	-0.760138	-0.897407	H	-7.496494	-0.820978	-0.864624
33	H	-5.162343	-1.348912	-0.855183	H	-5.078248	-1.375996	-0.806828
34	H	-4.175497	2.696907	0.232861	H	-4.158676	2.708767	0.190206
35	H	-0.335781	2.141204	0.318233	H	-0.327642	2.182669	0.335442
36	H	2.748352	4.127103	0.920387	H	2.767234	4.145844	0.948492
37	H	5.124446	3.304125	0.925894	H	5.134942	3.300125	0.944491
38	H	6.956834	-4.534988	-0.546573	H	6.858748	-4.552418	-0.571092
39	H	8.198988	-2.262807	0.022818	H	8.134269	-2.299117	-0.006146
40	H	6.475241	-0.271264	0.306469	H	6.440587	-0.283948	0.291324

Table 13
Molecular system 12: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-0.804165	0.021982	1.381671	C	-0.798016	0.021941	1.370109
2	C	0.578491	0.037186	1.503358	C	0.574409	0.037773	1.490917
3	C	1.403526	0.017442	0.364040	C	1.411734	0.018304	0.336591
4	C	0.790378	-0.018376	-0.904498	C	0.788992	-0.017733	-0.951209
5	C	-0.590996	-0.033689	-1.026079	C	-0.581434	-0.033476	-1.071846
6	C	-1.416903	-0.013911	0.115806	C	-1.420190	-0.014203	0.087313
7	C	-2.868781	-0.031307	-0.046039	C	-2.840313	-0.031467	-0.063006
8	S	-3.972808	-0.013485	1.323717	S	-3.938856	-0.009524	1.358656
9	C	-5.301828	-0.049576	0.238924	C	-5.273187	-0.047912	0.284754
10	C	-4.842774	-0.072288	-1.056209	C	-4.830662	-0.073979	-1.036683
11	N	-3.487480	-0.061997	-1.208928	N	-3.496377	-0.064876	-1.228661
12	C	2.861356	0.033226	0.458474	C	2.836284	0.033439	0.436850
13	N	3.674479	0.015212	-0.578133	N	3.686683	0.016254	-0.595994
14	C	4.982025	0.037177	-0.190652	C	4.966670	0.037198	-0.173607
15	C	5.206725	0.073036	1.164672	C	5.170529	0.071765	1.204812
16	S	3.707956	0.079506	2.000065	S	3.668427	0.078617	2.028716
17	H	-1.417168	0.038487	2.285629	H	-1.417392	0.037315	2.269813

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Table 13 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
18	H	1.023719	0.064897	2.500412	H	1.026650	0.065454	2.484896
19	H	1.426869	-0.033671	-1.789479	H	1.431569	-0.032385	-1.831680
20	H	-1.062713	-0.061462	-2.008508	H	-1.059880	-0.061078	-2.050931
21	H	-6.326386	-0.052226	0.599135	H	-6.296706	-0.049838	0.649159
22	H	-5.481558	-0.097229	-1.938646	H	-5.499902	-0.100711	-1.897678
23	H	5.765782	0.025780	-0.947607	H	5.776613	0.026609	-0.904222
24	H	6.152251	0.095386	1.698472	H	6.114356	0.092614	1.742532

Table 14
Molecular system 13: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-1.313758	0.626750	0.798389	C	-1.327445	0.622112	0.839584
2	C	-0.352808	0.001701	-0.005838	C	-0.367024	-0.017944	0.023927
3	C	-0.891623	-0.836055	-1.023356	C	-0.869412	-0.825515	-1.042338
4	C	-2.324990	-1.017791	-1.126520	C	-2.270515	-0.990006	-1.182160
5	C	-3.195626	-0.366193	-0.181087	C	-3.141365	-0.365265	-0.231577
6	N	-2.646377	0.453792	0.726414	N	-2.641959	0.475062	0.720831
7	C	-4.645200	-0.435971	-0.184168	C	-4.583517	-0.460610	-0.173050
8	N	-5.442018	-1.526462	-0.519779	N	-5.415739	-1.498200	-0.596232
9	C	-6.756332	-1.158086	-0.408325	C	-6.709649	-1.131846	-0.371471
10	C	-6.827423	0.172749	-0.016094	C	-6.747668	0.151023	0.176577
11	C	-5.505227	0.621880	0.142609	C	-5.420198	0.562582	0.324647
12	C	-5.028683	-2.905673	-0.740944	C	-5.041060	-2.870316	-0.927320
13	N	-2.686019	-1.765417	-2.190490	N	-2.639677	-1.717292	-2.290838
14	S	-1.308684	-2.202293	-2.933792	S	-1.207581	-2.149688	-3.019034
15	N	-0.199114	-1.479341	-1.987187	N	-0.101406	-1.420863	-1.984861
16	C	1.062386	0.245155	0.198305	C	1.026201	0.219465	0.235473
17	N	1.529682	1.027585	1.159129	N	1.512101	0.964445	1.241315
18	C	2.882510	1.087320	1.134311	C	2.847012	1.020227	1.198627
19	C	3.527232	0.351850	0.149886	C	3.486812	0.323202	0.154161
20	S	2.323398	-0.464132	-0.797228	S	2.274555	-0.444085	-0.823703
21	C	4.959185	0.236455	-0.116458	C	4.904620	0.228700	-0.113987
22	C	5.445613	-0.168138	-1.375438	C	5.393964	-0.447956	-1.258005
23	C	6.814225	-0.267001	-1.617073	C	6.757245	-0.534544	-1.508949
24	C	7.732865	0.041061	-0.610622	C	7.676412	0.050291	-0.629669
25	C	7.266056	0.443266	0.644086	C	7.213374	0.723317	0.507196
26	C	5.898705	0.534914	0.891877	C	5.851555	0.812929	0.764595
27	H	-0.964019	1.315505	1.571001	H	-0.977114	1.298487	1.623337
28	H	-7.543421	-1.883583	-0.591277	H	-7.516416	-1.825033	-0.592639
29	H	-7.738802	0.742828	0.134241	H	-7.645008	0.708908	0.425374
30	H	-5.164556	1.609798	0.434083	H	-5.046099	1.506371	0.705540
31	H	-5.861324	-3.564184	-0.465563	H	-5.942316	-3.393828	-1.267461
32	H	-4.169848	-3.148596	-0.102976	H	-4.647107	-3.382527	-0.036755
33	H	-4.746295	-3.077482	-1.786306	H	-4.279798	-2.869004	-1.715688
34	H	3.396427	1.718677	1.859353	H	3.372938	1.599200	1.958507
35	H	4.738749	-0.391176	-2.177480	H	4.687723	-0.903280	-1.954726
36	H	7.165664	-0.581081	-2.601523	H	7.109700	-1.060006	-2.397759
37	H	8.804513	-0.034975	-0.800904	H	8.746741	-0.018052	-0.829088
38	H	7.973747	0.677358	1.441451	H	7.923535	1.179862	1.198386
39	H	5.549920	0.820236	1.885503	H	5.512311	1.334931	1.659442

Table 15
System 14, cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-0.977609	1.095324	0.893178	C	-0.885036	1.438666	0.932032
2	C	0.388825	1.260922	1.037848	C	0.500509	1.516072	1.015497
3	C	1.319817	0.409126	0.401619	C	1.381260	0.524913	0.442320
4	C	0.773512	-0.614399	-0.385581	C	0.726900	-0.521170	-0.251602
5	C	-0.609448	-0.785235	-0.535341	C	-0.658267	-0.574477	-0.327776
6	C	-1.542300	0.066600	0.101371	C	-1.520299	0.372422	0.272172
7	C	-3.008995	0.016474	0.044278	C	-2.966491	0.191945	0.171523
8	S	-4.005297	-1.124984	-0.847279	S	-3.770528	0.134459	-1.511874
9	C	-5.406617	-0.338532	-0.261295	C	-5.237221	-0.225092	-0.773106
10	C	-5.059245	0.714798	0.554222	C	-5.105569	-0.211911	0.612488
11	N	-3.727095	0.905909	0.718796	N	-3.838298	-0.012995	1.104227
12	C	-0.821795	-1.948358	-1.426167	C	-1.033025	-1.708946	-1.134234
13	O	0.410618	-2.448856	-1.789322	O	0.065905	-2.386860	-1.532398
14	C	1.460808	-1.679376	-1.187372	C	1.248034	-1.705177	-1.012770
15	O	-1.842157	-2.460060	-1.832928	O	-2.173661	-2.066930	-1.487473
16	C	2.745164	0.653162	0.605983	C	2.795894	0.661791	0.593795
17	N	3.209660	1.634058	1.356756	N	3.373496	1.700150	1.218094
18	C	4.570546	1.648527	1.385123	C	4.721059	1.593551	1.204638
19	C	5.199539	0.670990	0.650842	C	5.259461	0.484352	0.584626
20	S	4.026615	-0.316663	-0.114079	S	3.986863	-0.511276	-0.027747
21	H	-1.663880	1.772091	1.400110	H	-1.489342	2.215425	1.404188
22	H	0.777519	2.068466	1.658464	H	0.967961	2.342502	1.548663
23	H	-6.399746	-0.681928	-0.538839	H	-6.135758	-0.453644	-1.340167
24	H	-5.762419	1.378909	1.056393	H	-5.932015	-0.344625	1.309837
25	H	2.077910	-2.354277	-0.570186	H	1.801139	-2.425554	-0.390748
26	H	2.098791	-1.272153	-1.990116	H	1.874113	-1.440816	-1.878632
27	H	5.086279	2.409729	1.969774	H	5.322757	2.373094	1.674331
28	H	6.262436	0.487180	0.524875	H	6.301596	0.207574	0.461223

Table 16
Molecular system 15: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	N	-0.823572	1.042664	-0.451684	N	-0.823852	1.100034	-0.479630
2	C	0.524513	1.083143	-0.451241	C	0.505997	1.133076	-0.475666
3	C	1.385368	0.075505	-0.003189	C	1.346378	0.091774	-0.011907
4	C	0.725036	-1.091961	0.492542	C	0.710214	-1.091370	0.492306
5	C	-0.719837	-1.150341	0.497922	C	-0.698412	-1.139329	0.493204
6	C	-1.475298	-0.028221	0.002750	C	-1.434268	-0.014650	-0.004255
7	C	-2.919801	-0.027371	-0.016923	C	-2.868552	-0.014006	-0.023047
8	C	-3.878559	-0.946891	0.369532	C	-3.820273	-0.952567	0.371421
9	C	-5.142672	-0.358167	0.097015	C	-5.084762	-0.383694	0.109201
10	C	-4.878759	0.876526	-0.435534	C	-4.838282	0.862041	-0.427159
11	O	-3.541353	1.096343	-0.512938	O	-3.512455	1.104966	-0.515779
12	N	-1.206162	-2.307346	0.990906	N	-1.243510	-2.301657	0.989411
13	S	0.086889	-3.205105	1.396208	S	0.085596	-3.221219	1.406825
14	N	1.304374	-2.208985	0.982615	N	1.344422	-2.194985	0.979815
15	C	2.820421	0.204835	-0.038985	C	2.764076	0.223948	-0.048393
16	O	3.328826	1.384467	-0.545368	O	3.303216	1.398783	-0.551680
17	C	4.687691	1.293863	-0.485249	C	4.651210	1.276158	-0.477546
18	C	5.067883	0.091805	0.044075	C	5.009657	0.056198	0.059354
19	C	3.866189	-0.615551	0.334055	C	3.808236	-0.624001	0.336864

(*continued on next page*)

Table 16 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
20	H	0.958044	2.005272	-0.844971	H	0.961947	2.046673	-0.865728
21	H	-3.675586	-1.922533	0.795946	H	-3.574770	-1.921048	0.793902
22	H	-6.123117	-0.789831	0.271262	H	-6.060406	-0.824563	0.287763
23	H	-5.508045	1.683937	-0.794773	H	-5.487001	1.657920	-0.779877
24	H	5.232188	2.156778	-0.852833	H	5.222908	2.125132	-0.838675
25	H	6.086304	-0.246328	0.206754	H	6.023384	-0.293306	0.227449
26	H	3.762245	-1.605397	0.763602	H	3.652510	-1.609200	0.763323

Table 17
Molecular system 16: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	1.500535	-0.982169	-0.958001	C	1.529904	-1.227541	-0.860956
2	C	2.878516	-1.041800	-0.788120	C	2.891059	-1.218769	-0.649396
3	C	3.477606	-0.304885	0.247737	C	3.476862	-0.293758	0.255533
4	N	2.748634	0.448027	1.093096	N	2.682900	0.602053	0.915858
5	C	1.427426	0.485133	0.926105	C	1.382370	0.582321	0.702850
6	C	0.726027	-0.198954	-0.088198	C	0.689973	-0.303311	-0.173387
7	C	-0.736945	-0.094238	-0.216338	C	-0.742121	-0.279054	-0.343183
8	C	-1.415180	1.113310	0.049438	C	-1.558535	0.761753	0.213853
9	N	-2.734875	1.276530	-0.031216	N	-2.854597	0.785905	0.053070
10	C	-3.486108	0.224042	-0.406461	C	-3.560191	-0.151785	-0.639301
11	C	-2.911324	-1.021387	-0.712246	C	-2.846975	-1.214689	-1.211681
12	C	-1.534442	-1.179855	-0.610410	C	-1.471061	-1.270894	-1.065049
13	C	-4.960053	0.430559	-0.477711	C	-4.952637	0.177452	-0.641545
14	N	-5.499929	1.281559	0.415177	N	-5.186021	1.322552	0.049755
15	C	-6.821010	1.478814	0.370461	C	-6.366461	1.876018	0.216565
16	C	-7.673093	0.859922	-0.549058	C	-7.507863	1.273198	-0.336981
17	C	-7.110771	-0.015820	-1.476689	C	-7.329908	0.089582	-1.059593
18	C	-5.735777	-0.236504	-1.441608	C	-6.063497	-0.465394	-1.220340
19	C	4.953827	-0.319929	0.449816	C	4.918962	-0.249784	0.507859
20	C	5.706193	-1.476909	0.183068	C	5.778511	-1.300610	0.096551
21	C	7.084147	-1.451490	0.386014	C	7.140492	-1.215867	0.346078
22	C	7.672510	-0.274002	0.845318	C	7.642793	-0.088522	1.007034
23	C	6.842444	0.825243	1.084621	C	6.723113	0.894909	1.389525
24	N	5.518906	0.816564	0.899320	N	5.412131	0.837948	1.160184
25	H	1.026972	-1.515125	-1.785264	H	1.114151	-1.925665	-1.589226
26	H	3.490985	-1.622113	-1.479666	H	3.516968	-1.908923	-1.215992
27	H	0.871927	1.078193	1.660448	H	0.817326	1.316494	1.290353
28	H	-0.841408	2.006158	0.320066	H	-1.126912	1.581842	0.788470
29	H	-3.541344	-1.868879	-0.986118	H	-3.376738	-1.990907	-1.766669
30	H	-1.079340	-2.153780	-0.802974	H	-0.935120	-2.111866	-1.503258
31	H	-7.224710	2.172238	1.115661	H	-6.408292	2.801221	0.794971
32	H	-8.744536	1.064699	-0.536484	H	-8.485460	1.728188	-0.194038
33	H	-7.731494	-0.513686	-2.223890	H	-8.193478	-0.406652	-1.505546
34	H	-5.263740	-0.896643	-2.170781	H	-5.916589	-1.384671	-1.786272
35	H	5.214086	-2.391284	-0.151614	H	5.376625	-2.189285	-0.391109
36	H	7.687111	-2.341538	0.196984	H	7.805996	-2.025150	0.038051
37	H	8.747281	-0.204968	1.019080	H	8.705505	0.023710	1.225123
38	H	7.266990	1.768291	1.444514	H	7.072862	1.791277	1.915913

Table 18
Molecular system 17: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-4.005228	-1.567560	2.506646	C	-3.926558	-1.415904	2.532926
2	C	-2.988091	-1.360100	1.556514	C	-2.928527	-1.077528	1.624999
3	C	-3.254288	-0.789772	0.312453	C	-3.241037	-0.608471	0.320323
4	C	-4.595010	-0.356971	0.012830	C	-4.631510	-0.350446	-0.001512
5	C	-5.631147	-0.606118	0.980178	C	-5.645219	-0.751169	0.936944
6	C	-5.307562	-1.219109	2.217864	C	-5.273018	-1.292875	2.189717
7	C	-6.963675	-0.210452	0.687259	C	-7.011216	-0.551094	0.606882
8	C	-7.274625	0.433233	-0.490676	C	-7.384678	0.066543	-0.578340
9	C	-6.250637	0.728148	-1.418085	C	-6.395560	0.530095	-1.456848
10	C	-4.947605	0.343752	-1.171236	C	-5.045570	0.331342	-1.165041
11	C	-2.166133	-0.680476	-0.650104	C	-2.179696	-0.450809	-0.621401
12	O	-0.900415	-0.532045	-0.126963	O	-0.889927	-0.405955	-0.091200
13	C	-0.002038	-0.543958	-1.167424	C	-0.002291	-0.335886	-1.129322
14	C	-0.689361	-0.705768	-2.352563	C	-0.707206	-0.364276	-2.338648
15	C	-2.065954	-0.789236	-2.023728	C	-2.070532	-0.437580	-2.013633
16	C	1.397286	-0.383256	-0.838909	C	1.399383	-0.251799	-0.807854
17	C	1.843917	-0.152372	0.474397	C	1.876451	-0.179256	0.526501
18	C	3.204347	-0.012704	0.715175	C	3.234478	-0.110131	0.752076
19	C	4.113580	-0.097266	-0.353197	C	4.149027	-0.114279	-0.340449
20	N	3.695664	-0.309973	-1.618485	N	3.685799	-0.170557	-1.627526
21	C	2.393309	-0.449191	-1.839156	C	2.379956	-0.235741	-1.827245
22	C	5.577975	0.051532	-0.135945	C	5.597486	-0.045346	-0.140845
23	C	6.176671	-0.375234	1.063246	C	6.185126	-0.231054	1.137864
24	C	7.550345	-0.218509	1.230465	C	7.561518	-0.151079	1.283834
25	C	8.290319	0.359313	0.199526	C	8.350547	0.115238	0.153765
26	C	7.609262	0.748649	-0.957650	C	7.688834	0.273174	-1.072370
27	N	6.292807	0.603969	-1.135693	N	6.371659	0.198229	-1.240552
28	H	-3.757426	-2.029421	3.463815	H	-3.648561	-1.804673	3.513788
29	H	-1.970823	-1.681794	1.780895	H	-1.882183	-1.226758	1.887225
30	H	-6.107509	-1.401504	2.938866	H	-6.054244	-1.582746	2.895093
31	H	-7.740327	-0.418825	1.426920	H	-7.770848	-0.882401	1.318353
32	H	-8.302770	0.733648	-0.699466	H	-8.440098	0.214162	-0.811325
33	H	-6.488768	1.275108	-2.332122	H	-6.676719	1.062895	-2.366306
34	H	-4.167576	0.611340	-1.882541	H	-4.294557	0.754611	-1.830289
35	H	-0.254682	-0.759305	-3.345642	H	-0.271751	-0.344526	-3.331482
36	H	-2.886214	-0.964721	-2.711284	H	-2.890764	-0.535822	-2.716635
37	H	1.124283	-0.070327	1.289440	H	1.174161	-0.157696	1.360953
38	H	3.557910	0.193106	1.726506	H	3.598662	-0.021826	1.775260
39	H	2.105640	-0.632880	-2.879930	H	2.065401	-0.287123	-2.877542
40	H	5.577738	-0.849656	1.841921	H	5.568827	-0.463404	2.007241
41	H	8.036403	-0.552623	2.149001	H	8.019807	-0.302029	2.263348
42	H	9.368459	0.503098	0.283405	H	9.436820	0.189711	0.216149
43	H	8.154791	1.206493	-1.789660	H	8.271170	0.474504	-1.980013

Table 19
Molecular system 18: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-3.825101	-2.323832	1.456824	C	-3.742356	-2.115609	1.573717
2	C	-2.738797	-1.770763	0.754849	C	-2.683519	-1.524447	0.879347
3	C	-2.931038	-0.897819	-0.316650	C	-2.908527	-0.747789	-0.276909
4	C	-4.271357	-0.508576	-0.673612	C	-4.268849	-0.480840	-0.686143
5	C	-5.372549	-1.110052	0.031493	C	-5.338861	-1.131234	0.019692

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Table 19 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
6	C	-5.119211	-2.021195	1.088730	C	-5.049166	-1.951605	1.138668
7	C	-6.701606	-0.760439	-0.328093	C	-6.678561	-0.910499	-0.391205
8	C	-6.953853	0.166481	-1.316003	C	-6.975227	-0.051806	-1.433208
9	C	-5.874991	0.801435	-1.970164	C	-5.934308	0.638515	-2.081590
10	C	-4.571100	0.472449	-1.655716	C	-4.613680	0.431091	-1.711144
11	C	-1.759743	-0.439433	-1.048662	C	-1.758924	-0.294877	-1.011174
12	O	-0.579971	-0.419542	-0.343217	O	-0.567522	-0.320363	-0.315640
13	C	0.427995	-0.061412	-1.200642	C	0.438112	0.017020	-1.164139
14	C	-0.104466	0.143410	-2.461589	C	-0.095247	0.258962	-2.430717
15	C	-1.495144	-0.094956	-2.363577	C	-1.484687	0.064994	-2.330145
16	C	1.769698	0.046546	-0.685033	C	1.789494	0.071567	-0.644722
17	C	2.217324	-0.515376	0.553614	C	2.218994	-0.567912	0.552315
18	C	3.601371	-0.352668	0.953471	C	3.585997	-0.426559	0.933078
19	C	4.511868	0.362821	0.100239	C	4.471790	0.347973	0.106424
20	N	4.048609	0.869180	-1.047869	N	4.031586	0.953633	-1.019464
21	C	2.761499	0.724435	-1.404734	C	2.747354	0.804976	-1.360811
22	C	5.909701	0.572650	0.404488	C	5.868706	0.530305	0.401297
23	C	6.674319	0.178306	1.496514	C	6.651159	0.049291	1.449690
24	C	8.022218	0.593613	1.402528	C	7.994456	0.466064	1.362420
25	C	8.276005	1.298698	0.244337	C	8.229742	1.260014	0.253072
26	S	6.880061	1.462773	-0.738411	S	6.823237	1.506132	-0.690557
27	N	3.888624	-0.936992	2.135375	N	3.936068	-1.082531	2.073108
28	S	2.505405	-1.620236	2.645961	S	2.532515	-1.816870	2.582781
29	N	1.490134	-1.229371	1.440114	N	1.464836	-1.339520	1.389289
30	H	-3.633634	-3.013576	2.280542	H	-3.529006	-2.729937	2.449513
31	H	-1.720593	-2.045841	1.031913	H	-1.655954	-1.693275	1.203966
32	H	-5.967771	-2.468415	1.611251	H	-5.875026	-2.435826	1.664021
33	H	-7.525600	-1.236850	0.208382	H	-7.478322	-1.424353	0.146739
34	H	-7.980667	0.426797	-1.578357	H	-8.011002	0.110663	-1.734637
35	H	-6.072540	1.567784	-2.721884	H	-6.166158	1.354239	-2.871841
36	H	-3.755408	1.002025	-2.145346	H	-3.831393	1.016747	-2.190893
37	H	0.448586	0.402755	-3.358841	H	0.465791	0.508801	-3.324782
38	H	-2.210526	-0.081425	-3.178407	H	-2.198097	0.106322	-3.145881
39	H	2.490629	1.203618	-2.349923	H	2.442915	1.328439	-2.272872
40	H	6.257118	-0.390001	2.324524	H	6.227969	-0.578485	2.231038
41	H	8.779363	0.383235	2.156777	H	8.766037	0.198533	2.083306
42	H	9.219030	1.731390	-0.079907	H	9.171525	1.711689	-0.049716

Table 20
Molecular system 19: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-3.468010	-3.140455	-0.487757	C	-3.487389	-2.353251	-1.628337
2	C	-2.468696	-2.247243	-0.061297	C	-2.481362	-1.650484	-0.974622
3	C	-2.784848	-0.980641	0.431549	C	-2.779585	-0.738443	0.071030
4	C	-4.161285	-0.556069	0.448933	C	-4.167298	-0.434333	0.360568
5	C	-5.173996	-1.493777	0.040937	C	-5.184955	-1.203955	-0.296046
6	C	-4.797972	-2.782968	-0.415890	C	-4.820133	-2.163596	-1.272668
7	C	-6.538998	-1.102485	0.078256	C	-6.548457	-0.955298	-0.002407
8	C	-6.907416	0.166998	0.467334	C	-6.914872	0.049332	0.876727
9	C	-5.912504	1.107669	0.813919	C	-5.923196	0.853691	1.461199
10	C	-4.577401	0.754575	0.803268	C	-4.577177	0.622477	1.199242
11	C	-1.701119	-0.151276	0.936797	C	-1.693458	-0.220488	0.829560

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Table 20 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
12	O	-0.458466	-0.398631	0.406507	O	-0.438233	-0.313455	0.266653
13	C	0.452328	0.394073	1.055640	C	0.474504	0.145846	1.170885
14	C	-0.208246	1.149534	2.010024	C	-0.194995	0.519525	2.337987
15	C	-1.576250	0.803585	1.933115	C	-1.555714	0.292904	2.133013
16	C	1.836974	0.323237	0.665728	C	1.885278	0.157824	0.793648
17	C	2.411987	-0.723988	-0.124435	C	2.713354	-0.958464	1.079156
18	C	3.829673	-0.692955	-0.437226	C	4.112830	-0.885706	0.697047
19	C	4.631656	0.387416	0.061702	C	4.582286	0.298143	0.050626
20	N	4.056047	1.343169	0.795261	N	3.742984	1.346571	-0.201908
21	C	2.742670	1.313608	1.069592	C	2.468823	1.266172	0.157861
22	C	6.059292	0.527243	-0.172526	C	5.946282	0.499219	-0.385173
23	N	6.838818	-0.282392	-0.858166	N	6.970425	-0.325385	-0.280489
24	C	8.123942	0.168714	-0.862443	C	8.098360	0.227019	-0.811784
25	C	8.348908	1.341091	-0.173468	C	7.965189	1.491306	-1.337799
26	S	6.891202	1.917894	0.517724	S	6.342667	2.038321	-1.167555
27	N	4.237491	-1.742550	-1.181236	N	4.811758	-1.996604	1.016800
28	S	2.917744	-2.651480	-1.424122	S	3.737243	-3.025522	1.742911
29	N	1.779176	-1.804103	-0.630985	N	2.339940	-2.101890	1.677293
30	H	-3.181656	-4.127638	-0.854166	H	-3.224000	-3.076357	-2.400142
31	H	-1.422626	-2.553932	-0.089804	H	-1.436722	-1.841357	-1.214615
32	H	-5.581061	-3.481390	-0.719442	H	-5.608098	-2.736212	-1.765553
33	H	-7.295127	-1.831424	-0.222774	H	-7.308682	-1.561629	-0.498536
34	H	-7.960187	0.453613	0.487355	H	-7.967431	0.234947	1.092103
35	H	-6.199636	2.126450	1.080332	H	-6.208452	1.679378	2.114121
36	H	-3.826255	1.507576	1.036156	H	-3.833811	1.302145	1.612384
37	H	0.246598	1.847114	2.706186	H	0.292152	0.885910	3.234573
38	H	-2.369771	1.163809	2.578289	H	-2.354728	0.413272	2.856677
39	H	2.374581	2.160216	1.655604	H	1.851764	2.143107	-0.068710
40	H	8.889091	-0.398413	-1.392166	H	9.027915	-0.343101	-0.795349
41	H	9.285910	1.876533	-0.046528	H	8.727556	2.108730	-1.804592

Table 21
Molecular system 20: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-6.710991	-0.056046	-0.663057	C	-6.285444	-0.255531	-0.929375
2	N	-5.377489	-0.084082	-0.745309	N	-5.017255	-0.133704	-0.580385
3	C	-4.671908	0.220494	0.360615	C	-4.619408	0.375634	0.606233
4	C	-5.292786	0.553008	1.577428	C	-5.585061	0.800573	1.524235
5	C	-6.683878	0.573488	1.646142	C	-6.932387	0.684006	1.181369
6	C	-7.416275	0.264972	0.500665	C	-7.301147	0.152543	-0.054542
7	C	-3.187185	0.185897	0.245867	C	-3.172932	0.376858	0.687997
8	N	-2.655151	-0.717114	-0.599719	N	-2.643589	-0.128922	-0.439780
9	C	-1.330474	-0.765049	-0.728306	C	-1.360640	-0.269426	-0.690835
10	C	-0.428199	0.071997	-0.035179	C	-0.388721	0.128770	0.274959
11	C	-1.000527	1.014689	0.835745	C	-0.921043	0.664419	1.468958
12	C	-2.380563	1.069877	0.982401	C	-2.290891	0.791325	1.683372
13	C	1.027923	-0.046112	-0.186136	C	1.046198	-0.019566	0.009151
14	C	1.684074	-0.395472	-1.405132	C	1.578649	-0.550570	-1.204806
15	C	3.127707	-0.475357	-1.443883	C	3.012087	-0.635261	-1.342206
16	C	3.894983	-0.205529	-0.259013	C	3.860003	-0.199136	-0.284756
17	N	3.244980	0.108631	0.863652	N	3.324177	0.299513	0.865286
18	C	1.896565	0.175034	0.883981	C	2.002528	0.371239	0.972528
19	C	5.345685	-0.253749	-0.206092	C	5.302037	-0.252311	-0.351953
20	S	6.366557	-0.625710	-1.567409	S	6.194215	-0.850424	-1.728267

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Table 21 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
21	C	7.785794	-0.455342	-0.622240	C	7.697595	-0.546647	-0.954776
22	C	7.503935	-0.126780	0.688507	C	7.537518	-0.009162	0.307483
23	C	6.119021	-0.012210	0.925065	C	6.180820	0.158101	0.650171
24	N	3.617478	-0.797816	-2.657315	N	3.432771	-1.146692	-2.523190
25	S	2.327054	-0.969288	-3.630366	S	2.059929	-1.491342	-3.384557
26	N	1.109679	-0.653785	-2.602023	N	0.900934	-1.000725	-2.284363
27	H	-7.250360	-0.303250	-1.583500	H	-6.492512	-0.680825	-1.912862
28	H	-4.693296	0.764952	2.463985	H	-5.279438	1.212990	2.485290
29	H	-7.187284	0.817539	2.583433	H	-7.699556	1.010725	1.884652
30	H	-8.507186	0.267918	0.504510	H	-8.343761	0.049893	-0.349369
31	H	-0.944919	-1.521340	-1.416374	H	-1.047444	-0.691799	-1.647446
32	H	-0.365929	1.726231	1.367582	H	-0.248602	0.995188	2.258197
33	H	-2.831597	1.823164	1.629873	H	-2.672183	1.208976	2.615829
34	H	1.469535	0.409185	1.863931	H	1.661119	0.782623	1.927592
35	H	8.759223	-0.607170	-1.081660	H	8.626025	-0.780297	-1.469853
36	H	8.269661	0.024569	1.447959	H	8.370205	0.253466	0.959307
37	H	5.661314	0.236634	1.880433	H	5.810373	0.562580	1.589774

Table 22
Molecular system 21: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	4.601892	-0.201461	-2.296752	C	4.556453	-0.188128	-2.330427
2	C	4.013346	-0.309822	-0.992876	C	4.001105	-0.215719	-1.005083
3	C	4.775098	-0.791396	0.064155	C	4.828813	-0.548927	0.070982
4	C	6.096912	-1.241205	-0.125963	C	6.160174	-0.950318	-0.118096
5	C	6.668500	-1.194766	-1.379469	C	6.696701	-0.987541	-1.391927
6	C	5.951039	-0.665555	-2.482959	C	5.924990	-0.591917	-2.513014
7	C	6.551633	-0.558076	-3.765971	C	6.496550	-0.555591	-3.811903
8	C	5.874356	0.009778	-4.822773	C	5.768944	-0.106055	-4.895615
9	C	4.564359	0.506169	-4.632148	C	4.441936	0.334546	-4.711717
10	C	3.946856	0.402692	-3.403038	C	3.851338	0.295148	-3.461578
11	C	2.615014	0.082054	-0.694549	C	2.594626	0.097981	-0.677992
12	C	1.481186	-0.434152	-1.407716	C	1.470036	-0.432676	-1.392109
13	C	0.143579	-0.044524	-1.017221	C	0.154750	-0.050497	-1.000286
14	C	-0.035544	0.852026	0.083346	C	0.008307	0.835343	0.100629
15	C	1.150948	1.240278	0.713389	C	1.179765	1.221988	0.767310
16	N	2.402966	0.876205	0.351847	N	2.425639	0.871345	0.412942
17	C	-1.331982	1.298720	0.521333	C	-1.294083	1.269137	0.554789
18	C	-2.624459	1.051368	0.098944	C	-2.586790	0.927531	0.175482
19	C	-3.481084	1.789808	0.950241	C	-3.455475	1.665661	1.000758
20	C	-2.681429	2.460315	1.856063	C	-2.672088	2.442590	1.849956
21	O	-1.365659	2.162717	1.595243	O	-1.346021	2.195328	1.568193
22	C	-3.016321	3.324589	2.981418	C	-3.032795	3.367497	2.896051
23	C	-4.201342	3.044958	3.660962	C	-4.329200	3.235705	3.429975
24	C	-4.629168	3.816453	4.756770	C	-4.792777	4.045495	4.469089
25	C	-3.862551	4.873634	5.197950	C	-3.966348	5.012829	5.017861
26	C	-2.652236	5.211888	4.540032	C	-2.658467	5.211651	4.513039
27	C	-2.213222	4.444304	3.403592	C	-2.170149	4.402948	3.425706
28	C	-1.027613	4.861355	2.740045	C	-0.881646	4.701421	2.914543
29	C	-0.300956	5.947438	3.185554	C	-0.101218	5.706700	3.463847
30	C	-0.717280	6.677400	4.320730	C	-0.568333	6.469064	4.551032
31	C	-1.872770	6.315802	4.977650	C	-1.828896	6.225823	5.059023
32	N	-0.822415	-0.628127	-1.758155	N	-0.857498	-0.611240	-1.724200
33	S	-0.048361	-1.586746	-2.822655	S	-0.067735	-1.593244	-2.828142

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Table 22 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
34	N	1.501246	-1.323427	-2.425690	N	1.520964	-1.324987	-2.425784
35	H	4.321751	-0.833225	1.055424	H	4.400329	-0.517806	1.072731
36	H	6.658746	-1.634332	0.722983	H	6.764286	-1.240337	0.743206
37	H	7.689134	-1.550113	-1.539784	H	7.730457	-1.303436	-1.551451
38	H	7.572872	-0.924831	-3.894083	H	7.533416	-0.877642	-3.934071
39	H	6.349886	0.090700	-5.801757	H	6.220728	-0.079497	-5.888702
40	H	4.039202	0.979444	-5.463781	H	3.872171	0.708235	-5.564153
41	H	2.941912	0.803078	-3.274116	H	2.826587	0.639002	-3.342038
42	H	1.095062	1.899980	1.582190	H	1.104431	1.852080	1.657960
43	H	-2.897707	0.413891	-0.734362	H	-2.819081	0.224912	-0.617106
44	H	-4.563059	1.852493	0.892166	H	-4.540324	1.662588	0.962552
45	H	-4.792622	2.181562	3.352195	H	-4.975164	2.445752	3.046633
46	H	-5.558565	3.556631	5.266033	H	-5.800201	3.895160	4.859559
47	H	-4.175217	5.468270	6.059196	H	-4.313312	5.638700	5.842621
48	H	-0.686558	4.316601	1.862428	H	-0.495334	4.137429	2.070081
49	H	0.603543	6.245160	2.652173	H	0.885091	5.907625	3.042740
50	H	-0.129823	7.529310	4.667312	H	0.056953	7.253574	4.979803
51	H	-2.216884	6.880556	5.847328	H	-2.216397	6.820640	5.889175

Table 23
Molecular system 22: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	4.408430	-3.318783	-1.248569	C	4.414145	-2.982796	-1.577326
2	C	5.756830	-3.786021	-1.406420	C	5.745181	-3.507119	-1.753085
3	C	6.823675	-3.020216	-0.867358	C	6.731700	-3.185435	-0.802526
4	C	5.312005	-1.464492	-0.084117	C	5.257966	-1.919904	0.428242
5	C	4.180480	-2.100285	-0.545081	C	4.189669	-2.163675	-0.444732
6	H	7.850094	-3.354599	-0.979421	H	7.747665	-3.572115	-0.922835
7	H	5.208624	-0.538507	0.470006	H	5.097245	-1.291724	1.311650
8	C	2.838141	-1.527513	-0.338333	C	2.849494	-1.572643	-0.214657
9	C	1.794992	-2.250685	0.310667	C	1.805748	-2.272663	0.471723
10	C	2.526765	-0.247418	-0.734025	C	2.520201	-0.303224	-0.664701
11	C	0.484968	-1.665953	0.505041	C	0.481204	-1.711444	0.655496
12	C	1.249085	0.325950	-0.552414	C	1.247082	0.270603	-0.465749
13	H	3.281075	0.341131	-1.241576	H	3.276230	0.263172	-1.207912
14	C	0.193541	-0.335223	0.051160	C	0.194330	-0.389548	0.175331
15	H	1.088240	1.324463	-0.938148	H	1.067907	1.268264	-0.874609
16	C	-1.101839	0.296411	0.236228	C	-1.088131	0.257931	0.335436
17	C	-2.388403	-0.216075	0.308402	C	-2.393129	-0.253127	0.523524
18	C	-2.920260	2.099332	0.470607	C	-2.905762	2.081719	0.464503
19	C	-3.372572	0.802037	0.428182	C	-3.364086	0.772448	0.578664
20	C	-3.132798	-1.448578	0.247334	C	-3.120732	-1.479713	0.616239
21	C	-4.431960	-1.094767	0.339850	C	-4.437073	-1.112026	0.723368
22	H	-2.749766	-2.449395	0.172566	H	-2.722798	-2.486340	0.628533
23	H	-5.337051	-1.678847	0.347367	H	-5.350504	-1.689105	0.823683
24	S	4.341359	-5.326135	-2.507577	S	4.394065	-4.295539	-3.594477
25	S	0.479057	-3.822550	1.508444	S	0.507723	-3.864851	1.667873
26	N	5.851179	-4.928550	-2.102538	N	5.897183	-4.278959	-2.868245
27	N	3.508147	-4.112083	-1.846323	N	3.516201	-3.327519	-2.526395
28	N	6.595782	-1.899871	-0.237725	N	6.497376	-2.407090	0.272829
29	N	1.906022	-3.472563	0.845809	N	1.933315	-3.501337	1.015024
30	N	-0.344034	-2.474531	1.174620	N	-0.359733	-2.522313	1.327387

(*continued on next page*)

Table 23 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
31	S	-1.185032	2.036937	0.354799	S	-1.161233	2.008767	0.288428
32	O	-4.620322	0.263717	0.453316	O	-4.612819	0.250660	0.704059
33	C	-3.656239	3.350455	0.598811	C	-3.632155	3.331732	0.485379
34	C	-3.015687	4.599465	0.575676	C	-2.985876	4.575018	0.315709
35	N	-4.987066	3.243107	0.740118	N	-4.968834	3.223451	0.678698
36	C	-3.776257	5.748097	0.705588	C	-3.750818	5.735449	0.349112
37	H	-1.942065	4.666512	0.455284	H	-1.907093	4.627972	0.158238
38	C	-5.702525	4.355985	0.860606	C	-5.681506	4.347718	0.705758
39	C	-5.153774	5.633522	0.851702	C	-5.127122	5.626761	0.547879
40	H	-3.300190	6.720882	0.691000	H	-3.279407	6.710406	0.220822
41	H	-6.774223	4.220590	0.971283	H	-6.757406	4.228213	0.862692
42	H	-5.786428	6.505046	0.955163	H	-5.765413	6.509927	0.580971

Table 24
Molecular system 23: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-2.556131	-1.174558	-0.008077	C	-2.265043	-0.909331	-1.152906
2	C	-1.150948	-1.404143	0.231080	C	-0.838073	-1.022159	-0.930411
3	C	-0.212581	-0.337805	0.028465	C	-0.235825	-0.079901	-0.081033
4	C	-1.990166	1.035667	-0.601236	C	-2.216853	1.005121	0.314197
5	C	-3.002837	0.107769	-0.438400	C	-2.981849	0.131759	-0.491644
6	H	-2.238155	2.029603	-0.957355	H	-2.714206	1.849428	0.798998
7	N	-0.678049	0.833937	-0.380548	N	-0.899394	0.926837	0.522482
8	N	-0.885969	-2.643986	0.645718	N	-0.230405	-2.052594	-1.576325
9	N	-3.303967	-2.258101	0.242853	N	-2.759459	-1.859217	-1.976447
10	S	-2.296315	-3.425629	0.721235	S	-1.461704	-2.808137	-2.416091
11	C	1.214170	-0.427473	0.234420	C	1.225110	-0.124762	0.206081
12	C	2.093225	-1.423864	0.646222	C	1.915172	-0.761635	1.223204
13	C	3.460692	-1.003251	0.694626	C	3.325799	-0.579935	1.233698
14	C	3.624727	0.324444	0.315381	C	3.742877	0.245766	0.154462
15	C	3.685292	-3.186874	1.378394	C	3.017642	-1.931118	3.076926
16	C	4.352028	-2.040416	1.119760	C	3.951923	-1.258282	2.304674
17	H	4.105897	-4.123322	1.713090	H	3.219875	-2.533453	3.960033
18	H	5.417353	-1.905944	1.216280	H	5.021589	-1.255657	2.498880
19	S	2.107534	1.035654	-0.092218	S	2.353354	0.733627	-0.789707
20	S	1.959609	-3.094232	1.130307	S	1.396530	-1.765166	2.538872
21	C	-4.412811	0.446892	-0.693380	C	-4.434932	0.330062	-0.619674
22	C	-4.926466	1.705149	-0.364770	C	-5.194332	0.890914	0.424111
23	C	-5.298001	-0.457767	-1.299477	C	-5.144303	-0.010279	-1.793981
24	C	-6.248946	2.001036	-0.653873	C	-6.559936	1.098317	0.254210
25	H	-4.300502	2.435400	0.133085	H	-4.717404	1.139593	1.374005
26	N	-6.568023	-0.181899	-1.580090	N	-6.456943	0.187883	-1.970720
27	H	-4.953884	-1.447378	-1.573375	H	-4.608556	-0.471380	-2.625371
28	C	-7.031682	1.026660	-1.260880	C	-7.146569	0.735701	-0.959151
29	H	-6.671299	2.965429	-0.402443	H	-7.165943	1.524692	1.055971
30	H	-8.073018	1.221169	-1.496775	H	-8.218132	0.884036	-1.127299
31	C	4.860524	1.064899	0.250087	C	5.062746	0.643430	-0.154895
32	S	4.937900	2.739019	-0.269825	S	5.447936	1.680053	-1.540526
33	C	7.024237	1.486328	0.413017	C	7.259700	0.811817	0.024984
34	C	6.636673	2.716810	-0.029277	C	7.092260	1.597258	-1.111763
35	H	8.043432	1.207624	0.641036	H	8.224144	0.610601	0.490358
36	H	7.244552	3.585465	-0.220710	H	7.855086	2.110282	-1.690698
37	N	6.031905	0.567687	0.567654	N	6.138116	0.285829	0.552498

Table 25
Molecular system 24: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	4.873905	-0.655688	-0.101052	C	4.898684	-0.683838	-0.059567
2	C	6.279343	-0.912075	0.109558	C	6.312620	-0.909377	0.129589
3	C	6.905976	-0.527526	1.331581	C	6.967259	-0.484726	1.304645
4	C	6.146887	0.080136	2.275607	C	6.187967	0.154950	2.261756
5	C	4.749133	0.324367	2.077632	C	4.804656	0.356991	2.094572
6	C	4.099986	-0.018333	0.927970	C	4.105624	-0.042932	0.940484
7	C	4.596749	-1.113373	-1.360009	C	4.609331	-1.168315	-1.332609
8	C	6.726375	-1.507537	-1.036092	C	6.756312	-1.532925	-1.033088
9	H	7.958547	-0.718762	1.494006	H	8.033996	-0.648055	1.453530
10	H	6.590940	0.380919	3.215372	H	6.653559	0.496749	3.187189
11	H	4.183823	0.774375	2.884049	H	4.241930	0.821959	2.903968
12	H	3.714007	-1.135335	-1.972841	H	3.707067	-1.199049	-1.933411
13	H	7.682782	-1.879261	-1.358469	H	7.720819	-1.900697	-1.366602
14	O	5.712958	-1.624507	-1.910351	O	5.725626	-1.685102	-1.907631
15	C	2.676957	0.265511	0.762565	C	2.683592	0.216136	0.794367
16	C	1.973208	1.337157	1.236213	C	1.978974	1.300723	1.277079
17	N	0.638015	1.346010	0.984400	N	0.648958	1.348056	1.002013
18	H	2.421726	2.164891	1.767104	H	2.437180	2.130130	1.818079
19	C	0.280226	0.293714	0.308745	C	0.255184	0.289927	0.314991
20	S	1.583243	-0.785687	-0.057720	S	1.568177	-0.834907	-0.047518
21	C	-1.083655	0.025744	-0.099658	C	-1.097781	0.018841	-0.100541
22	C	-1.564305	-1.031249	-0.831309	C	-1.578107	-1.031938	-0.860188
23	S	-2.328265	1.113005	0.353741	S	-2.380258	1.101833	0.369574
24	C	-2.957152	-0.960582	-1.029027	C	-2.977092	-0.972711	-1.062970
25	H	-0.938145	-1.827506	-1.210116	H	-0.943903	-1.823943	-1.262748
26	C	-3.513338	0.150764	-0.441844	C	-3.551217	0.132616	-0.454508
27	H	-3.533638	-1.689925	-1.575334	H	-3.570972	-1.689382	-1.625594
28	C	-4.900082	0.592331	-0.402031	C	-4.956390	0.576953	-0.414156
29	C	-5.970323	-0.128825	-1.036883	C	-6.002182	-0.123014	-1.061096
30	C	-7.302346	0.382331	-0.935468	C	-7.339945	0.399543	-0.954196
31	C	-6.440647	2.170518	0.335463	C	-6.436268	2.179561	0.378342
32	C	-7.535440	1.579386	-0.217748	C	-7.544732	1.583711	-0.210456
33	H	-6.541357	3.090188	0.898690	H	-6.550106	3.097340	0.961861
34	H	-8.528767	1.991673	-0.120250	H	-8.542818	2.010670	-0.105848
35	N	-5.168173	1.695928	0.247500	N	-5.179663	1.700340	0.285713
36	N	-5.899384	-1.259966	-1.741213	N	-5.902667	-1.271068	-1.799354
37	N	-8.200016	-0.380559	-1.567165	N	-8.285398	-0.325426	-1.600006
38	S	-7.389752	-1.602256	-2.205619	S	-7.458013	-1.589623	-2.285666

Table 26
Molecular system 25: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	3.284342	0.376354	-0.816108	C	3.317200	-0.065229	-0.915416
2	C	2.653923	-0.874152	-0.891077	C	2.630311	-1.277593	-0.953714
3	C	1.321429	-0.988514	-0.555282	C	1.285443	-1.298852	-0.593638
4	H	3.191347	-1.757110	-1.205463	H	3.144279	-2.189307	-1.261000
5	C	1.324840	1.345472	-0.097749	C	1.370850	1.064615	-0.180041
6	C	0.603834	0.140976	-0.141427	C	0.607581	-0.131474	-0.194302
7	H	0.816226	-1.942593	-0.605556	H	0.710498	-2.224796	-0.608974
8	H	0.840459	2.260065	0.213348	H	0.925192	2.014377	0.116000
9	C	-0.820127	0.006349	0.217823	C	-0.819002	-0.173309	0.184910
10	C	-1.677116	1.082591	0.633600	C	-1.568587	0.956119	0.596723

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Table 26 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
11	C	-3.056791	0.808097	0.959194	C	-2.950859	0.771605	0.938462
12	C	-2.635269	-1.452053	0.454016	C	-2.666354	-1.560614	0.431479
13	C	-3.572854	-0.519796	0.871856	C	-3.533532	-0.528552	0.858249
14	H	-2.930323	-2.489736	0.350964	H	-3.053954	-2.579845	0.349053
15	S	-2.696920	3.144821	1.255472	S	-2.453699	3.121454	1.236085
16	N	-1.369461	2.380356	0.768922	N	-1.135060	2.248409	0.717282
17	N	-3.733659	1.906907	1.326932	N	-3.592408	1.906470	1.321585
18	N	-1.350075	-1.202011	0.150382	N	-1.386321	-1.398977	0.112998
19	N	2.606762	1.457785	-0.420373	N	2.641727	1.031463	-0.529992
20	C	4.724011	0.563713	-1.168716	C	4.690925	0.283001	-1.221442
21	C	5.516917	-0.498435	-1.623710	C	5.758166	-0.508681	-1.656494
22	N	5.228946	1.795974	-1.031881	N	4.888290	1.605325	-1.028660
23	C	6.847778	-0.270596	-1.937645	C	6.995504	0.097201	-1.876999
24	H	5.109432	-1.492311	-1.737032	H	5.613805	-1.576629	-1.816524
25	C	6.503856	2.003687	-1.335100	C	6.048473	2.204333	-1.229591
26	C	7.362586	1.009240	-1.792752	C	7.157022	1.466541	-1.665432
27	H	7.471028	-1.082996	-2.290981	H	7.839508	-0.504767	-2.216460
28	H	6.863545	3.020611	-1.206562	H	6.093797	3.278374	-1.041797
29	H	8.395090	1.235339	-2.025326	H	8.109928	1.966254	-1.828938
30	C	-4.938917	-0.871283	1.185063	C	-4.912075	-0.781293	1.189412
31	C	-5.588119	-2.103139	1.169998	C	-5.682152	-1.956708	1.185178
32	N	-5.873415	0.060720	1.580877	N	-5.747505	0.237209	1.606498
33	C	-6.924287	-1.892183	1.562042	C	-6.984752	-1.616549	1.606295
34	H	-5.143845	-3.048428	0.906110	H	-5.331325	-2.945633	0.907002
35	C	-7.070739	-0.541648	1.810942	C	-6.994637	-0.246622	1.860875
36	H	-5.659210	1.041574	1.680119	H	-5.390993	1.196740	1.684890
37	H	-7.696052	-2.638269	1.654340	H	-7.831098	-2.287891	1.715873
38	H	-7.929170	0.024623	2.130741	H	-7.794185	0.403830	2.200568

Table 27
Molecular system 26: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	0.508377	-0.126563	0.644344	C	0.490607	0.081645	0.738669
2	C	1.948117	0.008690	0.722265	C	1.946120	0.121897	0.764147
3	C	2.684257	0.678307	-0.300517	C	2.671495	0.683499	-0.323438
4	C	0.524430	1.050621	-1.414376	C	0.501801	1.079401	-1.430796
5	C	-0.235382	0.396609	-0.462352	C	-0.272919	0.560042	-0.387523
6	H	0.034518	1.489720	-2.272560	H	0.001611	1.428621	-2.333290
7	N	2.456142	-0.517823	1.845490	N	2.474327	-0.377364	1.907286
8	N	-0.009259	-0.757172	1.703855	N	-0.034086	-0.434703	1.865566
9	S	1.219747	-1.121111	2.684943	S	1.202473	-0.829101	2.830019
10	C	-8.149375	-0.975000	0.970105	C	-8.070450	-1.395727	0.758609
11	C	-7.100002	-1.663465	1.629151	C	-6.983925	-1.969880	1.454250
12	C	-5.739342	-1.409971	1.242071	C	-5.652018	-1.520098	1.151405
13	C	-6.599294	0.140386	-0.326750	C	-6.658459	-0.031954	-0.439379
14	C	-5.471471	-0.467824	0.201038	C	-5.484082	-0.516201	0.161184
15	H	-6.482721	0.899773	-1.090007	H	-6.587017	0.752561	-1.198096
16	S	-5.715466	-3.028838	2.978751	S	-5.477761	-3.203800	2.861177
17	N	-7.216653	-2.569007	2.611524	N	-7.051219	-2.934949	2.410891
18	N	-4.857343	-2.135000	1.942669	N	-4.674958	-2.123113	1.867073
19	N	-7.887108	-0.106773	0.028547	N	-7.912191	-0.442604	-0.168225

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Table 27 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
20	C	1.928219	1.183957	-1.334641	C	1.907429	1.164448	-1.380563
21	H	2.434638	1.702049	-2.139564	H	2.421105	1.601951	-2.240710
22	H	-9.184406	-1.156584	1.239518	H	-9.091289	-1.727654	0.970153
23	C	-4.137405	-0.151138	-0.289132	C	-4.172441	0.005055	-0.227601
24	C	-3.820416	0.407580	-1.512107	C	-3.887195	0.946153	-1.217402
25	S	-2.699557	-0.406932	0.645837	S	-2.713146	-0.503089	0.560868
26	C	-2.449352	0.639437	-1.679807	C	-2.519188	1.227731	-1.343805
27	H	-4.554126	0.618447	-2.276871	H	-4.654020	1.414320	-1.831033
28	C	-1.682175	0.267113	-0.590286	C	-1.719590	0.521983	-0.449689
29	H	-2.033809	1.051873	-2.587419	H	-2.125927	1.950097	-2.059551
30	C	4.149674	0.875661	-0.248841	C	4.146291	0.822267	-0.330359
31	C	5.069437	-0.226396	-0.175575	C	5.034509	-0.260892	-0.082089
32	C	4.669457	2.144054	-0.310217	C	4.748463	2.055925	-0.627811
33	C	6.494129	0.035816	-0.151182	C	6.461744	-0.082995	-0.132104
34	C	4.801009	-1.584377	-0.160136	C	4.697482	-1.593965	0.210908
35	C	6.069917	2.397169	-0.280224	C	6.141517	2.225755	-0.698849
36	H	3.990896	2.986983	-0.357590	H	4.100691	2.914714	-0.805420
37	C	6.968993	1.376451	-0.197872	C	7.017653	1.174360	-0.445891
38	C	7.238259	-1.131237	-0.102321	C	7.144318	-1.280506	0.142180
39	H	3.843882	-2.076833	-0.164958	H	3.701218	-2.010917	0.316771
40	H	6.414151	3.423329	-0.316830	H	6.541791	3.209852	-0.945995
41	H	8.034101	1.571183	-0.171847	H	8.097718	1.313886	-0.489936
42	H	8.310896	-1.233914	-0.077353	H	8.219944	-1.434944	0.181883
43	S	6.231415	-2.499250	-0.098770	S	6.071576	-2.581706	0.436511

Table 28
Molecular system 27: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-6.505023	3.334368	2.605318	C	-6.560963	3.709026	2.008821
2	C	-5.846273	4.287232	1.792166	C	-5.366409	4.183173	2.580756
3	C	-4.601278	3.945331	1.149491	C	-4.108825	3.642872	2.121709
4	C	-4.823070	1.820857	2.171706	C	-5.431399	2.269677	0.617667
5	C	-4.049821	2.635225	1.349187	C	-4.171156	2.654476	1.105820
6	H	-4.491298	0.809572	2.376349	H	-5.489370	1.507488	-0.167271
7	S	-5.150908	6.187664	0.565307	S	-3.601217	5.270507	3.819059
8	N	-6.259685	5.535984	1.534283	N	-5.241893	5.127397	3.556246
9	N	-4.112749	4.957653	0.421900	N	-3.006492	4.145107	2.712779
10	N	-5.990708	2.144146	2.775066	N	-6.598117	2.767944	1.041785
11	C	-0.812409	0.603351	0.224963	C	-0.895980	0.561606	0.103420
12	C	-0.795101	1.839908	-0.369142	C	-1.037480	1.662795	-0.751885
13	C	-1.871587	2.721556	-0.090764	C	-2.149715	2.494883	-0.519732
14	C	-2.804556	2.157802	0.774790	C	-2.938560	2.068965	0.550662
15	C	-0.407303	3.667141	-1.487066	C	-0.960187	3.273164	-2.233481
16	C	-1.571342	3.912075	-0.851151	C	-2.073607	3.540946	-1.502653
17	H	0.187397	4.266960	-2.155350	H	-0.485467	3.768623	-3.073229
18	H	-2.148437	4.815025	-0.903795	H	-2.750125	4.378024	-1.636697
19	S	-2.260068	0.540827	1.188826	S	-2.250651	0.635581	1.231394
20	O	0.101770	2.415031	-1.221407	O	-0.298704	2.119411	-1.795574
21	H	-7.440872	3.577199	3.096493	H	-7.520812	4.106483	2.350067
22	C	0.120322	-0.504617	0.147014	C	0.088786	-0.463676	0.143823
23	C	1.286811	-0.425024	-0.634666	C	1.167361	-0.488747	-0.800479
24	C	-0.076151	-1.710694	0.836239	C	0.074883	-1.511253	1.100389
25	N	2.177272	-1.398592	-0.747387	N	2.116157	-1.405606	-0.828112

(*continued on next page*)

Table 28 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
26	H	1.500962	0.478082	-1.193202	H	1.230210	0.294644	-1.559637
27	C	0.845256	-2.728804	0.724164	C	1.061368	-2.471602	1.077582
28	H	-0.951089	-1.850760	1.459449	H	-0.713911	-1.554142	1.852728
29	C	1.979932	-2.550902	-0.082910	C	2.083462	-2.404385	0.098289
30	H	0.689436	-3.657201	1.257908	H	1.052902	-3.277579	1.813602
31	C	2.998386	-3.578493	-0.251986	C	3.146027	-3.368548	0.010529
32	C	4.145647	-3.532582	-1.000432	C	4.208670	-3.424772	-0.884662
33	C	4.840307	-2.547369	-1.897648	C	4.721381	-2.630072	-2.045059
34	C	4.922297	-4.727786	-0.937500	C	5.071984	-4.528982	-0.670126
35	C	4.370247	-5.691039	-0.140102	C	4.674124	-5.331356	0.396985
36	C	6.071810	-3.320261	-2.318412	C	5.950276	-3.405800	-2.447155
37	H	5.086163	-1.615740	-1.378645	H	4.947698	-1.585502	-1.771084
38	H	4.218877	-2.252044	-2.748739	H	3.981757	-2.551986	-2.860115
39	C	6.105966	-4.547005	-1.771076	C	6.140857	-4.490796	-1.652979
40	H	6.821163	-2.911232	-2.982639	H	6.590963	-3.111079	-3.277097
41	H	6.880977	-5.285896	-1.918948	H	6.951974	-5.211823	-1.732649
42	S	2.888450	-5.136207	0.540946	S	3.249325	-4.731589	1.130870
43	H	4.730281	-6.680742	0.091399	H	5.140875	-6.233495	0.784695

Table 29
Molecular system 28: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-3.956467	1.291876	1.668732	C	-3.919214	1.301850	1.646445
2	C	-4.523958	2.573672	2.004362	C	-4.482314	2.586503	1.983515
3	C	-5.866342	2.625553	2.532473	C	-5.829024	2.637587	2.516321
4	C	-5.947261	0.274283	2.356469	C	-5.909875	0.267944	2.331855
5	C	-6.592417	1.428885	2.709557	C	-6.556136	1.440162	2.692122
6	H	-6.444574	-0.683094	2.466126	H	-6.420732	-0.692234	2.444197
7	S	-5.054095	4.852912	2.415541	S	-5.014094	4.873662	2.400239
8	N	-3.963437	3.782041	1.894434	N	-3.908119	3.798067	1.868419
9	N	-6.277704	3.872363	2.804430	N	-6.249292	3.891975	2.795538
10	N	-4.690243	0.207387	1.859978	N	-4.658804	0.193571	1.835176
11	C	0.259520	-1.248232	-0.214863	C	0.241415	-1.302209	-0.212565
12	C	0.027292	-2.609127	-0.259641	C	-0.003366	-2.678612	-0.240413
13	C	2.081154	-2.665843	-1.059005	C	2.051243	-2.736192	-1.047108
14	N	1.031539	-3.382091	-0.724456	N	0.984598	-3.468660	-0.696554
15	H	-0.896923	-3.077231	0.050393	H	-0.941033	-3.134221	0.084562
16	S	1.870061	-0.949707	-0.806444	S	1.864222	-1.006717	-0.819064
17	C	-2.627296	1.070623	1.128123	C	-2.606038	1.072104	1.112521
18	C	-1.568396	1.880394	0.780320	C	-1.521988	1.868922	0.760649
19	C	-0.447041	1.161732	0.276038	C	-0.419205	1.131873	0.263717
20	C	-0.629334	-0.209099	0.229341	C	-0.634305	-0.270880	0.221804
21	C	0.173250	3.355035	0.216071	C	0.242744	3.311664	0.200519
22	C	0.604604	2.113155	-0.059604	C	0.653179	2.043031	-0.073745
23	H	0.740604	4.263577	0.068494	H	0.833519	4.214155	0.050887
24	H	1.573581	1.861824	-0.464393	H	1.623453	1.762499	-0.478314
25	S	-2.218063	-0.609114	0.822762	S	-2.233231	-0.636163	0.813444
26	H	-7.598908	1.432997	3.102363	H	-7.569968	1.444621	3.089855
27	C	-1.228915	3.349411	0.770455	C	-1.156298	3.326898	0.748439
28	H	-1.282233	3.795153	1.766920	H	-1.213136	3.783907	1.750369
29	H	-1.919930	3.931779	0.155708	H	-1.845024	3.928799	0.132421
30	C	3.284772	-3.243923	-1.583616	C	3.256544	-3.285162	-1.566734
31	C	4.475223	-2.631518	-1.980426	C	4.413251	-2.608613	-1.957236
32	C	5.457235	-3.571064	-2.457419	C	5.429591	-3.495086	-2.433458

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Table 29 (*continued*)

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
33	C	4.998719	-4.875438	-2.415412	C	4.992725	-4.835819	-2.383626
34	C	5.912284	-0.939270	-2.359814	C	5.788669	-0.858858	-2.336442
35	H	5.525731	-5.767612	-2.711522	H	5.567184	-5.708770	-2.686393
36	C	6.888795	-1.872567	-2.834018	C	6.783060	-1.731177	-2.802773
37	H	6.152133	0.119579	-2.342454	H	5.993316	0.216704	-2.319517
38	H	7.854191	-1.504116	-3.168578	H	7.738924	-1.319785	-3.138593
39	N	4.728134	-1.298284	-1.939753	N	4.571594	-1.242197	-1.896196
40	N	6.682818	-3.160150	-2.888344	N	6.646926	-3.078277	-2.870873
41	S	3.411895	-4.946746	-1.809328	S	3.415039	-5.006866	-1.783409

Table 30
Molecular system 29: Cartesian coordinates of the optimized molecular structure at ground and excited states.

	Ground state geometry				Excited state geometry			
No.	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-0.240416	2.508444	-0.344980	C	-0.675430	2.348670	-0.191083
2	C	-0.128482	1.158070	-0.850330	C	-0.532998	0.975084	-0.643622
3	C	-0.125421	0.038085	0.041499	C	0.011562	-0.006016	0.227834
4	C	-0.435161	1.646250	1.868311	C	0.235863	1.736835	1.929324
5	C	-0.368883	2.752763	1.054611	C	-0.248685	2.751550	1.115384
6	H	-0.566594	1.796440	2.931808	H	0.520232	2.002054	2.947424
7	N	-0.109191	1.101331	-2.186456	N	-1.002675	0.743185	-1.888935
8	N	-0.298669	3.424653	-1.320234	N	-1.293518	3.121387	-1.110512
9	S	-0.211538	2.619613	-2.715478	S	-1.593826	2.185773	-2.389740
10	C	-0.480871	4.108781	1.632082	C	-0.355889	4.136351	1.637708
11	C	0.426464	5.167273	1.295626	C	0.086216	5.268046	0.908903
12	C	0.248183	6.458770	1.901605	C	-0.033588	6.569844	1.536876
13	C	-1.575282	5.546157	3.096799	C	-0.936266	5.442500	3.459672
14	C	-0.805857	6.642786	2.823612	C	-0.576356	6.637671	2.837181
15	H	-2.386852	5.614079	3.812086	H	-1.342768	5.462903	4.476070
16	S	2.164062	6.570261	0.512630	S	0.992303	6.900804	-0.612945
17	N	1.497978	5.104594	0.494805	N	0.674697	5.292160	-0.316159
18	N	1.173583	7.353222	1.522091	N	0.425687	7.599905	0.792263
19	N	-1.422021	4.318860	2.524375	N	-0.822468	4.224917	2.907053
20	C	-0.305704	0.326870	1.379261	C	0.363769	0.392598	1.505927
21	H	-0.313498	-0.486469	2.094119	H	0.768742	-0.341104	2.206683
22	C	-0.793570	-5.173125	-0.693588	C	-0.918750	-5.065349	-0.985483
23	C	-1.571991	-5.806254	0.241447	C	-2.178368	-5.535863	-0.564351
24	C	-1.755135	-7.140572	-0.216544	C	-2.267586	-6.872041	-0.971606
25	H	-1.948331	-5.374158	1.153920	H	-2.925837	-4.957361	-0.030486
26	C	-1.077466	-7.232757	-1.389898	C	-1.076028	-7.158817	-1.615444
27	H	-2.308515	-7.927775	0.267430	H	-3.095514	-7.556719	-0.822493
28	C	0.940669	-1.881196	-1.325016	C	1.225169	-2.000419	-0.958145
29	C	2.752407	-1.920774	-2.666584	C	3.248437	-2.100062	-1.939750
30	C	0.766461	-3.298757	-1.525398	C	0.984144	-3.365461	-1.306298
31	C	0.013913	-1.329173	-0.443929	C	0.149731	-1.390394	-0.251426
32	C	2.564051	-3.322299	-2.885528	C	3.006040	-3.459506	-2.290922
33	H	3.587362	-1.414938	-3.143213	H	4.192162	-1.623935	-2.219199
34	C	-0.298388	-3.827829	-0.788208	C	-0.293876	-3.814874	-0.857225
35	H	3.251752	-3.857673	-3.533907	H	3.766369	-4.020972	-2.841811
36	S	-1.052147	-2.565126	0.100816	S	-1.113178	-2.509981	-0.039875
37	H	-0.977662	7.598505	3.298562	H	-0.687006	7.596531	3.344878
38	N	1.973890	-1.207920	-1.902691	N	2.373309	-1.363381	-1.275501
39	N	1.605839	-4.008056	-2.326498	N	1.891604	-4.108068	-1.984027
40	O	-0.490191	-6.049371	-1.695975	O	-0.254708	-6.085075	-1.632303
41	H	-0.918778	-8.031583	-2.093041	H	-0.690718	-8.053369	-2.093842

Table 31
Molecular system 30: Cartesian coordinates of the optimized molecular structure at ground and excited states.

No.	Ground state geometry				Excited state geometry			
	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-2.781485	-1.002420	0.612715	C	-2.784046	-0.968408	1.104864
2	C	-1.341359	-0.998580	0.596308	C	-1.336281	-0.951501	1.049794
3	C	-0.644452	0.137375	0.076082	C	-0.678780	0.046363	0.267662
4	C	-2.692336	1.164178	-0.320703	C	-2.723504	1.023284	-0.263836
5	C	-3.499595	0.125783	0.113557	C	-3.483422	0.036966	0.389237
6	H	-3.153440	2.061756	-0.717232	H	-3.238094	1.844114	-0.777005
7	S	-2.038781	-3.005801	1.643750	S	-2.006538	-2.746786	2.515860
8	N	-3.293478	-2.100894	1.181391	N	-3.321606	-1.934186	1.870672
9	N	-0.807450	-2.084862	1.168969	N	-0.766288	-1.897474	1.830714
10	N	-1.339907	1.177636	-0.330432	N	-1.395636	1.041981	-0.328018
11	C	0.828009	0.229360	0.031754	C	0.776990	0.136628	0.127974
12	C	1.662125	-0.801329	-0.493765	C	1.644846	-0.987420	-0.071769
13	C	1.466160	1.364168	0.472092	C	1.402902	1.381601	0.143984
14	C	3.102726	-0.653710	-0.503838	C	3.091000	-0.816511	-0.149657
15	C	2.873207	1.503613	0.468208	C	2.800121	1.542151	0.068671
16	H	0.863761	2.177154	0.855754	H	0.770692	2.263230	0.255249
17	C	3.729523	0.528795	0.004006	C	3.693054	0.479915	-0.056411
18	H	3.291958	2.413662	0.878344	H	3.203782	2.552828	0.156995
19	N	1.250131	-1.935063	-1.074815	N	1.250362	-2.257863	-0.291881
20	N	3.723290	-1.695129	-1.076957	N	3.748172	-1.974566	-0.388690
21	S	2.573802	-2.721801	-1.550853	S	2.603396	-3.123763	-0.521227
22	C	5.195274	0.717390	0.016578	C	5.151602	0.700463	-0.111424
23	C	6.068462	-0.327839	0.341876	C	6.062839	-0.209659	0.458668
24	C	5.744126	1.972667	-0.276308	C	5.673763	1.858484	-0.721198
25	C	7.439894	-0.117088	0.388390	C	7.434413	0.039731	0.432984
26	H	5.669234	-1.306841	0.564480	H	5.685727	-1.117667	0.927134
27	C	7.116055	2.179772	-0.236428	C	7.045462	2.104860	-0.748607
28	H	5.090044	2.786388	-0.563442	H	4.992028	2.561087	-1.204205
29	C	7.970355	1.135506	0.099818	C	7.934979	1.197306	-0.168107
30	H	8.097202	-0.936866	0.650998	H	8.118899	-0.678129	0.889445
31	H	7.518302	3.156210	-0.476885	H	7.422531	3.006164	-1.236160
32	H	9.041064	1.295054	0.130609	H	9.009616	1.387140	-0.190803
33	C	-4.952001	0.213763	0.088803	C	-4.949043	0.065914	0.384744
34	C	-5.935433	-0.734914	-0.123019	C	-5.864823	-0.503681	-0.474803
35	C	-7.268740	-0.201743	-0.164587	C	-7.241046	-0.286825	-0.171488
36	C	-7.293261	1.155409	0.049943	C	-7.387837	0.494686	0.983397
37	C	-7.691186	-2.423322	-0.629813	C	-7.382678	-1.592326	-2.083251
38	C	-8.253402	-1.208914	-0.451819	C	-8.103238	-0.916948	-1.101828
39	H	-8.198587	-3.349517	-0.853859	H	-7.793752	-2.159656	-2.915103
40	H	-9.315134	-1.020721	-0.522165	H	-9.191199	-0.892874	-1.072690
41	S	-5.952891	-2.452312	-0.436493	S	-5.686977	-1.484426	-1.902970
42	S	-5.716969	1.768460	0.281834	S	-5.868879	0.919422	1.637961
43	H	-8.144815	1.815568	0.087154	H	-8.313506	0.816352	1.455119

Table 32
Molecular system 31: Cartesian coordinates of the optimized molecular structure at ground and excited states.

No.	Ground state geometry				Excited state geometry			
	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-1.047881	-1.082317	-0.876364	C	-0.959303	-0.596600	-1.162635
2	C	-2.489665	-1.050486	-0.902082	C	-2.411133	-0.606461	-1.258894
3	C	-3.177153	-0.056219	-0.129495	C	-3.173759	-0.082329	-0.165510
4	C	-1.125168	0.796153	0.560718	C	-1.220758	0.422486	1.013062
5	C	-0.333556	-0.134817	-0.083814	C	-0.368671	-0.070107	0.011469
6	H	-0.656254	1.559253	1.172458	H	-0.789856	0.839357	1.930822
7	S	-1.774328	-2.734638	-2.405203	S	-1.503966	-1.552956	-3.291645

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Table 32 (*continued*)

No.	Ground state geometry				Excited state geometry			
	Atom	X	Y	Z	Atom	X	Y	Z
8	N	-0.524790	-2.001193	-1.696211	N	-0.297634	-1.090632	-2.223159
9	N	-3.014708	-1.952895	-1.743279	N	-2.850015	-1.130016	-2.428216
10	N	-2.475771	0.835831	0.536342	N	-2.543941	0.418859	0.938282
11	C	2.010234	-1.158743	0.258239	C	1.978543	-1.028239	0.680685
12	C	2.667245	-3.261532	0.743812	C	2.571833	-2.968748	1.660274
13	C	3.383745	-0.729292	0.294602	C	3.353682	-0.656242	0.596714
14	C	4.035595	-2.842015	0.740488	C	3.944079	-2.599277	1.569483
15	H	2.430794	-4.300616	0.954248	H	2.296981	-3.928009	2.107627
16	H	4.819630	-3.569231	0.929135	H	4.717499	-3.276055	1.944177
17	S	2.001063	1.350636	-0.168474	S	1.991666	1.281473	-0.432792
18	C	-4.654733	0.040857	-0.046202	C	-4.645341	-0.030660	-0.124729
19	C	-5.256110	1.275012	0.225027	C	-5.296865	0.495197	1.016742
20	C	-6.687041	-1.007395	-0.120812	C	-6.678655	-0.437776	-1.134569
21	C	-6.637016	1.338057	0.311539	C	-6.683479	0.539511	1.047360
22	H	-4.637153	2.149270	0.364879	H	-4.689808	0.853282	1.846837
23	C	-7.374846	0.173964	0.134628	C	-7.405332	0.063070	-0.052090
24	H	-7.226627	-1.939876	-0.254555	H	-7.202461	-0.821666	-2.017808
25	H	-7.130813	2.280808	0.513241	H	-7.201555	0.941644	1.921045
26	H	-8.455505	0.176330	0.194332	H	-8.496277	0.078090	-0.071861
27	C	1.118691	-0.119316	0.008631	C	1.090989	-0.049339	0.142527
28	C	3.550990	0.641997	0.080754	C	3.549979	0.620741	-0.001279
29	N	1.671007	-2.452324	0.514085	N	1.585007	-2.199065	1.226978
30	N	4.394219	-1.604799	0.531069	N	4.351391	-1.449768	1.047325
31	N	-5.362982	-1.080858	-0.213745	N	-5.345486	-0.490310	-1.185966
32	C	4.758656	1.425132	0.040948	C	4.758549	1.298624	-0.242304
33	C	4.870732	2.789251	-0.144058	C	4.932747	2.567579	-0.841581
34	S	6.340735	0.715631	0.223562	S	6.318986	0.611012	0.195739
35	C	6.204524	3.252004	-0.141227	C	6.269316	2.950610	-0.933892
36	H	4.015360	3.437886	-0.276716	H	4.094900	3.168209	-1.192702
37	C	7.105424	2.241174	0.046622	C	7.130487	1.988247	-0.410799
38	H	6.482850	4.288189	-0.271241	H	6.611875	3.889451	-1.364263
39	H	8.180603	2.311129	0.094116	H	8.215785	2.036811	-0.360455

Table 33
Molecular system 32: Cartesian coordinates of the optimized molecular structure at ground and excited states.

No.	Ground state geometry				Excited state geometry			
	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-2.528786	0.198152	-0.018322	C	-2.569932	0.177286	-0.577759
2	C	-1.099576	0.373502	0.040502	C	-1.142401	0.364750	-0.498409
3	C	-0.237589	-0.763876	-0.099596	C	-0.320754	-0.702608	-0.081046
4	C	-2.119697	-2.103476	-0.321725	C	-2.157729	-2.065300	0.177716
5	C	-3.071433	-1.104352	-0.218862	C	-3.104425	-1.102163	-0.244814
6	H	-2.448812	-3.129976	-0.438729	H	-2.523109	-3.045551	0.498363
7	S	-2.087952	2.516116	0.290582	S	-2.092753	2.445719	-1.261088
8	N	-3.194224	1.356580	0.110355	N	-3.241262	1.277057	-0.997010
9	N	-0.730624	1.646385	0.215475	N	-0.708484	1.600898	-0.856147
10	N	-0.779706	-1.951370	-0.271731	N	-0.837512	-1.902163	0.263634
11	C	-4.514198	-1.393864	-0.314342	C	-4.536378	-1.439535	-0.310986
12	C	-4.977407	-2.373840	-1.202901	C	-4.952709	-2.765654	-0.557485
13	C	-5.452133	-0.726000	0.483732	C	-5.539257	-0.465700	-0.121594
14	C	-6.327907	-2.683503	-1.282894	C	-6.303393	-3.106276	-0.593131
15	H	-4.275603	-2.879608	-1.853846	H	-4.204187	-3.535169	-0.752622
16	C	-6.801534	-1.041799	0.405823	C	-6.889757	-0.810588	-0.155021

(*continued on next page*)

Table 33 (*continued*)

No.	Ground state geometry				Excited state geometry			
	Atom	X	Y	Z	Atom	X	Y	Z
17	H	-5.120754	0.039418	1.170665	H	-5.243477	0.569172	0.043850
18	C	-7.246160	-2.020739	-0.476118	C	-7.282804	-2.130982	-0.387163
19	H	-6.664064	-3.436634	-1.984811	H	-6.593293	-4.139628	-0.795037
20	H	-7.508919	-0.520935	1.039369	H	-7.644157	-0.036169	-0.000124
21	H	-8.300304	-2.260569	-0.538875	H	-8.341303	-2.396050	-0.418835
22	C	1.220349	-0.668995	-0.063378	C	1.132845	-0.545859	-0.002375
23	C	3.588657	-0.019920	0.064898	C	3.435407	0.283948	-0.060686
24	C	3.310921	-1.361504	-0.133169	C	3.272718	-1.025475	0.332112
25	H	4.065394	-2.130945	-0.230416	H	4.085965	-1.698448	0.609733
26	N	2.012669	-1.704150	-0.202113	N	1.990768	-1.472185	0.367861
27	S	2.088965	0.837972	0.166905	S	1.892147	1.005630	-0.431477
28	C	4.868841	0.624451	0.177457	C	4.685627	1.016382	-0.186773
29	C	5.193288	1.945552	0.417380	C	5.361197	1.819966	0.709543
30	C	6.599790	2.216030	0.464545	C	6.588322	2.384826	0.253524
31	C	7.349407	1.083789	0.254850	C	6.871385	1.991895	-1.062314
32	C	5.743577	4.327906	0.856138	C	6.455898	3.224789	2.411362
33	C	6.875190	3.604202	0.719994	C	7.207572	3.190953	1.240423
34	H	5.664029	5.386464	1.051172	H	6.698894	3.765891	3.322965
35	H	7.867461	4.025232	0.796069	H	8.148408	3.725303	1.121350
36	S	6.349261	-0.283048	0.006433	S	5.650749	0.972166	-1.681549
37	S	4.267516	3.398732	0.686880	S	5.016069	2.305558	2.346197
38	H	8.422068	0.978622	0.232605	H	7.735105	2.263316	-1.665190

Table 34
Molecular system 33: Cartesian coordinates of the optimized molecular structure at ground and excited states.

No.	Ground state geometry				Excited state geometry			
	Atom	X	Y	Z	Atom	X	Y	Z
1	C	-0.001029	-0.850739	0.153016	C	0.008694	-0.794648	0.164930
2	C	0.820960	-1.992877	0.481033	C	0.789422	-1.924263	0.485352
3	C	2.244463	-1.826752	0.618386	C	2.231036	-1.768419	0.619282
4	C	1.963013	0.445280	0.122100	C	2.021839	0.494394	0.132595
5	C	0.585897	0.436271	-0.036146	C	0.633514	0.465007	-0.020389
6	H	2.504992	1.375641	-0.003378	H	2.557956	1.439443	0.000770
7	N	2.731366	-0.613621	0.427662	N	2.792480	-0.562612	0.436819
8	N	0.098010	-3.113853	0.620338	N	0.077196	-3.079921	0.638609
9	N	-1.304525	-1.154544	0.059251	N	-1.349309	-1.025922	0.055364
10	S	-1.442928	-2.737178	0.361213	S	-1.505745	-2.664022	0.371245
11	C	3.201867	-2.901982	0.957714	C	3.159878	-2.859818	0.949395
12	C	4.567393	-2.582959	1.046736	C	4.544067	-2.571512	1.035543
13	C	2.817010	-4.228875	1.199971	C	2.735253	-4.187589	1.186049
14	C	5.506160	-3.549236	1.366027	C	5.461108	-3.566850	1.343964
15	H	4.872095	-1.563461	0.860708	H	4.866217	-1.547256	0.852644
16	C	3.763930	-5.193902	1.520440	C	3.662358	-5.178793	1.495253
17	H	1.777756	-4.508939	1.139240	H	1.674401	-4.422244	1.122599
18	C	5.109998	-4.862515	1.606083	C	5.025210	-4.877424	1.575856
19	H	6.553002	-3.278002	1.428754	H	6.523722	-3.325333	1.405205
20	H	3.442972	-6.211910	1.704443	H	3.317886	-6.198561	1.675548
21	H	5.844396	-5.618043	1.856727	H	5.746671	-5.660180	1.818411
22	C	-0.172527	1.621522	-0.360747	C	-0.113538	1.659155	-0.350405
23	C	0.237500	2.936437	-0.574212	C	0.280319	3.001270	-0.578342
24	N	-1.537714	1.606039	-0.514528	N	-1.474575	1.603323	-0.497406
25	C	-0.902951	3.699868	-0.857519	C	-0.873777	3.727912	-0.861362

(*continued on next page*)

Table 34 (*continued*)

No.	Ground state geometry				Excited state geometry			
	Atom	X	Y	Z	Atom	X	Y	Z
26	H	1.250557	3.299545	-0.528314	H	1.294871	3.383839	-0.537720
27	C	-2.010302	2.854446	-0.817185	C	-1.980583	2.838826	-0.808809
28	H	-2.076260	0.759244	-0.413098	H	-1.944701	0.687775	-0.366487
29	H	-0.921984	4.755990	-1.067193	H	-0.926992	4.789038	-1.083198
30	C	-3.422248	3.131783	-1.032525	C	-3.385461	3.081713	-1.021550
31	C	-3.858459	4.428488	-1.356608	C	-3.855456	4.378534	-1.350274
32	C	-4.416626	2.151164	-0.932591	C	-4.360467	2.064918	-0.918571
33	N	-5.124414	4.764528	-1.566244	N	-5.132919	4.687671	-1.562383
34	H	-3.135953	5.232065	-1.449897	H	-3.143790	5.204100	-1.444212
35	C	-5.741682	2.493088	-1.150769	C	-5.694502	2.379807	-1.138640
36	H	-4.168140	1.126232	-0.685206	H	-4.078378	1.040628	-0.668647
37	C	-6.052100	3.810027	-1.464678	C	-6.037004	3.698229	-1.456886
38	H	-6.524646	1.749147	-1.077924	H	-6.467425	1.613527	-1.064795
39	H	-7.078848	4.112586	-1.641082	H	-7.079473	3.976257	-1.635355

Table 35
Electronic excitations giving rise the absorption spectra in OPV systems

System	Electronic transition (eV)				ΔEexc	Contribution (%)
1	HOMO -1	-5.52	LUMO +2	-2.13	3.39	68.4
2	HOMO	-4.44	LUMO +3	-1.34	3.10	68.4
3	HOMO	-4.76	LUMO +2	-0.83	3.93	46.6
4	HOMO	-4.59	LUMO +2	-1.75	2.84	63.6
5	HOMO	-4.68	LUMO +1	-2.00	2.68	92.4
6	HOMO	-5.42	LUMO +1	-1.90	3.52	90.9
7	HOMO	-5.56	LUMO +1	-2.09	3.47	66.4
8	HOMO	-5.26	LUMO +1	-2.66	2.60	80.0
9	HOMO	-5.41	LUMO	-3.30	2.11	92.8
10	HOMO	-5.16	LUMO +1	-2.47	2.69	55.2
11	HOMO	-4.89	LUMO	-3.77	1.12	91.0
12	HOMO	-5.38	LUMO	-2.84	2.54	96.8
13	HOMO	-4.97	LUMO +1	-2.38	2.59	84.7
14	HOMO	-5.63	LUMO	-3.18	2.45	93.8
15	HOMO	-5.05	LUMO +1	-2.02	3.03	73.6
16	HOMO -2	-5.84	LUMO	-2.74	3.10	41.1
17	HOMO	-4.99	LUMO	-2.70	2.29	92.4
18	HOMO	-4.86	LUMO +1	-2.44	2.42	78.0
19	HOMO	-4.99	LUMO +1	-2.50	2.49	81.9
20	HOMO	-5.41	LUMO +1	-2.47	2.94	87.3
21	HOMO	-4.99	LUMO +1	-2.49	2.50	80.6
22	HOMO -3	-6.20	LUMO +1	-3.34	2.86	44.5
23	HOMO	-5.01	LUMO	-3.68	1.33	93.2
24	HOMO	-5.01	LUMO +1	-2.72	2.29	80.4
25	HOMO	-5.09	LUMO +1	-2.45	2.64	88.8
26	HOMO -1	-5.33	LUMO	-3.60	1.73	83.5
27	HOMO	-4.94	LUMO +1	-2.74	2.20	81.4
28	HOMO	-4.92	LUMO	-3.62	1.30	92.8
29	HOMO	-5.01	LUMO +2	-3.05	1.96	52.7
30	HOMO	-5.03	LUMO	-3.51	1.52	96.7
31	HOMO	-5.04	LUMO	-3.53	1.51	71.9
32	HOMO	-4.98	LUMO +1	-2.56	2.42	79.3
33	HOMO	-4.99	LUMO +1	-2.27	2.72	90.2

Table 36
Dihedral angles $\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_2$ and $\boldsymbol{\theta}_3$ in degrees (°); $\boldsymbol{\lambda}$ maximum absorption wavelength in nm; Δ is the difference between ground and excited state values.

System	Ground State				Excited State				Δ Avg	Δλ Max
	θ_1	θ_2	θ_3	λ Max	θ_1	θ_2	θ_3	λ Max	Degree (°)	(nm)
1	49.7	42.9	-	337.3	40.2	41.0	-	422.5	5.7	85.2
2	43.2	37.8	40.7	375.3	35.8	15.2	76.7	336.3	2.0	-39.0
3	43.4	38.4	-	271.0	68.5	0.0	-	301.1	27.6	30.1
4	0.0	1.6	42.6	390.8	0.0	90.1	41.7	689.7	23.3	298.9
5	0.0	0.0	-	394.0	0.0	0.0	-	430.7	0.0	36.7
6	36.0	37.4	-	321.5	20.5	21.5	-	355.6	15.7	34.1
7	0.0	36.5	-	325.2	0.0	23.2	-	352.5	13.3	27.3
8	0.0	0.0	0.0	410.2	0.0	0.0	0.0	434.4	0.0	24.2
9	36.3	53.2	36.1	526.1	25.8	45.5	25.4	575.3	9.6	49.2
10	36.6	4.8	21.1	403.2	27.9	-	-	438.2	7.1	35.0
11	0.0	0.0	0.0	792.7	0.0	0.0	0.0	940.3	0.0	147.6
12	0.0	0.0	-	386.9	0.0	0.0	-	422.7	0.0	35.8
13	37.2	0.0	21.4	426.8	30.0	0.0	0.0	451.5	0.7	24.7
14	0.0	0.0	-	403.8	61.7	0.0	-	366.0	61.7	-37.8
15	0.0	0.0	-	347.0	0.0	0.0	-	366.4	0.0	19.4
16	33.9	36.8	33.8	356.4	13.7	8.3	0.0	419.2	23.8	62.8
17	35.9	0.0	31.9	455.7	24.3	0.0	12.1	512.7	15.7	57.0
18	32.6	16.4	0.0	457.5	26.1	19.8	0.0	476.6	6.6	19.1
19	32.4	15.2	0.0	446.3	25.5	91.8	0.0	415.0	34.9	-31.3
20	33.1	35.3	0.0	397.4	0.0	0.0	0.0	718.3	34.2	320.9
21	54.1	0.0	33.0	450.5	46.5	0.0	19.9	483.8	10.4	33.3
22	55.7	28.0	0.0	426.1	86.6	23.3	0.0	439.6	13.1	13.5
23	0.0	0.0	37.2	696.2	0.0	90.8	29.7	444.4	23.1	-251.8
24	35.0	0.0	0.0	481.5	34.6	0.0	0.0	540.6	0.4	59.1
25	0.0	0.0	0.0	432.2	0.0	0.0	0.0	442.4	0.0	10.2
26	21.1	6.1	57.6	630.5	0.0	18.6	51.5	736.7	6.8	106.2
27	2.5	0.2	0.2	478.4	88.8	0.0	0.0	479.3	88.8	0.9
28	0.0	0.0	0.0	756.0	0.0	0.0	0.0	500.8	0.0	-255.2
29	47.5	48.0	20.0	617.0	46.0	90.1	0.0	642.4	29.6	25.4
30	32.0	46.4	39.1	714.7	92.1	38.2	34.7	618.3	15.8	-96.4
31	26.6	47.5	0.0	694.4	0.0	91.5	0.0	475.6	54.5	-218.8
32	2.7	0.0	37.4	438.4	87.4	0.0	28.9	661.5	20.8	223.1
33	0.0	0.0	0.0	397.4	0.0	0.0	0.0	424.8	0.0	27.4

dihedral angle ϕ was evaluated by considering Eq. 1, in which ϕ stands for the dihedral angle in ground (θGrd) and excited (θExc) states.

$$cos\phi = \frac{|n_1 \cdot n_2|}{\|n_1\|\|n_2\|} \tag{1}$$

In Eq. 1, n_1 and n_2 represent normal vectors perpendicular to the planes 1 and 2, respectively (see Fig. 1 in [1]).

Ethics Statement

Not applicable.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi:10.1016/j.dib.2021.106952.

References

[1] C. Delesma, M. Robles, C. Amador-bedolla, J. Muñiz, The role of photoisomerization in the opto-electronic properties of organic photovoltaic materials: A DFT study, J. Photochem. Photobiol. A. 409 (2021) 113155, doi:10.1016/j.jphotochem.2021.113155.
[2] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77 (1996) 18, doi:10.1103/PhysRevLett.77.3865.
[3] F. Weigend, M. Häser, H. Patzelt, R. Ahlrichs, RI-MP2: optimized auxiliary basis sets and demonstration of efficiency, Chem. Phys. Lett. 294 (1998) 1, doi:10.1016/S0009-2614(98)00862-8.
[4] F. Weigend, R. Ahlrichs, Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: design and assessment of accuracy, Phys. Chem. Chem. Phys. 7 (2005) 18, doi:10.1039/B508541A.
[5] TURBOMOLE V7.3 2018, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.
[6] C. Steffen, K. Thomas, U. Huniar, A. Hellweg, O. Rubner, A. Schroer, TmoleX—A graphical user interface for TURBOMOLE, J. Comput. Chem. 31 (2010) 16, doi:10.1002/jcc.21576.
[7] G. Rossum, Python Reference Manual, CWI (Centre for Mathematics and Computer Science), 1995 Amsterdam, The Netherlands, The Netherlands.