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Data in Brief

Data Article

In silico geometric and energetic data of all possible simple rotamers made of non-metal elements

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A R T I C L E   I N F O

A B S T R A C T

This article presents theoretical data on geometric and energetic features of halogenated rotamers of the following backbone structures, C–C, N–N, P–P, O–O, S–S, N–P, O–S, C–N, C–P, C–O, C–S, N–O, N–S, P–O and P–S. The data is considered to be comprehensive combinations of non-metal elements in the form abcx–ydef whereby a,b,c,d,e,f are halogen (fluorine to iodine), hydrogen or a lone pair and x,y are carbon, nitrogen, phosphorus, oxygen and sulfur. Data were obtained from *ab initio* geometry optimization and frequency calculations at HF, B3LYP, MP2 and CCSD levels of theory on 6-311++G(d,p) basis set. In total, 8535 non-enantiomeric structures were produced by custom-made codes in Mathematica and Q-Chem quantum chemical package. Extracted geometric and energetic data as well as raw output files, codes and scripts associated with the data production are presented in the data repository.

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Specifications table

Subject	Chemistry
Specific subject area	Physical and theoretical chemistry/spectroscopy
Type of data	Tables and Q-Chem output files
How data were acquired	Quantum chemical computation on Q-Chem 5.2.1, developer version
Data format	Raw and analyzed
Parameters for data collection	Hartree-Fock (HF)/6-311++G(d,p),
	Becke, 3-parameter, Lee–Yang–Parr (B3LYP)/6-311++G(d,p),
	Second order Møller–Plesset perturbation theory (MP2)/6-311++G(d,p),
	Coupled Cluster Singles and Doubles (CCSD)/6-311++G(d,p)
Description of data collection	Data were obtained from ab initio geometry optimization and frequency calculations. In total, 8535 non-enantiomeric structures were produced and processed by custom-made codes.
Data source location	Mahidol University, Salaya, Thailand
	Latitude and longitude: 13.792790, 100.325707
Data accessibility	Repository name: mendeley.com
	Data identification number: DOI: 10.17632/m2h6yg9nzp
	Direct URL to data: https://data.mendeley.com/datasets/m2h6yg9nzp

Value of the data

- The origin of energetic preference for staggered structure in ethane [1-5] and gauche structure in 1,2-difluoroethane [6–11] has long been debated and sometimes controversial. The comprehensive data set presented in this article fills in the gap in the literature and can be used for further analysis and discussion in relevant topics such as gauche effect [7,8,12] and bent bond [7,13].
- Similar to cis effect where the *cis* or (*Z*) isomer is more stable than *trans* or (*E*) isomer [14] and relative stability of positional isomers of substituted benzenes [15], gauche effect is demonstrated in this data set by many examples where steric hindrance alone fails to account for the observed relative stability trend.
- For reference purpose, 15665 rotamers are identified with internal numbering, SMILES and PubChem CID. (Out of 15665 rotamers, 1713 rotamers (11%) are identified with CID, of which only 631 are unique.) These can be used in future theoretical or experimental work involving two-center non-metal rotamers.
- Source codes and raw data are available for reproduction of the work and further analysis. For example, molecular dipole moment and vibrational spectrum can be extracted from the raw output. Source codes can be used to generate molecules of related classes for further calculation.

1. Data description

There are 15 folders for C–C, N–N, P–P, O–O, S–S, N–P, O–S, C–N, C–P, C–O, C–S, N–O, N–S, P–O and P–S. In each folder, there are four subfolders for four different methodologies, HF, B3LYP, MP2 and CCSD. In addition to raw output files (.out) and geometry in *Z*-matrix and Cartesian coordinate format (.xyz), the following summary table files (.csv) are provided in each subfolder:

- A single csv file in xyz subfolder containing geometric data of 7 bond lengths in Å, 12 bond angles and 9 torsional angles in degree (If lone pair(s) are involved, there will be less numbers of geometric parameters and 'de' is shown in place of a numerical value.)
- Energetic data, in separate csv files, include electronic energy (E_{elec}) in a.u. (Hartree), thermal correction to enthalpy (H_{corr}) in kcal mol^{-1}, zero-point vibrational energy (E_{ZPE}) in kcal mol^{-1} and entropy (*S*) in cal mol^{-1} K^{-1}.

An example of these data is shown in Fig. 1. Names for compounds exist in two different formats and due to symmetry, there are up to six ways to write these out regardless of the format. Therefore, a rotamer name may not exactly match a file name in many instances. Source codes, scripts and examples are provided in a separate folder.
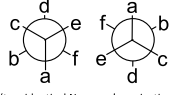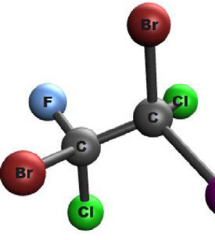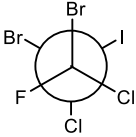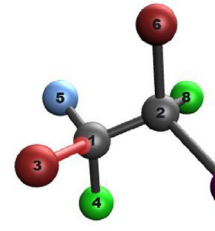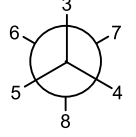
code/cidtable.csv
has the following fields presented in order:

1. Internal ID for this paper
2378

2. SMILES
[C@@](F)(Br)(Cl)[C@@](Br)(I)(Cl)

(two identical Newman's projections for two name formats below)

3. Benzene-equivalent name
CCFBrBrIClCl (in xyabcdef format)

4. Rotamer name
FBrClCClBrI (in acexyfbd format)

5. Empirical formula
C2Br2Cl2FI

6. PubChem CID
empty (does not exist as of December 30, 2019)

Energy information
CC/B3LYP/1_final_energy.csv
E_{elec} = -13164.31437 a.u.
CC/B3LYP/3_zero_point.csv
E_{ZPE} = 10.834 kcal mol^{-1}
CC/B3LYP/4_enthalpy.csv
H_{corr} = 17.641 kcal mol^{-1}
CC/B3LYP/5_entropy.csv
S = 104.922 cal mol^{-1} K^{-1}

Raw output file
CC/B3LYP/BrClFCCBrICl.out

Geometry file
CC/B3LYP/xyz/BrClFCCBrICl.xyz

Geometric data

CC/B3LYP/xyz/9_geotable.csv
has the following fields presented in order:

field #	atom #	atom list	value (length/angle)
1	12	CC	1.576972281
2	13	CBr	1.963928517
3	14	CCl	1.789244776
4	15	CF	1.351540593
5	26	CBr	1.965089634
6	27	CI	2.219998407
7	28	CCl	1.789640216
8	314	BrCCl	109.2371344
9	315	BrCF	107.2632773
10	415	ClCBr	107.5893669
11	627	BrCI	110.0685003
12	628	BrCCl	108.3994326
13	728	ICCl	109.705129
14	312	BrCC	112.742823
15	412	ClCC	111.6897445
16	512	FCC	108.0854286
17	621	BrCC	109.1643618
18	721	ICC	110.8733913
19	821	ClCC	108.5772857
20	3126	BrCCBr	-60.0664425
21	3127	BrCCI	61.35438007
22	3128	BrCCCl	-178.0574883
23	4126	ClCCBr	176.483838
24	4127	ClCCI	-62.09533944
25	4128	ClCCCl	58.49279221
26	5126	FCCBr	58.31890034
27	5127	FCCI	179.7397229
28	5128	FCCCl	-59.67214543

Fig. 1. An example of data for BrClFCCBrICl rotamer calculated at B3LYP/6-311++G(d,p) level of theory.

2. Experimental design, materials, and methods

Exhaustive listing of all rotamers can be done in many different approaches. We completed our comprehensive lists of all rotamers by extending the approach we have used for substituted benzenes [15]. Rotamers as viewed by Newman projection can be equivalent to substituted benzenes with two additional conditions. First, the list of substituent elements must include a lone pair of electrons. Second, rotamers are less symmetric compared to benzenes with regards to rotation and flipping. Q-Chem 5.2.1 [16], IQmol 2.13 [17] and Wolfram Mathematica 12.0 [18] were used in the same way as described previously [15]. In addition to compounds in Tables 1–8, Preliminary calculations were also completed for all combination of single atom of C, N, P, O, S and hydrogen/halogen atoms from F to I.

Tables 1–8 provide a comprehensive listing of all rotamers considered in this work. The listing is first arranged by the number of substituent elements and pattern of empirical formulas. An explanation on how to calculate the number of chemical empirical formulas in each table is given in Table 9. Rotamer structures are also listed for each pattern. Each rotamer structure can be rotated three times unless it is symmetric (cannot rotate) or has chiral center(s) (×2 for each center). Asterisks (*) shown in Tables 1, 2, 4, 6–8 indicate chiral centers. There are two special cases of meso compounds in Tables 1 and 2 which have a reduced number of rotamer structures. Similar symmetrical cases were also found in previous study of substituted benzenes [15]. Since enantiomeric structures are identical in energy, only one of the two enantiomeric structures is considered for each pair. Table 10 provides an overview of all computational jobs described in this paper.

All optimization jobs converged in Q-Chem before geometry information were extracted. The converged results are not necessarily the same conformer as the input. For example, some anti forms are turned into gauche forms during the geometry optimization. Almost all of the converged rotamers were confirmed to be local minima by frequency calculation (16,729 out of 16,840 jobs). However, there were 111 frequency jobs with exactly one imaginary frequency

Table 1
List of 2675 possible C–C rotamers in 210 formulas (1505 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula		Number of rotamers	
				Inclusive of enantiomers	Exclusive of enantiomers	Inclusive of enantiomers	Exclusive of enantiomers
1	$C_2\alpha_6$ (6)	5	$\alpha_3C-C\alpha_3$	1	1	5	5
2	$C_2\alpha_5\beta$ (1–5)	20	$\alpha_2\beta C-C\alpha_3$	1	1	20	20
	$C_2\alpha_2\beta_4$ (2–4)	20	$\alpha\beta_2C-C\alpha\beta_2$	3	2	60	40
			$\alpha_2\beta C-C\beta_3$	1	1	20	20
	$C_2\alpha_3\beta_3$ (3–3)	10	$\alpha\beta_2C-C\alpha_2\beta$	3	2	30	20
			$\alpha_3C-C\beta_3$	1	1	10	10
3	$C_2\alpha\beta\gamma_4$ (1–1–4)	30	$\alpha\beta\gamma C^*-C\gamma_3$	2	1	60	30
			$\alpha\gamma_2C-C\beta\gamma_2$	3	2	90	60
	$C_2\alpha\beta_2\gamma_3$ (1–2–3)	60	$\alpha\beta\gamma C^*-C\beta\gamma_2$	6	3	360	180
			$\alpha\gamma_2C-C\beta_2\gamma$	3	2	180	120
			$\alpha\beta_2C-C\gamma_3$	1	1	60	60
	$C_2\alpha_2\beta_2\gamma_2$ (2–2–2)	10	$\alpha\beta\gamma C^*-C^*\alpha\beta\gamma$ (meso compound)	9	5	90	50
			$\alpha\beta_2C-C\alpha\gamma_2$ $\alpha_2\beta C-C\beta\gamma_2$ $\alpha_2\gamma C-C\beta_2\gamma$	9	6	90	60
4	$C_2\alpha\beta\gamma\delta_3$ (1–1–1–3)	20	$\alpha\beta\delta C^*-C\gamma\delta_2$ $\alpha\gamma\delta C^*-C\beta\delta_2$ $\beta\gamma\delta C^*-C\alpha\delta_2$	18	9	360	180
			$\alpha\beta\gamma C^*-C\delta_3$	2	1	40	20
	$C_2\alpha\beta\gamma_2\delta_2$ (1–1–2–2)	30	$\alpha\gamma\delta C^*-C^*\beta\gamma\delta$	12	6	360	180
			$\alpha\beta\gamma C^*-C\gamma\delta_2$ $\alpha\beta\delta C^*-C\gamma_2\delta$	12	6	360	180
			$\alpha\gamma_2C-C\beta\delta_2$ $\alpha\delta_2C-C\beta\gamma_2$	6	4	180	120
5	$C_2\alpha\beta\gamma\delta\varepsilon_2$ (1–1–1–1–2)	5	$\alpha\beta\varepsilon C^*-C^*\gamma\delta\varepsilon$ $\alpha\gamma\varepsilon C^*-C^*\beta\delta\varepsilon$ $\alpha\delta\varepsilon C^*-C^*\beta\gamma\varepsilon$	36	18	180	90
			$\alpha\beta\gamma C^*-C\delta\varepsilon_2$ $\alpha\beta\delta C^*-C\gamma\varepsilon_2$ $\alpha\gamma\delta C^*-C\beta\varepsilon_2$ $\beta\gamma\delta C^*-C\alpha\varepsilon_2$	24	12	120	60

Table 2
List of 975 possible N–N (or P–P) rotamers in 70 formulas (500 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula		Number of rotamers	
				Inclusive of enantiomers	Exclusive of enantiomers	Inclusive of enantiomers	Exclusive of enantiomers
1	$N_2\alpha_4$ (4)	5	$\alpha_2N-N\alpha_2$	3	2	15	10
2	$N_2\alpha\beta_3$ (1–3)	20	$\alpha\beta N^*-N\beta_2$	6	3	120	60
	$N_2\alpha_2\beta_2$ (2–2)	10	$\alpha\beta N^*-N^*\alpha\beta$ (meso compound)	9	5	90	50
			$\alpha_2N-N\beta_2$	3	2	30	20
3	$N_2\alpha\beta\gamma_2$ (1–1–2)	30	$\alpha\gamma N^*-N^*\beta\gamma$	12	6	360	180
			$\alpha\beta N^*-N\gamma_2$	6	3	180	90
4	$N_2\alpha\beta\gamma\delta$ (1–1–1–1)	5	$\alpha\beta N^*-N^*\gamma\delta$ $\alpha\gamma N^*-N^*\beta\delta$ $\alpha\delta N^*-N^*\beta\gamma$	36	18	180	90

Table 3

List of 45 possible O–O (or S–S) rotamers in 15 formulas (30 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula		Number of rotamers	
				Inclusive of enantiomers	Exclusive of enantiomers	Inclusive of enantiomers	Exclusive of enantiomers
1	$O_2\alpha_2$ (2)	5	$\alpha O{-}O\alpha$	3	2	15	10
2	$O_2\alpha\beta$ (1–1)	10	$\alpha O{-}O\beta$	3	2	30	20

Table 4

List of 1875 possible N–P rotamers in 70 formulas (950 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula		Number of rotamers	
				Inclusive of enantiomers	Exclusive of enantiomers	Inclusive of enantiomers	Exclusive of enantiomers
1	$NP\alpha_4$ (4)	5	$\alpha_2 N{-}P\alpha_2$	3	2	15	10
2	$NP\alpha\beta_3$ (1–3)	20	$\alpha\beta N^*{-}P\beta_2$	12	6	240	120
	$NP\alpha_2\beta_2$ (2–2)	10	$\alpha\beta N^*{-}P^*\alpha\beta$	12	6	120	60
			$\alpha_2 N{-}P\beta_2$ $\alpha_2 P{-}N\beta_2$	6	4	60	40
3	$NP\alpha\beta\gamma_2$ (1–1–2)	30	$\alpha\gamma N^*{-}P^*\beta\gamma$ $\alpha\gamma P^*{-}N^*\beta\gamma$	24	12	720	360
			$\alpha\beta N^*{-}P\gamma_2$ $\alpha\beta P^*{-}N\gamma_2$	12	6	360	180
4	$NP\alpha\beta\gamma\delta$ (1–1–1–1)	5	$\alpha\beta N^*{-}P^*\gamma\delta$ $\binom{4}{2}=6$ structures	72	36	360	180

Table 5

List of 75 possible O–S rotamers in 15 formulas (50 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula		Number of rotamers	
				Inclusive of enantiomers	Exclusive of enantiomers	Inclusive of enantiomers	Exclusive of enantiomers
1	$OS\alpha_2$ (2)	5	$\alpha O{-}S\alpha$	3	2	15	10
2	$OS\alpha\beta$ (1–1)	10	$\alpha O{-}S\beta$ $\alpha S{-}O\beta$	6	4	60	40

ranging from 4.9i cm^{-1} to 513.1i cm^{-1}. The list of files is provided in data folder. Most of them (74) are HF calculations and the rest (37) are B3LYP. Upon closer inspection, all rotamers of O–O, S–S and O–S with an imaginary frequency (55) are in an anti form. Similarly, 28 of 34 rotamers of N–N, P–P and N–P with an imaginary frequency are in an anti form from the perspective of the two lone pairs. As these observations suggest that the anti form is not stable, gauche effect is evident in these classes of compounds.

Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Table 6
List of 3125 possible C–N (or C–P) rotamers in 126 formulas (1625 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula		Number of rotamers	
				Inclusive of enantiomers	Exclusive of enantiomers	Inclusive of enantiomers	Exclusive of enantiomers
1	$CN\alpha_5$ (5)	5	$\alpha_3C{-}N\alpha_2$	1	1	5	5
2	$CN\alpha\beta_4$ (1–4)	20	$\alpha\beta_2C{-}N\beta_2$	3	2	60	40
			$\beta_3C{-}N^*\alpha\beta$	2	1	40	20
	$CN\alpha_2\beta_3$ (2–3)	20	$\alpha\beta_2C{-}N^*\alpha\beta$	6	3	120	60
			$\alpha_2\beta C{-}N\beta_2$	3	2	60	40
			$\beta_3C{-}N\alpha_2$	1	1	20	20
3	$CN\alpha\beta\gamma_3$ (1–1–3)	30	$\alpha\beta\gamma C^*{-}N\gamma_2$	6	3	180	90
			$\alpha\gamma_2C{-}N^*\beta\gamma$ $\beta\gamma_2C{-}N^*\alpha\gamma$	12	6	360	180
			$\gamma_3C{-}N^*\alpha\beta$	2	1	60	30
	$CN\alpha\beta_2\gamma_2$ (1–2–2)	30	$\alpha\beta\gamma C^*{-}N^*\beta\gamma$	12	6	360	180
			$\beta_2\gamma C{-}N^*\alpha\gamma$ $\beta\gamma_2C{-}N^*\alpha\beta$	12	6	360	180
			$\alpha\beta_2C{-}N\gamma_2$ $\alpha\gamma_2C{-}N\beta_2$	6	4	180	120
4	$CN\alpha\beta\gamma\delta_2$ (1–1–1–2)	20	$\alpha\beta\delta C^*{-}N^*\gamma\delta$ $\alpha\gamma\delta C^*{-}N^*\beta\delta$ $\beta\gamma\delta C^*{-}N^*\alpha\delta$	36	18	720	360
			$\alpha\beta\gamma C^*{-}N\delta_2$	6	3	120	60
			$\alpha\delta_2C{-}N^*\beta\gamma$ $\beta\delta_2C{-}N^*\alpha\gamma$ $\gamma\delta_2C{-}N^*\alpha\beta$	18	9	360	180
5	$CN\alpha\beta\gamma\delta\varepsilon$ (1–1–1–1–1)	1	$\alpha\beta\gamma C^*{-}N^*\delta\varepsilon$ $\binom{5}{3}=10$ structures	120	60	120	60

Table 7
List of 625 possible C–O (or C–S) rotamers in 70 formulas (375 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula		Number of rotamers	
				Inclusive of enantiomers	Exclusive of enantiomers	Inclusive of enantiomers	Exclusive of enantiomers
1	$CO\alpha_4$ (4)	5	$\alpha_3C{-}O\alpha$	1	1	5	5
2	$CO\alpha\beta_3$ (1–3)	20	$\alpha\beta_2C{-}O\beta$	3	2	60	40
			$\beta_3C{-}O\alpha$	1	1	20	20
	$CO\alpha_2\beta_2$ (2–2)	10	$\alpha\beta_2C{-}O\alpha$ $\alpha_2\beta C{-}O\beta$	6	4	60	40
3	$CO\alpha\beta\gamma_2$ (1–1–2)	30	$\alpha\beta\gamma C^*{-}O\gamma$	6	3	180	90
			$\alpha\gamma_2C{-}O\beta$ $\beta\gamma_2C{-}O\alpha$	6	4	180	120
4	$CO\alpha\beta\gamma\delta$ (1–1–1–1)	5	$\alpha\beta\gamma C^*{-}O\delta$ $\alpha\beta\delta C^*{-}O\gamma$ $\alpha\gamma\delta C^*{-}O\beta$ $\beta\gamma\delta C^*{-}O\alpha$	24	12	120	60

Table 8
List of 375 possible N–O (or N–S, P–O, P–S) rotamers in 35 formulas (200 non-enantiomeric rotamers).

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas	Rotamer structure	Rotamers per formula Inclusive of enantiomers	Rotamers per formula Exclusive of enantiomers	Number of rotamers Inclusive of enantiomers	Number of rotamers Exclusive of enantiomers
1	$NO\alpha_3$ (3)	5	$\alpha_2N{-}O\alpha$	3	2	15	10
2	$NO\alpha\beta_2$ (1-2)	20	$\alpha\beta N^*{-}O\beta$ $\beta_2N{-}O\alpha$	6 3	3 2	120 60	60 40
3	$NO\alpha\beta\gamma$ (1-1-1)	10	$\alpha\beta N^*{-}O\gamma$ $\alpha\gamma N^*{-}O\beta$ $\beta\gamma N^*{-}O\alpha$	18	9	180	90

Table 9
Examples for number of empirical formula calculation.

Number of elements	Empirical formula (Distribution of elements)	Number of empirical formulas[a]
3	$C_2\alpha\beta_2\gamma_3$ (1-2-3)	$k=3$, $n_1=1$, $n_2=1$, $n_3=1$ therefore $\binom{5}{3}\frac{3!}{1!1!1!}=60$
3	$C_2\alpha_2\beta_2\gamma_2$ (2-2-2)	$k=3$, $n_1=3$ therefore $\binom{5}{3}\frac{3!}{3!}=10$
4	$C_2\alpha\beta\gamma_2\delta_2$ (1-1-2-2)	$k=4$, $n_1=2$, $n_2=2$ therefore $\binom{5}{4}\frac{4!}{2!2!}=30$
5	$C_2\alpha\beta\gamma\delta\varepsilon_2$ (1-1-1-1-2)	$k=5$, $n_1=4$, $n_2=1$ therefore $\binom{5}{5}\frac{5!}{4!1!}=5$

[a] The number of empirical formulas is calculated by using the expression $\binom{5}{k}\frac{k!}{\prod n_i!}$, where
- 5 is the number of possible substituent elements (H, F, Cl, Br, I),
- k is the actual number of substituent elements and
- $\prod n_i!$ is the product of the factorial of the number of substituent elements with the same subscript.

Table 10
Summary of 43450 computational jobs included in this paper (opt for geometry optimization and freq for frequency calculation).

Class of compound	Number of rotamers All	Number of rotamers non-enantiomeric	HF opt	HF freq	B3LYP opt	B3LYP freq	MP2 opt	MP2 freq	CCSD opt	CCSD freq
Preliminary CNPOS	175	170	All	All	All	All	All	–	All	–
C–C	2675	1505	All	All	All	All	All	–	23	–
N–N	975	500	All	All	All	All	All	–	30	–
P–P	975	500	All	All	All	All	All	–	30	–
O–O	45	30	All	All	All	All	All	All	All	–
S–S	45	30	All	All	All	All	All	All	all	–
C–N	3125	1625	All	All	All	All	All	–	33	–
C–P	3125	1625	All	All	All	All	All	–	33	–
C–O	625	375	All	All	All	All	All	–	33	–
C–S	625	375	All	All	All	All	All	–	33	–
N–P	1875	950	All	All	All	All	All	–	34	–
N–O	375	200	All	All	All	All	All	–	34	–
N–S	375	200	All	All	All	All	All	–	34	–
P–O	375	200	All	All	All	All	All	–	34	–
P–S	375	200	All	All	All	All	All	–	34	–
O–S	75	50	All	All	All	All	All	All	All	–
Total	15840	8535	8535	8535	8535	8535	8535	110	665	–

Acknowledgments

References

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