Electronic Supplementary Material (ESI) for Dalton Transactions.

The Global Electrophilicity Index as a Metric for Lewis Acidity

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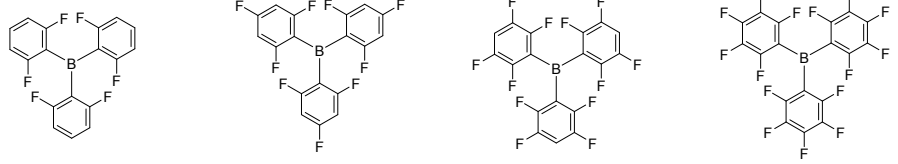
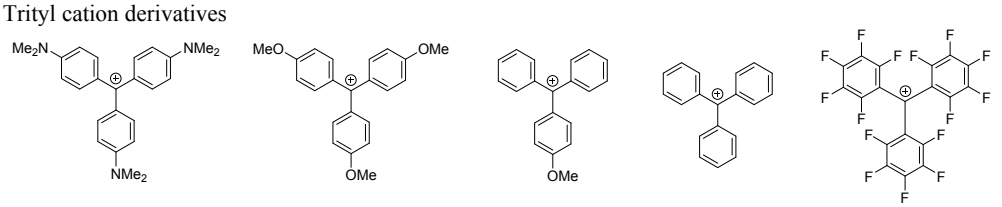
Diagrams of Lewis acids included in study

Fluoroaryl boranes



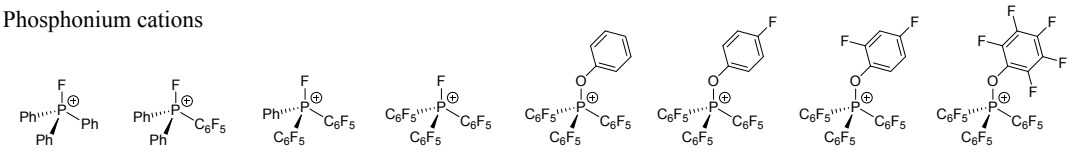
1 **2** **3** **4**

Trityl cation derivatives



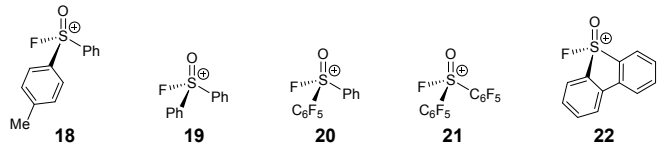
5 **6** **7** **8** **9**

Phosphonium cations



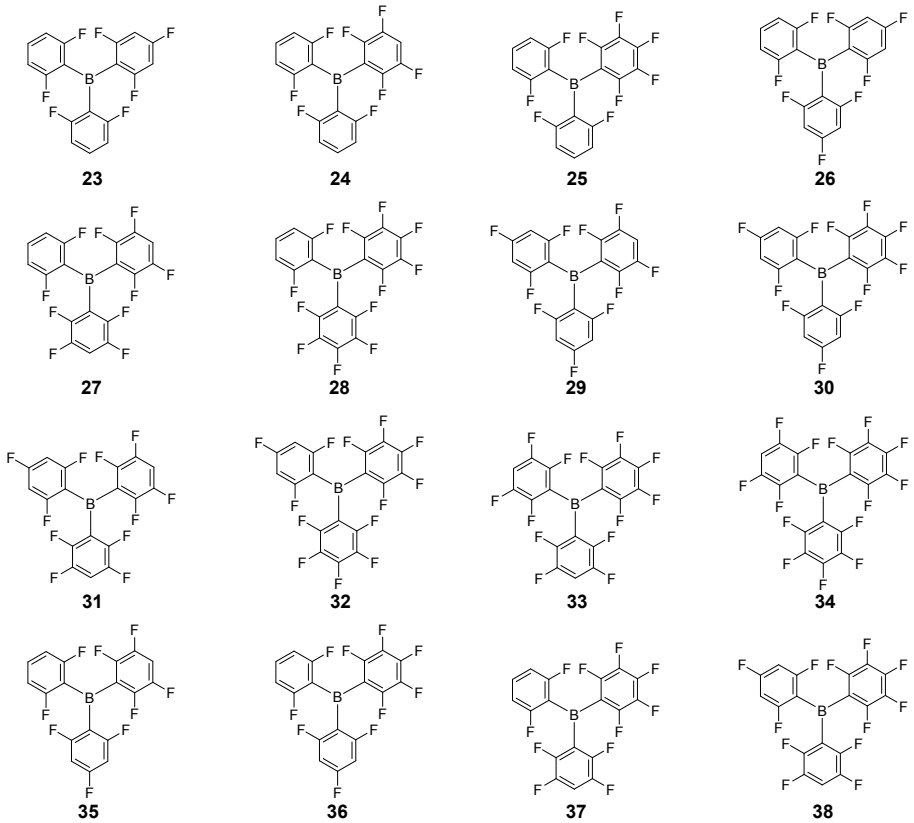
10 **11** **12** **13** **14** **15** **16** **17**

Sulfoxonium cations



18 **19** **20** **21** **22**

Library of fluoroaryl boranes



23 **24** **25** **26**

27 **28** **29** **30**

31 **32** **33** **34**

35 **36** **37** **38**

Figure S1: Depictions of Lewis acids considered in this study.

Computational details

Geometry optimizations were carried out on Gaussian 09[1] using the BP86 functional and the def2-TZVP basis set.[2–5] Frequency calculations were carried out on all optimized structures, and the absence of any imaginary frequencies confirmed that each optimized structure was located at a minimum on its potential energy hypersurface. Energies were subsequently recalculated on the optimized structures at the MP2/def2-TZVPP level of theory.[6–8] This model chemistry was chosen based on previous reports detailing its applicability to molecules comprising atoms from across the periodic table,[4,5] and based on a screening of different basis sets carried out on a subset of Lewis acids from this paper (see *Basis set dependence* section later in SI for full details). Calculations were carried out in the gas phase unless otherwise stated; a study on the effect of solvent (toluene and dichloromethane) on the GEI values of Lewis acids **1**–**9** was carried out (see *Solvent dependence* section later in SI). The effect of dispersion was also examined on Lewis acids **1**–**9** (see *Dispersion dependence* section later in SI).

GEI values, ω, were calculated using the chemical potential, μ, and chemical hardness, η, according to equation (1). These latter values can be related to the energies of the highest occupied molecular orbital (E_{HOMO}) and lowest unoccupied molecular orbital (E_{LUMO}) according to equations (2) and (3), respectively, at the level of theory outlined above. A full derivation of the GEI can be found in Parr's original publication,[9] and is further discussed in a review by Chattaraj et al.[10] The GEI values are reported in eV by convention.[11,12]

$$\omega = \mu^2/2\eta \quad (1)$$

$$\mu = \tfrac{1}{2}(E_{HOMO} + E_{LUMO}) \quad (2)$$

$$\eta = (E_{LUMO} - E_{HOMO}) \quad (3)$$

Due to the difficulties of obtaining accurate energies for the F^- anion, FIA values were obtained by initially calculating the energy change for reaction (4), where LA is the Lewis acid in question. This was combined with the experimentally obtained energy change for (5) of –209 kJ/mol to obtain a value for the energy change of (6), the negative of which is the FIA (in kJ/mol); this is the same method employed originally by Christe[13] and other researchers since.[14–17] Although the FIA has previously been calculated for a number of the Lewis acids discussed in this paper,[14,18–20] they were all recalculated at the same level of theory for internal consistency and ease of comparison.

$$[F_3CO]^- + LA \rightarrow F_2CO + [LA\text{-}F]^- \quad (4)$$

$$F_2CO + F^- \rightarrow [F_3CO]^- \quad (5)$$

$$LA + F^- \rightarrow [LA\text{-}F]^- \quad (6)$$

Tables of data for GEI and FIA calculations

The data for both the FIA and GEI calculations are compiled and grouped for each series discussed in the main paper. The energies of the Lewis acid and the fluoride adduct are used to calculate FIA, and the energies of the HOMO and LUMO are used to calculate GEI.

Table S1: FIA and GEI data for boranes **1**–**4**.

Lewis acid	Energy (kJ/mol)	Energy of F-adduct (kJ/mol)	Energy of HOMO (eV)	Energy of LUMO (eV)	FIA (kJ/mol)	GEI (eV)
1	-3447380.9	-3709585.2	-9.366	1.039	362.3	0.833
2	-4228196.3	-4490426.0	-9.798	0.780	387.7	0.961
3	-5008887.3	-5271161.5	-9.972	-0.009	432.2	1.250
4	-5789595.6	-6051890.2	-10.494	-0.249	452.6	1.408

Table S2: FIA and GEI data for trityl derivatives **5**–**9**.

Lewis acid	Energy (kJ/mol)	Energy of F-adduct (kJ/mol)	Energy of HOMO (eV)	Energy of LUMO (eV)	FIA (kJ/mol)	GEI (eV)
5	-2972993.3	-3235358.8	-10.125	-2.362	523.5	2.511
6	-2820437.6	-3082880.8	-11.477	-3.131	601.2	3.196
7	-2220034.2	-2482519.1	-11.945	-3.631	642.9	3.647
8	-1919825.6	-2182338.1	-12.593	-3.975	670.5	3.982
9	-5823491.3	-6086101.5	-14.148	-5.915	768.1	6.111

Table S3: FIA and GEI data for phosphonium derivatives **10**–**17**.

Lewis acid	Energy (kJ/mol)	Energy of F-adduct (kJ/mol)	Energy of HOMO (eV)	Energy of LUMO (eV)	FIA (kJ/mol)	GEI (eV)
10	-2977042.3	-3239540.9	-12.788	-1.862	656.5	2.455
11	-4278266.7	-4540808.9	-13.018	-2.435	700.1	2.820
12	-5579490.2	-5842074.2	-13.341	-2.942	742.0	3.187
13	-6880712.7	-7143334.1	-14.077	-3.461	779.3	3.622
14	-7422983.1	-7685542.8	-12.662	-2.734	717.7	2.984
15	-7683246.6	-7945813.3	-12.639	-2.903	724.7	3.102
16	-7943504.5	-8206075.1	-12.856	-2.943	728.6	3.147
17	-8724206.7	-8986798.4	-13.511	-3.067	749.7	3.290

Table S4: FIA and GEI data for sulfoxonium derivatives **18**–**22**.

Lewis acid	Energy (kJ/mol)	Energy of F-adduct (kJ/mol)	Energy of HOMO (eV)	Energy of LUMO (eV)	FIA (kJ/mol)	GEI (eV)
18	-2819261.8	-3081724.7	-13.407	-2.582	620.9	2.952
19	-2716260.5	-2978732.9	-13.593	-2.743	630.3	3.075
20	-4017453.8	-4279969.9	-13.946	-3.098	674.1	3.347
21	-5318644.4	-5581206.2	-14.620	-3.906	719.8	4.004
22	-2713143.4	-2975614.0	-12.878	-3.668	628.6	3.716

Table S5: GEI data for all fluoroarylboranes considered in this study.

Lewis acid	No. of F atoms	Energy of HOMO (eV)	Energy of LUMO (eV)	GEI (eV)
1	6	-9.366	1.039	0.833
2	9	-9.798	0.780	0.961
3	12	-9.972	-0.009	1.250
4	15	-10.494	-0.249	1.408
23	7	-9.464	0.955	0.869
24	8	-9.574	0.708	0.956
25	9	-9.651	0.611	0.995
26	8	-9.560	0.871	0.905
27	10	-9.775	0.349	1.097
28	12	-9.945	0.179	1.178
29	10	-9.773	0.553	1.029
30	11	-9.993	0.448	1.091
31	11	-9.881	0.276	1.135
32	13	-10.279	0.099	1.248
33	13	-10.059	-0.085	1.290
34	14	-10.145	-0.164	1.331
35	9	-9.677	0.633	0.992
36	10	-9.752	0.525	1.035
37	11	-9.858	0.269	1.135
38	12	-9.957	0.192	1.174

Basis set dependence

A range of basis sets were screened to calculate the energies of the Lewis acids **4**, **8**, **9**, **10**, and **13**. This selection incorporates a mixture of neutral and cationic Lewis acids centred on B, C and P, with combinations of C_6F_5 and C_6H_5 rings, in order to be representative of a large number of main-group Lewis acids. The five structures were initially optimized at the same level of theory (BP86/def2-TZVP), and the energies were subsequently computed using the MP2 method and six different basis sets: def2-SV, def2-SVP, def2-TZV, def2-TZVPP, def2-QZV and def2-QZVPP.[2–5]

The split valence basis set, def2-SV, was the simplest employed in this study, and def2-SVP has additional polarization functions on hydrogen atoms. For this reason, the energies and GEI values calculated using these two basis sets is identical for non-hydrogen containing molecules (**4**, **9**, and **13**). def2-TZV is a valence triple-zeta basis set, and def2-TZVPP is the same with two sets of polarization functions added. Similarly, def2-QZV is a valence quadruple-zeta basis set, and def2-QZVPP has two sets of polarization functions. The latter is a very large basis set, and thus should give the best results of those surveyed, but calculations using it take significantly longer.

The energy for each Lewis acid was calculated for the six basis sets, and are compiled in Table S6. For all five Lewis acids, the energy was lowest (i.e. most negative) when calculated using the most expensive def2-QZVPP basis set. Interestingly, the energies calculated using def2-TZVPP were only slightly higher than def2-QZVPP, and both of these were significantly lower than the other four basis sets. This result is highlighted in Figure S2, which shows the energies for the different acids relative to that calculated using def2-QZVPP.

Table S6: Energies (in Hartrees) of selected Lewis acids calculated using different basis sets.

	4	**8**	**9**	**10**	**13**
def2-SV	-2201.040758	-729.790131	-2213.934579	-1132.16345	-2616.308443
def2-SVP	-2201.040758	-729.932747	-2213.934579	-1132.306217	-2616.308443
def2-TZV	-2201.648464	-729.7002324	-2214.501484	-1132.124838	-2616.927364
def2-TZVPP	-2205.140199	-731.2228536	-2218.050384	-1133.895386	-2620.724713
def2-QZV	-2201.866983	-729.7905065	-2214.717867	-1132.241973	-2617.174221
def2-QZVPP	-2205.767831	-731.4350712	-2218.678055	-1134.149469	-2621.394886

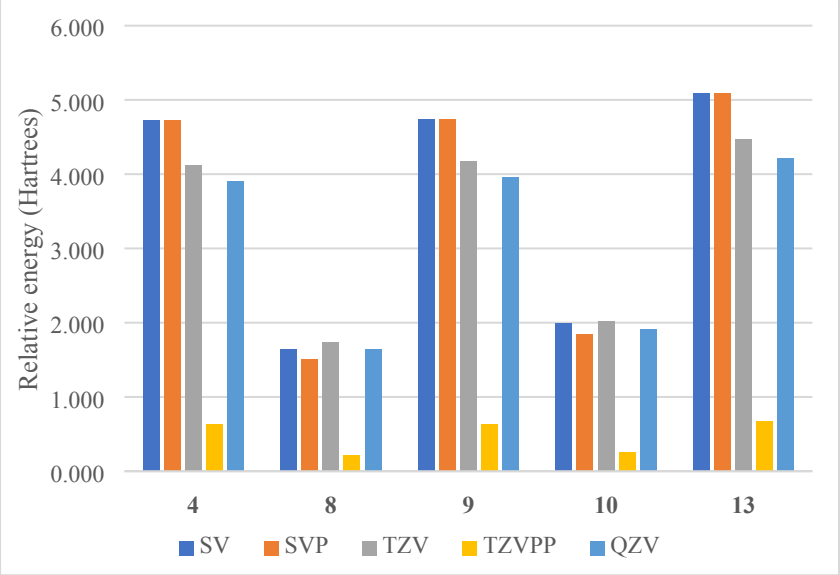


Figure S2: Relative energies (in Hartrees) of a range of Lewis acids using different basis sets, relative to the def2-QZVPP basis set.

The GEI values were subsequently calculated as detailed in the main paper, and are compiled in Table S7 and Figure S3. The triple-zeta basis set def2-TZVPP gave remarkably similar energies to those obtained using the more computationally expensive quadruple-zeta def2-QZVPP, but in significantly shorter times. The energies obtained when polarization functions were omitted (def2-TZV and def2-QZV) were significantly higher.

Table S7: GEI values calculated using different basis sets for selected Lewis acids.

	4	**8**	**9**	**10**	**13**
def2-SV	1.519	4.103	6.605	2.475	3.848
def2-SVP	1.519	4.071	6.605	2.456	3.848
def2-TZV	1.795	4.066	7.238	2.503	4.258
def2-TZVPP	1.408	3.982	6.111	2.455	3.622
def2-QZV	1.762	4.044	7.116	2.505	4.209
def2-QZVPP	1.413	3.986	6.099	2.469	3.627

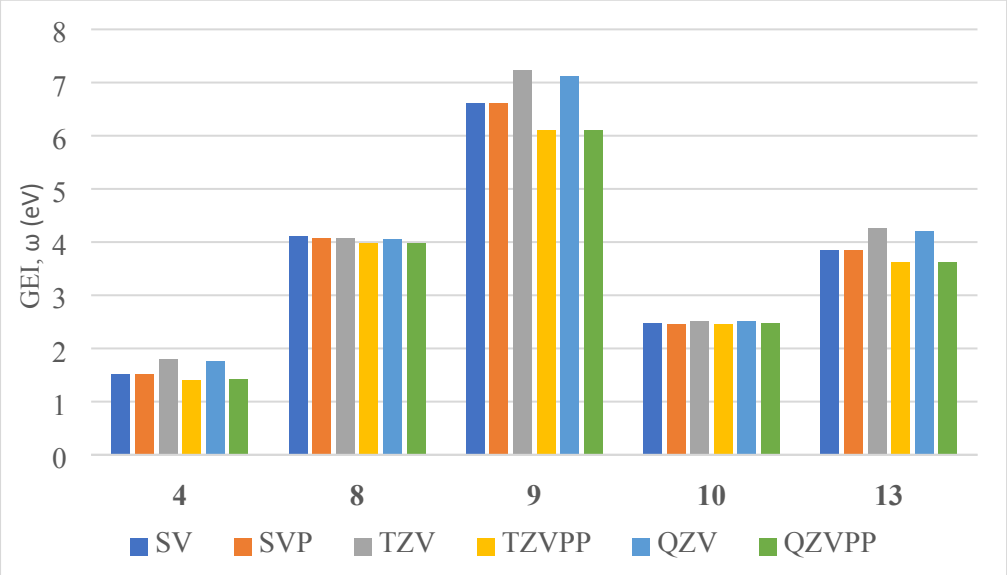


Figure S3: GEI values for a range of Lewis acids using different basis sets.

These results guided the choice of the def2-TZVPP basis set for the rest of the Lewis acids studied in this paper; def2-TZVPP gave very similar results to def2-QZVPP but in a much shorter time, while the other smaller basis sets did not yield satisfactory results.

Solvent dependence

The effect of solvent on the GEI values of the neutral boranes **1**–**4** and the cationic trityl derivatives **5**–**9** was explored. Solvent interactions for toluene (ε = 2.3741) and dichloromethane (ε = 8.93) were treated implicitly using a polarizable continuum model.[1,21] The geometries of the nine Lewis acids were re-optimized in each solvent at the BP86/def2-TZVP level of theory, and the energy recalculated at the MP2/def2-TZVPP level, again with solvent interactions present. The energies of the frontier molecular orbitals and the GEI for Lewis acids **1**–**9** are tabulated in Table S8.

Table S8: FIA data for Lewis acids **1**–**9** in toluene and dichloromethane.

Lewis acid	Toluene			Dichloromethane		
	Energy of HOMO (eV)	Energy of LUMO (eV)	GEI (eV)	Energy of HOMO (eV)	Energy of LUMO (eV)	GEI (eV)
1	-9.425	0.988	0.855	-9.501	0.922	0.883
2	-9.759	0.827	0.942	-9.746	0.849	0.934
3	-9.890	0.118	1.193	-9.839	0.213	1.152
4	-10.335	-0.048	1.310	-10.205	0.127	1.229
5	-8.713	-0.943	1.500	-7.984	-0.210	1.080
6	-9.946	-1.562	1.974	-9.133	-0.712	1.439
7	-10.275	-1.931	2.232	-9.386	-1.015	1.615
8	-10.841	-2.197	2.458	-9.912	-1.242	1.794
9	-12.285	-4.001	4.003	-11.205	-2.870	2.971

In general, the presence of solvent leads to a decrease in Lewis acidity compared to the gas phase calculations, and the more polar solvent (dichloromethane) leads to a greater decrease in Lewis acidity (see Figures S4–S6). As expected, the cationic substrates are affected to a greater extent than the neutral Lewis acids; this is highlighted in Figure S6, which shows the decreases in Lewis acidity for the boranes is significantly smaller than for the trityl cation derivatives. Interestingly the presence of solvent appears to reverse the order for borane **1**, where the acid in dichloromethane is actually slightly more acidic than in the gas phase. This does not fit the trend for the rest of the Lewis acids, but the absolute changes in acidity for **1** are very small.

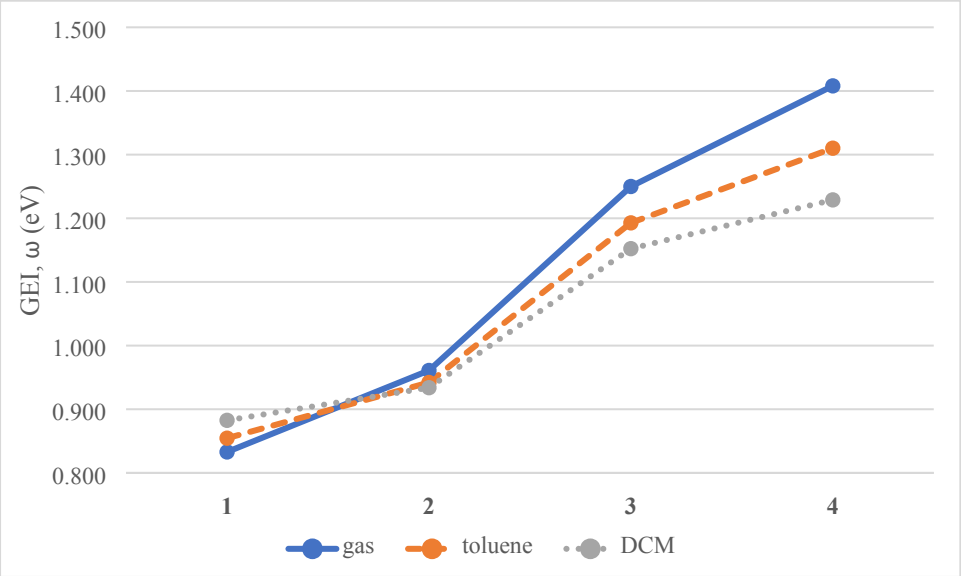


Figure S4: GEI values for boranes **1**–**4** in the gas phase, in toluene and in DCM.

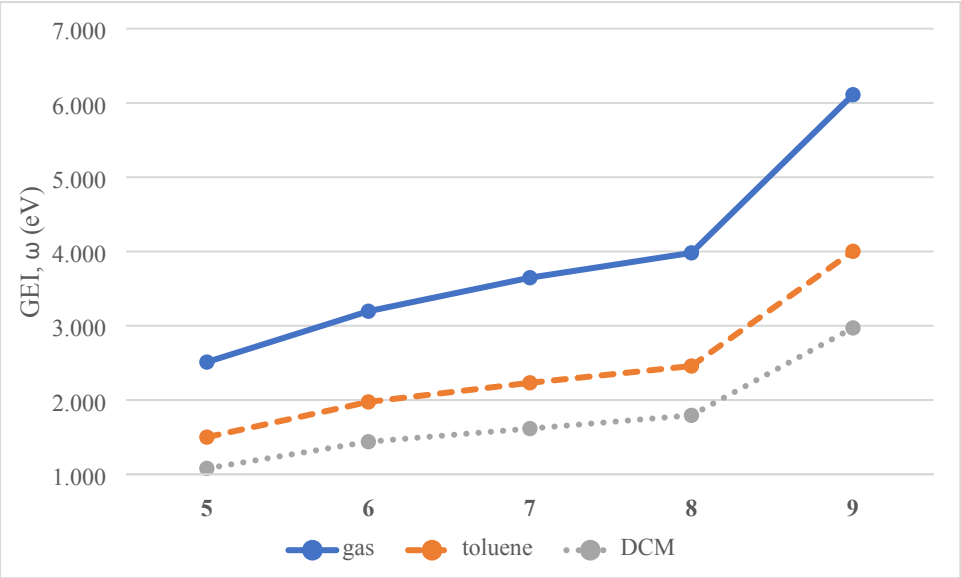


Figure S5: GEI values for trityl cation derivatives **5**–**9** in the gas phase, in toluene and in DCM.

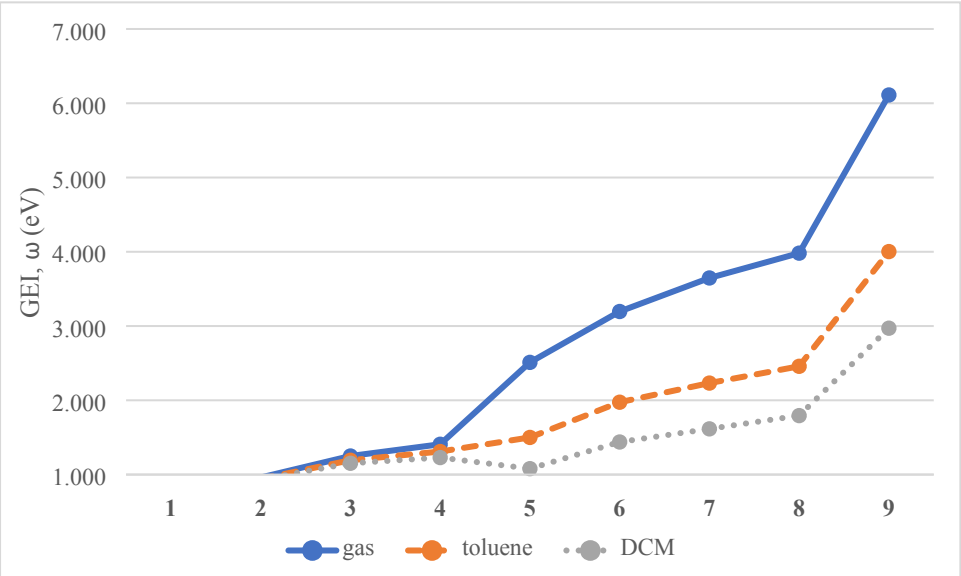


Figure S6: GEI values for Lewis acids **1**–**9** in the gas phase, in toluene and in DCM.

Dispersion dependence

The effect of dispersion on the GEI was explored, to assess if there was significant interaction between the peripheral substituents and the Lewis acidic centre. For example, in the fluoroaryl boranes the *ortho*-fluorine substituents could potentially interact with the vacant 2p orbital on boron and diminish the Lewis acidity.

Dispersion corrections are applied to density functional methods to account for nonlocal interactions.[22] The geometries of Lewis acids **1**–**9** were re-optimized at BP86/def2-TZVP with Grimme's D3BJ dispersion correction with Becke-Johnson damping.[23] Our model chemistry uses MP2, a post-Hartree-Fock method, to subsequently assess the energies of the frontier molecular orbitals, and thus the GEI, and dispersion corrections are not applicable. Nevertheless, the single point energy calculations at MP2/def2-TZVPP was carried out on the newly optimized structures. The data for these values are tabulated in Table S9, alongside the dispersion-free values for comparison. It is evident that the dispersion correction only has a small effect on the GEI values of these Lewis acids, and this is further supported by the graph in Figure S7.

Table S9: FIA data for Lewis acids **1**–**9** in with and without dispersion.

Lewis acid	**Dispersion-corrected**			**No dispersion**		
	Energy of HOMO (eV)	Energy of LUMO (eV)	GEI (eV)	Energy of HOMO (eV)	Energy of LUMO (eV)	GEI (eV)
1	-9.348	1.016	0.837	-9.366	1.039	0.833
2	-9.774	0.768	0.962	-9.798	0.780	0.961
3	-9.955	-0.032	1.257	-9.972	-0.009	1.250
4	-10.480	-0.263	1.412	-10.494	-0.249	1.408
5	-10.120	-2.339	2.493	-10.125	-2.362	2.511
6	-11.478	-3.115	3.183	-11.477	-3.131	3.196
7	-11.946	-3.618	3.636	-11.945	-3.631	3.647
8	-12.596	-3.963	3.970	-12.593	-3.975	3.982
9	-14.149	-5.901	6.093	-14.148	-5.915	6.111

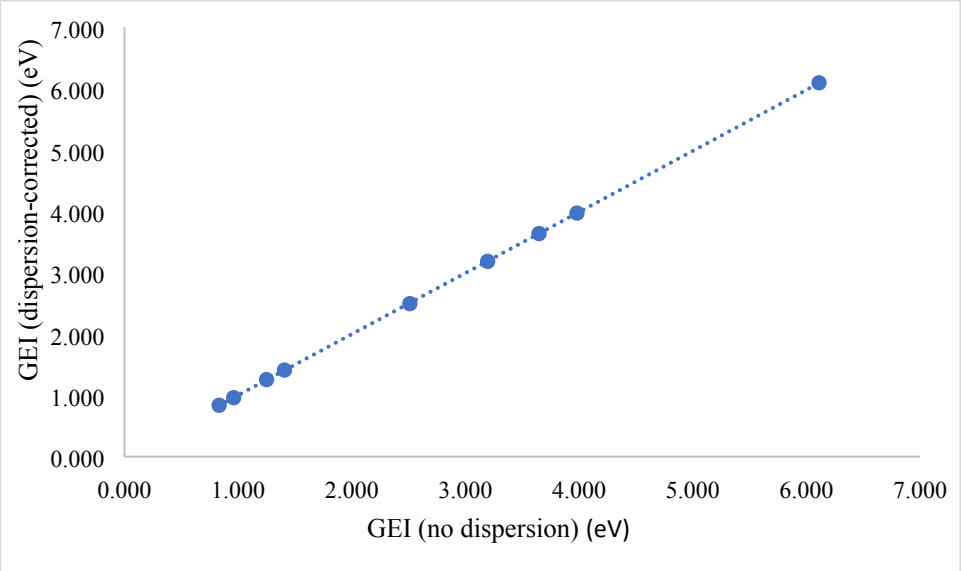


Figure S7: Comparison of GEI values for Lewis acids **1**–**9** with and without the dispersion correction.

Tables of optimized coordinates

The following tables contain the optimized coordinates of the Lewis acids **1**–**22** and their fluoride adducts (always denoted for simplicity as [**x**-F]$^-$, even though **5**–**22** are cations and their adducts would be neutral), followed by the remainder of the fluoroarylboranes **23**–**38**. All calculations were carried out in the gas phase, unless otherwise indicated. The re-optimized coordinates for the Lewis acids **1**–**9** in toluene and dichloromethane are included at the end.

Table S10: Optimized Cartesian coordinates of **1**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000416	-0.005489	0.001566
2	6	0	1.529482	0.353048	0.002187
3	6	0	2.479225	-0.321480	-0.788612
4	6	0	2.076869	1.383844	0.790175
5	6	0	3.835443	-0.016529	-0.822254
6	6	0	3.425023	1.722633	0.817811
7	6	0	4.304370	1.013782	-0.003920
8	6	0	-0.456434	-1.507904	0.000759
9	6	0	-1.518969	-1.987666	-0.789113
10	6	0	0.155993	-2.499689	0.790518
11	6	0	-1.941962	-3.311757	-0.819742
12	6	0	-0.233835	-3.834009	0.821148
13	6	0	-1.290552	-4.235645	0.000715
14	6	0	-1.072236	1.141921	0.000375
15	6	0	-2.238961	1.108166	0.787989
16	6	0	-0.953614	2.303054	-0.787423
17	6	0	-3.197837	2.114683	0.818880
18	6	0	-1.886926	3.333107	-0.817996
19	6	0	-3.014031	3.231879	0.000856
20	9	0	-2.434035	0.041795	1.607816
21	9	0	1.246931	2.078393	1.612485
22	9	0	2.047457	-1.314683	-1.609953
23	9	0	1.174051	-2.132887	1.612859
24	9	0	-2.158952	-1.113884	-1.610248
25	9	0	0.124251	2.419849	-1.607264
26	1	0	3.765240	2.524752	1.472445
27	1	0	5.365818	1.266776	-0.006665
28	1	0	4.497468	-0.579402	-1.479984
29	1	0	0.285885	-4.531591	1.477632
30	1	0	-1.609642	-5.279122	0.000710
31	1	0	-2.763319	-3.599338	-1.475780
32	1	0	-4.062670	2.013916	1.474331
33	1	0	-3.756510	4.031476	0.001594
34	1	0	-1.723173	4.188678	-1.472879

Table S11: Optimized Cartesian coordinates of [**1**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.195306	0.974538	1.620280
2	6	0	2.379822	1.504770	2.627211
3	6	0	4.553022	1.265150	1.831546
4	6	0	2.817051	2.272700	3.709234
5	6	0	5.067331	2.024156	2.883824
6	6	0	4.181111	2.538575	3.832229
7	1	0	2.087353	2.641604	4.431646
8	1	0	6.143988	2.189887	2.946753
9	1	0	4.552787	3.137565	4.666641
10	6	0	1.092437	0.360945	-0.071357
11	6	0	0.075166	-0.591331	0.064960
12	6	0	0.613727	1.573995	-0.593152
13	6	0	-1.261135	-0.415175	-0.301830
14	6	0	-0.702357	1.827030	-0.983547
15	6	0	-1.650110	0.812057	-0.839286
16	1	0	-1.967235	-1.234019	-0.155690
17	1	0	-0.961773	2.809745	-1.380543
18	1	0	-2.687590	0.979527	-1.137170
19	6	0	3.145448	-1.452558	0.297661
20	6	0	3.263745	-2.198036	-0.886638
21	6	0	3.480777	-2.205509	1.429486
22	6	0	3.705565	-3.519521	-0.973908
23	6	0	3.929852	-3.527975	1.424934
24	6	0	4.048451	-4.189174	0.202037
25	1	0	3.762358	-3.999936	-1.951987
26	1	0	4.170974	-4.013261	2.371933
27	1	0	4.398295	-5.223340	0.166266
28	5	0	2.712691	0.155052	0.252511
29	9	0	1.031292	1.261714	2.593923
30	9	0	5.478029	0.757881	0.964486
31	9	0	2.900606	-1.620939	-2.069721
32	9	0	3.355152	-1.638487	2.670803
33	9	0	1.476020	2.625265	-0.717870
34	9	0	0.369747	-1.810205	0.618007
35	9	0	3.432169	0.745948	-0.847371

Table S12: Optimized Cartesian coordinates of **2**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000563	-0.002709	0.001693
2	6	0	1.527575	0.353702	0.000226
3	6	0	2.482295	-0.342391	-0.767613
4	6	0	2.076699	1.403411	0.763509
5	6	0	3.840413	-0.047842	-0.808905
6	6	0	3.423763	1.745240	0.795930
7	6	0	4.282239	1.001817	-0.008836
8	6	0	-0.455987	-1.504268	0.002100
9	6	0	-1.533276	-1.984144	-0.769079
10	6	0	0.171826	-2.501846	0.773985
11	6	0	-1.960504	-3.306537	-0.805606
12	6	0	-0.209327	-3.838314	0.811505
13	6	0	-1.279155	-4.211512	0.003169
14	6	0	-1.072588	1.143114	0.001299
15	6	0	-2.259990	1.092665	0.758891
16	6	0	-0.939033	2.324398	-0.755840
17	6	0	-3.225048	2.092753	0.796332
18	6	0	-1.867946	3.357937	-0.791546
19	6	0	-3.001623	3.214384	0.003140
20	9	0	-2.479625	0.012932	1.549219
21	9	0	1.251714	2.123334	1.563637
22	9	0	2.059959	-1.354140	-1.565834
23	9	0	1.203124	-2.145128	1.579168
24	9	0	-2.192987	-1.113647	-1.572988
25	9	0	0.153065	2.467709	-1.546889
26	1	0	3.787758	2.555985	1.424647
27	1	0	4.523301	-0.611529	-1.442176
28	1	0	0.305175	-4.556541	1.447546
29	1	0	-2.788488	-3.617190	-1.440476
30	1	0	-4.111451	2.001138	1.421627
31	1	0	-1.714306	4.236516	-1.415701
32	9	0	5.597590	1.311816	-0.013724
33	9	0	-1.672434	-5.504442	0.003814
34	9	0	-3.922018	4.203791	0.004634

Table S13: Optimized Cartesian coordinates of [**2**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.194108	0.977354	1.621070
2	6	0	2.376371	1.508803	2.624149
3	6	0	4.550933	1.265716	1.836537
4	6	0	2.803836	2.276882	3.712973
5	6	0	5.071965	2.023160	2.889350
6	6	0	4.164982	2.522443	3.813806
7	1	0	2.094158	2.657744	4.446068
8	1	0	6.142771	2.200923	2.979288
9	6	0	1.097856	0.359751	-0.074550
10	6	0	0.081170	-0.590615	0.069372
11	6	0	0.619583	1.569399	-0.602538
12	6	0	-1.260008	-0.423051	-0.292126
13	6	0	-0.697069	1.829855	-0.993949
14	6	0	-1.617482	0.804236	-0.829830
15	1	0	-1.985534	-1.222635	-0.149238
16	1	0	-0.982458	2.800365	-1.397666
17	6	0	3.150262	-1.450060	0.298477
18	6	0	3.256915	-2.195250	-0.886233
19	6	0	3.493142	-2.202678	1.426985
20	6	0	3.691915	-3.520305	-0.985820
21	6	0	3.937505	-3.529267	1.427672
22	6	0	4.032318	-4.161435	0.196921
23	1	0	3.747448	-4.023464	-1.950222
24	1	0	4.190201	-4.037593	2.357125
25	5	0	2.717338	0.157008	0.252536
26	9	0	1.029848	1.272514	2.590187
27	9	0	5.478359	0.760392	0.976573
28	9	0	2.889382	-1.621112	-2.065311
29	9	0	3.383776	-1.640210	2.668437
30	9	0	1.477153	2.618758	-0.736769
31	9	0	0.370859	-1.805224	0.626631
32	9	0	3.439281	0.747182	-0.845312
33	9	0	-2.919885	1.013973	-1.200484
34	9	0	4.629508	3.272639	4.862138
35	9	0	4.465017	-5.460710	0.148176

Table S14: Optimized Cartesian coordinates of **3**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000787	-0.004592	0.001125
2	6	0	1.530566	0.353861	0.001366
3	6	0	2.461948	-0.341948	-0.790977
4	6	0	2.053254	1.394376	0.791416
5	6	0	3.818543	-0.014321	-0.805263
6	6	0	3.412398	1.710830	0.800412
7	6	0	4.307655	1.012545	-0.003812
8	6	0	-0.456349	-1.507742	0.000117
9	6	0	-1.524411	-1.962113	-0.795213
10	6	0	0.174629	-2.482031	0.794995
11	6	0	-1.927062	-3.298247	-0.807156
12	6	0	-0.239195	-3.814842	0.806441
13	6	0	-1.291203	-4.236862	-0.000537
14	6	0	-1.072743	1.143015	0.000794
15	6	0	-2.233669	1.082503	0.793415
16	6	0	-0.930343	2.297258	-0.791205
17	6	0	-3.180196	2.108080	0.806038
18	6	0	-1.885341	3.314813	-0.802052
19	6	0	-3.017397	3.232369	0.002673
20	9	0	-2.443084	0.025367	1.607630
21	9	0	1.239296	2.100971	1.605411
22	9	0	2.048734	-1.338021	-1.604300
23	9	0	1.191704	-2.133581	1.612588
24	9	0	-2.173393	-1.103695	-1.611534
25	9	0	0.138810	2.431634	-1.605733
26	9	0	4.660494	-0.703374	-1.601813
27	9	0	3.858296	2.705506	1.594156
28	9	0	-1.704400	4.388148	-1.597915
29	9	0	-4.262714	2.004023	1.603251
30	9	0	-2.944661	-3.678926	-1.605797
31	9	0	0.390965	-4.699831	1.605125
32	1	0	-1.609962	-5.278969	-0.000829
33	1	0	5.367981	1.264133	-0.005974
34	1	0	-3.759724	4.030186	0.003960

Table S15: Optimized Cartesian coordinates of [**3**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.196017	0.978046	1.619247
2	6	0	2.354121	1.490913	2.611835
3	6	0	4.557405	1.261255	1.807864
4	6	0	2.818305	2.251558	3.688971
5	6	0	5.036288	2.019605	2.878138
6	6	0	4.170436	2.532935	3.837330
7	1	0	4.537970	3.124136	4.674944
8	6	0	1.096520	0.359950	-0.076580
9	6	0	0.099622	-0.610507	0.070714
10	6	0	0.644940	1.582415	-0.597238
11	6	0	-1.232219	-0.400661	-0.298019
12	6	0	-0.682011	1.807036	-0.970534
13	6	0	-1.644838	0.813818	-0.831019
14	1	0	-2.681295	0.983808	-1.119146
15	6	0	3.151002	-1.453813	0.298889
16	6	0	3.249210	-2.179173	-0.898277
17	6	0	3.490557	-2.179803	1.445602
18	6	0	3.683955	-3.505446	-0.951691
19	6	0	3.926561	-3.507239	1.408375
20	6	0	4.035650	-4.192156	0.204803
21	1	0	4.373424	-5.226988	0.169953
22	5	0	2.720157	0.156974	0.246781
23	9	0	1.013854	1.254093	2.582914
24	9	0	5.487248	0.772059	0.950185
25	9	0	2.887451	-1.615570	-2.077644
26	9	0	3.389877	-1.620272	2.682304
27	9	0	1.494681	2.630830	-0.731133
28	9	0	0.383186	-1.826778	0.612139
29	9	0	3.437242	0.742085	-0.846906
30	9	0	6.373660	2.255311	2.994612
31	9	0	1.933343	2.724236	4.611563
32	9	0	4.246665	-4.144579	2.569939
33	9	0	3.755850	-4.144786	-2.153269
34	9	0	-2.144013	-1.399752	-0.129874
35	9	0	-1.046927	3.021635	-1.469857

Table S16: Optimized Cartesian coordinates of **4**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000242	-0.002620	0.001135
2	6	0	1.528587	0.354175	-0.000035
3	6	0	2.465703	-0.358733	-0.771190
4	6	0	2.053944	1.410667	0.767582
5	6	0	3.824444	-0.046454	-0.797971
6	6	0	3.409416	1.736722	0.786733
7	6	0	4.298692	1.005600	-0.007670
8	6	0	-0.456108	-1.504912	0.001162
9	6	0	-1.537834	-1.960719	-0.775354
10	6	0	0.188279	-2.485635	0.777992
11	6	0	-1.950391	-3.292397	-0.798151
12	6	0	-0.211118	-3.821385	0.801393
13	6	0	-1.284637	-4.226950	0.001725
14	6	0	-1.073046	1.143654	0.001146
15	6	0	-2.252068	1.070904	0.766796
16	6	0	-0.918942	2.315568	-0.763417
17	6	0	-3.207732	2.086042	0.791246
18	6	0	-1.864037	3.340399	-0.784842
19	6	0	-3.013230	3.225823	0.004248
20	9	0	-3.923790	4.204077	0.006354
21	9	0	-4.304858	1.984495	1.556764
22	9	0	-2.482244	0.002130	1.557592
23	9	0	1.243417	2.138166	1.564266
24	9	0	3.869081	2.737381	1.553193
25	9	0	5.599615	1.311900	-0.011683
26	9	0	4.677626	-0.738038	-1.568583
27	9	0	2.060231	-1.370787	-1.566334
28	9	0	1.217992	-2.145523	1.581088
29	9	0	0.417774	-4.717546	1.576965
30	9	0	-1.673940	-5.505543	0.002155
31	9	0	-2.972376	-3.686423	-1.573035
32	9	0	-2.204645	-1.104390	-1.577303
33	9	0	0.162640	2.471434	-1.555116
34	9	0	-1.686118	4.429253	-1.548202

Table S17: Optimized Cartesian coordinates of [**4**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.195132	0.981147	1.619600
2	6	0	2.353803	1.496079	2.609544
3	6	0	4.555093	1.261196	1.813804
4	6	0	2.801625	2.256626	3.695150
5	6	0	5.049038	2.016260	2.880706
6	6	0	4.162277	2.523647	3.830025
7	6	0	1.100025	0.359222	-0.079777
8	6	0	0.103002	-0.607853	0.075087
9	6	0	0.646430	1.577073	-0.605974
10	6	0	-1.234525	-0.414890	-0.286314
11	6	0	-0.678202	1.815778	-0.982476
12	6	0	-1.628834	0.807746	-0.825312
13	6	0	3.155361	-1.451064	0.298431
14	6	0	3.247522	-2.176957	-0.897365
15	6	0	3.497705	-2.178672	1.441484
16	6	0	3.676644	-3.505151	-0.969800
17	6	0	3.931414	-3.508387	1.418787
18	6	0	4.026796	-4.177541	0.200510
19	5	0	2.723794	0.159714	0.245682
20	9	0	1.013377	1.266657	2.579770
21	9	0	5.487444	0.771859	0.961074
22	9	0	2.884339	-1.614925	-2.075516
23	9	0	3.406024	-1.623062	2.679454
24	9	0	1.492713	2.625321	-0.748912
25	9	0	0.383263	-1.821326	0.621779
26	9	0	3.442252	0.744804	-0.845753
27	9	0	6.375909	2.254469	3.015107
28	9	0	1.933036	2.735649	4.618079
29	9	0	4.255877	-4.157009	2.563279
30	9	0	3.746002	-4.154553	-2.156786
31	9	0	-2.152812	-1.396577	-0.116701
32	9	0	-1.057460	3.015224	-1.485440
33	9	0	4.617654	3.257522	4.870598
34	9	0	-2.916268	1.017098	-1.182294
35	9	0	4.443897	-5.463097	0.154503

Table S18: Optimized Cartesian coordinates of **5**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.052507	10.286779	-2.151003
2	1	0	6.361808	11.276704	-2.501289
3	1	0	4.952796	10.230379	-2.207362
4	1	0	6.477372	9.533351	-2.833310
5	6	0	6.324502	8.912230	-0.137623
6	6	0	6.828753	8.686120	1.177772
7	1	0	7.424827	9.450573	1.673661
8	6	0	6.598709	7.492594	1.831779
9	1	0	7.028300	7.345011	2.823847
10	6	0	5.879155	6.424235	1.227673
11	6	0	5.647749	5.173889	1.916768
12	6	0	5.493717	5.157752	3.355241
13	6	0	5.924957	4.054129	4.142622
14	1	0	6.423863	3.217670	3.650819
15	6	0	5.794108	4.036262	5.516525
16	1	0	6.183688	3.183647	6.070660
17	6	0	5.186024	5.124170	6.211311
18	6	0	5.395852	6.652650	-0.090732
19	1	0	4.802067	5.877397	-0.577348
20	6	0	5.594534	7.849452	-0.748820
21	1	0	5.162272	7.982198	-1.739439
22	6	0	5.566231	3.938588	1.167978
23	6	0	4.724732	2.868406	1.580348
24	1	0	4.093900	3.002655	2.460311
25	6	0	4.628733	1.691810	0.865219
26	1	0	3.933099	0.925706	1.203982
27	6	0	5.400786	1.485007	-0.316647
28	6	0	6.258182	2.547597	-0.730717
29	1	0	6.892894	2.426684	-1.607097
30	6	0	6.321225	3.728757	-0.019284
31	1	0	7.013560	4.505135	-0.348610
32	6	0	4.737470	6.229494	5.428620
33	1	0	4.235343	7.069388	5.906114
34	6	0	4.901745	6.243635	4.058195
35	1	0	4.515359	7.091905	3.491045
36	6	0	4.451836	6.248178	8.265489
37	1	0	3.401819	6.408253	7.969408
38	1	0	4.476938	6.057235	9.343067
39	1	0	5.016772	7.173176	8.068355
40	6	0	4.474939	-0.774594	-0.554080
41	1	0	3.409715	-0.489687	-0.550858
42	1	0	4.597179	-1.630929	-1.224944
43	1	0	4.755329	-1.093213	0.462565
44	6	0	5.465285	3.944600	8.343709
45	1	0	4.956412	3.028238	8.004743
46	1	0	6.554370	3.787440	8.273513
47	1	0	5.210596	4.106400	9.395914
48	6	0	7.234598	11.190620	-0.119756
49	1	0	6.741387	11.466623	0.825665
50	1	0	8.284011	10.928886	0.095302
51	1	0	7.228628	12.066973	-0.775663
52	6	0	6.089020	0.145120	-2.253682
53	1	0	5.841558	0.923217	-2.993262
54	1	0	7.174816	0.173909	-2.064102
55	1	0	5.844390	-0.828829	-2.689275
56	7	0	5.039127	5.106854	7.566707
57	7	0	5.323172	0.320251	-1.021096
58	7	0	6.530884	10.095066	-0.783487

Table S19: Optimized Cartesian coordinates of [**5**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.104272	2.123875	0.412205
2	6	0	3.621316	1.961168	1.837903
3	6	0	2.770703	1.834933	2.942558
4	1	0	1.689704	1.825438	2.790946
5	6	0	3.267346	1.709455	4.240875
6	1	0	2.557597	1.604914	5.060664
7	6	0	4.659726	1.704000	4.492560
8	6	0	5.517826	1.813002	3.368785
9	1	0	6.599409	1.787953	3.497453
10	6	0	5.003882	1.950529	2.083192
11	1	0	5.694471	2.030951	1.242050
12	6	0	3.284709	3.537890	-0.130454
13	6	0	3.423386	4.657176	0.698782
14	1	0	3.428943	4.526858	1.782604
15	6	0	3.566465	5.943869	0.177024
16	1	0	3.680642	6.775956	0.870778
17	6	0	3.577472	6.168345	-1.219863
18	6	0	3.456077	5.029457	-2.056209
19	1	0	3.484723	5.136253	-3.140113
20	6	0	3.301324	3.756112	-1.517535
21	1	0	3.211942	2.902684	-2.191781
22	6	0	1.686765	1.591428	0.228200
23	6	0	0.575875	2.429990	0.078111
24	1	0	0.716681	3.512443	0.064058
25	6	0	-0.715099	1.919311	-0.065751
26	1	0	-1.540135	2.619912	-0.189064
27	6	0	-0.952665	0.524471	-0.066187
28	6	0	0.177747	-0.321441	0.066770
29	1	0	0.060656	-1.404456	0.046508
30	6	0	1.455603	0.206439	0.222350
31	1	0	2.302155	-0.475114	0.320904
32	6	0	-2.411641	-1.419857	-0.415020
33	1	0	-1.964412	-2.009715	0.400595
34	1	0	-3.484517	-1.647788	-0.437632
35	1	0	-1.963264	-1.762368	-1.368687
36	6	0	3.936945	7.610462	-3.174774
37	1	0	3.956093	8.681213	-3.412790
38	1	0	4.895880	7.163708	-3.504427
39	1	0	3.128830	7.153459	-3.767402
40	6	0	6.587493	1.368475	5.976349
41	1	0	7.186079	2.174107	5.522621
42	1	0	6.804546	1.361217	7.051692
43	1	0	6.929579	0.406312	5.546163
44	6	0	4.268030	1.268138	6.875784
45	1	0	3.461647	2.013197	6.966895
46	1	0	3.798213	0.271157	6.759556
47	1	0	4.832812	1.275123	7.816249
48	6	0	4.040457	8.553461	-0.873106
49	1	0	3.295903	8.666640	-0.069076
50	1	0	5.035993	8.436032	-0.400470
51	1	0	4.043065	9.483321	-1.455259
52	6	0	-3.332397	0.889754	-0.542228
53	1	0	-3.441632	1.700520	0.195578
54	1	0	-3.205998	1.353541	-1.540820
55	1	0	-4.267569	0.316186	-0.544738
56	7	0	-2.236569	0.004730	-0.184607
57	7	0	3.694771	7.447829	-1.750676
58	7	0	5.165916	1.603303	5.783330
59	9	0	3.952179	1.276378	-0.412059

Table S20: Optimized Cartesian coordinates of **6**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.542489	10.026083	-0.762924
2	6	0	6.064640	10.280045	-2.099859
3	1	0	6.412351	11.288784	-2.343482
4	1	0	4.965252	10.246952	-2.134116
5	1	0	6.491527	9.556433	-2.810358
6	6	0	6.279306	8.841810	-0.187311
7	6	0	6.804588	8.662232	1.114293
8	1	0	7.400606	9.465228	1.549737
9	6	0	6.576867	7.485606	1.797021
10	1	0	7.016146	7.347668	2.785780
11	6	0	5.840501	6.416262	1.208437
12	6	0	5.608744	5.177082	1.919278
13	6	0	5.459383	5.184630	3.358702
14	6	0	5.901776	4.089613	4.157230
15	1	0	6.406190	3.250454	3.676698
16	6	0	5.769302	4.102221	5.529921
17	1	0	6.142793	3.281672	6.143840
18	6	0	5.157512	5.202781	6.175562
19	6	0	5.337156	6.615026	-0.104771
20	1	0	4.732112	5.832946	-0.565393
21	6	0	5.533773	7.803972	-0.789598
22	1	0	5.098038	7.933172	-1.779456
23	6	0	5.529174	3.929428	1.189927
24	6	0	4.679666	2.876778	1.622968
25	1	0	4.047269	3.031773	2.498144
26	6	0	4.578501	1.684775	0.922497
27	1	0	3.885453	0.916958	1.263595
28	6	0	5.359563	1.488843	-0.238109
29	6	0	6.225780	2.516437	-0.680806
30	1	0	6.840333	2.333727	-1.563198
31	6	0	6.295187	3.709218	0.008004
32	1	0	6.992036	4.479385	-0.324988
33	6	0	4.695625	6.294844	5.407731
34	1	0	4.195333	7.137866	5.882310
35	6	0	4.861281	6.283359	4.031495
36	1	0	4.470758	7.116087	3.444895
37	8	0	5.063467	5.113348	7.511876
38	8	0	5.352330	0.373874	-0.986199
39	6	0	4.475572	6.203164	8.251748
40	1	0	3.425794	6.353017	7.957799
41	1	0	4.525928	5.898569	9.301742
42	1	0	5.050185	7.129830	8.104376
43	6	0	4.516016	-0.733722	-0.593473
44	1	0	3.454316	-0.444530	-0.604786
45	1	0	4.695837	-1.510386	-1.343327
46	1	0	4.801089	-1.103987	0.402639

Table S21: Optimized Cartesian coordinates of [**6**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.058018	1.447701	5.709893
2	8	0	3.846770	7.373977	-1.635978
3	8	0	-2.165054	0.116927	-0.332458
4	6	0	3.174803	2.050458	0.343464
5	6	0	3.677748	1.873839	1.775217
6	6	0	2.805497	1.774358	2.870870
7	1	0	1.726883	1.797765	2.707019
8	6	0	3.291886	1.640658	4.169291
9	1	0	2.612472	1.562177	5.019675
10	6	0	4.674960	1.591878	4.402647
11	6	0	5.561044	1.686941	3.317791
12	1	0	6.639586	1.648352	3.468623
13	6	0	5.056132	1.833920	2.022979
14	1	0	5.751736	1.905046	1.185490
15	6	0	3.368939	3.471146	-0.184017
16	6	0	3.477874	4.581723	0.667977
17	1	0	3.448348	4.438719	1.749439
18	6	0	3.628680	5.869193	0.157796
19	1	0	3.714440	6.731207	0.821484
20	6	0	3.685685	6.075942	-1.229134
21	6	0	3.581264	4.975797	-2.095124
22	1	0	3.625732	5.105818	-3.176160
23	6	0	3.417070	3.692618	-1.566648
24	1	0	3.338953	2.843100	-2.246766
25	6	0	1.750466	1.533861	0.146665
26	6	0	0.648567	2.395899	0.028392
27	1	0	0.802297	3.476075	0.050641
28	6	0	-0.643363	1.897377	-0.122536
29	1	0	-1.498567	2.568850	-0.215594
30	6	0	-0.863531	0.512121	-0.170365
31	6	0	0.227743	-0.363792	-0.056670
32	1	0	0.087232	-1.443777	-0.094092
33	6	0	1.515675	0.153218	0.107715
34	1	0	2.358195	-0.534624	0.193211
35	6	0	-2.430833	-1.284656	-0.389168
36	1	0	-2.129043	-1.791275	0.543367
37	1	0	-3.515652	-1.377203	-0.518702
38	1	0	-1.918502	-1.758596	-1.243735
39	6	0	3.912765	7.626182	-3.039675
40	1	0	4.040270	8.710371	-3.141902
41	1	0	4.771929	7.111438	-3.502536
42	1	0	2.984572	7.317120	-3.549864
43	6	0	6.456999	1.390605	5.988897
44	1	0	6.969210	2.317075	5.677985
45	1	0	6.539571	1.276677	7.076268
46	1	0	6.932743	0.527196	5.493304
47	9	0	4.017508	1.206890	-0.477392

Table S22: Optimized Cartesian coordinates of **7**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.484217	10.061618	-0.740148
2	6	0	6.068967	10.306120	-2.103925
3	1	0	6.384732	11.331372	-2.318808
4	1	0	4.976089	10.224140	-2.195255
5	1	0	6.568589	9.607659	-2.790663
6	6	0	6.249221	8.872401	-0.179583
7	6	0	6.715427	8.720350	1.151530
8	1	0	7.251132	9.551573	1.611528
9	6	0	6.506578	7.539658	1.825475
10	1	0	6.902133	7.422479	2.834675
11	6	0	5.851557	6.431605	1.200172
12	6	0	5.639573	5.196931	1.896323
13	6	0	5.506427	5.178802	3.346895
14	6	0	6.025433	4.097858	4.106103
15	1	0	6.562618	3.296377	3.597615
16	6	0	5.908383	4.087280	5.491779
17	1	0	6.338019	3.265618	6.066638
18	6	0	5.244826	5.132166	6.148594
19	1	0	5.142828	5.113565	7.235112
20	6	0	5.408756	6.605322	-0.144936
21	1	0	4.860236	5.797503	-0.630368
22	6	0	5.583929	7.798530	-0.819651
23	1	0	5.191919	7.910344	-1.829647
24	6	0	5.552966	3.940469	1.163709
25	6	0	4.665256	2.918003	1.588412
26	1	0	4.017006	3.095676	2.447383
27	6	0	4.574153	1.723516	0.882221
28	1	0	3.866188	0.957050	1.200839
29	6	0	5.385973	1.506603	-0.239199
30	1	0	5.321966	0.562013	-0.782266
31	6	0	6.284046	2.495426	-0.662129
32	1	0	6.932917	2.313847	-1.520190
33	6	0	6.360455	3.704895	0.020560
34	1	0	7.087026	4.459229	-0.284660
35	6	0	4.706754	6.197984	5.415087
36	1	0	4.169247	6.997611	5.926887
37	6	0	4.845180	6.231571	4.031725
38	1	0	4.393779	7.042532	3.458565

Table S23: Optimized Cartesian coordinates of [**7**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.087346	0.298420	-0.453845
2	6	0	3.283554	2.077162	0.368724
3	6	0	3.742521	1.903711	1.818767
4	6	0	2.832132	1.856674	2.882624
5	1	0	1.761556	1.915411	2.679910
6	6	0	3.284467	1.727942	4.200869
7	1	0	2.561415	1.692025	5.018430
8	6	0	4.651806	1.635248	4.468755
9	6	0	5.566774	1.677470	3.410551
10	1	0	6.637865	1.602297	3.609846
11	6	0	5.116688	1.817065	2.096719
12	1	0	5.831527	1.847995	1.273378
13	6	0	3.527186	3.492571	-0.162040
14	6	0	3.617585	4.602373	0.688387
15	1	0	3.541707	4.465166	1.768329
16	6	0	3.811765	5.885750	0.164428
17	1	0	3.881123	6.739850	0.841278
18	6	0	3.927686	6.071802	-1.214539
19	6	0	3.842387	4.967090	-2.069493
20	1	0	3.934699	5.102278	-3.149217
21	6	0	3.637479	3.688684	-1.548518
22	1	0	3.572795	2.828737	-2.216444
23	6	0	1.850968	1.602434	0.133263
24	6	0	0.777160	2.496020	-0.009092
25	1	0	0.959345	3.571526	0.021144
26	6	0	-0.523468	2.034415	-0.195157
27	1	0	-1.356613	2.729976	-0.308437
28	6	0	-0.780865	0.655864	-0.255336
29	6	0	0.282253	-0.250783	-0.117443
30	1	0	0.112787	-1.326210	-0.163641
31	6	0	1.579549	0.229011	0.081957
32	1	0	2.399678	-0.482976	0.185375
33	6	0	-2.390125	-1.094768	-0.535554
34	1	0	-2.131487	-1.620188	0.399461
35	1	0	-3.472564	-1.155020	-0.698975
36	1	0	-1.865129	-1.572700	-1.380010
37	1	0	5.004865	1.527467	5.496370
38	1	0	4.087028	7.071730	-1.623183
39	9	0	4.127319	1.210281	-0.415465

Table S24: Optimized Cartesian coordinates of **8**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.253605	8.848074	-0.158496
2	6	0	6.794965	8.670077	1.122619
3	1	0	7.390202	9.461907	1.579385
4	6	0	6.582933	7.480104	1.807477
5	1	0	7.032782	7.327406	2.789116
6	6	0	5.845413	6.422955	1.206641
7	6	0	5.632443	5.174030	1.910329
8	6	0	5.484642	5.170044	3.352251
9	6	0	5.962761	4.078865	4.129047
10	1	0	6.487390	3.260193	3.635349
11	6	0	5.833022	4.087907	5.512215
12	1	0	6.233175	3.261489	6.101204
13	6	0	5.199041	5.163177	6.150827
14	1	0	5.088537	5.160503	7.236747
15	6	0	5.319703	6.618411	-0.100227
16	1	0	4.712328	5.835219	-0.555157
17	6	0	5.510883	7.824107	-0.763421
18	1	0	5.074904	7.976335	-1.751742
19	6	0	5.566378	3.928422	1.171885
20	6	0	4.717580	2.872296	1.603609
21	1	0	4.075410	3.023855	2.471845
22	6	0	4.647682	1.685544	0.884594
23	1	0	3.968351	0.894616	1.205462
24	6	0	5.440688	1.509393	-0.258210
25	1	0	5.391728	0.570681	-0.813056
26	6	0	6.295682	2.532187	-0.692680
27	1	0	6.925739	2.381895	-1.570412
28	6	0	6.349517	3.734944	0.000687
29	1	0	7.040182	4.517333	-0.315898
30	6	0	4.706207	6.241694	5.402603
31	1	0	4.194824	7.065349	5.902696
32	6	0	4.858414	6.257325	4.021765
33	1	0	4.443809	7.078622	3.436185
34	1	0	6.411534	9.789242	-0.688312

Table S25: Optimized Cartesian coordinates of [**8**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.281343	2.077809	0.377205
2	6	0	3.738572	1.912635	1.828623
3	6	0	2.829992	1.877067	2.894503
4	1	0	1.759014	1.940810	2.695594
5	6	0	3.284813	1.752853	4.212263
6	1	0	2.563358	1.724977	5.031468
7	6	0	4.652150	1.653642	4.477529
8	6	0	5.564965	1.684445	3.417172
9	1	0	6.636008	1.603926	3.614351
10	6	0	5.112831	1.818881	2.103551
11	1	0	5.826022	1.840188	1.278515
12	6	0	3.526463	3.488079	-0.165950
13	6	0	3.636829	4.602358	0.676200
14	1	0	3.574616	4.472849	1.757945
15	6	0	3.834555	5.880702	0.141362
16	1	0	3.920105	6.738416	0.811713
17	6	0	3.933752	6.056937	-1.240122
18	6	0	3.828239	4.947603	-2.086860
19	1	0	3.907617	5.075158	-3.168501
20	6	0	3.620008	3.674297	-1.555112
21	1	0	3.540607	2.810991	-2.217171
22	6	0	1.843410	1.603006	0.153325
23	6	0	0.774061	2.503259	0.054998
24	1	0	0.964032	3.576646	0.105832
25	6	0	-0.534279	2.036976	-0.115549
26	1	0	-1.356129	2.751899	-0.191951
27	6	0	-0.786328	0.665978	-0.199763
28	6	0	0.277528	-0.238195	-0.106742
29	1	0	0.090821	-1.311969	-0.175037
30	6	0	1.581625	0.225602	0.074928
31	1	0	2.409368	-0.481082	0.145309
32	1	0	5.006800	1.549180	5.504896
33	1	0	4.095987	7.052860	-1.657259
34	1	0	-1.806012	0.302041	-0.340987
35	9	0	4.116153	1.203316	-0.402810

Table S26: Optimized Cartesian coordinates of **9**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.261677	8.869472	-0.166516
2	6	0	6.893848	8.646502	1.070049
3	6	0	6.667285	7.454385	1.745771
4	6	0	5.845723	6.419503	1.208286
5	6	0	5.632426	5.171688	1.909651
6	6	0	5.484337	5.169714	3.349461
7	6	0	6.043373	4.140629	4.163462
8	6	0	5.923816	4.143617	5.547254
9	6	0	5.191983	5.167952	6.174680
10	6	0	5.244858	6.683267	-0.058178
11	6	0	5.424973	7.887304	-0.726668
12	6	0	5.566241	3.928365	1.172021
13	6	0	4.657832	2.887971	1.529089
14	6	0	4.574199	1.699826	0.814561
15	6	0	5.439454	1.486177	-0.273553
16	6	0	6.366937	2.473923	-0.650776
17	6	0	6.407082	3.673614	0.048008
18	6	0	4.604051	6.193218	5.412230
19	6	0	4.770408	6.198145	4.033287
20	9	0	4.163530	7.169016	3.343167
21	9	0	3.893824	7.139838	6.015899
22	9	0	5.056538	5.167031	7.486131
23	9	0	6.496047	3.196360	6.282204
24	9	0	6.779147	3.171240	3.610533
25	9	0	3.792245	3.065540	2.532129
26	9	0	3.685447	0.768698	1.143146
27	9	0	5.380510	0.352829	-0.944489
28	9	0	7.195669	2.248191	-1.664206
29	9	0	7.328944	4.569085	-0.319506
30	9	0	4.412601	5.792205	-0.606163
31	9	0	4.813635	8.122818	-1.882420
32	9	0	6.454548	10.006843	-0.804826
33	9	0	7.702197	9.572310	1.574311
34	9	0	7.316645	7.266971	2.899185

Table S27: Optimized Cartesian coordinates of [**9**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.205362	2.153395	0.439021
2	6	0	3.695243	1.962451	1.884679
3	6	0	2.858392	1.787478	2.996987
4	6	0	3.359304	1.554889	4.281416
5	6	0	4.737057	1.501544	4.491351
6	6	0	5.601675	1.697988	3.412174
7	6	0	5.079610	1.935357	2.139739
8	6	0	3.473544	3.559818	-0.123737
9	6	0	3.719219	4.699936	0.656157
10	6	0	4.023931	5.941846	0.090887
11	6	0	4.080000	6.079617	-1.295878
12	6	0	3.813916	4.972577	-2.104945
13	6	0	3.506023	3.743830	-1.519163
14	6	0	1.770491	1.652662	0.200383
15	6	0	0.671118	2.476579	-0.083564
16	6	0	-0.599626	1.961347	-0.356687
17	6	0	-0.809228	0.582605	-0.340461
18	6	0	0.255679	-0.267801	-0.034634
19	6	0	1.514307	0.268766	0.240707
20	9	0	4.025220	1.288730	-0.340179
21	9	0	2.481991	-0.600555	0.578094
22	9	0	0.061217	-1.593594	0.008131
23	9	0	-2.020689	0.080119	-0.601953
24	9	0	-1.617884	2.791152	-0.627750
25	9	0	0.775347	3.821016	-0.078268
26	9	0	1.516349	1.866668	2.891261
27	9	0	2.517009	1.389903	5.312065
28	9	0	5.225888	1.278265	5.715978
29	9	0	6.928100	1.673818	3.605593
30	9	0	5.965189	2.169160	1.156347
31	9	0	3.644169	4.664996	2.002243
32	9	0	4.256566	7.001286	0.879745
33	9	0	4.372643	7.262868	-1.846147
34	9	0	3.840714	5.098189	-3.439425
35	9	0	3.209891	2.732660	-2.353226

Table S28: Optimized Cartesian coordinates of **10**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000726	-0.000474	0.793124
2	6	0	-1.230052	-1.195232	0.312318
3	6	0	-2.510404	-1.137580	0.903208
4	6	0	-0.932679	-2.175055	-0.654268
5	6	0	-3.478827	-2.065684	0.526489
6	6	0	-1.916684	-3.092039	-1.026852
7	6	0	-3.183511	-3.038468	-0.437277
8	6	0	1.653414	-0.466911	0.318052
9	6	0	2.267348	-1.563169	0.959790
10	6	0	2.328553	0.237224	-0.696854
11	6	0	3.555703	-1.939704	0.585554
12	6	0	3.614822	-0.158699	-1.066730
13	6	0	4.226315	-1.241153	-0.426504
14	6	0	-0.420751	1.663700	0.317055
15	6	0	0.266151	2.740708	0.916932
16	6	0	-1.415247	1.899969	-0.651107
17	6	0	-0.055233	4.045474	0.548866
18	6	0	-1.718728	3.212698	-1.015618
19	6	0	-1.043135	4.280215	-0.416193
20	9	0	0.003007	-0.002999	2.377516
21	1	0	-1.947578	1.066499	-1.111702
22	1	0	-2.488352	3.401420	-1.765215
23	1	0	-1.288708	5.304902	-0.700346
24	1	0	0.464034	4.882575	1.017450
25	1	0	1.033035	2.560679	1.672751
26	1	0	1.855127	1.088094	-1.189139
27	1	0	4.142378	0.384432	-1.851949
28	1	0	5.235039	-1.541968	-0.714498
29	1	0	4.039952	-2.778863	1.086881
30	1	0	1.749606	-2.105871	1.752938
31	1	0	0.058398	-2.221709	-1.108108
32	1	0	-1.690598	-3.852905	-1.775054
33	1	0	-3.947597	-3.761473	-0.727810
34	1	0	-4.466848	-2.032839	0.987704
35	1	0	-2.742873	-0.384496	1.658589

Table S29: Optimized Cartesian coordinates of [**10**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.001416	0.008424	0.000245
2	9	0	-0.002539	0.006347	1.701382
3	9	0	-0.001540	0.017510	-1.700874
4	6	0	0.031715	1.848422	0.006449
5	6	0	-0.625381	2.576112	-1.000113
6	6	0	0.715876	2.543634	1.018001
7	6	0	-0.611282	3.972981	-0.983356
8	6	0	0.755141	3.940074	1.010925
9	6	0	0.085344	4.658243	0.016202
10	6	0	1.575240	-0.942151	-0.001686
11	6	0	1.859543	-1.850804	1.032460
12	6	0	2.510175	-0.773722	-1.037627
13	6	0	3.046782	-2.586697	1.019579
14	6	0	3.710306	-1.488879	-1.028725
15	6	0	3.978601	-2.402883	-0.005819
16	6	0	-1.608574	-0.889247	-0.004124
17	6	0	-1.920563	-1.783188	-1.043127
18	6	0	-2.539247	-0.695306	1.031173
19	6	0	-3.131567	-2.479386	-1.036110
20	6	0	-3.762496	-1.370144	1.016422
21	6	0	-4.058916	-2.269561	-0.011681
22	1	0	2.297023	-0.082180	-1.851685
23	1	0	4.434495	-1.335277	-1.831418
24	1	0	4.911608	-2.970384	-0.007949
25	1	0	3.246164	-3.301295	1.820771
26	1	0	1.150224	-1.982428	1.848491
27	1	0	1.217456	1.990052	1.810955
28	1	0	1.305155	4.467907	1.792710
29	1	0	0.106138	5.750088	0.019926
30	1	0	-1.140671	4.526815	-1.761387
31	1	0	-1.147717	2.047662	-1.796792
32	1	0	-1.213945	-1.934462	-1.858062
33	1	0	-2.304870	-0.015294	1.849097
34	1	0	-4.482833	-1.196629	1.818499
35	1	0	-3.352811	-3.183344	-1.840952
36	1	0	-5.010260	-2.805732	-0.014156

Table S30: Optimized Cartesian coordinates of **11**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.014739	-0.013325	0.755821
2	6	0	-1.233517	-1.195528	0.240484
3	6	0	-2.502344	-1.165773	0.862064
4	6	0	-1.013356	-2.180170	-0.746585
5	6	0	-3.499567	-2.084783	0.542644
6	6	0	-2.002148	-3.106724	-1.081765
7	6	0	-3.244090	-3.060136	-0.433300
8	6	0	1.677609	-0.462347	0.323078
9	6	0	2.311641	-1.512142	1.019764
10	6	0	2.343854	0.221008	-0.711905
11	6	0	3.614456	-1.865434	0.676401
12	6	0	3.645914	-0.150595	-1.046498
13	6	0	4.278084	-1.189281	-0.355399
14	6	0	-0.413059	1.646588	0.292318
15	6	0	0.324627	2.709103	0.858478
16	6	0	-1.456743	1.903221	-0.616953
17	6	0	0.002601	4.020172	0.515538
18	6	0	-1.759521	3.221581	-0.957383
19	6	0	-1.034612	4.275036	-0.390897
20	9	0	-0.018191	-0.086456	2.332598
21	9	0	-2.768023	-0.233507	1.786977
22	9	0	-4.684288	-2.040233	1.147178
23	9	0	-4.185568	-3.936427	-0.749776
24	9	0	-1.774003	-4.027041	-2.016705
25	9	0	0.149526	-2.246832	-1.405998
26	1	0	-2.026167	1.082254	-1.055207
27	1	0	-2.566469	3.426520	-1.661960
28	1	0	-1.280053	5.304876	-0.655719
29	1	0	0.560315	4.846461	0.958227
30	1	0	1.130426	2.513578	1.568677
31	1	0	1.851905	1.033861	-1.248011
32	1	0	4.169073	0.375680	-1.845902
33	1	0	5.298266	-1.473140	-0.619070
34	1	0	4.115741	-2.669153	1.217326
35	1	0	1.800227	-2.035703	1.829431

Table S31: Optimized Cartesian coordinates of [**11**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.024488	-0.013301	-0.000162
2	9	0	-0.049634	-0.135102	1.685223
3	9	0	-0.144453	0.033572	-1.684352
4	6	0	0.034250	1.820977	0.087871
5	6	0	-0.439038	2.612646	-0.973066
6	6	0	0.585095	2.451075	1.218010
7	6	0	-0.375338	4.005901	-0.895307
8	6	0	0.670724	3.843262	1.277040
9	6	0	0.184334	4.624850	0.225306
10	6	0	1.562239	-0.935547	-0.087676
11	6	0	1.993138	-1.736542	0.984339
12	6	0	2.379167	-0.822168	-1.227174
13	6	0	3.210027	-2.418268	0.910277
14	6	0	3.606630	-1.485021	-1.283072
15	6	0	4.022807	-2.289926	-0.218894
16	6	0	-1.643949	-0.912975	-0.000418
17	6	0	-1.799567	-2.139002	-0.659263
18	6	0	-2.767705	-0.396129	0.656274
19	6	0	-3.014111	-2.830226	-0.662365
20	6	0	-3.998005	-1.059096	0.653155
21	6	0	-4.119781	-2.284379	-0.006201
22	9	0	-0.764053	-2.713650	-1.298466
23	9	0	-3.124745	-4.014134	-1.287419
24	9	0	-5.292165	-2.933868	-0.008815
25	9	0	-5.062529	-0.526232	1.275680
26	9	0	-2.706974	0.784478	1.299021
27	1	0	2.053855	-0.216310	-2.071009
28	1	0	4.235883	-1.376643	-2.168603
29	1	0	4.977847	-2.816813	-0.270253
30	1	0	3.524417	-3.048780	1.744292
31	1	0	1.376009	-1.827887	1.876050
32	1	0	0.946115	1.851178	2.051432
33	1	0	1.112708	4.317924	2.155226
34	1	0	0.240712	5.713993	0.279566
35	1	0	-0.761604	4.608362	-1.719793
36	1	0	-0.858394	2.139683	-1.859173

Table S32: Optimized Cartesian coordinates of **12**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.034053	0.024755	0.735686
2	6	0	-1.205204	-1.177236	0.270268
3	6	0	-2.461114	-1.122418	0.917820
4	6	0	-1.012501	-2.185279	-0.699023
5	6	0	-3.472101	-2.038928	0.637949
6	6	0	-2.015289	-3.108260	-0.995674
7	6	0	-3.244158	-3.036209	-0.323029
8	6	0	1.683261	-0.452729	0.244715
9	6	0	2.267338	-1.593822	0.839703
10	6	0	2.454302	0.263095	-0.697356
11	6	0	3.566154	-1.994843	0.542063
12	6	0	3.757195	-0.127211	-1.010222
13	6	0	4.312889	-1.254139	-0.388227
14	6	0	-0.431660	1.674286	0.291915
15	6	0	0.121008	2.753359	1.012966
16	6	0	-1.321857	1.896894	-0.775843
17	6	0	-0.231449	4.053590	0.659073
18	6	0	-1.655361	3.205888	-1.121071
19	6	0	-1.112466	4.278868	-0.406220
20	9	0	0.093853	-0.002965	2.307367
21	9	0	1.554168	-2.323614	1.709481
22	9	0	4.096350	-3.068969	1.119653
23	9	0	5.547639	-1.626645	-0.684228
24	9	0	4.470205	0.561512	-1.898076
25	9	0	1.956067	1.330080	-1.331434
26	9	0	-2.694337	-0.171807	1.831292
27	9	0	-4.642006	-1.972461	1.266084
28	9	0	-4.197851	-3.909816	-0.602216
29	9	0	-1.814584	-4.048878	-1.915156
30	9	0	0.138608	-2.276198	-1.379319
31	1	0	-1.749129	1.060567	-1.331555
32	1	0	-2.344756	3.388128	-1.946315
33	1	0	-1.381396	5.300989	-0.677820
34	1	0	0.180123	4.894610	1.218529
35	1	0	0.801848	2.580369	1.848106

Table S33: Optimized Cartesian coordinates of [**12**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.002030	-0.000278	0.001999
2	9	0	-0.119484	-0.047411	1.674967
3	9	0	-0.018181	0.126564	-1.670619
4	6	0	0.034430	1.842817	0.093539
5	6	0	-0.904359	2.640003	-0.575821
6	6	0	1.021462	2.506925	0.835391
7	6	0	-0.873465	4.034890	-0.508019
8	6	0	1.084142	3.901119	0.902593
9	6	0	0.128974	4.667844	0.231199
10	6	0	1.569496	-0.941150	0.001069
11	6	0	1.985059	-1.632870	1.153569
12	6	0	2.375336	-0.982130	-1.151516
13	6	0	3.177963	-2.357588	1.146377
14	6	0	3.577021	-1.692422	-1.142953
15	6	0	3.979154	-2.385529	0.001859
16	6	0	-1.610686	-0.899922	-0.089038
17	6	0	-1.737033	-2.073403	-0.845991
18	6	0	-2.753220	-0.453283	0.589620
19	6	0	-2.939264	-2.781626	-0.918490
20	6	0	-3.970854	-1.134240	0.517155
21	6	0	-4.062227	-2.306528	-0.237090
22	9	0	-0.685200	-2.581573	-1.511494
23	9	0	-3.020128	-3.914907	-1.632837
24	9	0	-5.221399	-2.972379	-0.306108
25	9	0	-5.052028	-0.667252	1.160331
26	9	0	-2.728277	0.679923	1.313515
27	9	0	-1.900948	2.083108	-1.287143
28	9	0	-1.800812	4.768789	-1.142100
29	9	0	0.173912	6.004147	0.295388
30	9	0	2.056541	4.506373	1.602108
31	9	0	1.972416	1.817842	1.489979
32	1	0	2.061834	-0.462877	-2.054737
33	1	0	4.197534	-1.708133	-2.040868
34	1	0	4.915627	-2.947024	0.001771
35	1	0	3.483539	-2.897484	2.044488
36	1	0	1.378301	-1.601441	2.056034

Table S34: Optimized Cartesian coordinates of **13**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.003687	-0.007611	0.700740
2	6	0	-1.226054	-1.215676	0.237491
3	6	0	-2.494558	-1.157594	0.859577
4	6	0	-1.001389	-2.244995	-0.702897
5	6	0	-3.487175	-2.094742	0.589721
6	6	0	-1.986108	-3.190245	-0.988119
7	6	0	-3.227552	-3.116162	-0.338624
8	6	0	1.656105	-0.454656	0.238547
9	6	0	2.257893	-1.564421	0.875208
10	6	0	2.420878	0.248092	-0.718619
11	6	0	3.569161	-1.943341	0.603000
12	6	0	3.734382	-0.120674	-1.006707
13	6	0	4.308889	-1.214822	-0.342628
14	6	0	-0.439914	1.656775	0.245354
15	6	0	0.235834	2.724827	0.879727
16	6	0	-1.429587	1.980767	-0.708559
17	6	0	-0.074646	4.054054	0.608004
18	6	0	-1.750137	3.307014	-0.996384
19	6	0	-1.074240	4.343235	-0.334852
20	9	0	-0.002104	-0.012649	2.269176
21	9	0	1.551643	-2.282532	1.758535
22	9	0	4.116476	-2.985873	1.218669
23	9	0	5.553580	-1.567468	-0.614413
24	9	0	4.440097	0.555277	-1.908505
25	9	0	1.903018	1.285293	-1.389462
26	9	0	1.210787	2.460252	1.759807
27	9	0	0.569807	5.040947	1.221412
28	9	0	-1.375461	5.601375	-0.606689
29	9	0	-2.687387	3.591977	-1.895527
30	9	0	-2.083776	1.022482	-1.377385
31	9	0	-2.759683	-0.170997	1.726675
32	9	0	-4.670022	-2.024068	1.190748
33	9	0	-4.163147	-4.010259	-0.608144
34	9	0	-1.755798	-4.154872	-1.873854
35	9	0	0.161936	-2.337804	-1.359603

Table S35: Optimized Cartesian coordinates of [**13**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.000002	-0.001479	-0.000378
2	9	0	0.002054	0.001011	1.666265
3	9	0	-0.003455	-0.000291	-1.666910
4	6	0	0.031485	1.835186	-0.000346
5	6	0	-0.914206	2.582808	-0.716979
6	6	0	1.001796	2.549071	0.717891
7	6	0	-0.906783	3.979346	-0.714208
8	6	0	1.040556	3.945046	0.719304
9	6	0	0.078382	4.662538	0.003703
10	6	0	1.574996	-0.945774	-0.001852
11	6	0	1.715468	-2.133102	0.731961
12	6	0	2.689708	-0.509602	-0.733347
13	6	0	2.905949	-2.863219	0.734358
14	6	0	3.896079	-1.213417	-0.730050
15	6	0	4.002227	-2.397881	0.003508
16	6	0	-1.605815	-0.892712	0.001416
17	6	0	-1.784173	-2.077952	-0.727335
18	6	0	-2.707321	-0.415123	0.726780
19	6	0	-2.998877	-2.766983	-0.730849
20	6	0	-3.937096	-1.077151	0.722169
21	6	0	-4.081194	-2.260772	-0.006322
22	9	0	-0.768509	-2.619895	-1.421315
23	9	0	-3.129468	-3.911884	-1.415841
24	9	0	-5.251212	-2.907535	-0.009688
25	9	0	-4.979210	-0.580438	1.403672
26	9	0	-2.629791	0.731619	1.423547
27	9	0	-1.896827	1.974212	-1.403326
28	9	0	-1.841375	4.665862	-1.386794
29	9	0	0.100315	5.999290	0.005869
30	9	0	1.997372	4.598270	1.393815
31	9	0	1.963875	1.906437	1.402334
32	9	0	0.684608	-2.637416	1.431756
33	9	0	2.999726	-4.008820	1.424189
34	9	0	5.149302	-3.084496	0.005642
35	9	0	4.952002	-0.755881	-1.417690
36	9	0	2.649439	0.636037	-1.435007

Table S36: Optimized Cartesian coordinates of **14**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.094390	0.039541	0.337819
2	9	0	4.231469	-3.452236	-1.783685
3	9	0	-1.443971	2.521219	1.223903
4	9	0	-1.769131	4.862386	-0.069784
5	9	0	-0.831687	5.161679	-2.618850
6	9	0	0.426797	3.092068	-3.873317
7	9	0	0.764889	0.747279	-2.622639
8	9	0	-1.950975	-0.475854	-1.905300
9	9	0	-4.452419	-1.500708	-1.863581
10	9	0	-5.527867	-2.374774	0.493596
11	9	0	-4.087173	-2.222732	2.801666
12	9	0	-1.613142	-1.219484	2.803110
13	9	0	-0.192137	-3.015329	-0.277407
14	9	0	1.796392	-4.542375	-1.216700
15	9	0	4.670221	-0.783512	-1.406108
16	9	0	2.684663	0.794156	-0.483506
17	8	0	0.249404	0.391504	1.843283
18	6	0	3.255204	-2.682046	-1.329043
19	6	0	2.003247	-3.239470	-1.037819
20	6	0	0.978848	-2.424541	-0.553263
21	6	0	1.165516	-1.038150	-0.359286
22	6	0	1.530580	0.645754	2.431661
23	6	0	1.955158	1.964335	2.556000
24	1	0	1.346197	2.783089	2.173257
25	6	0	3.166699	2.206640	3.210922
26	1	0	3.516717	3.233393	3.325626
27	6	0	3.916849	1.144572	3.725327
28	1	0	4.858153	1.342372	4.239511
29	6	0	-0.267469	1.561261	-0.620120
30	6	0	-0.946547	2.644136	-0.016702
31	6	0	-1.134932	3.859166	-0.673624
32	6	0	-0.656789	4.013474	-1.981872
33	6	0	-0.006111	2.950239	-2.622202
34	6	0	0.173455	1.742469	-1.947825
35	6	0	-1.708069	-0.743664	0.448857
36	6	0	-2.476272	-0.864165	-0.728126
37	6	0	-3.759410	-1.402488	-0.730846
38	6	0	-4.309258	-1.855530	0.476778
39	6	0	-3.566743	-1.774169	1.661421
40	6	0	-2.277383	-1.234604	1.645745
41	6	0	3.479115	-1.311267	-1.134335
42	6	0	2.443703	-0.515070	-0.653633
43	6	0	2.244103	-0.431883	2.947709
44	1	0	1.852070	-1.446544	2.871361
45	6	0	3.454989	-0.168510	3.597752
46	1	0	4.027851	-0.996422	4.017925

Table S37: Optimized Cartesian coordinates of [**14**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.446151	-2.147810	4.090124
2	6	0	-1.095803	-1.641516	2.955449
3	6	0	-1.432953	-0.292221	2.833685
4	6	0	-1.143736	0.588166	3.879848
5	6	0	0.155363	-5.049478	2.723508
6	6	0	0.781887	-4.620286	1.544266
7	6	0	0.904610	-5.449340	0.426692
8	6	0	0.408522	-6.753996	0.473778
9	6	0	-0.215635	-7.213285	1.635402
10	6	0	-0.345544	-6.359926	2.733480
11	9	0	-1.414229	-2.449840	1.927609
12	9	0	-2.038174	0.161305	1.725936
13	9	0	-1.468639	1.882196	3.777765
14	9	0	1.254196	-3.367102	1.420110
15	9	0	1.486940	-4.995874	-0.693641
16	9	0	0.527813	-7.557959	-0.588860
17	9	0	-0.681047	-8.469982	1.693565
18	9	0	-0.939538	-6.865987	3.829203
19	15	0	-0.037263	-3.954474	4.199293
20	6	0	-0.176739	-1.242043	5.122329
21	6	0	-0.519773	0.109516	5.033260
22	6	0	-0.026472	-4.738163	5.870634
23	9	0	-1.697505	-4.247533	4.109614
24	9	0	0.395382	-1.653060	6.270209
25	9	0	-0.254861	0.945477	6.047580
26	6	0	-0.932151	-4.355354	6.874294
27	6	0	0.845800	-5.794640	6.178693
28	6	0	-0.944661	-4.960099	8.133224
29	9	0	-1.814636	-3.363741	6.672988
30	6	0	0.836431	-6.427818	7.424079
31	9	0	1.704351	-6.278588	5.263161
32	6	0	-0.057717	-6.003140	8.409116
33	9	0	-1.802091	-4.545969	9.077173
34	9	0	1.673374	-7.446026	7.673946
35	9	0	-0.068234	-6.595365	9.607899
36	8	0	1.660013	-3.740838	4.118047
37	6	0	2.530909	-2.822151	4.674665
38	6	0	3.205111	-3.123605	5.865509
39	6	0	2.828888	-1.642777	3.977445
40	6	0	4.154844	-2.231137	6.367697
41	1	0	3.000310	-4.062630	6.379568
42	6	0	3.779639	-0.756494	4.491286
43	1	0	2.332438	-1.442611	3.027680
44	6	0	4.441646	-1.042767	5.688630
45	1	0	4.679519	-2.472637	7.294234
46	1	0	4.011786	0.158185	3.942028
47	1	0	5.186711	-0.350407	6.083838

Table S38: Optimized Cartesian coordinates of **15**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.616130	1.561730	3.919391
2	9	0	0.628518	1.025317	0.863436
3	9	0	2.589233	-0.090131	-0.581305
4	9	0	3.138052	0.181254	4.844314
5	9	0	4.832215	-1.052664	0.640559
6	9	0	0.624013	-1.572636	4.076451
7	9	0	-1.688698	2.297461	5.655884
8	9	0	1.511771	4.151713	2.736947
9	9	0	-2.311997	1.289167	2.835314
10	9	0	-0.978886	-3.113324	5.564049
11	9	0	5.093316	-0.907202	3.352787
12	9	0	-2.926519	-1.999588	7.114538
13	8	0	1.532518	2.401481	4.911454
14	9	0	-3.272492	0.709705	7.159372
15	9	0	-3.671918	3.090137	1.387754
16	6	0	2.997794	0.176689	3.512087
17	6	0	3.877326	-0.489845	1.364524
18	6	0	1.721909	0.593077	1.509901
19	6	0	-0.308338	-0.969210	4.825656
20	9	0	0.111828	5.935142	1.282812
21	6	0	2.725973	0.005861	0.739478
22	6	0	4.012329	-0.408534	2.758029
23	6	0	1.838202	0.718142	2.911201
24	6	0	1.234554	2.925823	6.206427
25	6	0	-1.695928	2.435504	2.509784
26	9	0	-2.482809	5.417225	0.604381
27	6	0	-1.477844	0.971164	5.640609
28	9	0	0.647832	4.506191	9.927394
29	6	0	-0.365451	2.684111	2.908683
30	6	0	0.228217	3.882329	2.453261
31	6	0	1.412721	2.104849	7.317667
32	1	0	1.733248	1.069963	7.198934
33	6	0	-2.415840	3.350975	1.743109
34	6	0	-1.137475	-1.791964	5.590358
35	6	0	-2.139526	-1.222601	6.386888
36	6	0	-0.452173	0.435352	4.831302
37	6	0	-2.313641	0.168926	6.411736
38	6	0	-0.475231	4.810809	1.687433
39	6	0	0.886927	4.269933	6.315516
40	1	0	0.796916	4.894938	5.427442
41	6	0	1.207173	2.644098	8.590016
42	1	0	1.343655	2.041836	9.488340
43	6	0	-1.805599	4.545138	1.335330
44	6	0	0.685190	4.809469	7.586985
45	1	0	0.418035	5.857832	7.720413
46	6	0	0.842449	3.985468	8.701844

Table S39: Optimized Cartesian coordinates of [**15**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.445508	-2.148309	4.089182
2	6	0	-1.095894	-1.643240	2.954183
3	6	0	-1.435691	-0.294594	2.832132
4	6	0	-1.148314	0.586728	3.878131
5	6	0	0.156693	-5.049405	2.723167
6	6	0	0.783571	-4.619502	1.544388
7	6	0	0.906573	-5.447712	0.426320
8	6	0	0.410402	-6.752469	0.472528
9	6	0	-0.213952	-7.212591	1.633780
10	6	0	-0.344038	-6.359947	2.732404
11	9	0	-1.412933	-2.452414	1.926762
12	9	0	-2.041558	0.157276	1.724406
13	9	0	-1.475636	1.879731	3.775760
14	9	0	1.255986	-3.365924	1.421172
15	9	0	1.489193	-4.993542	-0.693381
16	9	0	0.529901	-7.555570	-0.590437
17	9	0	-0.679202	-8.469161	1.691140
18	9	0	-0.937704	-6.866520	3.828015
19	15	0	-0.037897	-3.955435	4.199166
20	6	0	-0.178239	-1.241579	5.121119
21	6	0	-0.523507	0.109436	5.031783
22	6	0	-0.024604	-4.738198	5.870746
23	9	0	-1.696934	-4.248507	4.110357
24	9	0	0.393693	-1.651102	6.270163
25	9	0	-0.260239	0.945660	6.045991
26	6	0	-0.931102	-4.356460	6.874251
27	6	0	0.848263	-5.794314	6.178794
28	6	0	-0.944145	-4.962138	8.132752
29	9	0	-1.813758	-3.365158	6.672932
30	6	0	0.838461	-6.428377	7.423764
31	9	0	1.708123	-6.276851	5.263549
32	6	0	-0.056764	-6.004961	8.408501
33	9	0	-1.802250	-4.549162	9.076196
34	9	0	1.675826	-7.446081	7.673354
35	9	0	-0.067720	-6.597941	9.606572
36	8	0	1.662609	-3.741964	4.116405
37	6	0	2.528265	-2.821655	4.675727
38	6	0	3.197405	-3.117084	5.871629
39	6	0	2.833560	-1.644822	3.976497
40	6	0	4.146532	-2.230083	6.383034
41	1	0	2.991166	-4.052646	6.390756
42	6	0	3.780608	-0.751509	4.483769
43	1	0	2.344606	-1.445626	3.022964
44	6	0	4.417229	-1.057216	5.683087
45	1	0	4.680359	-2.444124	7.309511
46	1	0	4.036577	0.165480	3.951934
47	9	0	5.342368	-0.193447	6.177627

Table S40: Optimized Cartesian coordinates of **16**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.616130	1.561730	3.919391
2	9	0	0.628518	1.025317	0.863436
3	9	0	2.589233	-0.090131	-0.581305
4	9	0	3.138052	0.181254	4.844314
5	9	0	4.832215	-1.052664	0.640559
6	9	0	0.624013	-1.572636	4.076451
7	9	0	-1.688698	2.297461	5.655884
8	9	0	1.511771	4.151713	2.736947
9	9	0	-2.311997	1.289167	2.835314
10	9	0	-0.978886	-3.113324	5.564049
11	9	0	5.093316	-0.907202	3.352787
12	9	0	-2.926519	-1.999588	7.114538
13	8	0	1.532518	2.401481	4.911454
14	9	0	-3.272492	0.709705	7.159372
15	9	0	-3.671918	3.090137	1.387754
16	6	0	2.997794	0.176689	3.512087
17	6	0	3.877326	-0.489845	1.364524
18	6	0	1.721909	0.593077	1.509901
19	6	0	-0.308338	-0.969210	4.825656
20	9	0	0.111828	5.935142	1.282812
21	6	0	2.725973	0.005861	0.739478
22	6	0	4.012329	-0.408534	2.758029
23	6	0	1.838202	0.718142	2.911201
24	6	0	1.234554	2.925823	6.206427
25	6	0	-1.695928	2.435504	2.509784
26	9	0	-2.482809	5.417225	0.604381
27	6	0	-1.477844	0.971164	5.640609
28	9	0	0.647832	4.506191	9.927394
29	6	0	-0.365451	2.684111	2.908683
30	6	0	0.228217	3.882329	2.453261
31	6	0	1.412721	2.104849	7.317667
32	1	0	1.733248	1.069963	7.198934
33	6	0	-2.415840	3.350975	1.743109
34	6	0	-1.137475	-1.791964	5.590358
35	6	0	-2.139526	-1.222601	6.386888
36	6	0	-0.452173	0.435352	4.831302
37	6	0	-2.313641	0.168926	6.411736
38	6	0	-0.475231	4.810809	1.687433
39	6	0	0.886927	4.269933	6.315516
40	6	0	1.207173	2.644098	8.590016
41	1	0	1.343655	2.041836	9.488340
42	6	0	-1.805599	4.545138	1.335330
43	6	0	0.685190	4.809469	7.586985
44	1	0	0.418035	5.857832	7.720413
45	6	0	0.842449	3.985468	8.701844
46	9	0	0.775413	5.044247	5.215288

Table S41: Optimized Cartesian coordinates of [**16**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.461401	-2.130067	4.073839
2	6	0	-1.110042	-1.626246	2.937856
3	6	0	-1.446923	-0.277711	2.813614
4	6	0	-1.156244	0.604811	3.857557
5	6	0	0.136471	-5.056126	2.716355
6	6	0	0.745342	-4.658347	1.516049
7	6	0	0.844128	-5.516886	0.417439
8	6	0	0.341055	-6.816327	0.502974
9	6	0	-0.267033	-7.243473	1.685257
10	6	0	-0.373188	-6.363705	2.764213
11	9	0	-1.423972	-2.437753	1.911827
12	9	0	-2.049204	0.174119	1.704495
13	9	0	-1.478977	1.898797	3.752809
14	9	0	1.219720	-3.415256	1.352465
15	9	0	1.410530	-5.093925	-0.722357
16	9	0	0.437992	-7.646376	-0.541320
17	9	0	-0.739721	-8.495103	1.781609
18	9	0	-0.954032	-6.842402	3.879485
19	15	0	-0.047563	-3.933556	4.172961
20	6	0	-0.193262	-1.223977	5.105933
21	6	0	-0.534014	0.127989	5.012662
22	6	0	0.008608	-4.713648	5.844410
23	9	0	-1.703016	-4.234340	4.112487
24	9	0	0.373721	-1.632904	6.259889
25	9	0	-0.271864	0.964941	6.027258
26	6	0	-0.889275	-4.348564	6.862051
27	6	0	0.894555	-5.764237	6.133706
28	6	0	-0.880106	-4.963877	8.116092
29	9	0	-1.786876	-3.368137	6.678611
30	6	0	0.907684	-6.407115	7.373928
31	9	0	1.748143	-6.231105	5.203905
32	6	0	0.021080	-5.999647	8.373095
33	9	0	-1.730963	-4.567378	9.072644
34	9	0	1.758977	-7.417418	7.605189
35	9	0	0.031389	-6.601157	9.566621
36	8	0	1.662627	-3.690679	4.051817
37	6	0	2.516855	-2.804719	4.661065
38	6	0	3.197153	-3.137724	5.841538
39	6	0	2.851645	-1.585251	4.041138
40	6	0	4.149199	-2.285251	6.403084
41	1	0	2.988323	-4.097887	6.311301
42	6	0	3.796414	-0.714548	4.576233
43	6	0	4.427703	-1.082716	5.760510
44	1	0	4.677545	-2.549797	7.318757
45	1	0	4.035351	0.220773	4.071064
46	9	0	5.351374	-0.243582	6.291216
47	9	0	2.255678	-1.239823	2.876340

Table S42: Optimized Cartesian coordinates of **17**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	3.856141	17.679119	2.529397
2	9	0	5.080031	19.364922	0.810762
3	9	0	7.663335	18.904379	0.053816
4	9	0	9.015979	16.739996	1.012779
5	9	0	7.832642	15.044091	2.720968
6	6	0	5.817618	16.339967	2.747042
7	6	0	5.134951	17.450276	2.198866
8	6	0	5.746261	18.322907	1.301072
9	6	0	7.071439	18.085685	0.909169
10	6	0	7.766729	16.974940	1.407717
11	6	0	7.139243	16.113478	2.306965
12	15	0	4.909263	15.293014	3.893601
13	8	0	4.093778	16.238005	4.902074
14	9	0	5.243415	18.719757	5.296596
15	9	0	5.688935	19.674245	7.819836
16	9	0	5.116011	18.113443	9.990605
17	9	0	4.097394	15.598033	9.645980
18	9	0	3.635367	14.646853	7.122923
19	6	0	4.445741	16.669372	6.181924
20	6	0	4.147801	15.875831	7.296141
21	6	0	4.375841	16.360457	8.587341
22	6	0	4.895590	17.649613	8.763260
23	6	0	5.190238	18.449665	7.650947
24	6	0	4.964239	17.956994	6.362697
25	9	0	4.688272	12.224969	4.401565
26	9	0	6.333622	10.710031	5.873849
27	9	0	8.494406	11.816467	7.114716
28	9	0	9.013148	14.485646	6.868171
29	9	0	7.389746	16.044295	5.370589
30	6	0	5.988912	14.197121	4.815269
31	6	0	5.741854	12.815168	4.976961
32	6	0	6.585551	12.009227	5.742921
33	6	0	7.696329	12.575755	6.382708
34	6	0	7.961984	13.948099	6.255101
35	6	0	7.112356	14.733681	5.483195
36	9	0	5.298290	13.716189	1.464420
37	9	0	3.469107	12.488596	-0.115034
38	9	0	0.828233	12.516170	0.591630
39	9	0	0.026949	13.769174	2.873561
40	9	0	1.797973	14.993185	4.453969
41	6	0	3.619137	14.440708	2.986007
42	6	0	2.251384	14.415086	3.341291
43	6	0	1.311944	13.773259	2.528632
44	6	0	1.720541	13.128686	1.354092
45	6	0	3.075064	13.119680	0.988378
46	6	0	3.996151	13.766744	1.804971

Table S43: Optimized Cartesian coordinates of [**17**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.434486	-2.137065	4.107290
2	6	0	-1.067303	-1.616302	2.969475
3	6	0	-1.393560	-0.264130	2.858094
4	6	0	-1.105398	0.604531	3.914864
5	6	0	0.157640	-5.060683	2.748187
6	6	0	0.816676	-4.676517	1.570387
7	6	0	0.937973	-5.535932	0.474811
8	6	0	0.402885	-6.823635	0.538981
9	6	0	-0.260322	-7.236775	1.696445
10	6	0	-0.386858	-6.356630	2.772696
11	9	0	-1.370199	-2.414078	1.930485
12	9	0	-1.980742	0.204627	1.749048
13	9	0	-1.417564	1.900691	3.821914
14	9	0	1.319906	-3.442970	1.423926
15	9	0	1.554991	-5.123479	-0.641666
16	9	0	0.519810	-7.654283	-0.501641
17	9	0	-0.766649	-8.475766	1.772237
18	9	0	-1.023511	-6.823555	3.860505
19	15	0	-0.064642	-3.946470	4.203025
20	6	0	-0.164579	-1.244175	5.150388
21	6	0	-0.493896	0.111280	5.069308
22	6	0	-0.043989	-4.761101	5.850117
23	9	0	-1.716856	-4.212501	4.093209
24	9	0	0.395759	-1.671668	6.301504
25	9	0	-0.229917	0.934967	6.093275
26	6	0	-0.938685	-4.384753	6.866159
27	6	0	0.793817	-5.856360	6.114934
28	6	0	-0.966638	-5.030723	8.103387
29	9	0	-1.797567	-3.366599	6.692141
30	6	0	0.765045	-6.531342	7.336752
31	9	0	1.631249	-6.330781	5.178672
32	6	0	-0.111541	-6.110263	8.339047
33	9	0	-1.810695	-4.624559	9.062372
34	9	0	1.569169	-7.582111	7.549359
35	9	0	-0.137784	-6.741489	9.516578
36	8	0	1.686498	-3.710112	4.143207
37	6	0	2.519262	-2.770524	4.664453
38	6	0	3.246471	-3.016777	5.846850
39	6	0	2.819274	-1.573292	3.981169
40	6	0	4.202442	-2.122568	6.331282
41	6	0	3.770683	-0.668093	4.460911
42	6	0	4.467289	-0.938307	5.639734
43	9	0	5.379067	-0.071464	6.103582
44	9	0	2.201309	-1.273760	2.824449
45	9	0	4.018302	0.463440	3.780792
46	9	0	4.868337	-2.400285	7.463740
47	9	0	3.039861	-4.151889	6.539930

Table S44: Optimized Cartesian coordinates of **18**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.497040	-2.233117	0.783390
2	6	0	0.451409	-1.465393	-0.393033
3	6	0	-0.356707	-1.803255	-1.491195
4	6	0	-1.145575	-2.948884	-1.392523
5	6	0	-1.121072	-3.725588	-0.227748
6	6	0	-0.303059	-3.372627	0.852079
7	16	0	1.472679	-0.040852	-0.414731
8	8	0	2.744000	-0.204562	0.236313
9	6	0	0.634444	1.407315	0.058678
10	6	0	-0.742069	1.556502	-0.189238
11	6	0	-1.349956	2.750862	0.175682
12	6	0	-0.618171	3.793518	0.781813
13	6	0	0.757943	3.603284	1.017011
14	6	0	1.399056	2.421648	0.663327
15	9	0	1.668643	0.152095	-1.986063
16	1	0	-0.350963	-1.207986	-2.403671
17	1	0	-1.772468	-3.241437	-2.235709
18	1	0	-1.739553	-4.622322	-0.164962
19	1	0	2.463717	2.280564	0.851106
20	1	0	1.152592	-1.956956	1.610033
21	1	0	-1.325503	0.756470	-0.645971
22	1	0	-2.417952	2.880620	-0.009317
23	1	0	1.338569	4.399283	1.486901
24	1	0	-0.278913	-3.990685	1.750290
25	6	0	-1.299685	5.065416	1.192519
26	1	0	-1.767512	4.939816	2.183796
27	1	0	-0.590929	5.900078	1.267785
28	1	0	-2.100001	5.338490	0.491185

Table S45: Optimized Cartesian coordinates of [**18**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.620734	-2.846901	0.601087
2	6	0	0.427136	-1.621485	-0.040517
3	6	0	-0.390032	-1.494522	-1.164389
4	6	0	-1.047344	-2.631471	-1.644230
5	6	0	-0.858193	-3.870286	-1.024950
6	6	0	-0.018292	-3.977826	0.088436
7	8	0	2.649014	-0.351142	1.189204
8	6	0	0.505620	1.417941	0.605312
9	6	0	-0.845783	1.560741	0.920520
10	6	0	-1.410049	2.838818	0.895947
11	6	0	-0.640839	3.972735	0.595748
12	6	0	0.722778	3.792369	0.306025
13	6	0	1.300223	2.524030	0.290144
14	9	0	1.829358	0.138874	-0.991023
15	1	0	-0.501913	-0.532523	-1.662491
16	1	0	-1.697500	-2.546242	-2.516730
17	1	0	-1.363831	-4.756267	-1.413363
18	1	0	2.353539	2.390891	0.045593
19	1	0	1.261390	-2.910085	1.480333
20	1	0	-1.446072	0.694825	1.194938
21	1	0	-2.469855	2.954550	1.135082
22	1	0	1.346135	4.661125	0.080747
23	1	0	0.136254	-4.945123	0.569674
24	6	0	-1.258192	5.347959	0.565990
25	1	0	-0.592510	6.096051	1.020765
26	1	0	-1.447323	5.670232	-0.471196
27	1	0	-2.217925	5.370331	1.100062
28	16	0	1.315981	-0.197047	0.636198
29	9	0	0.463868	-0.510098	2.118860

Table S46: Optimized Cartesian coordinates of **19**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.501646	-2.238103	0.778255
2	6	0	0.451025	-1.460980	-0.392261
3	6	0	-0.364274	-1.787320	-1.489241
4	6	0	-1.154715	-2.931955	-1.395434
5	6	0	-1.125775	-3.717867	-0.236663
6	6	0	-0.301288	-3.375816	0.841824
7	16	0	1.473358	-0.039507	-0.408186
8	8	0	2.741091	-0.204684	0.247743
9	6	0	0.635246	1.420009	0.070050
10	6	0	-0.740098	1.563915	-0.178192
11	6	0	-1.349997	2.758859	0.197198
12	6	0	-0.598016	3.772855	0.804990
13	6	0	0.770643	3.604837	1.048278
14	6	0	1.409045	2.421102	0.682328
15	9	0	1.665570	0.171005	-1.974619
16	1	0	-0.361923	-1.185055	-2.397208
17	1	0	-1.786541	-3.216675	-2.237609
18	1	0	-1.746269	-4.613484	-0.177742
19	1	0	2.472411	2.269840	0.868915
20	1	0	1.162315	-1.970394	1.603586
21	1	0	-1.320882	0.763678	-0.637595
22	1	0	-2.417235	2.896466	0.020293
23	1	0	-1.087250	4.703069	1.098303
24	1	0	1.346129	4.397307	1.528063
25	1	0	-0.274217	-4.001105	1.734924

Table S47: Optimized Cartesian coordinates of [**19**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.565321	-2.761572	0.721000
2	6	0	0.409627	-1.589352	-0.023003
3	6	0	-0.402189	-1.534619	-1.157027
4	6	0	-1.093383	-2.687825	-1.540597
5	6	0	-0.941704	-3.874705	-0.818192
6	6	0	-0.106440	-3.912305	0.303303
7	8	0	2.685182	-0.276911	1.059848
8	6	0	0.554664	1.486532	0.409317
9	6	0	-0.808104	1.647058	0.663130
10	6	0	-1.359492	2.928085	0.563932
11	6	0	-0.548879	4.022824	0.250354
12	6	0	0.818813	3.841162	0.019752
13	6	0	1.380685	2.564089	0.081262
14	9	0	1.814639	0.083578	-1.126627
15	1	0	-0.484117	-0.616090	-1.736039
16	1	0	-1.739926	-2.657268	-2.419366
17	1	0	-1.473103	-4.775063	-1.131978
18	1	0	2.440270	2.402987	-0.115702
19	1	0	1.202175	-2.769831	1.605085
20	1	0	-1.423906	0.794470	0.945902
21	1	0	-2.425736	3.068378	0.749862
22	1	0	-0.983195	5.022357	0.189025
23	1	0	1.454880	4.695384	-0.218603
24	1	0	0.018834	-4.839487	0.865164
25	16	0	1.341261	-0.138993	0.530313
26	9	0	0.521411	-0.322400	2.051760

Table S48: Optimized Cartesian coordinates of **20**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.143970	-1.806540	0.685361
2	6	0	0.345285	-1.369799	-0.645571
3	6	0	-0.144303	-2.163915	-1.710869
4	6	0	-0.840474	-3.343769	-1.433834
5	6	0	-1.042955	-3.750012	-0.106461
6	6	0	-0.550321	-2.980458	0.960420
7	16	0	1.333109	0.073903	-0.822108
8	8	0	2.724432	-0.111050	-0.530141
9	6	0	0.608091	1.445101	-0.033496
10	6	0	-0.752038	1.733796	-0.246284
11	6	0	-1.278499	2.865051	0.370201
12	6	0	-0.461626	3.673004	1.174789
13	6	0	0.889345	3.363411	1.372198
14	6	0	1.447424	2.238359	0.767260
15	9	0	1.110721	0.387426	-2.351427
16	1	0	2.496254	1.977207	0.908578
17	1	0	-1.376945	1.102152	-0.879533
18	1	0	-2.328443	3.119461	0.221708
19	1	0	1.514167	3.998503	2.001103
20	1	0	-0.886940	4.555781	1.655021
21	9	0	0.032356	-1.830155	-2.984965
22	9	0	-1.307838	-4.084933	-2.431134
23	9	0	-1.700131	-4.867975	0.143047
24	9	0	-0.740712	-3.373891	2.213816
25	9	0	0.630356	-1.083857	1.700257

Table S49: Optimized Cartesian coordinates of [**20**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.577042	-2.817072	0.744457
2	6	0	0.381632	-1.595049	0.084883
3	6	0	-0.433748	-1.565218	-1.053037
4	6	0	-1.042262	-2.729610	-1.528990
5	6	0	-0.826172	-3.944749	-0.874164
6	6	0	-0.013131	-3.989120	0.261078
7	8	0	2.482895	-0.222813	1.423864
8	6	0	0.489520	1.520034	0.438679
9	6	0	-0.856992	1.774183	0.706027
10	6	0	-1.342780	3.069962	0.511173
11	6	0	-0.485099	4.090077	0.090937
12	6	0	0.865096	3.817463	-0.151771
13	6	0	1.362256	2.522587	0.003780
14	9	0	1.906212	-0.006385	-0.866032
15	1	0	2.407162	2.294647	-0.201042
16	1	0	-1.512101	0.983642	1.065886
17	1	0	-2.396103	3.280086	0.703690
18	1	0	1.538659	4.613466	-0.473265
19	1	0	-0.869262	5.102506	-0.046040
20	9	0	-0.682367	-0.421403	-1.707410
21	9	0	-1.833437	-2.683504	-2.610698
22	9	0	-1.399191	-5.063145	-1.332379
23	9	0	0.197683	-5.155400	0.886426
24	9	0	1.344144	-2.908369	1.833938
25	16	0	1.226053	-0.110655	0.716592
26	9	0	0.197245	-0.288035	2.086872

Table S50: Optimized Cartesian coordinates of **21**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.313289	-1.862947	0.689628
2	6	0	0.381966	-1.375478	-0.638493
3	6	0	-0.255854	-2.099904	-1.675924
4	6	0	-0.942778	-3.278314	-1.372349
5	6	0	-1.000558	-3.743544	-0.049402
6	6	0	-0.372639	-3.034655	0.989545
7	16	0	1.369005	0.053787	-0.847516
8	8	0	2.753516	-0.127002	-0.544387
9	6	0	0.649897	1.434107	-0.076907
10	6	0	-0.691398	1.780543	-0.378875
11	6	0	-1.293384	2.883354	0.214449
12	6	0	-0.555990	3.658029	1.129447
13	6	0	0.771687	3.329816	1.446540
14	6	0	1.381762	2.224152	0.849624
15	9	0	1.143580	0.365419	-2.369317
16	9	0	-0.226160	-1.702030	-2.941423
17	9	0	-1.541753	-3.960505	-2.339421
18	9	0	-1.652347	-4.857602	0.223281
19	9	0	-0.436104	-3.479386	2.237529
20	9	0	0.912467	-1.181516	1.672989
21	9	0	-1.387257	1.044153	-1.250012
22	9	0	-2.545952	3.208120	-0.076203
23	9	0	-1.121522	4.705850	1.694900
24	9	0	1.447142	4.071297	2.313345
25	9	0	2.632661	1.941819	1.176517

Table S51: Optimized Cartesian coordinates of [**21**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.580138	-2.806394	0.723854
2	6	0	0.409574	-1.596980	0.030507
3	6	0	-0.433268	-1.572438	-1.089712
4	6	0	-1.095138	-2.728276	-1.510807
5	6	0	-0.905478	-3.929594	-0.822592
6	6	0	-0.063453	-3.969816	0.291823
7	8	0	2.633549	-0.275984	1.200568
8	6	0	0.554433	1.488959	0.414314
9	6	0	-0.826083	1.700217	0.542081
10	6	0	-1.366276	2.983083	0.424236
11	6	0	-0.525353	4.074955	0.193233
12	6	0	0.852539	3.879798	0.068381
13	6	0	1.387868	2.591993	0.165311
14	9	0	1.852117	0.031245	-1.009730
15	9	0	-0.666765	-0.443374	-1.772116
16	9	0	-1.914088	-2.685941	-2.569713
17	9	0	-1.529557	-5.038107	-1.229528
18	9	0	0.126479	-5.123107	0.944354
19	9	0	1.378125	-2.894803	1.789655
20	9	0	-1.680107	0.687808	0.741647
21	9	0	-2.688786	3.167552	0.527714
22	9	0	-1.038838	5.303570	0.090464
23	9	0	1.659139	4.926917	-0.143586
24	9	0	2.709744	2.456934	0.044926
25	16	0	1.325989	-0.141232	0.605531
26	9	0	0.427683	-0.276030	2.051875

Table S52: Optimized Cartesian coordinates of **22**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000775	0.055178	-3.524819
2	6	0	-1.102563	-0.032129	-2.666770
3	6	0	-0.828862	-0.053200	-1.301155
4	6	0	0.465893	0.018639	-0.739516
5	6	0	1.542229	0.105557	-1.621511
6	6	0	1.298292	0.119375	-3.004019
7	6	0	0.465893	0.018639	0.739516
8	6	0	-0.828862	-0.053200	1.301155
9	16	0	-1.984674	-0.145729	0.000000
10	6	0	-1.102563	-0.032129	2.666770
11	6	0	-0.000775	0.055178	3.524819
12	6	0	1.298292	0.119375	3.004019
13	6	0	1.542229	0.105557	1.621511
14	8	0	-3.158952	0.680892	0.000000
15	9	0	-2.459711	-1.664663	-0.000000
16	1	0	-2.122478	-0.079318	-3.050271
17	1	0	-0.159300	0.075231	-4.603310
18	1	0	2.144243	0.187890	-3.689812
19	1	0	2.564990	0.167527	-1.247540
20	1	0	2.564990	0.167527	1.247540
21	1	0	2.144243	0.187890	3.689812
22	1	0	-0.159300	0.075231	4.603310
23	1	0	-2.122478	-0.079318	3.050271

Table S53: Optimized Cartesian coordinates of [**22**-F]$^{-}$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029850	0.023570	-3.527001
2	6	0	-1.089007	-0.057286	-2.684970
3	6	0	-0.856729	-0.038985	-1.322290
4	6	0	0.420092	0.054859	-0.738553
5	6	0	1.518845	0.134237	-1.602321
6	6	0	1.317115	0.117927	-2.987004
7	6	0	0.420087	0.054858	0.738540
8	6	0	-0.856734	-0.038984	1.322286
9	6	0	-1.089012	-0.057283	2.684967
10	6	0	0.029843	0.023572	3.526998
11	6	0	1.317106	0.117927	2.986995
12	6	0	1.518836	0.134236	1.602311
13	8	0	-3.513309	-0.240029	-0.000029
14	9	0	-1.798157	-1.847093	0.000056
15	1	0	-2.100121	-0.131583	-3.086111
16	1	0	-0.109307	0.012270	-4.609055
17	1	0	2.178147	0.179670	-3.654658
18	1	0	2.530538	0.208163	-1.199400
19	1	0	2.530527	0.208162	1.199386
20	1	0	2.178138	0.179670	3.654648
21	1	0	-0.109314	0.012270	4.609052
22	1	0	-2.100125	-0.131580	3.086113
23	16	0	-2.066581	-0.129552	-0.000008
24	9	0	-2.061420	1.608229	0.000050

Table S54: Optimized Cartesian coordinates of **23**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.010767	0.000661	0.001043
2	6	0	1.537529	0.356923	-0.000168
3	6	0	2.496623	-0.355949	-0.747933
4	6	0	2.083183	1.422403	0.744442
5	6	0	3.855305	-0.063261	-0.786642
6	6	0	3.430592	1.763367	0.777667
7	6	0	4.293053	1.002332	-0.005846
8	6	0	-0.450507	-1.501192	-0.011652
9	6	0	-1.504887	-1.973907	-0.815914
10	6	0	0.142568	-2.495915	0.788480
11	6	0	-1.938127	-3.294698	-0.849958
12	6	0	-0.258196	-3.826834	0.816722
13	6	0	-1.306319	-4.221876	-0.018031
14	6	0	-1.066456	1.144352	0.014258
15	6	0	-2.227221	1.099199	0.809822
16	6	0	-0.966358	2.305045	-0.776382
17	6	0	-3.197730	2.094476	0.844569
18	6	0	-1.911501	3.324102	-0.803463
19	6	0	-3.032422	3.211590	0.022595
20	9	0	-2.403768	0.032552	1.633676
21	9	0	1.256032	2.159244	1.525197
22	9	0	2.079712	-1.382750	-1.528079
23	9	0	1.153586	-2.134655	1.623176
24	9	0	-2.125002	-1.095972	-1.648167
25	9	0	0.106446	2.432911	-1.602253
26	1	0	-1.633731	-5.262734	-0.020370
27	1	0	-3.784235	4.002367	0.025908
28	9	0	5.609097	1.310871	-0.008818
29	1	0	-1.761791	4.180035	-1.461216
30	1	0	-4.057175	1.985177	1.505698
31	1	0	-2.752019	-3.577214	-1.517391
32	1	0	0.246425	-4.527105	1.482060
33	1	0	4.541601	-0.640731	-1.403626
34	1	0	3.791531	2.586709	1.391642

Table S55: Optimized Cartesian coordinates of **24**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.024898	-0.012666	0.003671
2	6	0	1.512560	0.347601	0.004236
3	6	0	2.425899	-0.277468	-0.859608
4	6	0	2.047539	1.319444	0.865260
5	6	0	3.781664	0.054477	-0.875371
6	6	0	3.406100	1.639372	0.873256
7	6	0	4.286870	1.013596	-0.003192
8	6	0	-0.465015	-1.515617	0.024784
9	6	0	-1.549582	-2.011560	-0.726982
10	6	0	0.194088	-2.500402	0.787908
11	6	0	-1.949384	-3.342484	-0.746280
12	6	0	-0.171391	-3.840995	0.827623
13	6	0	-1.251071	-4.257352	0.045476
14	6	0	-1.081460	1.144021	-0.021547
15	6	0	-2.273061	1.119936	0.731022
16	6	0	-0.918586	2.314995	-0.789022
17	6	0	-3.213279	2.143466	0.747415
18	6	0	-1.832263	3.361590	-0.832377
19	6	0	-2.984620	3.268418	-0.048626
20	9	0	-2.512473	0.046621	1.527408
21	9	0	1.244935	1.954275	1.749507
22	9	0	1.994196	-1.208115	-1.740886
23	9	0	1.234003	-2.119540	1.574724
24	9	0	-2.235185	-1.147754	-1.518970
25	9	0	0.183896	2.423576	-1.575813
26	1	0	-1.551826	-5.306198	0.053085
27	1	0	-3.712543	4.081191	-0.058095
28	1	0	-1.634511	4.223154	-1.469649
29	1	0	-4.099146	2.049945	1.375168
30	1	0	-2.789605	-3.642865	-1.371899
31	1	0	0.384118	-4.531870	1.461372
32	1	0	5.346275	1.268165	-0.006488
33	9	0	4.609322	-0.565434	-1.744091
34	9	0	3.867014	2.568862	1.737939

Table S56: Optimized Cartesian coordinates of **25**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.011774	-0.008220	0.003098
2	6	0	1.522899	0.350953	0.002921
3	6	0	2.452437	-0.328629	-0.802918
4	6	0	2.051850	1.377645	0.804214
5	6	0	3.810651	-0.011632	-0.831275
6	6	0	3.407034	1.707348	0.822497
7	6	0	4.290482	1.010540	-0.007130
8	6	0	-0.457974	-1.510622	0.006935
9	6	0	-1.532296	-1.995268	-0.765694
10	6	0	0.175555	-2.501287	0.782869
11	6	0	-1.945908	-3.321951	-0.792326
12	6	0	-0.204461	-3.837812	0.816420
13	6	0	-1.273096	-4.243540	0.013495
14	6	0	-1.074631	1.143993	-0.003088
15	6	0	-2.257251	1.107152	0.762491
16	6	0	-0.933927	2.315564	-0.773330
17	6	0	-3.209278	2.119698	0.788136
18	6	0	-1.859677	3.351534	-0.807936
19	6	0	-3.002493	3.246212	-0.011550
20	9	0	-2.474588	0.032048	1.563268
21	9	0	1.246753	2.072681	1.635748
22	9	0	2.041328	-1.311483	-1.632210
23	9	0	1.205759	-2.129643	1.588211
24	9	0	-2.192398	-1.123702	-1.571438
25	9	0	0.160350	2.436237	-1.571068
26	9	0	4.659164	-0.672174	-1.637018
27	9	0	3.872185	2.681456	1.622687
28	1	0	-1.584845	-5.289159	0.015733
29	1	0	-3.739649	4.050625	-0.013939
30	9	0	5.593014	1.321406	-0.012457
31	1	0	-1.678618	4.214680	-1.448053
32	1	0	-4.087014	2.016633	1.425763
33	1	0	-2.776787	-3.613809	-1.434271
34	1	0	0.331391	-4.534072	1.461137

Table S57: Optimized Cartesian coordinates of **26**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.011585	-0.008436	0.001308
2	6	0	1.518824	0.350006	0.001505
3	6	0	2.463470	-0.305916	-0.809705
4	6	0	2.070294	1.362283	0.809395
5	6	0	3.819367	0.000010	-0.844884
6	6	0	3.418307	1.701224	0.837055
7	6	0	4.292898	1.011701	-0.006070
8	6	0	-0.462549	-1.510378	0.014783
9	6	0	-1.547484	-1.998362	-0.741063
10	6	0	0.184582	-2.503969	0.776589
11	6	0	-1.964372	-3.324073	-0.772905
12	6	0	-0.185405	-3.843653	0.817588
13	6	0	-1.263730	-4.224433	0.024501
14	6	0	-1.078941	1.140936	-0.013960
15	6	0	-2.271988	1.101884	0.735580
16	6	0	-0.927341	2.322162	-0.768205
17	6	0	-3.225992	2.112576	0.768893
18	6	0	-1.844853	3.365955	-0.807600
19	6	0	-2.984827	3.233372	-0.020324
20	9	0	-2.509363	0.023102	1.521860
21	9	0	1.242721	2.038068	1.650994
22	9	0	2.025278	-1.281989	-1.649475
23	9	0	1.222840	-2.140708	1.568431
24	9	0	-2.226681	-1.133169	-1.533983
25	9	0	0.169923	2.454615	-1.552837
26	1	0	3.762292	2.488368	1.507656
27	1	0	4.477611	-0.547403	-1.519206
28	1	0	0.344021	-4.558406	1.445217
29	1	0	-2.799160	-3.640707	-1.395782
30	1	0	-4.117350	2.029580	1.388312
31	1	0	-1.677648	4.243967	-1.429042
32	9	0	-1.646739	-5.520572	0.029249
33	9	0	-3.894356	4.233069	-0.022442
34	1	0	5.354191	1.265208	-0.009559

Table S58: Optimized Cartesian coordinates of **27**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.023760	0.005034	-0.001562
2	6	0	1.545638	0.360041	-0.002211
3	6	0	2.506661	-0.368094	-0.734798
4	6	0	2.086564	1.437834	0.730059
5	6	0	3.863807	-0.071243	-0.763332
6	6	0	3.435434	1.769956	0.758911
7	6	0	4.323556	1.005938	-0.001968
8	6	0	-0.448551	-1.497508	-0.018643
9	6	0	-1.495585	-1.940188	-0.845474
10	6	0	0.141252	-2.475313	0.801074
11	6	0	-1.918222	-3.270316	-0.864002
12	6	0	-0.292476	-3.801807	0.806005
13	6	0	-1.323814	-4.213848	-0.032225
14	6	0	-1.064231	1.143921	0.017324
15	6	0	-2.202124	1.074929	0.839925
16	6	0	-0.963634	2.286904	-0.795120
17	6	0	-3.167898	2.082568	0.861633
18	6	0	-1.937435	3.286610	-0.796562
19	6	0	-3.047498	3.196865	0.037524
20	9	0	-2.369852	0.026277	1.676320
21	9	0	1.249079	2.185059	1.493505
22	9	0	2.084863	-1.407231	-1.499601
23	9	0	1.138415	-2.136723	1.647608
24	9	0	-2.104019	-1.075479	-1.687873
25	9	0	0.083141	2.428453	-1.637536
26	9	0	-1.796486	4.351698	-1.613194
27	9	0	-4.228260	1.970513	1.688588
28	9	0	-2.915321	-3.640476	-1.694449
29	9	0	0.298910	-4.692260	1.629745
30	1	0	-1.657913	-5.251038	-0.037256
31	1	0	5.386315	1.252991	-0.001631
32	1	0	-3.804397	3.980717	0.045144
33	1	0	4.534476	-0.676644	-1.372639
34	1	0	3.770161	2.609268	1.368081

Table S59: Optimized Cartesian coordinates of **28**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.005134	0.002646	0.001843
2	6	0	1.528432	0.352084	-0.000942
3	6	0	2.457966	-0.351264	-0.787953
4	6	0	2.060984	1.394762	0.779010
5	6	0	3.817708	-0.042518	-0.819357
6	6	0	3.417696	1.717069	0.793680
7	6	0	4.299994	0.996197	-0.017089
8	6	0	-0.454029	-1.504761	0.003199
9	6	0	-1.523770	-1.968155	-0.784005
10	6	0	0.182831	-2.478061	0.793647
11	6	0	-1.932505	-3.301351	-0.802772
12	6	0	-0.212902	-3.815117	0.821159
13	6	0	-1.275003	-4.228969	0.011275
14	6	0	-1.074172	1.145291	0.001613
15	6	0	-2.266004	1.087550	0.753099
16	6	0	-0.933750	2.330499	-0.749522
17	6	0	-3.226173	2.091506	0.783232
18	6	0	-1.867767	3.358661	-0.778487
19	6	0	-3.018818	3.231496	0.002894
20	9	0	-2.483683	-0.001839	1.534846
21	9	0	1.257889	2.112457	1.591460
22	9	0	2.044409	-1.350829	-1.596091
23	9	0	1.202068	-2.129887	1.607961
24	9	0	-2.182950	-1.119304	-1.599581
25	9	0	0.167974	2.471922	-1.531704
26	9	0	4.664379	-0.725422	-1.606366
27	9	0	3.885488	2.706074	1.572099
28	9	0	-2.944758	-3.703632	-1.587924
29	9	0	0.409214	-4.704876	1.611061
30	9	0	5.602855	1.299764	-0.025229
31	9	0	-1.661575	-5.509694	0.015422
32	1	0	-4.110427	1.972046	1.408766
33	1	0	-1.687004	4.233047	-1.403179
34	1	0	-3.762555	4.029772	0.003841

Table S60: Optimized Cartesian coordinates of **29**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.035058	-0.013572	0.002121
2	6	0	1.503567	0.346333	0.002538
3	6	0	2.412452	-0.261925	-0.877058
4	6	0	2.042553	1.299415	0.881043
5	6	0	3.768731	0.068119	-0.891099
6	6	0	3.401558	1.617604	0.891092
7	6	0	4.278294	1.008544	-0.001144
8	6	0	-0.470643	-1.515542	0.036110
9	6	0	-1.575117	-2.018790	-0.683572
10	6	0	0.218452	-2.502358	0.772327
11	6	0	-1.971154	-3.350349	-0.704512
12	6	0	-0.129231	-3.847138	0.821697
13	6	0	-1.228814	-4.241997	0.065206
14	6	0	-1.087183	1.144029	-0.034817
15	6	0	-2.298944	1.115794	0.687299
16	6	0	-0.900717	2.330354	-0.775387
17	6	0	-3.237828	2.139881	0.706377
18	6	0	-1.802003	3.386995	-0.827250
19	6	0	-2.962045	3.263636	-0.067937
20	9	0	-2.569545	0.035138	1.457959
21	9	0	1.241849	1.917407	1.779962
22	9	0	1.974654	-1.175586	-1.774087
23	9	0	1.276908	-2.125871	1.529598
24	9	0	-2.294666	-1.163567	-1.448938
25	9	0	0.215561	2.452938	-1.533712
26	1	0	0.432463	-4.555534	1.428103
27	1	0	-2.821938	-3.678962	-1.298893
28	1	0	-4.144692	2.065460	1.303994
29	1	0	-1.608275	4.267654	-1.437123
30	9	0	-1.591291	-5.542409	0.079005
31	9	0	-3.856559	4.274797	-0.083145
32	1	0	5.338128	1.261622	-0.002893
33	9	0	4.591929	-0.535308	-1.774901
34	9	0	3.866212	2.528430	1.772828

Table S61: Optimized Cartesian coordinates of **30**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.021935	-0.010361	0.001809
2	6	0	1.514063	0.348862	0.001851
3	6	0	2.439240	-0.312656	-0.822738
4	6	0	2.046426	1.357092	0.823090
5	6	0	3.797467	0.004502	-0.850557
6	6	0	3.401697	1.686494	0.842902
7	6	0	4.281341	1.008204	-0.006084
8	6	0	-0.462948	-1.512046	0.019095
9	6	0	-1.558991	-2.004338	-0.719917
10	6	0	0.202901	-2.504787	0.767495
11	6	0	-1.968211	-3.331886	-0.747463
12	6	0	-0.158786	-3.845919	0.811545
13	6	0	-1.248819	-4.230420	0.035845
14	6	0	-1.079884	1.143389	-0.017438
15	6	0	-2.284589	1.103336	0.715441
16	6	0	-0.911972	2.331345	-0.759250
17	6	0	-3.233255	2.118330	0.743482
18	6	0	-1.823430	3.379340	-0.802685
19	6	0	-2.975432	3.244915	-0.032783
20	9	0	-2.537469	0.019657	1.488307
21	9	0	1.243070	2.033973	1.672358
22	9	0	2.022470	-1.278639	-1.670088
23	9	0	1.253000	-2.137398	1.542203
24	9	0	-2.255523	-1.141308	-1.498362
25	9	0	0.197597	2.465163	-1.526800
26	9	0	4.641693	-0.638532	-1.674265
27	9	0	3.870065	2.642606	1.662192
28	9	0	5.583688	1.318877	-0.010402
29	1	0	-1.643482	4.262095	-1.413782
30	1	0	-4.133836	2.034880	1.349381
31	1	0	-2.811571	-3.652211	-1.356794
32	1	0	0.385066	-4.559545	1.428035
33	9	0	-3.879275	4.247660	-0.039239
34	9	0	-1.624274	-5.527153	0.043819

Table S62: Optimized Cartesian coordinates of **31**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.033611	0.010761	-0.002801
2	6	0	1.553052	0.363485	-0.004659
3	6	0	2.521565	-0.392965	-0.701091
4	6	0	2.093735	1.466613	0.692230
5	6	0	3.880559	-0.107524	-0.733871
6	6	0	3.441208	1.801945	0.727109
7	6	0	4.311334	0.996228	-0.002602
8	6	0	-0.442773	-1.491183	-0.030247
9	6	0	-1.483310	-1.927561	-0.867937
10	6	0	0.130250	-2.471331	0.798013
11	6	0	-1.916287	-3.254500	-0.887962
12	6	0	-0.313615	-3.794358	0.801623
13	6	0	-1.338814	-4.200481	-0.047091
14	6	0	-1.058689	1.145984	0.028520
15	6	0	-2.190438	1.067255	0.858485
16	6	0	-0.975314	2.287800	-0.787189
17	6	0	-3.167253	2.064297	0.883088
18	6	0	-1.959748	3.276931	-0.785725
19	6	0	-3.064027	3.177350	0.055044
20	9	0	-2.341096	0.019226	1.699000
21	9	0	1.260137	2.245120	1.421156
22	9	0	2.112022	-1.456528	-1.431510
23	9	0	1.122359	-2.137740	1.653470
24	9	0	-2.074637	-1.059434	-1.719228
25	9	0	0.066320	2.438821	-1.635119
26	9	0	-1.834819	4.341215	-1.605747
27	9	0	-4.221086	1.942884	1.716731
28	9	0	-2.906501	-3.618786	-1.728918
29	9	0	0.261873	-4.687085	1.633903
30	1	0	-1.680858	-5.235070	-0.053370
31	1	0	-3.829345	3.952963	0.064813
32	1	0	4.574094	-0.719039	-1.308468
33	1	0	3.797995	2.654489	1.302447
34	9	0	5.626011	1.297706	-0.001241

Table S63: Optimized Cartesian coordinates of **32**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.011843	0.010570	0.001995
2	6	0	1.523280	0.355773	-0.011996
3	6	0	2.444096	-0.349082	-0.807503
4	6	0	2.067090	1.387870	0.773781
5	6	0	3.806476	-0.051758	-0.840835
6	6	0	3.426356	1.698892	0.786754
7	6	0	4.300100	0.976624	-0.032193
8	6	0	-0.456868	-1.498614	0.014578
9	6	0	-1.518155	-1.973154	-0.777020
10	6	0	0.182656	-2.463882	0.812323
11	6	0	-1.916412	-3.309436	-0.793902
12	6	0	-0.202459	-3.804135	0.841945
13	6	0	-1.256296	-4.229203	0.027097
14	6	0	-1.079082	1.151155	0.001595
15	6	0	-2.293018	1.077005	0.718536
16	6	0	-0.921612	2.357020	-0.715560
17	6	0	-3.258731	2.074846	0.753500
18	6	0	-1.850278	3.389247	-0.750228
19	6	0	-3.009930	3.220286	0.001905
20	9	0	-2.536707	-0.024785	1.468059
21	9	0	1.271534	2.106985	1.593392
22	9	0	2.018877	-1.338748	-1.621932
23	9	0	1.194054	-2.104219	1.631594
24	9	0	-2.180225	-1.131099	-1.598305
25	9	0	0.194317	2.524286	-1.465295
26	9	0	4.644538	-0.735743	-1.635806
27	9	0	3.904541	2.678286	1.570745
28	9	0	-2.921087	-3.721972	-1.583218
29	9	0	0.421914	-4.685900	1.638730
30	9	0	5.605289	1.269443	-0.042318
31	9	0	-1.632949	-5.512748	0.033482
32	9	0	-3.929636	4.206761	0.002520
33	1	0	-4.165533	1.964899	1.345743
34	1	0	-1.678122	4.286683	-1.341924

Table S64: Optimized Cartesian coordinates of **33**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.013077	0.001997	0.000540
2	6	0	1.540145	0.358075	-0.000642
3	6	0	2.481769	-0.373970	-0.749432
4	6	0	2.062411	1.431928	0.745954
5	6	0	3.840979	-0.064023	-0.774211
6	6	0	3.418301	1.755945	0.766410
7	6	0	4.311378	1.005179	-0.004995
8	6	0	-0.449466	-1.500528	-0.013933
9	6	0	-1.509080	-1.946315	-0.824471
10	6	0	0.160357	-2.478669	0.791875
11	6	0	-1.924132	-3.278784	-0.839956
12	6	0	-0.265782	-3.807493	0.800028
13	6	0	-1.309484	-4.221550	-0.021883
14	6	0	-1.065918	1.145393	0.015742
15	6	0	-2.218782	1.073497	0.818691
16	6	0	-0.945013	2.298091	-0.781522
17	6	0	-3.178520	2.086873	0.835366
18	6	0	-1.912742	3.303449	-0.788241
19	6	0	-3.037064	3.209824	0.026220
20	9	0	-2.407005	0.016881	1.639034
21	9	0	1.249864	2.178145	1.521451
22	9	0	2.081517	-1.402419	-1.524406
23	9	0	1.170129	-2.137178	1.622534
24	9	0	-2.136846	-1.082661	-1.652234
25	9	0	0.116809	2.443111	-1.604710
26	9	0	4.698678	-0.773905	-1.523114
27	9	0	3.875167	2.773023	1.512921
28	9	0	-1.751877	4.375845	-1.589548
29	9	0	-4.252616	1.971887	1.642221
30	9	0	-2.932818	-3.651424	-1.653426
31	9	0	0.344336	-4.696424	1.609739
32	1	0	-1.637774	-5.260672	-0.025000
33	1	0	-3.789424	3.998155	0.030513
34	9	0	5.612842	1.309318	-0.007230

Table S65: Optimized Cartesian coordinates of **34**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.007006	-0.010303	0.001321
2	6	0	1.533913	0.350994	0.013398
3	6	0	2.480958	-0.359828	-0.747951
4	6	0	2.046530	1.417925	0.775730
5	6	0	3.836895	-0.035991	-0.770641
6	6	0	3.399260	1.755296	0.798840
7	6	0	4.298362	1.025913	0.014120
8	6	0	-0.453202	-1.510321	-0.011936
9	6	0	-1.545291	-1.952552	-0.782338
10	6	0	0.189258	-2.501092	0.754166
11	6	0	-1.969118	-3.280705	-0.809067
12	6	0	-0.221499	-3.833296	0.773389
13	6	0	-1.304925	-4.225191	-0.019793
14	6	0	-1.067665	1.138047	0.001540
15	6	0	-2.217724	1.086542	0.809603
16	6	0	-0.936485	2.282245	-0.805906
17	6	0	-3.165046	2.111453	0.822300
18	6	0	-1.891903	3.299449	-0.816697
19	6	0	-3.013489	3.226209	0.003524
20	9	0	-2.415547	0.037469	1.638234
21	9	0	1.226985	2.143555	1.563863
22	9	0	2.088512	-1.381185	-1.537482
23	9	0	1.228176	-2.174894	1.550876
24	9	0	-2.210193	-1.087256	-1.575184
25	9	0	0.123584	2.406890	-1.634940
26	9	0	4.699930	-0.725787	-1.531889
27	9	0	3.847126	2.765057	1.560349
28	9	0	-1.721447	4.362982	-1.627563
29	9	0	-4.236970	2.015723	1.634404
30	9	0	-3.000179	-3.662115	-1.578222
31	9	0	0.405782	-4.739430	1.538663
32	1	0	-3.756281	4.023574	0.004822
33	9	0	5.596777	1.342942	0.014185
34	9	0	-1.704791	-5.500569	-0.023502

Table S66: Optimized Cartesian coordinates of **35**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.028555	-0.022329	0.001623
2	6	0	1.508375	0.342699	0.014243
3	6	0	2.426869	-0.264153	-0.856636
4	6	0	2.034912	1.307482	0.887799
5	6	0	3.779828	0.078715	-0.867964
6	6	0	3.390960	1.638432	0.900472
7	6	0	4.276950	1.030991	0.016458
8	6	0	-0.467492	-1.522726	0.023594
9	6	0	-1.581910	-2.014021	-0.689490
10	6	0	0.220351	-2.518518	0.749198
11	6	0	-1.988373	-3.342552	-0.712916
12	6	0	-0.137439	-3.860698	0.795246
13	6	0	-1.246598	-4.243317	0.046430
14	6	0	-1.082003	1.137789	-0.035190
15	6	0	-2.269562	1.129477	0.723625
16	6	0	-0.912913	2.301635	-0.811731
17	6	0	-3.200319	2.161417	0.738585
18	6	0	-1.817192	3.356362	-0.857081
19	6	0	-2.965756	3.279071	-0.066158
20	9	0	-2.514601	0.062216	1.527527
21	9	0	1.226083	1.923496	1.779947
22	9	0	2.002135	-1.189143	-1.748166
23	9	0	1.288349	-2.154569	1.498916
24	9	0	-2.300185	-1.150817	-1.445732
25	9	0	0.186403	2.393962	-1.605151
26	9	0	4.612513	-0.523842	-1.743724
27	9	0	3.843777	2.560182	1.777264
28	9	0	-1.618994	-5.541102	0.057345
29	1	0	-4.083539	2.080188	1.371760
30	1	0	-1.615196	4.211855	-1.501161
31	1	0	5.334351	1.294011	0.016907
32	1	0	-3.686222	4.098436	-0.076839
33	1	0	0.423951	-4.576388	1.393312
34	1	0	-2.846637	-3.661804	-1.301626

Table S67: Optimized Cartesian coordinates of **36**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.002476	0.014706	0.000950
2	6	0	1.527518	0.358092	-0.014861
3	6	0	2.466547	-0.344201	-0.795670
4	6	0	2.092017	1.393800	0.756025
5	6	0	3.826913	-0.061321	-0.835276
6	6	0	3.444837	1.711320	0.776731
7	6	0	4.312003	0.974866	-0.033964
8	6	0	-0.456404	-1.495100	0.012021
9	6	0	-1.504157	-1.967769	-0.796751
10	6	0	0.164023	-2.459204	0.824561
11	6	0	-1.907879	-3.302628	-0.816945
12	6	0	-0.227135	-3.798061	0.851161
13	6	0	-1.267116	-4.222215	0.018782
14	6	0	-1.078993	1.150602	0.004649
15	6	0	-2.283175	1.075114	0.735566
16	6	0	-0.936464	2.351570	-0.722142
17	6	0	-3.254708	2.067961	0.775782
18	6	0	-1.871604	3.379022	-0.752596
19	6	0	-3.021167	3.209436	0.014041
20	9	0	-2.512881	-0.023382	1.495965
21	9	0	1.273250	2.114864	1.566011
22	9	0	2.017918	-1.344076	-1.600327
23	9	0	1.161853	-2.100990	1.660553
24	9	0	-2.148048	-1.125314	-1.633367
25	9	0	0.168976	2.520129	-1.486176
26	9	0	-2.900255	-3.713948	-1.623920
27	9	0	0.379541	-4.680487	1.662562
28	9	0	-1.649103	-5.505533	0.022405
29	9	0	-3.947020	4.192190	0.019030
30	1	0	-4.153749	1.956584	1.379400
31	1	0	-1.711023	4.273149	-1.352436
32	1	0	5.377240	1.210997	-0.041293
33	1	0	4.479794	-0.645083	-1.483799
34	1	0	3.798764	2.518439	1.417761

Table S68: Optimized Cartesian coordinates of **37**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.018358	-0.001863	0.001661
2	6	0	1.517971	0.349157	0.000357
3	6	0	2.433930	-0.308062	-0.838223
4	6	0	2.054314	1.345519	0.834036
5	6	0	3.791589	0.015463	-0.856612
6	6	0	3.414628	1.657664	0.839257
7	6	0	4.296432	0.999095	-0.011928
8	6	0	-0.461135	-1.509873	0.018788
9	6	0	-1.540980	-1.983522	-0.749116
10	6	0	0.200236	-2.478066	0.796257
11	6	0	-1.936225	-3.320660	-0.762108
12	6	0	-0.181557	-3.819170	0.828827
13	6	0	-1.254130	-4.242607	0.038154
14	6	0	-1.081719	1.144804	-0.016182
15	6	0	-2.281475	1.099586	0.723946
16	6	0	-0.920196	2.329828	-0.764042
17	6	0	-3.229678	2.114867	0.747097
18	6	0	-1.842039	3.368957	-0.799576
19	6	0	-3.001445	3.253851	-0.029013
20	9	0	-2.520022	0.011613	1.501134
21	9	0	1.251929	2.012746	1.692704
22	9	0	2.002727	-1.263113	-1.693373
23	9	0	1.228931	-2.121604	1.593677
24	9	0	-2.224451	-1.141403	-1.551004
25	9	0	0.188682	2.459284	-1.536864
26	9	0	4.619575	-0.635717	-1.699820
27	9	0	3.875509	2.610890	1.675869
28	9	0	-2.958871	-3.732535	-1.528699
29	9	0	0.463577	-4.703673	1.606137
30	9	0	-1.627871	-5.527079	0.047757
31	1	0	-4.121086	2.004821	1.364113
32	1	0	-1.645388	4.242205	-1.421015
33	1	0	5.357437	1.247471	-0.016775
34	1	0	-3.735787	4.060839	-0.033286

Table S69: Optimized Cartesian coordinates of **38**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.024964	0.006884	0.002299
2	6	0	1.512970	0.353127	-0.010950
3	6	0	2.419350	-0.305596	-0.858379
4	6	0	2.061567	1.338004	0.827994
5	6	0	3.780072	0.005296	-0.879237
6	6	0	3.424604	1.637625	0.830837
7	6	0	4.297180	0.977373	-0.028665
8	6	0	-0.463796	-1.502907	0.030655
9	6	0	-1.533781	-1.988277	-0.743270
10	6	0	0.199225	-2.462477	0.816974
11	6	0	-1.918188	-3.328497	-0.754408
12	6	0	-0.171716	-3.806707	0.851695
13	6	0	-1.234632	-4.241976	0.054442
14	6	0	-1.086756	1.151135	-0.015259
15	6	0	-2.308917	1.088462	0.689188
16	6	0	-0.908567	2.357224	-0.727940
17	6	0	-3.263800	2.096719	0.716632
18	6	0	-1.825934	3.399465	-0.769456
19	6	0	-2.994784	3.241178	-0.029618
20	9	0	-2.572595	-0.011915	1.433503
21	9	0	1.267301	2.007286	1.693514
22	9	0	1.975414	-1.249674	-1.719339
23	9	0	1.218691	-2.093939	1.620941
24	9	0	-2.218895	-1.153680	-1.552649
25	9	0	0.215338	2.513945	-1.466604
26	9	0	4.598526	-0.646836	-1.730686
27	9	0	3.897020	2.580241	1.672757
28	9	0	-2.931819	-3.751208	-1.526824
29	9	0	0.474585	-4.682594	1.637478
30	9	0	-1.598146	-5.529246	0.066256
31	9	0	-3.904008	4.237426	-0.036099
32	1	0	-4.177775	1.995412	1.299246
33	1	0	-1.638192	4.296309	-1.357226
34	1	0	5.360427	1.215976	-0.035539

Table S70: Optimized Cartesian coordinates of **1** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000722	-0.005821	0.001331
2	6	0	1.529723	0.353127	0.002375
3	6	0	2.480447	-0.319042	-0.789338
4	6	0	2.077843	1.382482	0.791856
5	6	0	3.836403	-0.014455	-0.822992
6	6	0	3.425432	1.722093	0.820762
7	6	0	4.305181	1.014712	-0.002454
8	6	0	-0.456364	-1.508155	0.000390
9	6	0	-1.519016	-1.988684	-0.789053
10	6	0	0.155120	-2.501008	0.789741
11	6	0	-1.943075	-3.312077	-0.820139
12	6	0	-0.234494	-3.835024	0.821075
13	6	0	-1.291770	-4.236384	0.000573
14	6	0	-1.071898	1.141718	0.000044
15	6	0	-2.237342	1.110469	0.789656
16	6	0	-0.955750	2.301588	-0.789992
17	6	0	-3.196489	2.116264	0.820987
18	6	0	-1.888411	3.331781	-0.821410
19	6	0	-3.014217	3.232107	0.000089
20	9	0	-2.429912	0.044126	1.613312
21	9	0	1.246042	2.075565	1.616679
22	9	0	2.047472	-1.311718	-1.613825
23	9	0	1.174447	-2.133363	1.613236
24	9	0	-2.158848	-1.113153	-1.611548
25	9	0	0.121943	2.415798	-1.613585
26	1	0	3.766987	2.522745	1.476537
27	1	0	5.366405	1.267891	-0.004669
28	1	0	4.499794	-0.574963	-1.481407
29	1	0	0.284010	-4.533879	1.477199
30	1	0	-1.611257	-5.279557	0.000698
31	1	0	-2.764356	-3.600910	-1.475764
32	1	0	-4.060477	2.018241	1.478007
33	1	0	-3.756592	4.031563	0.000649
34	1	0	-1.727438	4.186600	-1.478002

Table S71: Optimized Cartesian coordinates of **2** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000447	-0.003169	0.001616
2	6	0	1.527769	0.353432	0.000271
3	6	0	2.482317	-0.339118	-0.770872
4	6	0	2.077621	1.400391	0.766722
5	6	0	3.840167	-0.044555	-0.813043
6	6	0	3.424120	1.743421	0.799584
7	6	0	4.280955	1.002641	-0.009264
8	6	0	-0.455939	-1.504816	0.002181
9	6	0	-1.531209	-1.985698	-0.771142
10	6	0	0.169299	-2.502024	0.776566
11	6	0	-1.959435	-3.307516	-0.807845
12	6	0	-0.211521	-3.838314	0.815080
13	6	0	-1.279539	-4.210704	0.004069
14	6	0	-1.072463	1.142774	0.001021
15	6	0	-2.258770	1.094196	0.760416
16	6	0	-0.940317	2.322968	-0.758044
17	6	0	-3.223871	2.093875	0.798449
18	6	0	-1.868295	3.357001	-0.794363
19	6	0	-3.000194	3.213669	0.002816
20	9	0	-2.476656	0.014541	1.553430
21	9	0	1.251706	2.116932	1.571025
22	9	0	2.058283	-1.348589	-1.573168
23	9	0	1.199217	-2.143457	1.584770
24	9	0	-2.188324	-1.114472	-1.578462
25	9	0	0.151626	2.463958	-1.551795
26	1	0	3.788760	2.551865	1.431022
27	1	0	4.522966	-0.605270	-1.449173
28	1	0	0.300829	-4.556313	1.453251
29	1	0	-2.785864	-3.619015	-1.444486
30	1	0	-4.109369	2.003819	1.425373
31	1	0	-1.715902	4.234770	-1.420107
32	9	0	5.597180	1.313698	-0.014605
33	9	0	-1.673502	-5.504561	0.005240
34	9	0	-3.921052	4.204097	0.004325

Table S72: Optimized Cartesian coordinates of **3** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000261	-0.005283	0.001408
2	6	0	1.530051	0.353283	0.001800
3	6	0	2.461721	-0.339206	-0.792671
4	6	0	2.054229	1.391610	0.793335
5	6	0	3.817664	-0.010331	-0.807648
6	6	0	3.412941	1.708487	0.801211
7	6	0	4.308957	1.014219	-0.005118
8	6	0	-0.456781	-1.508433	0.000814
9	6	0	-1.523323	-1.964718	-0.795105
10	6	0	0.172541	-2.482812	0.796537
11	6	0	-1.925046	-3.300792	-0.806569
12	6	0	-0.240968	-3.815368	0.807819
13	6	0	-1.291260	-4.239928	0.000509
14	6	0	-1.073033	1.142607	0.000386
15	6	0	-2.234338	1.084175	0.792248
16	6	0	-0.930960	2.297028	-0.791076
17	6	0	-3.179436	2.110639	0.804751
18	6	0	-1.885092	3.314948	-0.801624
19	6	0	-3.017550	3.235323	0.002290
20	9	0	-2.445905	0.027020	1.607501
21	9	0	1.241203	2.096486	1.611365
22	9	0	2.048967	-1.334327	-1.609032
23	9	0	1.188948	-2.134351	1.616558
24	9	0	-2.172498	-1.107273	-1.613883
25	9	0	0.138469	2.431698	-1.606777
26	9	0	4.657721	-0.698575	-1.608880
27	9	0	3.857291	2.702387	1.598828
28	9	0	-1.700932	4.388010	-1.599163
29	9	0	-4.262027	2.005259	1.603720
30	9	0	-2.942349	-3.680522	-1.608094
31	9	0	0.390352	-4.698714	1.609435
32	1	0	-1.609546	-5.282189	0.000223
33	1	0	5.369194	1.266364	-0.007912
34	1	0	-3.759253	4.033802	0.003616

Table S73: Optimized Cartesian coordinates of **4** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000960	-0.003911	0.000927
2	6	0	1.527931	0.353338	0.000378
3	6	0	2.465132	-0.355836	-0.773684
4	6	0	2.053281	1.407528	0.770776
5	6	0	3.823125	-0.041855	-0.800766
6	6	0	3.408112	1.734732	0.789310
7	6	0	4.297273	1.007669	-0.007967
8	6	0	-0.456722	-1.506293	0.001396
9	6	0	-1.536777	-1.963242	-0.776469
10	6	0	0.186203	-2.486436	0.779839
11	6	0	-1.948591	-3.294794	-0.798832
12	6	0	-0.212813	-3.821929	0.803174
13	6	0	-1.284340	-4.228556	0.002287
14	6	0	-1.073498	1.142809	0.000042
15	6	0	-2.251297	1.072871	0.767470
16	6	0	-0.919638	2.313529	-0.766070
17	6	0	-3.204921	2.089443	0.792510
18	6	0	-1.863175	3.339322	-0.786754
19	6	0	-3.010642	3.227806	0.004343
20	9	0	-3.920026	4.207822	0.007175
21	9	0	-4.301290	1.990094	1.560920
22	9	0	-2.482388	0.005140	1.560256
23	9	0	1.243057	2.132015	1.571314
24	9	0	3.867658	2.733838	1.559402
25	9	0	5.598333	1.315632	-0.012446
26	9	0	4.676523	-0.730323	-1.575425
27	9	0	2.060262	-1.366161	-1.572189
28	9	0	1.214653	-2.145950	1.585203
29	9	0	0.415470	-4.717735	1.581122
30	9	0	-1.673312	-5.507768	0.002808
31	9	0	-2.969618	-3.689812	-1.575981
32	9	0	-2.203046	-1.107913	-1.580697
33	9	0	0.160941	2.467707	-1.560300
34	9	0	-1.684815	4.427553	-1.552423

Table S74: Optimized Cartesian coordinates of **5** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.269382	-1.788710	0.634711
2	1	0	-7.353456	-1.738420	0.492625
3	1	0	-6.064874	-1.819886	1.717438
4	1	0	-5.905489	-2.725148	0.182885
5	6	0	-4.298347	-0.475055	0.000353
6	6	0	-3.673952	0.629210	-0.653577
7	1	0	-4.277532	1.357939	-1.192367
8	6	0	-2.301888	0.778993	-0.641235
9	1	0	-1.860252	1.618386	-1.180511
10	6	0	-1.442236	-0.161156	-0.007330
11	6	0	-0.005093	-0.001415	-0.007081
12	6	0	0.576635	1.323319	-0.006033
13	6	0	1.813072	1.598379	-0.653861
14	1	0	2.312285	0.797390	-1.201258
15	6	0	2.369547	2.861402	-0.669553
16	1	0	3.295760	3.021162	-1.219311
17	6	0	1.735748	3.952421	-0.002453
18	6	0	-2.073367	-1.266720	0.628344
19	1	0	-1.457412	-1.990911	1.163602
20	6	0	-3.445089	-1.418657	0.647550
21	1	0	-3.872737	-2.262548	1.186825
22	6	0	0.853601	-1.165880	-0.004963
23	6	0	2.117621	-1.161611	0.647765
24	1	0	2.425859	-0.269783	1.195355
25	6	0	2.937863	-2.271597	0.668602
26	1	0	3.873787	-2.223784	1.223012
27	6	0	2.560947	-3.476631	0.003274
28	6	0	1.300485	-3.486275	-0.666030
29	1	0	0.981022	-4.370327	-1.215463
30	6	0	0.480315	-2.375967	-0.653234
31	1	0	-0.460863	-2.411290	-1.204076
32	6	0	0.501875	3.683207	0.662328
33	1	0	-0.004827	4.472673	1.215189
34	6	0	-0.055031	2.420161	0.643461
35	1	0	-0.982955	2.247050	1.190738
36	6	0	1.604480	6.312979	0.653755
37	1	0	1.517040	6.152764	1.741090
38	1	0	2.180553	7.228664	0.487554
39	1	0	0.594947	6.462200	0.239414
40	6	0	4.679825	-4.525427	0.655708
41	1	0	4.587868	-4.356816	1.741323
42	1	0	5.188123	-5.482064	0.499748
43	1	0	5.309069	-3.727794	0.229960
44	6	0	3.576609	5.439756	-0.644860
45	1	0	4.361580	4.791709	-0.223921
46	1	0	3.524181	5.265534	-1.732213
47	1	0	3.867500	6.481534	-0.478221
48	6	0	-6.510618	0.380732	-0.621792
49	1	0	-6.338678	1.379137	-0.189795
50	1	0	-6.340204	0.435518	-1.709724
51	1	0	-7.557370	0.110073	-0.452193
52	6	0	2.947478	-5.811772	-0.642128
53	1	0	1.999783	-6.181273	-0.219423
54	1	0	2.817177	-5.676194	-1.728334
55	1	0	3.714358	-6.576060	-0.482322
56	7	0	2.287365	5.198336	0.000088
57	7	0	3.371007	-4.572248	0.006598
58	7	0	-5.652775	-0.622024	0.006461

Table S75: Optimized Cartesian coordinates of **6** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.542202	10.025912	-0.762591
2	6	0	6.068524	10.267792	-2.104136
3	1	0	6.412149	11.276277	-2.354052
4	1	0	4.969908	10.227502	-2.142583
5	1	0	6.501377	9.539965	-2.806096
6	6	0	6.277840	8.841659	-0.183704
7	6	0	6.798884	8.663871	1.119347
8	1	0	7.392968	9.466359	1.558186
9	6	0	6.569976	7.487149	1.802151
10	1	0	7.006708	7.350476	2.792022
11	6	0	5.836137	6.417757	1.211378
12	6	0	5.605090	5.178122	1.920802
13	6	0	5.455526	5.183529	3.359964
14	6	0	5.899821	4.087779	4.155672
15	1	0	6.404060	3.249310	3.674036
16	6	0	5.768900	4.099012	5.528811
17	1	0	6.143761	3.276988	6.139764
18	6	0	5.157677	5.198588	6.175672
19	6	0	5.335841	6.615568	-0.102992
20	1	0	4.732336	5.833652	-0.565581
21	6	0	5.534170	7.804202	-0.787795
22	1	0	5.101874	7.931980	-1.779083
23	6	0	5.527121	3.931482	1.189839
24	6	0	4.677687	2.878055	1.620407
25	1	0	4.044059	3.030313	2.494922
26	6	0	4.578300	1.687122	0.917739
27	1	0	3.885135	0.918626	1.256488
28	6	0	5.361826	1.494095	-0.241151
29	6	0	6.227588	2.522420	-0.681576
30	1	0	6.843613	2.343541	-1.563666
31	6	0	6.295012	3.714605	0.009059
32	1	0	6.990928	4.485933	-0.322573
33	6	0	4.692976	6.290750	5.410492
34	1	0	4.193202	7.133055	5.886579
35	6	0	4.857038	6.281004	4.034029
36	1	0	4.465598	7.114472	3.449430
37	8	0	5.065672	5.109819	7.513861
38	8	0	5.355353	0.377897	-0.990422
39	6	0	4.482179	6.205395	8.250074
40	1	0	3.434099	6.360553	7.953952
41	1	0	4.529675	5.904104	9.301093
42	1	0	5.061555	7.128221	8.099188
43	6	0	4.517738	-0.727794	-0.592680
44	1	0	3.457398	-0.435012	-0.596645
45	1	0	4.690487	-1.505053	-1.343446
46	1	0	4.807576	-1.097722	0.401903

Table S76: Optimized Cartesian coordinates of **7** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.486424	10.058903	-0.743269
2	6	0	6.079050	10.287109	-2.113010
3	1	0	6.406275	11.305467	-2.342074
4	1	0	4.986197	10.213847	-2.207508
5	1	0	6.572856	9.571669	-2.785718
6	6	0	6.246334	8.872529	-0.176264
7	6	0	6.707240	8.723962	1.156655
8	1	0	7.241553	9.554594	1.618898
9	6	0	6.496769	7.544177	1.831803
10	1	0	6.889928	7.429145	2.841945
11	6	0	5.844977	6.435087	1.205211
12	6	0	5.637160	5.199976	1.899617
13	6	0	5.505449	5.179041	3.350485
14	6	0	6.026067	4.097631	4.107079
15	1	0	6.562208	3.296484	3.597409
16	6	0	5.910156	4.084890	5.492949
17	1	0	6.339883	3.261872	6.065622
18	6	0	5.247513	5.128837	6.152063
19	1	0	5.147247	5.108937	7.238585
20	6	0	5.403036	6.607631	-0.140405
21	1	0	4.853669	5.801019	-0.626288
22	6	0	5.580088	7.799681	-0.815830
23	1	0	5.189079	7.910333	-1.825920
24	6	0	5.552964	3.944657	1.164319
25	6	0	4.670325	2.918481	1.588984
26	1	0	4.026035	3.090491	2.451765
27	6	0	4.579924	1.726259	0.878690
28	1	0	3.876080	0.956460	1.198078
29	6	0	5.387067	1.516327	-0.247392
30	1	0	5.323017	0.574029	-0.794208
31	6	0	6.280432	2.509360	-0.669974
32	1	0	6.925270	2.334086	-1.532244
33	6	0	6.357055	3.716121	0.017836
34	1	0	7.079529	4.473812	-0.287904
35	6	0	4.708326	6.195213	5.420481
36	1	0	4.172583	6.995028	5.933640
37	6	0	4.844207	6.230287	4.036690
38	1	0	4.392529	7.042268	3.465603

Table S77: Optimized Cartesian coordinates of **8** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.022172	-3.003685	-0.000370
2	6	0	3.238360	-1.798103	0.681828
3	1	0	4.168824	-1.637910	1.227774
4	6	0	2.262474	-0.809425	0.672197
5	1	0	2.415374	0.113802	1.231658
6	6	0	1.027867	-1.021619	-0.000161
7	6	0	0.000280	-0.000226	-0.000947
8	6	0	0.370677	1.400692	-0.000872
9	6	0	-0.430562	2.363258	0.672163
10	1	0	-1.306343	2.033803	1.231841
11	6	0	-0.062098	3.702728	0.682576
12	1	0	-0.666316	4.428080	1.228832
13	6	0	1.090268	4.119171	0.001252
14	1	0	1.369462	5.174162	0.002444
15	6	0	0.822382	-2.257648	-0.672015
16	1	0	-0.100167	-2.416153	-1.231197
17	6	0	1.817391	-3.227203	-0.681669
18	1	0	1.662672	-4.158915	-1.227158
19	6	0	-1.398166	-0.380047	-0.001754
20	6	0	-2.365655	0.414017	-0.676006
21	1	0	-2.041055	1.290425	-1.237364
22	6	0	-3.703127	0.038167	-0.684158
23	1	0	-4.432376	0.636682	-1.231530
24	6	0	-4.112696	-1.114258	0.001193
25	1	0	-5.166196	-1.399179	0.002082
26	6	0	-3.176826	-1.902877	0.685137
27	1	0	-3.503867	-2.787042	1.233684
28	6	0	-1.832277	-1.553177	0.674082
29	1	0	-1.109331	-2.145945	1.235076
30	6	0	1.886009	3.188165	-0.681100
31	1	0	2.770456	3.520366	-1.226124
32	6	0	1.543533	1.841787	-0.672643
33	1	0	2.142671	1.122649	-1.231767
34	1	0	3.796161	-3.773116	-0.000651

Table S78: Optimized Cartesian coordinates of **9** in toluene.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.266648	8.866118	-0.165153
2	6	0	6.898550	8.641720	1.069491
3	6	0	6.670983	7.450627	1.745347
4	6	0	5.845822	6.418817	1.208758
5	6	0	5.633947	5.171280	1.910010
6	6	0	5.486049	5.170758	3.349352
7	6	0	6.049867	4.145780	4.164090
8	6	0	5.924193	4.148098	5.546703
9	6	0	5.184919	5.166974	6.171168
10	6	0	5.242067	6.684655	-0.055290
11	6	0	5.426399	7.887730	-0.723082
12	6	0	5.567407	3.928311	1.173330
13	6	0	4.663160	2.885933	1.534861
14	6	0	4.579654	1.698917	0.819813
15	6	0	5.437270	1.488784	-0.273117
16	6	0	6.359461	2.477896	-0.654449
17	6	0	6.403116	3.676088	0.045257
18	6	0	4.595345	6.188632	5.408043
19	6	0	4.766003	6.196177	4.030230
20	9	0	4.159689	7.166394	3.339705
21	9	0	3.877069	7.132627	6.010686
22	9	0	5.044931	5.164670	7.484115
23	9	0	6.500426	3.203108	6.284991
24	9	0	6.795588	3.182924	3.614002
25	9	0	3.801171	3.060039	2.541002
26	9	0	3.693352	0.763993	1.152207
27	9	0	5.375955	0.354731	-0.946237
28	9	0	7.183888	2.254268	-1.674338
29	9	0	7.322050	4.572006	-0.326805
30	9	0	4.404937	5.797826	-0.602085
31	9	0	4.813521	8.126299	-1.879716
32	9	0	6.463135	10.003958	-0.805339
33	9	0	7.711573	9.566482	1.573586
34	9	0	7.323884	7.261630	2.896076

Table S79: Optimized Cartesian coordinates of **1** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000653	-0.006269	0.001099
2	6	0	1.529630	0.352888	0.002324
3	6	0	2.480661	-0.315945	-0.791980
4	6	0	2.078723	1.379776	0.794487
5	6	0	3.836352	-0.011319	-0.826170
6	6	0	3.425822	1.720271	0.824007
7	6	0	4.305397	1.015660	-0.002387
8	6	0	-0.456374	-1.508589	0.000343
9	6	0	-1.517634	-1.990466	-0.790368
10	6	0	0.153158	-2.501524	0.791318
11	6	0	-1.942231	-3.313419	-0.821598
12	6	0	-0.236085	-3.835374	0.823554
13	6	0	-1.292266	-4.237308	0.001284
14	6	0	-1.071874	1.141372	-0.000372
15	6	0	-2.236388	1.112456	0.790901
16	6	0	-0.957302	2.300409	-0.792057
17	6	0	-3.195318	2.118101	0.822789
18	6	0	-1.889065	3.331068	-0.824003
19	6	0	-3.013844	3.232937	-0.000287
20	9	0	-2.427137	0.046203	1.617688
21	9	0	1.245748	2.069679	1.623388
22	9	0	2.045953	-1.306674	-1.620507
23	9	0	1.171689	-2.131973	1.617521
24	9	0	-2.155631	-1.114074	-1.615935
25	9	0	0.120246	2.412042	-1.618772
26	1	0	3.769014	2.518559	1.481827
27	1	0	5.366352	1.269216	-0.004553
28	1	0	4.500657	-0.568470	-1.486539
29	1	0	0.280097	-4.534875	1.480840
30	1	0	-1.611819	-5.280280	0.001746
31	1	0	-2.762140	-3.604215	-1.478094
32	1	0	-4.058715	2.022860	1.481020
33	1	0	-3.755797	4.032557	0.000285
34	1	0	-1.730268	4.185401	-1.481782

Table S80: Optimized Cartesian coordinates of **2** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000403	-0.003583	0.001683
2	6	0	1.527840	0.353223	0.000551
3	6	0	2.482556	-0.337234	-0.772266
4	6	0	2.078037	1.398796	0.768679
5	6	0	3.840193	-0.042662	-0.814975
6	6	0	3.424069	1.742846	0.801896
7	6	0	4.280035	1.003394	-0.009138
8	6	0	-0.455974	-1.505274	0.002033
9	6	0	-1.529678	-1.986805	-0.773123
10	6	0	0.167322	-2.502452	0.778060
11	6	0	-1.958558	-3.308192	-0.810352
12	6	0	-0.213192	-3.838617	0.816962
13	6	0	-1.279808	-4.210331	0.003744
14	6	0	-1.072424	1.142484	0.001020
15	6	0	-2.257243	1.096019	0.762905
16	6	0	-0.941938	2.321328	-0.760468
17	6	0	-3.222278	2.095469	0.801477
18	6	0	-1.869186	3.355734	-0.797263
19	6	0	-2.999134	3.213322	0.002902
20	9	0	-2.472956	0.017116	1.559194
21	9	0	1.251171	2.113218	1.575516
22	9	0	2.057420	-1.345655	-1.576930
23	9	0	1.196086	-2.142585	1.588760
24	9	0	-2.184678	-1.114888	-1.583021
25	9	0	0.149179	2.459753	-1.557448
26	1	0	3.789028	2.550112	1.434752
27	1	0	4.523123	-0.601689	-1.452549
28	1	0	0.297536	-4.556592	1.456556
29	1	0	-2.783686	-3.620221	-1.448523
30	1	0	-4.106485	2.007207	1.430571
31	1	0	-1.718255	4.232344	-1.425076
32	9	0	5.596693	1.315139	-0.014583
33	9	0	-1.674146	-5.504680	0.004844
34	9	0	-3.920123	4.204417	0.004468

Table S81: Optimized Cartesian coordinates of **3** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000128	-0.006140	0.001478
2	6	0	1.529864	0.352846	0.002506
3	6	0	2.462476	-0.337026	-0.792758
4	6	0	2.054456	1.389935	0.795049
5	6	0	3.817847	-0.006874	-0.807520
6	6	0	3.412756	1.707490	0.802847
7	6	0	4.310050	1.016303	-0.004250
8	6	0	-0.456962	-1.509212	0.000733
9	6	0	-1.523646	-1.966244	-0.794307
10	6	0	0.171874	-2.484496	0.795457
11	6	0	-1.925229	-3.302097	-0.805590
12	6	0	-0.241873	-3.816708	0.806395
13	6	0	-1.292237	-4.242420	0.000259
14	6	0	-1.073005	1.142022	-0.000060
15	6	0	-2.233367	1.086452	0.793005
16	6	0	-0.932324	2.295342	-0.793008
17	6	0	-3.177346	2.113618	0.805253
18	6	0	-1.885824	3.313518	-0.803556
19	6	0	-3.017393	3.237317	0.001474
20	9	0	-2.445366	0.030449	1.611038
21	9	0	1.241490	2.093884	1.615304
22	9	0	2.050913	-1.331920	-1.611371
23	9	0	1.189283	-2.137167	1.616047
24	9	0	-2.174066	-1.108942	-1.613560
25	9	0	0.136247	2.429013	-1.611376
26	9	0	4.657132	-0.694678	-1.611578
27	9	0	3.855085	2.701243	1.603430
28	9	0	-1.700355	4.385107	-1.604428
29	9	0	-4.258779	2.008452	1.607472
30	9	0	-2.943784	-3.680009	-1.608008
31	9	0	0.391331	-4.699413	1.608846
32	1	0	-1.610666	-5.284631	-0.000043
33	1	0	5.370088	1.269250	-0.007060
34	1	0	-3.758587	4.036259	0.002683

Table S82: Optimized Cartesian coordinates of **4** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.001376	-0.005571	0.000559
2	6	0	1.527468	0.352480	0.001244
3	6	0	2.465394	-0.353267	-0.774649
4	6	0	2.051879	1.405100	0.774043
5	6	0	3.822584	-0.037131	-0.801289
6	6	0	3.406003	1.733889	0.792595
7	6	0	4.295743	1.010659	-0.006548
8	6	0	-0.457167	-1.507928	0.000970
9	6	0	-1.536775	-1.965073	-0.777121
10	6	0	0.185102	-2.488202	0.779497
11	6	0	-1.948440	-3.296339	-0.799268
12	6	0	-0.214107	-3.823303	0.802410
13	6	0	-1.284969	-4.230036	0.001625
14	6	0	-1.073716	1.141631	-0.001247
15	6	0	-2.248945	1.075555	0.769980
16	6	0	-0.921180	2.309845	-0.771000
17	6	0	-3.200429	2.093724	0.795665
18	6	0	-1.863227	3.336595	-0.790987
19	6	0	-3.007567	3.229424	0.004276
20	9	0	-3.915697	4.211444	0.007907
21	9	0	-4.294793	1.997937	1.568968
22	9	0	-2.479560	0.010127	1.566601
23	9	0	1.241335	2.127006	1.577160
24	9	0	3.864682	2.732146	1.565877
25	9	0	5.596947	1.320641	-0.010844
26	9	0	4.677076	-0.722908	-1.578707
27	9	0	2.062104	-1.362595	-1.575780
28	9	0	1.213619	-2.148440	1.585606
29	9	0	0.414245	-4.719636	1.581245
30	9	0	-1.674162	-5.509785	0.002008
31	9	0	-2.969860	-3.691485	-1.577391
32	9	0	-2.203270	-1.110097	-1.582048
33	9	0	0.157009	2.460912	-1.569665
34	9	0	-1.685866	4.423015	-1.561046

Table S83: Optimized Cartesian coordinates of **5** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.908520	-2.753119	0.637821
2	1	0	-6.987015	-2.873116	0.496159
3	1	0	-5.700293	-2.749726	1.720151
4	1	0	-5.401817	-3.621037	0.187160
5	6	0	-4.169287	-1.147308	-0.000637
6	6	0	-3.726623	0.041643	-0.655382
7	1	0	-4.437865	0.666735	-1.192967
8	6	0	-2.395145	0.405642	-0.643392
9	1	0	-2.092318	1.304923	-1.181988
10	6	0	-1.397503	-0.387224	-0.009816
11	6	0	-0.003500	-0.002505	-0.008868
12	6	0	0.361470	1.397557	-0.006608
13	6	0	1.540913	1.865447	-0.650728
14	1	0	2.163451	1.154068	-1.195567
15	6	0	1.890499	3.200755	-0.665506
16	1	0	2.782085	3.505150	-1.211448
17	6	0	1.089249	4.178029	-0.001168
18	6	0	-1.846518	-1.578863	0.625541
19	1	0	-1.124207	-2.198039	1.159660
20	6	0	-3.177221	-1.945230	0.645679
21	1	0	-3.466070	-2.846627	1.184081
22	6	0	1.028162	-1.016962	-0.006672
23	6	0	2.276288	-0.813273	0.645389
24	1	0	2.441232	0.116585	1.191675
25	6	0	3.261471	-1.779975	0.666838
26	1	0	4.178908	-1.584307	1.219674
27	6	0	3.078730	-3.030500	0.002811
28	6	0	1.835162	-3.238868	-0.666712
29	1	0	1.658762	-4.162776	-1.215148
30	6	0	0.850392	-2.271428	-0.654246
31	1	0	-0.073662	-2.455932	-1.204353
32	6	0	-0.088560	3.716391	0.660503
33	1	0	-0.716341	4.415669	1.210530
34	6	0	-0.437809	2.380858	0.640653
35	1	0	-1.328720	2.063693	1.184915
36	6	0	0.582051	6.487437	0.651986
37	1	0	0.516761	6.314095	1.738668
38	1	0	1.007333	7.482292	0.487713
39	1	0	-0.436617	6.474363	0.233679
40	6	0	5.335965	-3.732060	0.655571
41	1	0	5.218647	-3.578999	1.740916
42	1	0	5.987702	-4.597083	0.499080
43	1	0	5.830787	-2.845285	0.229125
44	6	0	2.671277	5.938247	-0.641598
45	1	0	3.548482	5.425084	-0.217118
46	1	0	2.649745	5.753881	-1.728159
47	1	0	2.790036	7.013586	-0.477578
48	6	0	-6.488926	-0.648754	-0.618827
49	1	0	-6.473049	0.364454	-0.187747
50	1	0	-6.331445	-0.568752	-1.706970
51	1	0	-7.479547	-1.080124	-0.445821
52	6	0	3.826232	-5.276879	-0.638626
53	1	0	2.943709	-5.785415	-0.219767
54	1	0	3.682917	-5.165877	-1.725889
55	1	0	4.700655	-5.912977	-0.470732
56	7	0	1.435525	5.494935	0.001430
57	7	0	4.050099	-3.984752	0.007580
58	7	0	-5.483013	-1.504876	0.007281

Table S84: Optimized Cartesian coordinates of **6** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.541981	10.026248	-0.762055
2	6	0	6.065894	10.264831	-2.104255
3	1	0	6.408571	11.272941	-2.357139
4	1	0	4.967531	10.223298	-2.140745
5	1	0	6.497731	9.535357	-2.804729
6	6	0	6.277539	8.840880	-0.181768
7	6	0	6.798594	8.663702	1.121016
8	1	0	7.391736	9.465896	1.561770
9	6	0	6.570189	7.486715	1.804147
10	1	0	7.006333	7.350825	2.794272
11	6	0	5.836865	6.417829	1.212651
12	6	0	5.606154	5.177875	1.921259
13	6	0	5.456179	5.182202	3.360132
14	6	0	5.897895	4.084814	4.154469
15	1	0	6.399656	3.245035	3.672793
16	6	0	5.766474	4.095774	5.527878
17	1	0	6.138985	3.271144	6.136853
18	6	0	5.157877	5.196444	6.174697
19	6	0	5.335912	6.615447	-0.101342
20	1	0	4.732184	5.834009	-0.564136
21	6	0	5.533870	7.804203	-0.786202
22	1	0	5.101480	7.931247	-1.777410
23	6	0	5.528490	3.931917	1.189406
24	6	0	4.678916	2.878618	1.619446
25	1	0	4.044572	3.030134	2.493438
26	6	0	4.579997	1.687694	0.916487
27	1	0	3.887258	0.919154	1.255714
28	6	0	5.364316	1.495833	-0.241524
29	6	0	6.229884	2.523967	-0.681665
30	1	0	6.846285	2.347525	-1.564022
31	6	0	6.296895	3.716438	0.009127
32	1	0	6.992165	4.488050	-0.322897
33	6	0	4.695308	6.289884	5.410855
34	1	0	4.197715	7.133499	5.886588
35	6	0	4.859400	6.280348	4.034337
36	1	0	4.469140	7.114911	3.450762
37	8	0	5.065315	5.108335	7.514460
38	8	0	5.358018	0.377965	-0.991185
39	6	0	4.482271	6.207659	8.247059
40	1	0	3.435562	6.363978	7.947833
41	1	0	4.527159	5.909261	9.299034
42	1	0	5.063370	7.128738	8.094088
43	6	0	4.516557	-0.725087	-0.591361
44	1	0	3.457298	-0.429351	-0.598779
45	1	0	4.689515	-1.505631	-1.338715
46	1	0	4.802509	-1.091228	0.405446

Table S85: Optimized Cartesian coordinates of **7** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.485837	10.059605	-0.742576
2	6	0	6.080631	10.283599	-2.114454
3	1	0	6.403704	11.303076	-2.344481
4	1	0	4.988703	10.204448	-2.211114
5	1	0	6.579289	9.569098	-2.784071
6	6	0	6.246036	8.872363	-0.174981
7	6	0	6.703735	8.725657	1.159074
8	1	0	7.235483	9.556757	1.623337
9	6	0	6.493499	7.546062	1.834365
10	1	0	6.884600	7.432126	2.845244
11	6	0	5.844918	6.436318	1.205704
12	6	0	5.637571	5.201975	1.899058
13	6	0	5.507175	5.179638	3.350417
14	6	0	6.031211	4.099375	4.105478
15	1	0	6.569385	3.300144	3.595085
16	6	0	5.914923	4.085020	5.491536
17	1	0	6.346550	3.262323	6.063228
18	6	0	5.248890	5.126333	6.151554
19	1	0	5.148303	5.105014	7.238041
20	6	0	5.405899	6.607427	-0.141227
21	1	0	4.858522	5.800465	-0.628386
22	6	0	5.583068	7.799094	-0.816615
23	1	0	5.195203	7.908165	-1.827897
24	6	0	5.552199	3.946447	1.163990
25	6	0	4.668590	2.921847	1.589325
26	1	0	4.024389	3.094739	2.451911
27	6	0	4.577398	1.729129	0.879641
28	1	0	3.873227	0.960038	1.199997
29	6	0	5.384310	1.517997	-0.246488
30	1	0	5.319350	0.575564	-0.793009
31	6	0	6.278298	2.510207	-0.669511
32	1	0	6.922038	2.335281	-1.532637
33	6	0	6.356312	3.717239	0.018152
34	1	0	7.078569	4.474519	-0.288652
35	6	0	4.706697	6.191604	5.420723
36	1	0	4.169052	6.990061	5.933953
37	6	0	4.842373	6.228005	4.036653
38	1	0	4.388563	7.038936	3.466031

Table S86: Optimized Cartesian coordinates of **8** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.254154	8.845574	-0.157755
2	6	0	6.793952	8.668107	1.123913
3	1	0	7.387456	9.460030	1.582177
4	6	0	6.581732	7.478166	1.808897
5	1	0	7.030564	7.325897	2.790620
6	6	0	5.844379	6.422417	1.207064
7	6	0	5.631361	5.174147	1.910460
8	6	0	5.484075	5.170220	3.351713
9	6	0	5.960537	4.077936	4.126757
10	1	0	6.483462	3.258571	3.633171
11	6	0	5.829680	4.086626	5.509909
12	1	0	6.226334	3.258116	6.097901
13	6	0	5.198289	5.163141	6.148680
14	1	0	5.087539	5.160218	7.234340
15	6	0	5.319251	6.616281	-0.099518
16	1	0	4.712361	5.833214	-0.554518
17	6	0	5.512145	7.821592	-0.763151
18	1	0	5.078478	7.972114	-1.752479
19	6	0	5.565462	3.929317	1.172125
20	6	0	4.719634	2.872700	1.606230
21	1	0	4.079550	3.022472	2.475809
22	6	0	4.651495	1.685568	0.887549
23	1	0	3.976030	0.892852	1.211380
24	6	0	5.442053	1.511451	-0.257085
25	1	0	5.394027	0.572825	-0.811776
26	6	0	6.293564	2.536116	-0.693507
27	1	0	6.920901	2.388453	-1.573354
28	6	0	6.347145	3.738715	0.000292
29	1	0	7.035046	4.522425	-0.317602
30	6	0	4.708702	6.243250	5.400908
31	1	0	4.201109	7.069154	5.900661
32	6	0	4.860388	6.258824	4.019953
33	1	0	4.448738	7.081386	3.434848
34	1	0	6.412861	9.786327	-0.687686

Table S87: Optimized Cartesian coordinates of **9** in dichloromethane.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.268827	8.866049	-0.164475
2	6	0	6.901398	8.639145	1.067752
3	6	0	6.671514	7.449370	1.744150
4	6	0	5.842935	6.420740	1.207643
5	6	0	5.629658	5.173552	1.907883
6	6	0	5.483622	5.171813	3.347028
7	6	0	6.050200	4.146751	4.159086
8	6	0	5.925848	4.148015	5.541311
9	6	0	5.186309	5.163700	6.167391
10	6	0	5.238518	6.688362	-0.055369
11	6	0	5.425747	7.891477	-0.721264
12	6	0	5.562683	3.930929	1.171648
13	6	0	4.658597	2.889156	1.533904
14	6	0	4.580306	1.700228	0.822445
15	6	0	5.441568	1.487464	-0.265351
16	6	0	6.361412	2.476271	-0.647685
17	6	0	6.401159	3.677354	0.046372
18	6	0	4.594814	6.184441	5.407077
19	6	0	4.763256	6.195406	4.029464
20	9	0	4.154691	7.165845	3.342191
21	9	0	3.874516	7.127383	6.013517
22	9	0	5.047225	5.159313	7.482632
23	9	0	6.506090	3.202252	6.279194
24	9	0	6.796416	3.185373	3.608117
25	9	0	3.793694	3.063648	2.536885
26	9	0	3.693156	0.763376	1.155258
27	9	0	5.385241	0.348455	-0.934774
28	9	0	7.190727	2.249560	-1.665628
29	9	0	7.318938	4.572860	-0.327580
30	9	0	4.399367	5.804735	-0.602983
31	9	0	4.810532	8.133750	-1.878261
32	9	0	6.468222	10.005694	-0.805090
33	9	0	7.719687	9.562621	1.571095
34	9	0	7.325159	7.259160	2.893632

Table S88: Optimized Cartesian coordinates of **1** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000187	-0.001953	0.001321
2	6	0	1.521776	0.352692	-0.000677
3	6	0	2.470912	-0.350731	-0.763956
4	6	0	2.063966	1.405734	0.758089
5	6	0	3.827505	-0.051524	-0.798100
6	6	0	3.412024	1.741216	0.783048
7	6	0	4.293495	1.003121	-0.009999
8	6	0	-0.453968	-1.497388	0.001588
9	6	0	-1.530547	-1.970175	-0.769931
10	6	0	0.176877	-2.489138	0.773490
11	6	0	-1.952309	-3.293735	-0.799561
12	6	0	-0.209912	-3.823430	0.803693
13	6	0	-1.282479	-4.220722	0.002168
14	6	0	-1.068206	1.138962	0.001850
15	6	0	-2.252733	1.080464	0.758313
16	6	0	-0.929216	2.317807	-0.753066
17	6	0	-3.213814	2.083612	0.789759
18	6	0	-1.862790	3.346445	-0.780640
19	6	0	-3.010239	3.221392	0.005815
20	9	0	-2.465709	-0.007757	1.543072
21	9	0	1.229484	2.127655	1.550669
22	9	0	2.039761	-1.368390	-1.554086
23	9	0	1.210865	-2.123280	1.575376
24	9	0	-2.186842	-1.090292	-1.570658
25	9	0	0.169956	2.456120	-1.539447
26	1	0	3.751422	2.562937	1.412721
27	1	0	5.355430	1.252606	-0.013867
28	1	0	4.492648	-0.637016	-1.431906
29	1	0	0.323578	-4.524865	1.444233
30	1	0	-1.599938	-5.264352	0.002299
31	1	0	-2.786491	-3.579427	-1.439451
32	1	0	-4.095599	1.965262	1.418522
33	1	0	-3.753953	4.019395	0.007869
34	1	0	-1.684503	4.219433	-1.407530

Table S89: Optimized Cartesian coordinates of **2** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.001397	-0.000165	0.001142
2	6	0	1.519597	0.353265	-0.001211
3	6	0	2.473960	-0.366166	-0.744821
4	6	0	2.062778	1.420736	0.738301
5	6	0	3.832220	-0.076254	-0.784639
6	6	0	3.409510	1.760362	0.769603
7	6	0	4.270607	0.993393	-0.009742
8	6	0	-0.453952	-1.494695	0.002096
9	6	0	-1.546442	-1.967125	-0.748826
10	6	0	0.193347	-2.492960	0.753701
11	6	0	-1.972785	-3.288926	-0.784260
12	6	0	-0.184704	-3.829433	0.790061
13	6	0	-1.271892	-4.197742	0.003076
14	6	0	-1.068550	1.139671	0.001453
15	6	0	-2.268242	1.070863	0.734954
16	6	0	-0.918873	2.332726	-0.730881
17	6	0	-3.234624	2.068458	0.771924
18	6	0	-1.847232	3.365647	-0.764207
19	6	0	-2.995980	3.205023	0.005040
20	9	0	-2.500611	-0.024873	1.498091
21	9	0	1.232957	2.162014	1.512493
22	9	0	2.052637	-1.398169	-1.516202
23	9	0	1.242034	-2.138229	1.536083
24	9	0	-2.223494	-1.090431	-1.530334
25	9	0	0.188888	2.490175	-1.495952
26	1	0	3.772291	2.586692	1.377791
27	1	0	4.518660	-0.657996	-1.396772
28	1	0	0.344464	-4.552084	1.408193
29	1	0	-2.814392	-3.597273	-1.401493
30	1	0	-4.133667	1.964766	1.376308
31	1	0	-1.682931	4.256810	-1.366814
32	9	0	5.586458	1.300065	-0.014246
33	9	0	-1.663319	-5.490990	0.003567
34	9	0	-3.917173	4.193306	0.007381

Table S90: Optimized Cartesian coordinates of **3** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.000164	-0.001262	0.000908
2	6	0	1.522498	0.353322	-0.001212
3	6	0	2.452301	-0.367983	-0.769527
4	6	0	2.040350	1.412907	0.763254
5	6	0	3.809142	-0.045453	-0.784912
6	6	0	3.399289	1.725892	0.770180
7	6	0	4.295838	1.002127	-0.009554
8	6	0	-0.454087	-1.497404	0.001263
9	6	0	-1.535487	-1.945214	-0.776230
10	6	0	0.194986	-2.470954	0.779115
11	6	0	-1.936375	-3.280882	-0.787205
12	6	0	-0.215650	-3.803750	0.790764
13	6	0	-1.282589	-4.221950	0.001842
14	6	0	-1.068847	1.139945	0.001737
15	6	0	-2.246228	1.056334	0.764840
16	6	0	-0.906658	2.310323	-0.759529
17	6	0	-3.194293	2.079170	0.778270
18	6	0	-1.861712	3.326479	-0.768379
19	6	0	-3.012628	3.222204	0.006308
20	9	0	-2.472486	-0.021425	1.545772
21	9	0	1.222151	2.143224	1.550701
22	9	0	2.038671	-1.385379	-1.554867
23	9	0	1.227532	-2.122677	1.576417
24	9	0	-2.200409	-1.080966	-1.572569
25	9	0	0.182810	2.464066	-1.542019
26	9	0	4.654210	-0.758834	-1.555859
27	9	0	3.844740	2.741357	1.536903
28	9	0	-1.663535	4.419862	-1.531661
29	9	0	-4.296634	1.955152	1.544333
30	9	0	-2.969126	-3.659663	-1.566637
31	9	0	0.431339	-4.692938	1.570683
32	1	0	-1.599471	-5.264290	0.001916
33	1	0	5.356600	1.250447	-0.012862
34	1	0	-3.755864	4.018738	0.008617

Table S91: Optimized Cartesian coordinates of **4** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.001474	-0.000212	0.000675
2	6	0	1.520230	0.353506	-0.001543
3	6	0	2.456088	-0.380866	-0.750850
4	6	0	2.039927	1.426053	0.744193
5	6	0	3.814820	-0.072943	-0.776967
6	6	0	3.394940	1.749756	0.762318
7	6	0	4.286017	0.997012	-0.009427
8	6	0	-0.454232	-1.495495	0.001631
9	6	0	-1.549869	-1.944437	-0.755901
10	6	0	0.208794	-2.475982	0.759772
11	6	0	-1.960941	-3.275557	-0.777724
12	6	0	-0.187218	-3.811715	0.782601
13	6	0	-1.276556	-4.213034	0.002610
14	6	0	-1.069192	1.140142	0.001137
15	6	0	-2.260374	1.049362	0.742758
16	6	0	-0.898414	2.323626	-0.738731
17	6	0	-3.216881	2.062328	0.767022
18	6	0	-1.842580	3.347971	-0.758184
19	6	0	-3.006711	3.216653	0.005873
20	9	0	-3.917721	4.194128	0.008764
21	9	0	-4.329736	1.946145	1.506780
22	9	0	-2.503533	-0.035567	1.506258
23	9	0	1.224653	2.173149	1.516680
24	9	0	3.853650	2.767960	1.505359
25	9	0	5.587417	1.300225	-0.013492
26	9	0	4.671713	-0.784796	-1.524131
27	9	0	2.050628	-1.411451	-1.520985
28	9	0	1.254797	-2.136765	1.541127
29	9	0	0.458959	-4.712620	1.537697
30	9	0	-1.663675	-5.492070	0.003127
31	9	0	-2.998514	-3.667439	-1.532204
32	9	0	-2.233183	-1.082221	-1.536542
33	9	0	0.199227	2.493149	-1.504116
34	9	0	-1.650973	4.452337	-1.494937

Table S92: Optimized Cartesian coordinates of **5** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.502130	-3.462216	0.635288
2	1	0	-6.555976	-3.719747	0.491424
3	1	0	-5.298335	-3.434271	1.718292
4	1	0	-4.888373	-4.257395	0.183403
5	6	0	-3.979634	-1.652928	-0.002241
6	6	0	-3.692533	-0.418627	-0.655916
7	1	0	-4.477292	0.110527	-1.193150
8	6	0	-2.417902	0.107588	-0.646103
9	1	0	-2.223636	1.036473	-1.183751
10	6	0	-1.333474	-0.557748	-0.013179
11	6	0	-0.002483	-0.003522	-0.010852
12	6	0	0.183867	1.426646	-0.008115
13	6	0	1.299525	2.033233	-0.645679
14	1	0	2.005431	1.400652	-1.185202
15	6	0	1.479385	3.400361	-0.658267
16	1	0	2.327599	3.815874	-1.199141
17	6	0	0.556502	4.266262	-0.000939
18	6	0	-1.624822	-1.795384	0.621276
19	1	0	-0.827223	-2.314893	1.153708
20	6	0	-2.898204	-2.324137	0.640788
21	1	0	-3.074730	-3.253660	1.178848
22	6	0	1.144036	-0.878593	-0.006994
23	6	0	2.353802	-0.515410	0.643533
24	1	0	2.395481	0.429250	1.186960
25	6	0	3.451089	-1.350317	0.664472
26	1	0	4.337735	-1.042865	1.215666
27	6	0	3.422262	-2.613660	0.003882
28	6	0	2.215904	-2.980539	-0.661961
29	1	0	2.158425	-3.920188	-1.207996
30	6	0	1.119156	-2.144567	-0.651577
31	1	0	0.222881	-2.438712	-1.199117
32	6	0	-0.559143	3.664636	0.652186
33	1	0	-1.271228	4.281688	1.196823
34	6	0	-0.737801	2.297317	0.633238
35	1	0	-1.582532	1.865862	1.171689
36	6	0	-0.241275	6.490869	0.645194
37	1	0	-0.295726	6.307200	1.730836
38	1	0	0.056674	7.532149	0.488566
39	1	0	-1.245583	6.351980	0.214838
40	6	0	5.748104	-3.024531	0.653169
41	1	0	5.613779	-2.887908	1.738825
42	1	0	6.505655	-3.798541	0.496264
43	1	0	6.125222	-2.082229	0.225300
44	6	0	1.908959	6.207845	-0.631794
45	1	0	2.839879	5.807777	-0.199984
46	1	0	1.917319	6.021045	-1.718197
47	1	0	1.894060	7.290011	-0.469934
48	6	0	-6.343770	-1.441792	-0.607435
49	1	0	-6.445504	-0.434562	-0.173887
50	1	0	-6.206855	-1.342952	-1.696940
51	1	0	-7.274850	-1.987724	-0.426828
52	6	0	4.442341	-4.747028	-0.636192
53	1	0	3.633023	-5.362023	-0.211945
54	1	0	4.280666	-4.654993	-1.722762
55	1	0	5.389980	-5.269624	-0.473833
56	7	0	0.735215	5.616174	0.003244
57	7	0	4.505678	-3.438503	0.008041
58	7	0	-5.238969	-2.170637	0.008220

Table S93: Optimized Cartesian coordinates of **6** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.536544	10.019302	-0.751790
2	6	0	6.063212	10.261673	-2.091530
3	1	0	6.404846	11.270827	-2.340531
4	1	0	4.964346	10.219536	-2.129217
5	1	0	6.497750	9.535202	-2.794289
6	6	0	6.275722	8.835010	-0.176834
7	6	0	6.793985	8.659455	1.127377
8	1	0	7.383270	9.465753	1.564834
9	6	0	6.568412	7.482091	1.807596
10	1	0	7.000870	7.341331	2.798533
11	6	0	5.839650	6.413589	1.212299
12	6	0	5.608930	5.177390	1.919333
13	6	0	5.459645	5.182903	3.354295
14	6	0	5.895693	4.083027	4.146476
15	1	0	6.394372	3.244138	3.660424
16	6	0	5.761292	4.092836	5.518031
17	1	0	6.127839	3.269528	6.131700
18	6	0	5.157037	5.196617	6.163815
19	6	0	5.341763	6.606954	-0.101969
20	1	0	4.743068	5.820344	-0.562262
21	6	0	5.538592	7.795287	-0.785343
22	1	0	5.109281	7.923751	-1.777516
23	6	0	5.529690	3.934504	1.190578
24	6	0	4.684857	2.882421	1.628405
25	1	0	4.058167	3.038369	2.507023
26	6	0	4.584572	1.691863	0.927727
27	1	0	3.896514	0.920906	1.270190
28	6	0	5.360060	1.502202	-0.237220
29	6	0	6.220512	2.531777	-0.684421
30	1	0	6.829624	2.350799	-1.570417
31	6	0	6.291092	3.722232	0.006378
32	1	0	6.982673	4.497242	-0.325044
33	6	0	4.703058	6.294338	5.399965
34	1	0	4.208883	7.138847	5.877130
35	6	0	4.868009	6.284254	4.024842
36	1	0	4.484322	7.118282	3.436294
37	8	0	5.060926	5.106523	7.499212
38	8	0	5.350971	0.388296	-0.985578
39	6	0	4.479620	6.203306	8.232047
40	1	0	3.432808	6.360467	7.931662
41	1	0	4.522981	5.903312	9.283363
42	1	0	5.062659	7.124105	8.081400
43	6	0	4.518547	-0.716907	-0.581598
44	1	0	3.457348	-0.425867	-0.583256
45	1	0	4.690591	-1.496574	-1.329718
46	1	0	4.812941	-1.081912	0.413693

Table S94: Optimized Cartesian coordinates of **7** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	6.482196	10.054503	-0.734156
2	6	0	6.067505	10.287728	-2.099050
3	1	0	6.379133	11.312294	-2.321496
4	1	0	4.975153	10.199497	-2.189631
5	1	0	6.570091	9.585081	-2.779183
6	6	0	6.248134	8.866222	-0.172716
7	6	0	6.711028	8.717106	1.159072
8	1	0	7.243697	9.549926	1.618718
9	6	0	6.503477	7.536504	1.831785
10	1	0	6.895428	7.415565	2.841546
11	6	0	5.851473	6.431259	1.202588
12	6	0	5.639981	5.199717	1.896156
13	6	0	5.506695	5.180629	3.341868
14	6	0	6.016085	4.093494	4.095657
15	1	0	6.545467	3.290438	3.582333
16	6	0	5.896570	4.080724	5.480134
17	1	0	6.316973	3.254371	6.054352
18	6	0	5.242812	5.131288	6.137279
19	1	0	5.139708	5.111638	7.223331
20	6	0	5.410357	6.600498	-0.141682
21	1	0	4.864261	5.789914	-0.624361
22	6	0	5.586498	7.792557	-0.815903
23	1	0	5.197625	7.904731	-1.826514
24	6	0	5.554126	3.947839	1.165006
25	6	0	4.673820	2.924248	1.596687
26	1	0	4.032566	3.102117	2.460371
27	6	0	4.584581	1.730297	0.891214
28	1	0	3.883563	0.959566	1.213547
29	6	0	5.389350	1.519819	-0.236256
30	1	0	5.326135	0.575757	-0.779647
31	6	0	6.279380	2.512824	-0.665654
32	1	0	6.922076	2.334711	-1.528576
33	6	0	6.355728	3.720559	0.018169
34	1	0	7.075384	4.480728	-0.287549
35	6	0	4.715623	6.204134	5.406452
36	1	0	4.185955	7.007350	5.919967
37	6	0	4.854159	6.238222	4.024092
38	1	0	4.411707	7.051840	3.448446

Table S95: Optimized Cartesian coordinates of **8** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.251331	8.839494	-0.153130
2	6	0	6.785654	8.665864	1.131303
3	1	0	7.374390	9.460767	1.590238
4	6	0	6.575368	7.475926	1.814856
5	1	0	7.018575	7.321436	2.798815
6	6	0	5.844995	6.419207	1.208663
7	6	0	5.632659	5.174106	1.910087
8	6	0	5.485197	5.170091	3.347487
9	6	0	5.956483	4.074729	4.119431
10	1	0	6.474549	3.255114	3.621223
11	6	0	5.825760	4.082883	5.501564
12	1	0	6.218803	3.253422	6.090343
13	6	0	5.200399	5.162993	6.140054
14	1	0	5.090037	5.160272	7.225650
15	6	0	5.324851	6.608319	-0.099512
16	1	0	4.723484	5.820382	-0.553342
17	6	0	5.516572	7.812849	-0.762740
18	1	0	5.086948	7.963201	-1.753704
19	6	0	5.566675	3.932352	1.174000
20	6	0	4.723147	2.877033	1.612290
21	1	0	4.086777	3.030777	2.483938
22	6	0	4.654210	1.690326	0.894928
23	1	0	3.980224	0.896694	1.219055
24	6	0	5.441235	1.518144	-0.252365
25	1	0	5.392308	0.579562	-0.806769
26	6	0	6.290230	2.543142	-0.692722
27	1	0	6.914976	2.394288	-1.574005
28	6	0	6.345041	3.744698	0.000779
29	1	0	7.030424	4.531287	-0.315524
30	6	0	4.715741	6.246395	5.393914
31	1	0	4.211315	7.072940	5.895455
32	6	0	4.866524	6.261359	4.013855
33	1	0	4.458829	7.083581	3.425412
34	1	0	6.408742	9.780565	-0.682601

Table S96: Optimized Cartesian coordinates of **9** with Grimme's D3BJ dispersion correction.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.260038	8.860448	-0.160953
2	6	0	6.883907	8.642745	1.080629
3	6	0	6.658319	7.450778	1.754856
4	6	0	5.844901	6.415904	1.210176
5	6	0	5.631891	5.171927	1.909202
6	6	0	5.484409	5.169806	3.344583
7	6	0	6.036414	4.135207	4.152994
8	6	0	5.916633	4.137211	5.535751
9	6	0	5.193972	5.167735	6.163395
10	6	0	5.250931	6.672138	-0.058874
11	6	0	5.431889	7.874841	-0.727435
12	6	0	5.565912	3.932392	1.173987
13	6	0	4.663556	2.892228	1.539177
14	6	0	4.581223	1.703912	0.826761
15	6	0	5.440324	1.494991	-0.266973
16	6	0	6.360972	2.486058	-0.651705
17	6	0	6.401329	3.684723	0.046825
18	6	0	4.614286	6.199280	5.403314
19	6	0	4.778890	6.203432	4.025179
20	9	0	4.181845	7.178748	3.333387
21	9	0	3.913941	7.151329	6.009308
22	9	0	5.059143	5.166707	7.474701
23	9	0	6.479314	3.184347	6.270267
24	9	0	6.762207	3.161300	3.595543
25	9	0	3.805715	3.069349	2.548486
26	9	0	3.700277	0.767952	1.161346
27	9	0	5.381866	0.361407	-0.937136
28	9	0	7.182212	2.263243	-1.671454
29	9	0	7.314878	4.586494	-0.324812
30	9	0	4.427780	5.774752	-0.609469
31	9	0	4.830153	8.107023	-1.888530
32	9	0	6.452937	9.997756	-0.798934
33	9	0	7.682887	9.573634	1.589622
34	9	0	7.297078	7.264450	2.913999

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