Supporting Information

All metallagermoxane with an adamantanoid cage structure: $[(Cp^*Ru(CO)_2Ge)_4(\mu-O)_6]$ ($Cp^* = \eta^5-C_5Me_5$)

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III Supplementary Data

I Solid state X-ray structure and spectroscopic data of 2

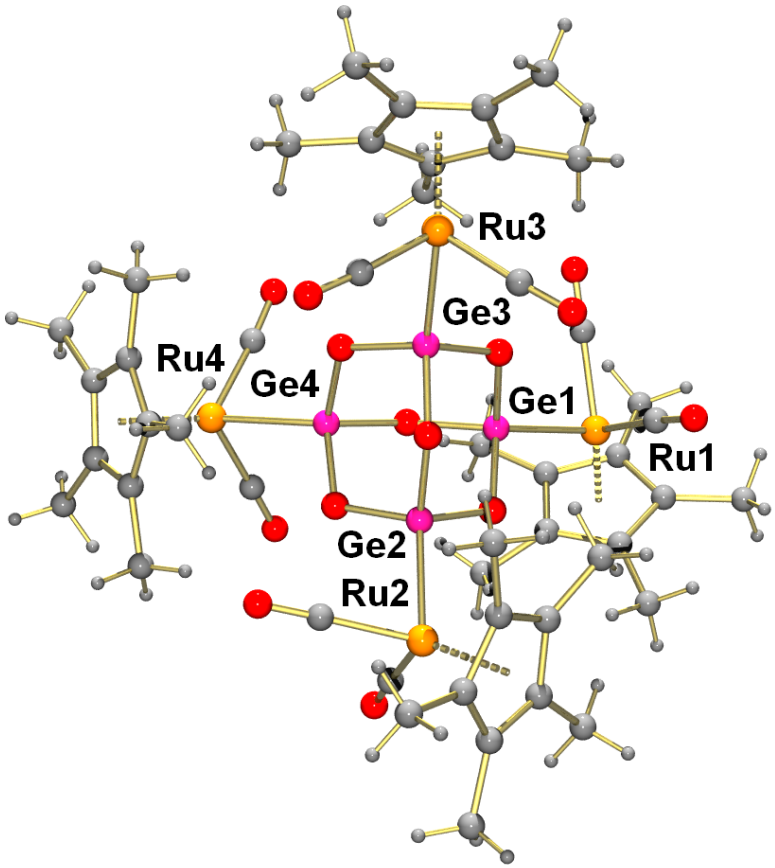


Figure S1. Molecular structure of **2**. Selected bond lengths (Å) and angels (°): O9−Ge2 1.787(5), O9−Ge1 1.798(5), O10−Ge2 1.797(5), O10−Ge3 1.797(5), O11−Ge4 1.790(5), O11−Ge3 1.793(5), O12−Ge1 1.795(5), Ge1−Ru1 2.3960(11), Ge2−Ru2 2.4042(11), Ge3−Ru3 2.3993(11), Ge4−Ru4 2.4021(11); O13−Ge1−O9 104.2(2), O12−Ge1−Ru1−115.62(17), O9−Ge1−Ru1 112.40(17), O9−Ge2−O10 104.4(2), O9−Ge2−Ru2 113.72(16), O14−Ge2−Ru2 113.66(17), O11−Ge3−O10 104.5(2), O13−Ge3−Ru3 112.46(17), O11−Ge3−Ru3 113.06(16).

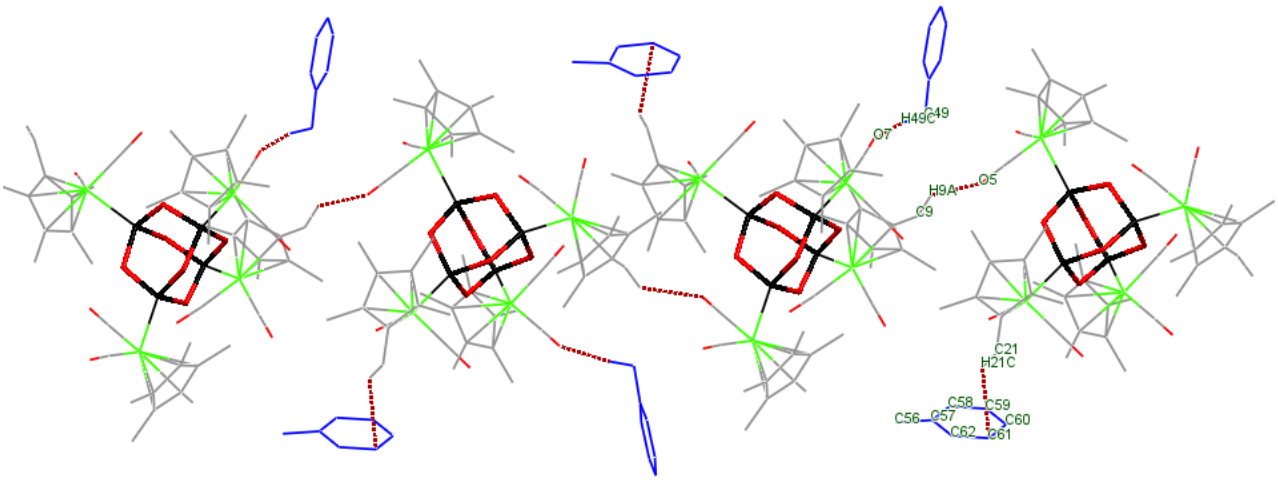


Figure S2. C–H…π interaction of compound **2**, (color code: C: gray; O: red; Ge: black, Ru: green; H: gray, toluene: blue).

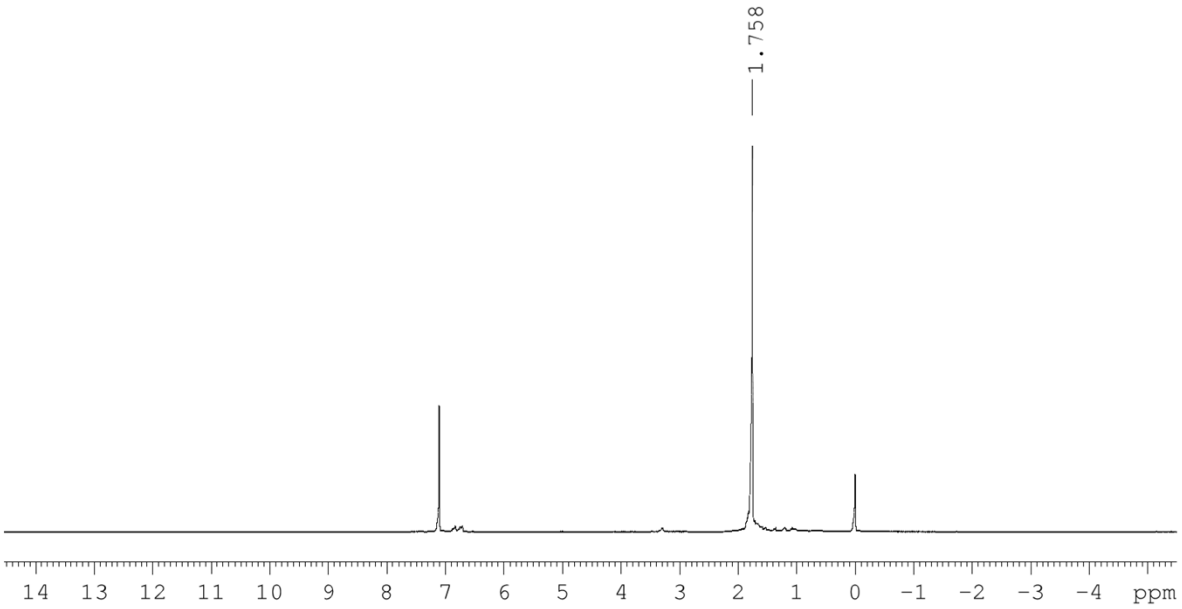


Figure S3. ^{1}H NMR spectrum of **2**.

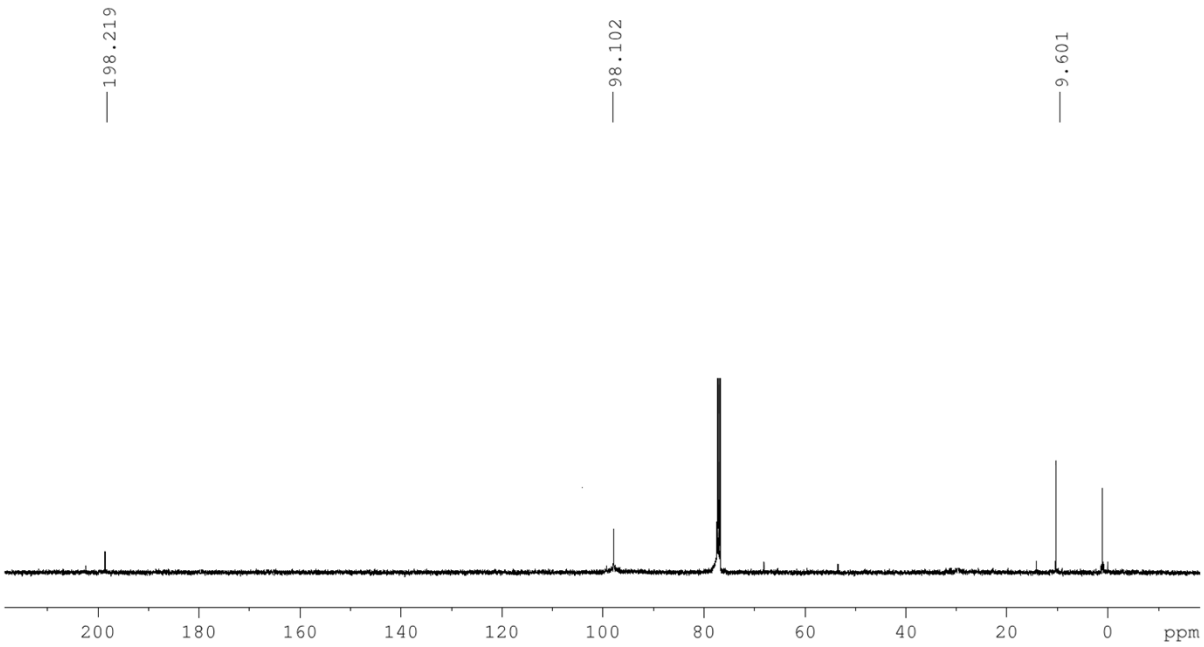


Figure S4. ^{13}C NMR spectrum of **2**.

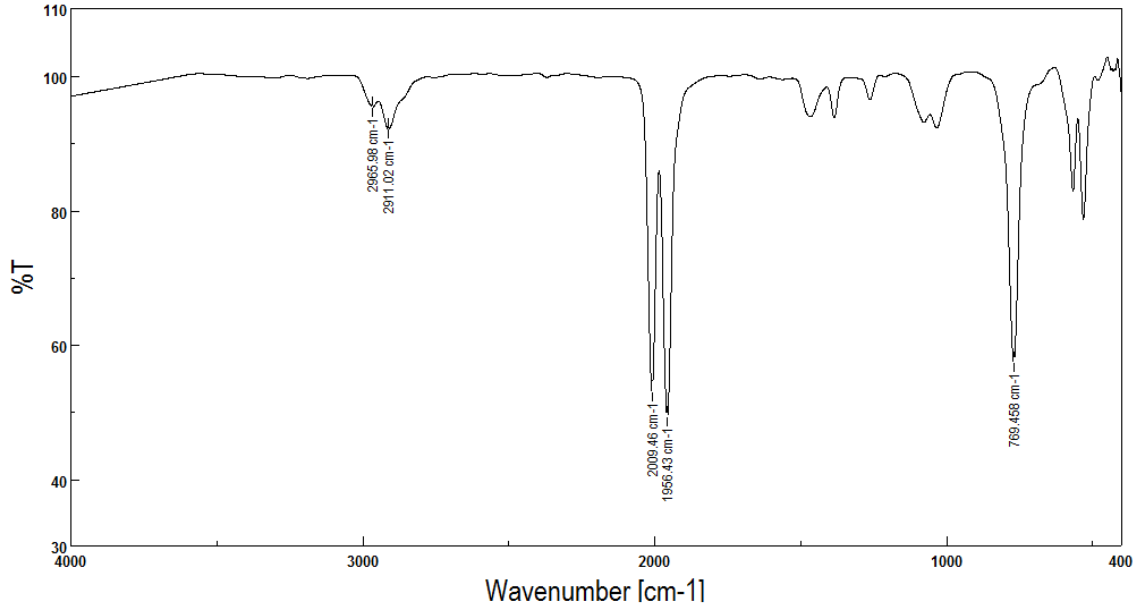


Figure S5. IR spectrum of **2**.

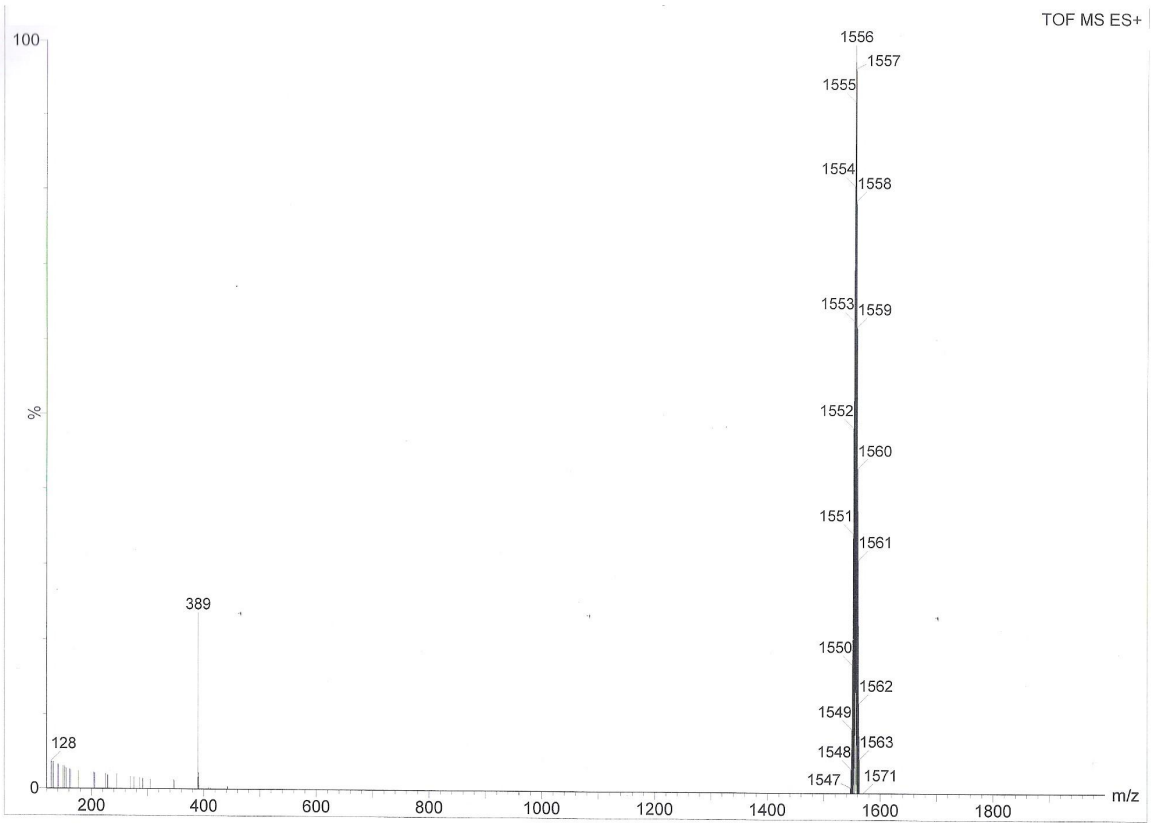


Figure S6. Mass spectrum of **2**.

II Computational details

Geometry optimizations without symmetry constraints were carried out using Gaussin09[1] software suite. The calculations were performed using density functional theory at the BP86[2] level in conjunction with def2-TZVP[3] basis sets. The 28 core electrons of ruthenium were replaced by the quasi-relativistic effective core potential def2-ECP[4] for ruthenium. To save computing time all the calculations were carried out with the Cp analogue model compounds, instead of Cp*. The model compounds were fully optimized in gaseous state (no solvent effect). Stationary points were characterized as minima by calculating the Hessian matrix analytically at the same level. Thermodynamic corrections and Kohn-Sham orbitals have been taken from these calculations. The standard state for all thermodynamic data is 298.15 K and 1 atm. NBO analysis was carried out using the NBO routine within the Gaussian09 package. For NBO analysis, BP86 functional and 6-31g* basis set[5] (SDD-ECP[6] on Ru) was employed. Wiberg bond indexes (WBI)[7] and NBO second order perturbation energy values on some selected bonds are obtained on natural bond orbital (NBO) analysis.[8,9]

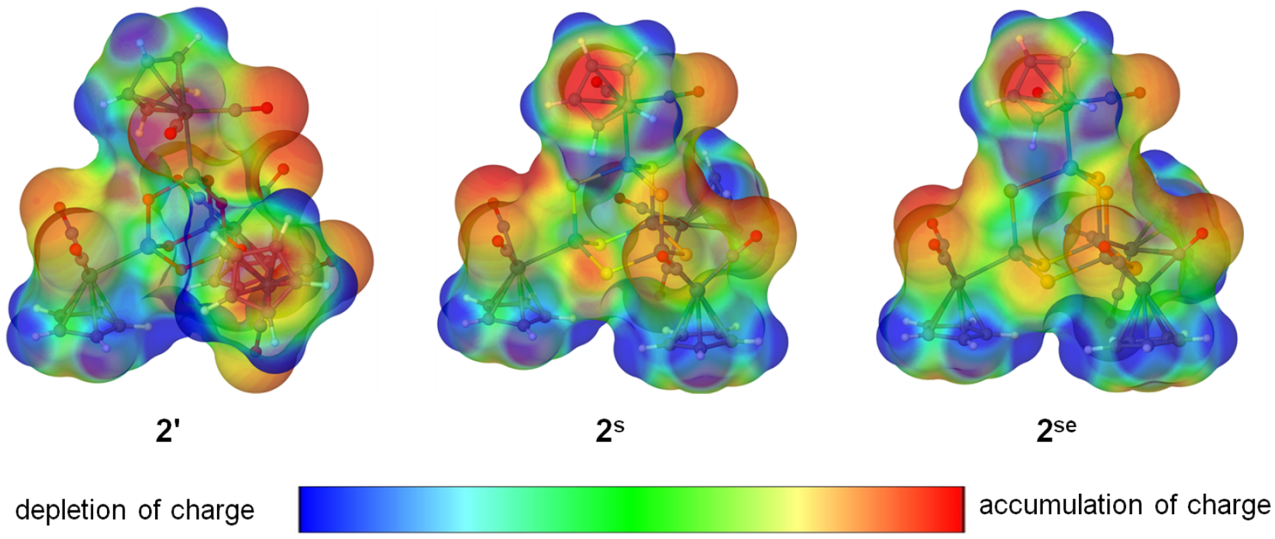


Figure S7. Electrostatic potential analysis of **2'**, **2^{S}** (S-analogue of **2**) and **2^{Se}** (Se-analogue of **2**).

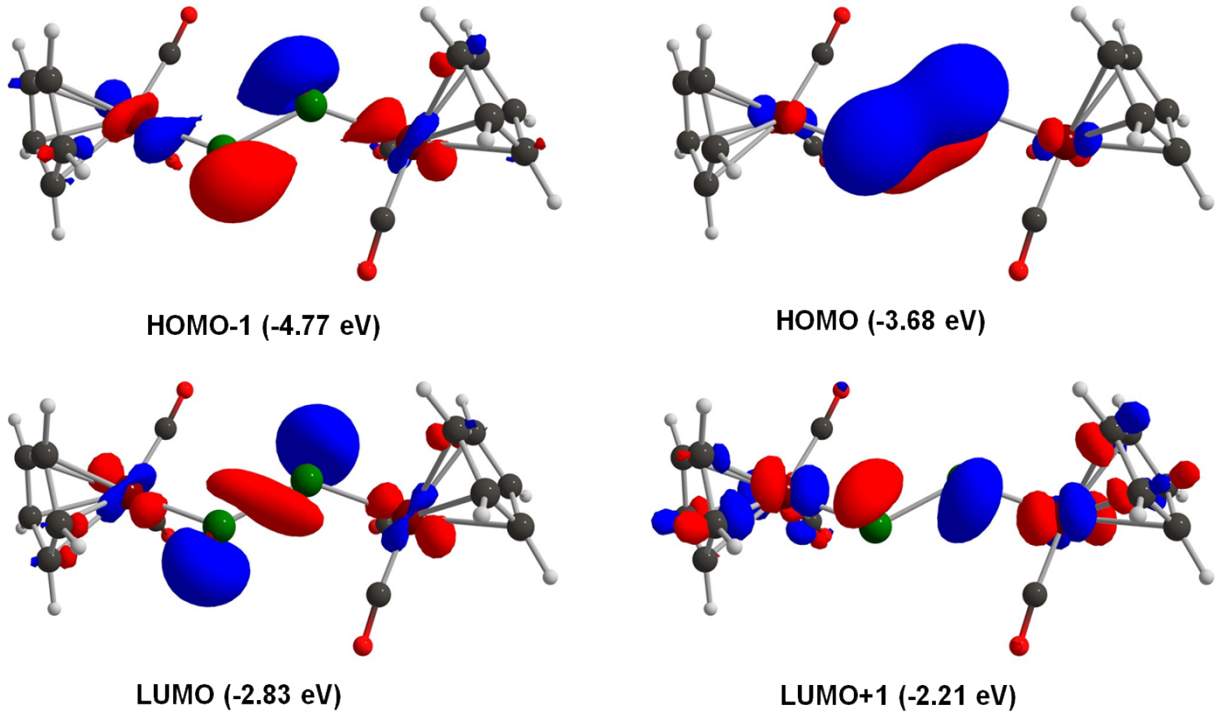


Figure S8. Computed Kohn–Sham (KS) MO of intermediate **B**, showing π-bond orthogonal to the Ge_2Ru_2 plane (HOMO), slipped π orbital (HOMO–1) that lies in the Ge_2Ru_2 plane and the LUMO+1 and LUMO represents the antibonding counterparts of these two orbitals.

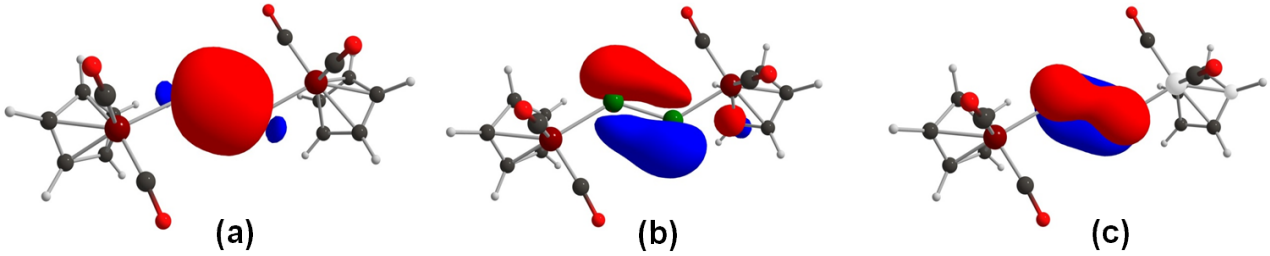


Figure S9. Key natural bond orbitals of **B**, showing (a) σ(Ge–Ge), (b) and (c) π(Ge–Ge) bonding interactions.

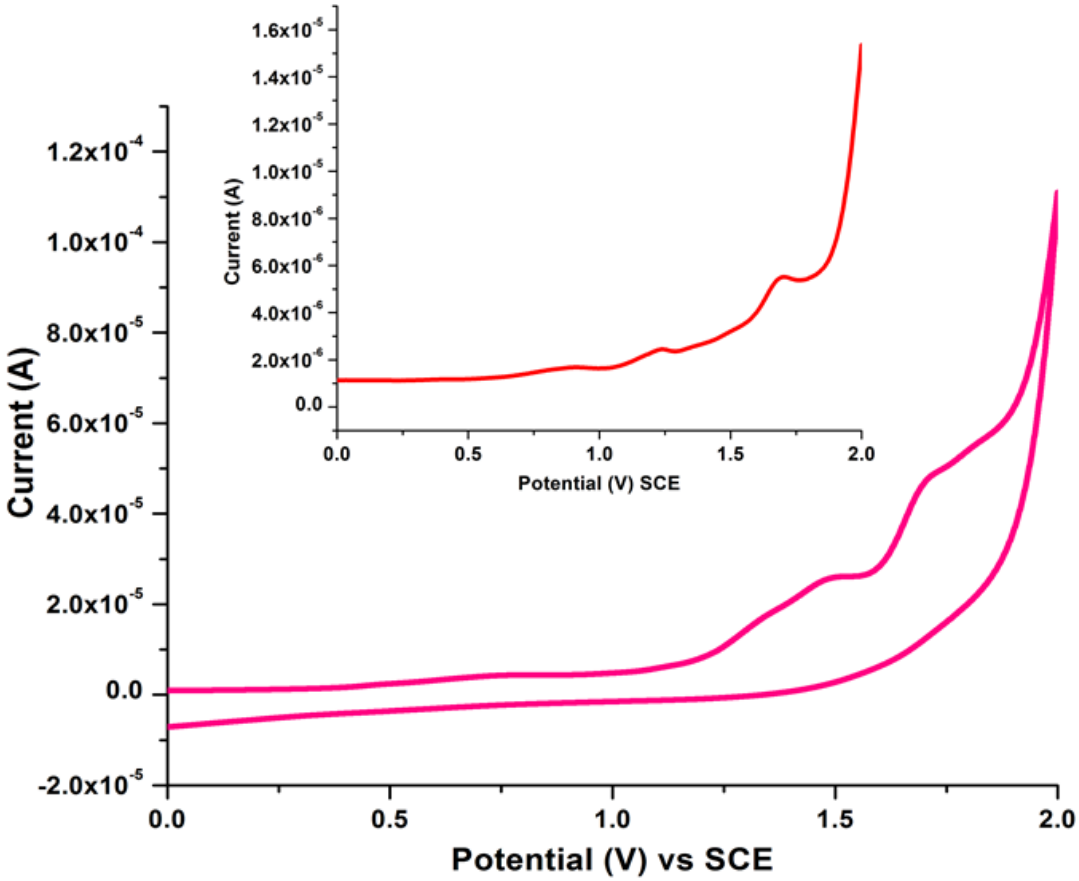
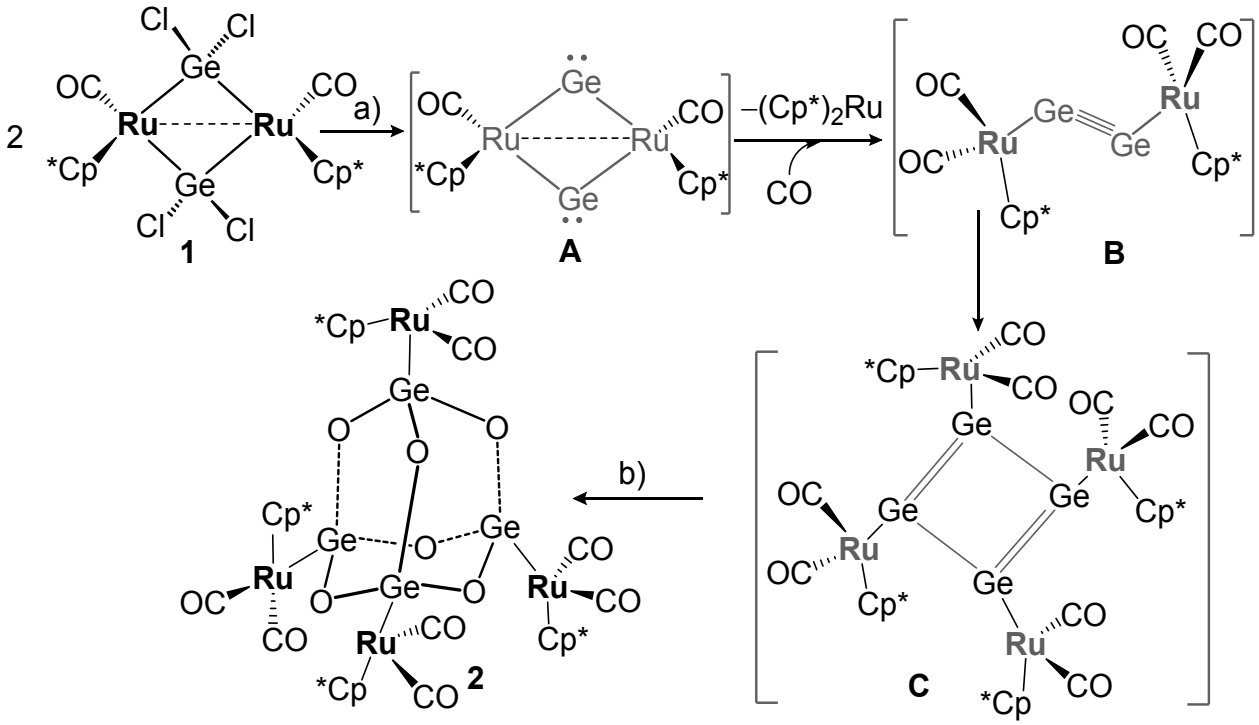
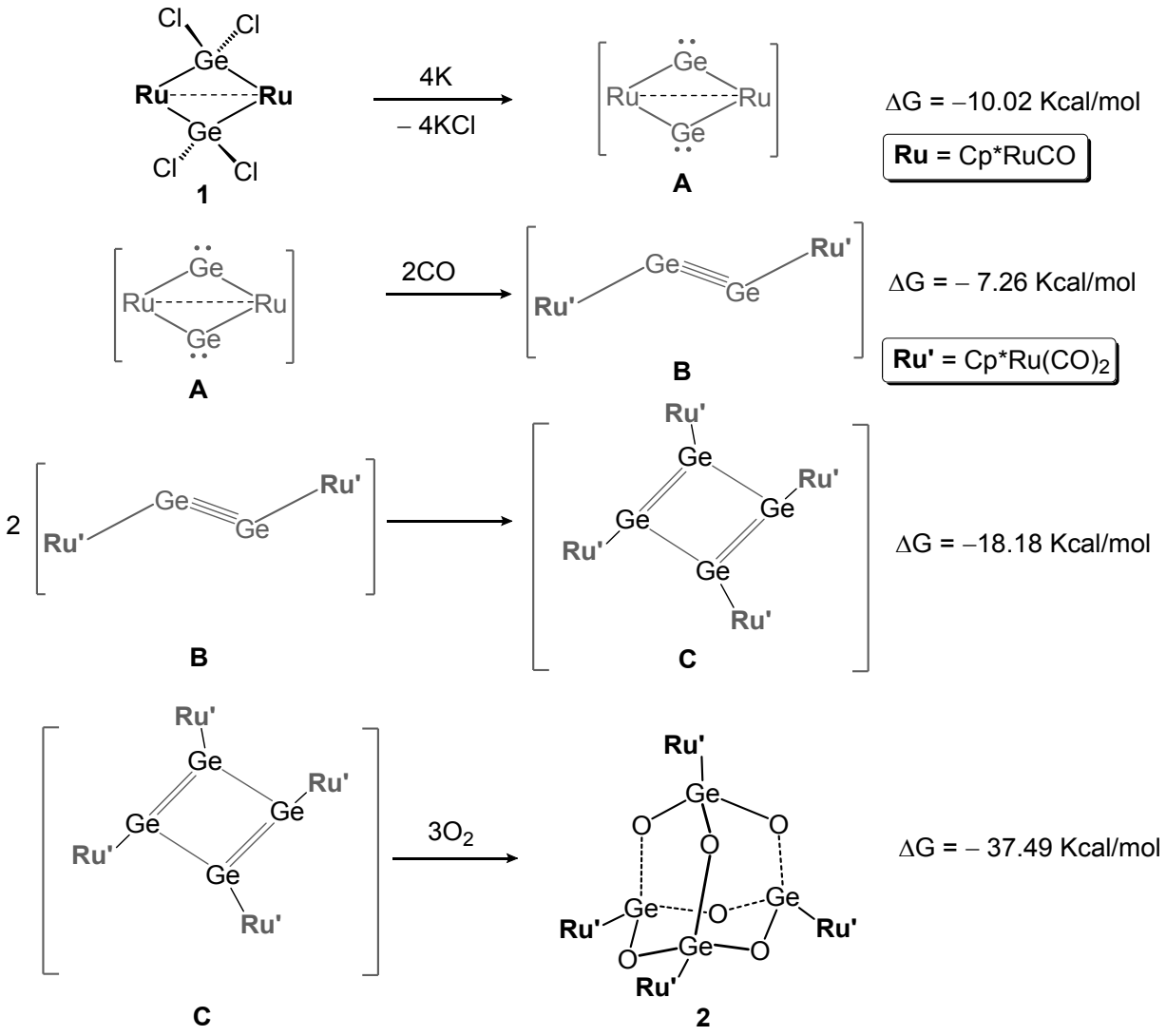


Figure S10. Cyclic voltammogram and differential pulse voltammogram (inset) for **2** in CH_3CN containing 10^{-4} M [*n*-Bu_4NPClO_4]. The cyclic voltammogram and the differential pulse voltammogram are scanned from 0 to 2 V at a scan rate of 0.10 V/s.



Scheme S1. Syntheses of tetrametallagermoxane, **2**. Key reagents: a) K metal (4.2 equiv), thf, rt, 48 h; b) O_2, thf, rt, 10 min.



Scheme S2. The calculated ΔG for each step of the proposed reaction pathway.

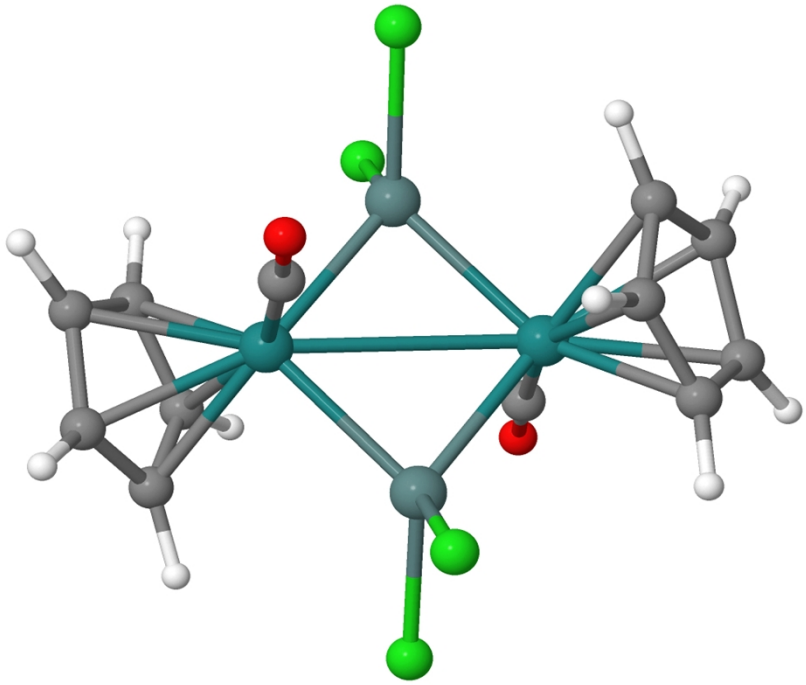
III Supplementary data

Table S1: **Calculated natural charges (q_{Ru}, q_{Ge}, and q_E), natural valence population (Pop), HOMO – LUMO gaps and vertical ionization potential (IP_v) of 2', 2^S and 2^{Se}. The chalcogen atoms are indicated by E.**

	q_{Ru}	q_{Ge}	q_E	Pop (Ru_{val})	Pop (Ge_{val})	Pop (E_{val})	ΔE_{H-L} (eV)	IP_v (eV)
2'	–1.098	1.936	–1.150	9.092	2.042	7.144	3.36	7.89
2^S	–1.038	0.953	–0.556	9.031	2.999	6.541	2.66	6.58
2^{Se}	–1.031	0.705	–0.393	9.024	3.250	6.380	2.25	6.32

IP_v: The vertical ionization potential computed for the compounds **2'**, $\mathbf{2^S}$ and $\mathbf{2^{Se}}$, corresponds to the removal of one electron from the fixed geometry of the neutral molecule.

Cartesian coordinates of the optimized molecules along with their total energies (T.E, in hartrees) including zero point vibrational correction.



T.E = –6799.899339

Figure S11. Optimized geometry of **1'.**

Cartesian coordinates for the calculated structure of **1'** (in Å).

Center Number	*Atomic Number*	*Atomic Type*	*Coordinates (Angstroms) X*	*Y*	*Z*
1	*6*	*0*	*1.187697*	*-3.503071*	*0.596717*
2	*6*	*0*	*-0.188252*	*-3.648813*	*0.132202*
3	*6*	*0*	*-0.267141*	*-3.080894*	*-1.185329*
4	*6*	*0*	*1.033552*	*-2.562966*	*-1.536453*
5	*6*	*0*	*1.936656*	*-2.837176*	*-0.445619*
6	*6*	*0*	*0.187075*	*-1.089733*	*2.169840*
7	*17*	*0*	*-3.309903*	*-0.241463*	*1.659133*
8	*17*	*0*	*-3.197998*	*-1.078083*	*-1.610018*
9	*32*	*0*	*-1.845612*	*-0.398965*	*0.004899*

10	8	0	0.130822	-0.914352	3.326071
11	44	0	0.308583	-1.470994	0.364310
12	6	0	-1.397357	3.403954	-0.573987
13	6	0	0.027360	3.676222	-0.414953
14	6	0	0.411416	3.232531	0.900269
15	6	0	-0.750973	2.664612	1.545336
16	6	0	-1.870442	2.794472	0.643238
17	6	0	-0.201025	1.038868	-2.188455
18	17	0	3.339269	0.224661	-1.591454
19	17	0	3.144186	1.094657	1.666982
20	32	0	1.842702	0.396715	0.029244
21	8	0	-0.145325	0.839589	-3.325598
22	44	0	-0.311972	1.470938	-0.380757
23	1	0	1.579139	-3.854793	1.550560
24	1	0	3.002505	-2.602018	-0.422050
25	1	0	1.303723	-2.061866	-2.470537
26	1	0	-1.162468	-3.022963	-1.814393
27	1	0	-1.001356	-4.146589	0.680076
28	1	0	1.414748	3.290803	1.331590
29	1	0	0.672803	4.165576	-1.148200
30	1	0	-2.005451	3.650085	-1.447373
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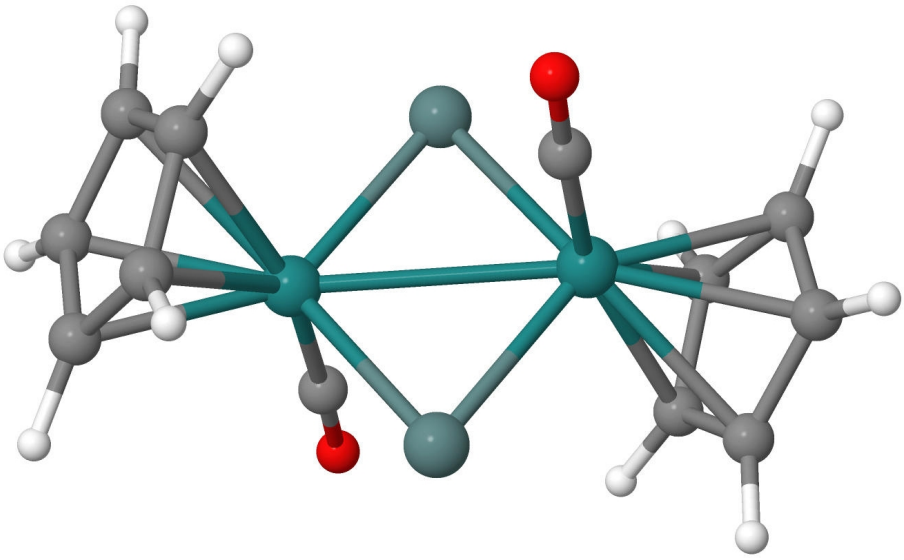
32	1	0	-0.784708	2.239545	2.546288

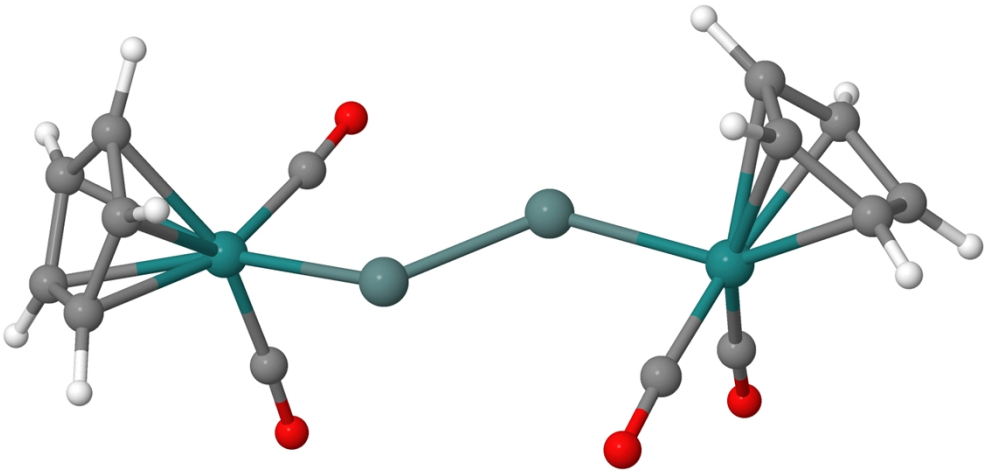


T.E = –4958.648618

Figure S12. Optimized geometry of **A.**

Cartesian coordinates for the calculated structure of **A** (in Å).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.646788	0.101528	-0.610578
2	6	0	-3.489719	-0.816434	0.487128
3	6	0	-2.861842	-0.111704	1.557846
4	6	0	-2.625354	1.235369	1.124091
5	6	0	-3.139185	1.372518	-0.206724
6	6	0	-0.955502	-1.283428	-1.689411
7	32	0	-0.003497	-1.561878	1.181826
8	8	0	-0.703547	-1.976218	-2.599923
9	44	0	-1.422012	-0.200962	-0.266289
10	6	0	3.647317	-0.106533	0.603822
11	6	0	3.489004	0.811806	-0.493377
12	6	0	2.856156	0.108576	-1.562144
13	6	0	2.617839	-1.237958	-1.127677
14	6	0	3.135510	-1.376328	0.201535
15	6	0	0.962798	1.284554	1.691094
16	32	0	0.002386	1.565282	-1.177410
17	8	0	0.716446	1.977598	2.602958
18	44	0	1.422199	0.201136	0.266453
19	1	0	-4.107878	-0.127204	-1.567670
20	1	0	-3.146432	2.284514	-0.797631
21	1	0	-2.176359	2.023836	1.722314
22	1	0	-2.639977	-0.509553	2.545376
23	1	0	-3.809429	-1.854524	0.501865
24	1	0	2.632165	0.506970	-2.548970
25	1	0	3.811090	1.849145	-0.509096
26	1	0	4.111899	0.121107	1.559485
27	1	0	3.142442	-2.288339	0.792418
28	1	0	2.165198	-2.025387	-1.724525



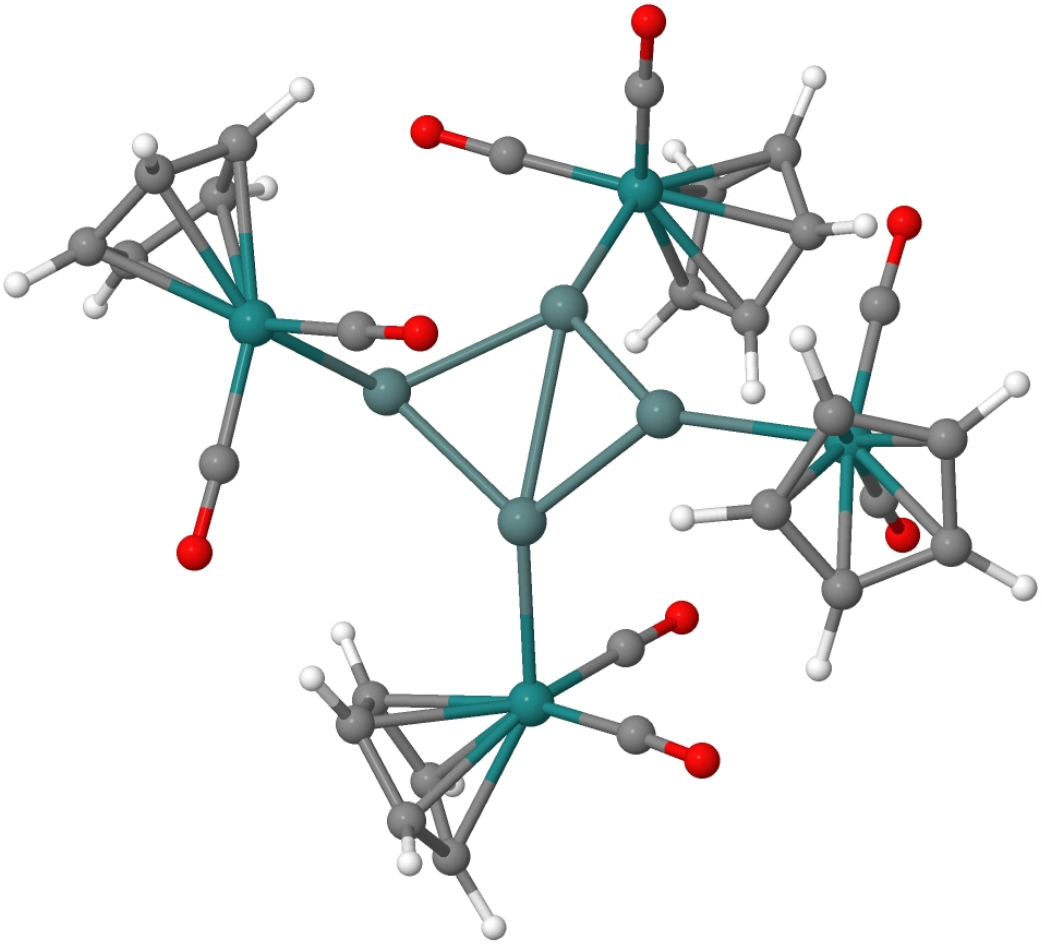
T.E = –5185.396318

Figure S13. Optimized geometry of **B.**

Cartesian coordinates for the calculated structure of **B** (in Å).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.987516	-0.130390	0.618908
2	32	0	-0.971670	-0.175865	-0.542096
3	44	0	-3.348043	0.094477	0.133110
4	6	0	-4.619778	-0.656263	-1.630702
5	6	0	-5.510060	-0.218441	-0.585804
6	6	0	-5.304530	-1.054251	0.546055
7	6	0	-4.287049	-2.016240	0.209769
8	6	0	-3.885992	-1.779053	-1.138495
9	6	0	-3.129024	1.917073	-0.180531
10	6	0	-2.694295	0.316814	1.867352
11	1	0	-4.549838	-0.233966	-2.629369
12	1	0	-6.215416	0.605479	-0.653525
13	1	0	-5.825069	-0.981728	1.497160
14	1	0	-3.909019	-2.801302	0.858793
15	1	0	-3.131664	-2.338302	-1.685199
16	8	0	-3.045325	3.058086	-0.375919
17	8	0	-2.370297	0.445161	2.974487
18	44	0	3.344740	0.086463	-0.149094
19	6	0	4.591873	-0.633835	1.646361

20	*6*	*0*	*5.491832*	*-0.163571*	*0.625498*
21	*6*	*0*	*5.345514*	*-1.000838*	*-0.515632*
22	*6*	*0*	*4.349266*	*-1.994177*	*-0.207994*
23	*6*	*0*	*3.904827*	*-1.775888*	*1.129130*
24	*6*	*0*	*3.136687*	*1.925005*	*0.057863*
25	*6*	*0*	*2.637435*	*0.204176*	*-1.872407*
26	*1*	*0*	*4.485221*	*-0.219739*	*2.645128*
27	*1*	*0*	*6.168027*	*0.682696*	*0.714150*
28	*1*	*0*	*5.890113*	*-0.908869*	*-1.451299*
29	*1*	*0*	*4.009001*	*-2.785382*	*-0.870592*
30	*1*	*0*	*3.152658*	*-2.360008*	*1.652161*
31	*8*	*0*	*3.061309*	*3.076373*	*0.184648*
32	*8*	*0*	*2.279811*	*0.264986*	*-2.975071*



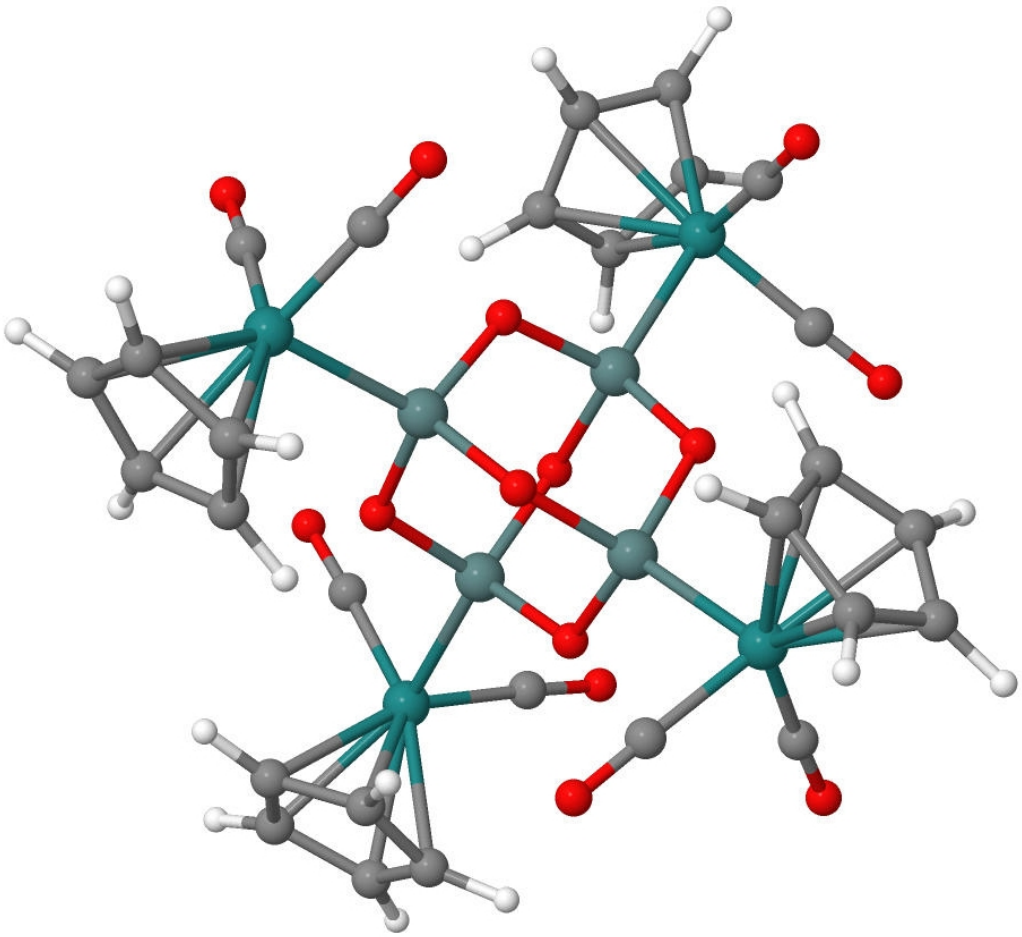
T.E = –10370.892349

Figure S14. Optimized geometry of **C.**

Cartesian coordinates for the calculated structure of **C** (in Å).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.126669	0.228342	-0.040343
2	32	0	0.069798	0.060691	2.811371
3	32	0	2.066701	0.225963	1.416611
4	32	0	-1.763374	1.092292	1.405168
5	44	0	-0.397082	-1.447399	4.774190
6	6	0	-1.888173	0.115625	5.605956
7	6	0	-1.183249	-0.469293	6.701278
8	6	0	-1.507348	-1.868835	6.757485
9	6	0	-2.391115	-2.144857	5.673560
10	6	0	-2.627325	-0.923946	4.955148
11	6	0	1.422054	-1.445854	5.157555
12	6	0	-0.171235	-2.840046	3.558649
13	1	0	-1.871007	1.163758	5.318696
14	1	0	-0.533148	0.061010	7.392551
15	1	0	-1.145457	-2.583226	7.491396
16	1	0	-2.815998	-3.115879	5.431613
17	1	0	-3.264162	-0.801229	4.083306
18	8	0	2.545665	-1.459188	5.461495
19	8	0	-0.073864	-3.742688	2.832901
20	44	0	-0.119169	-1.064028	-2.201694
21	6	0	1.462505	-2.736430	-2.232062
22	6	0	0.658058	-2.851249	-3.421198
23	6	0	-0.678423	-3.131963	-3.022166
24	6	0	-0.711015	-3.190063	-1.583511
25	6	0	0.618022	-2.966788	-1.104895
26	6	0	0.768279	0.360858	-3.021095
27	6	0	-1.746090	-0.189839	-2.399796
28	1	0	2.529184	-2.533897	-2.202407
29	1	0	1.011845	-2.743788	-4.443051
30	1	0	-1.527126	-3.275824	-3.685541
31	1	0	-1.580965	-3.408380	-0.970682
32	1	0	0.925655	-2.965776	-0.063046
33	8	0	1.320326	1.218618	-3.577101
34	8	0	-2.778596	0.322313	-2.563664
35	44	0	-1.943047	3.672772	1.422322
36	6	0	-2.274831	4.348746	-0.755825
37	6	0	-2.462836	5.490415	0.100553
38	6	0	-3.577449	5.222221	0.943241
39	6	0	-4.090892	3.919876	0.607244

40	*6*	*0*	*-3.294674*	*3.395343*	*-0.455944*
41	*6*	*0*	*-0.095522*	*3.765131*	*1.589916*
42	*6*	*0*	*-2.090257*	*3.529321*	*3.262027*
43	*1*	*0*	*-1.510365*	*4.244549*	*-1.520976*
44	*1*	*0*	*-1.859275*	*6.393828*	*0.103520*
45	*1*	*0*	*-3.976297*	*5.886515*	*1.705323*
46	*1*	*0*	*-4.953100*	*3.436273*	*1.058004*
47	*1*	*0*	*-3.431835*	*2.435230*	*-0.946880*
48	*8*	*0*	*1.056719*	*3.896697*	*1.690736*
49	*8*	*0*	*-2.197393*	*3.476789*	*4.424366*
50	*44*	*0*	*4.465001*	*-0.583471*	*1.491393*
51	*6*	*0*	*5.656038*	*1.356341*	*1.864376*
52	*6*	*0*	*6.590559*	*0.261902*	*1.786543*
53	*6*	*0*	*6.321336*	*-0.624089*	*2.865150*
54	*6*	*0*	*5.214234*	*-0.088325*	*3.614845*
55	*6*	*0*	*4.831745*	*1.147700*	*3.010851*
56	*6*	*0*	*4.412676*	*-0.730845*	*-0.359355*
57	*6*	*0*	*3.812155*	*-2.318817*	*1.659069*
58	*1*	*0*	*5.613350*	*2.210497*	*1.194225*
59	*1*	*0*	*7.364909*	*0.137974*	*1.034122*
60	*1*	*0*	*6.850942*	*-1.547596*	*3.082648*
61	*1*	*0*	*4.768603*	*-0.527754*	*4.502779*
62	*1*	*0*	*4.034163*	*1.803753*	*3.349213*
63	*8*	*0*	*4.444134*	*-0.830876*	*-1.519555*
64	*8*	*0*	*3.463330*	*-3.423656*	*1.766527*



T. E = –10822.737525

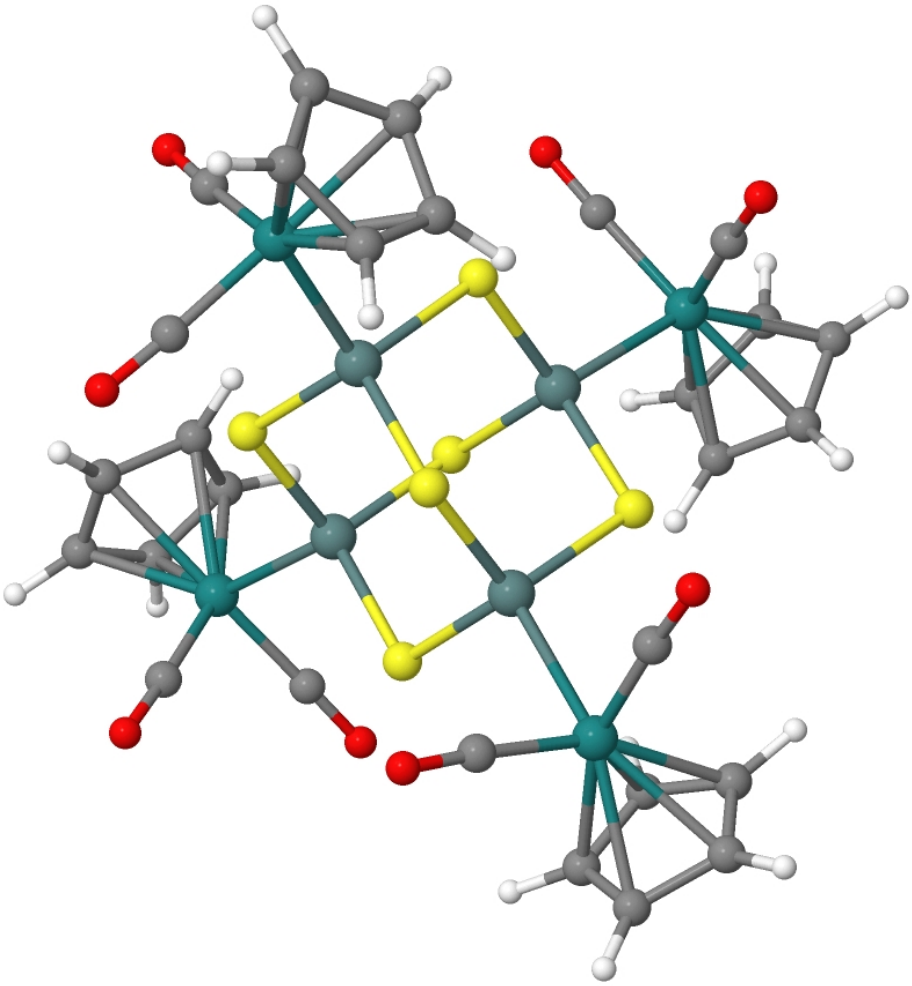
Figure S15. Optimized geometry of **2'.**

Cartesian coordinates for the calculated structure of **2'** (in Å).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.998719	0.591151	-1.775561
2	8	0	-0.593651	1.742293	0.856279
3	8	0	1.009827	-0.530000	1.612100
4	8	0	0.612189	-1.688553	-1.020121
5	8	0	-1.678447	-0.922668	0.592858
6	8	0	1.680939	0.975655	-0.777261

7	32	0	-1.106735	-1.110999	-1.127152
8	32	0	0.037212	1.766223	-0.843875
9	32	0	-0.688581	0.127190	1.696556
10	32	0	1.769763	-0.687061	-0.027910
11	44	0	0.120173	3.975286	-1.889492
12	6	0	1.952316	3.759524	-3.226170
13	6	0	1.493042	5.119915	-3.324131
14	6	0	0.186930	5.110548	-3.890959
15	6	0	-0.171532	3.738752	-4.145801
16	6	0	0.923542	2.912570	-3.751345
17	6	0	0.766078	4.614483	-0.259739
18	6	0	-1.641194	4.224757	-1.319028
19	1	0	2.912749	3.430202	-2.841381
20	1	0	2.047927	6.002140	-3.015442
21	1	0	-0.428470	5.981569	-4.098828
22	1	0	-1.103566	3.390480	-4.582134
23	1	0	0.958679	1.828865	-3.821543
24	8	0	1.193537	5.052445	0.726060
25	8	0	-2.743629	4.413012	-1.011380
26	44	0	-2.637250	-2.502827	-2.428785
27	6	0	-4.519980	-2.693238	-1.152486
28	6	0	-4.770965	-3.348934	-2.410786
29	6	0	-4.692531	-2.367949	-3.439557
30	6	0	-4.393193	-1.099571	-2.825874
31	6	0	-4.306316	-1.304933	-1.413088
32	6	0	-1.645894	-3.992792	-1.890319
33	6	0	-1.502962	-2.237677	-3.885124
34	1	0	-4.514890	-3.161769	-0.172428
35	1	0	-4.984115	-4.405512	-2.548765
36	1	0	-4.833048	-2.544521	-4.502669
37	1	0	-4.277045	-0.148489	-3.337265
38	1	0	-4.089334	-0.548043	-0.663898
39	8	0	-1.078087	-4.950151	-1.565423
40	8	0	-0.832632	-2.074789	-4.819865
41	44	0	4.032327	-1.611116	-0.076594
42	6	0	4.091662	-3.013276	-1.878067
43	6	0	5.417965	-2.960376	-1.317978
44	6	0	5.887503	-1.621116	-1.427772
45	6	0	4.857412	-0.835825	-2.057235
46	6	0	3.758769	-1.705716	-2.347079
47	6	0	3.522402	-2.766251	1.301015
48	6	0	4.506119	-0.301384	1.165429
49	1	0	3.457962	-3.892601	-1.950473
50	1	0	5.963195	-3.796846	-0.889220
51	1	0	6.854381	-1.253676	-1.094093
52	1	0	4.909807	0.223580	-2.290251
53	1	0	2.821981	-1.425179	-2.820955

54	*8*	*0*	*3.248874*	*-3.520047*	*2.138273*
55	*8*	*0*	*4.848356*	*0.510801*	*1.920711*
56	*44*	*0*	*-1.455199*	*0.338699*	*4.002178*
57	*6*	*0*	*0.541330*	*0.537887*	*5.081414*
58	*6*	*0*	*-0.499670*	*0.521016*	*6.075257*
59	*6*	*0*	*-1.326295*	*1.663626*	*5.874828*
60	*6*	*0*	*-0.800138*	*2.395971*	*4.751193*
61	*6*	*0*	*0.358738*	*1.709059*	*4.277927*
62	*6*	*0*	*-1.812601*	*-1.494620*	*3.980076*
63	*6*	*0*	*-3.163046*	*0.702584*	*3.339984*
64	*1*	*0*	*1.336157*	*-0.192824*	*4.964967*
65	*1*	*0*	*-0.632284*	*-0.235438*	*6.844443*
66	*1*	*0*	*-2.195764*	*1.938014*	*6.465835*
67	*1*	*0*	*-1.199538*	*3.320389*	*4.343415*
68	*1*	*0*	*0.984490*	*2.014731*	*3.443621*
69	*8*	*0*	*-2.029689*	*-2.633193*	*4.020568*
70	*8*	*0*	*-4.233500*	*0.952600*	*2.967280*



T. E = –24782.229097

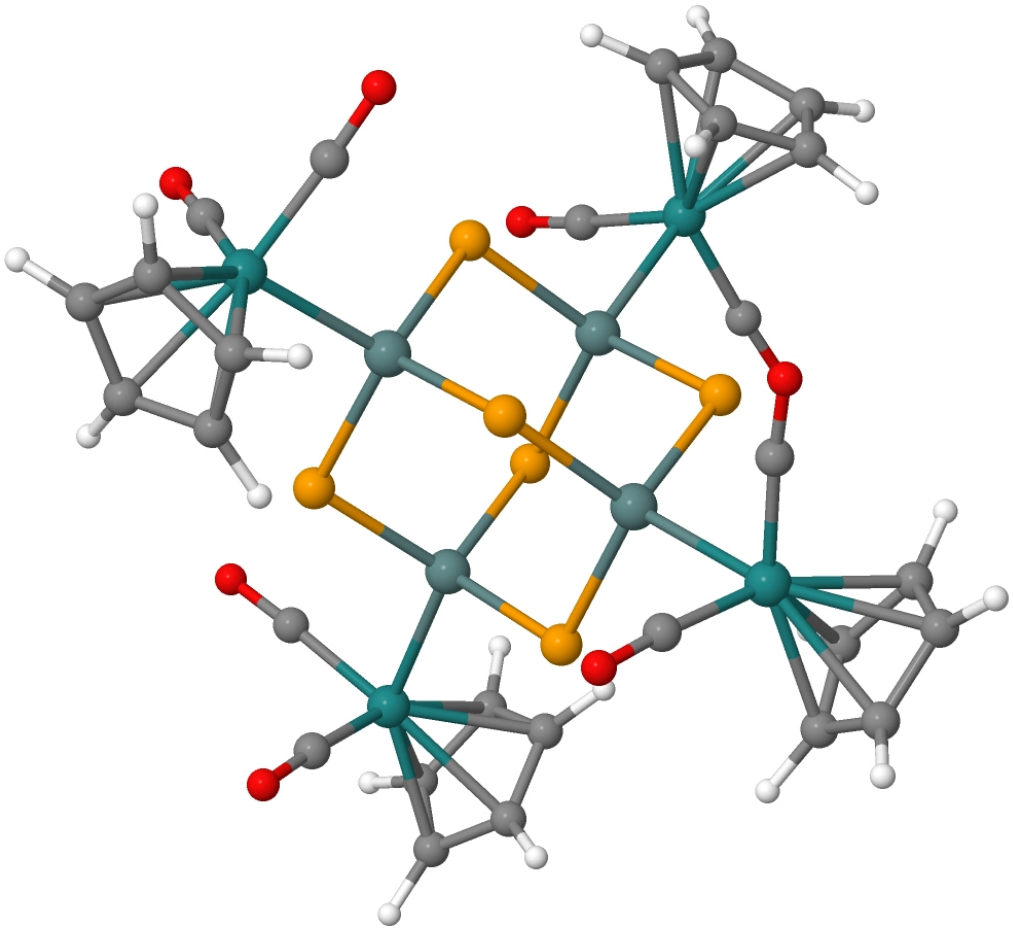
Figure S16. Optimized geometry of $\mathbf{2^S}$.

Cartesian coordinates for the calculated structure of $\mathbf{2^S}$ (in Å).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.733014	1.762466	-1.194348
2	32	0	0.764003	0.030784	2.057340
3	32	0	-2.299531	0.105906	0.039000
4	32	0	0.565980	-1.901324	-1.073176
5	44	0	1.815260	0.061775	4.307487

6	6	0	3.691025	-1.228840	4.101067
7	6	0	3.630184	-0.744607	5.456416
8	6	0	3.725742	0.674913	5.422527
9	6	0	3.846255	1.080030	4.044898
10	6	0	3.841389	-0.098843	3.238351
11	6	0	0.519679	-1.161648	4.868847
12	6	0	0.703761	1.498344	4.746332
13	1	0	3.652747	-2.267861	3.786372
14	1	0	3.527237	-1.356652	6.348546
15	1	0	3.709764	1.337528	6.283795
16	1	0	3.948782	2.098218	3.680439
17	1	0	3.911381	-0.128055	2.153747
18	8	0	-0.238971	-1.941660	5.269956
19	8	0	0.064676	2.410287	5.069540
20	44	0	1.521965	3.815857	-2.341758
21	6	0	-0.129340	5.354320	-1.973228
22	6	0	0.904224	5.984119	-2.754608
23	6	0	2.095679	6.005445	-1.976109
24	6	0	1.807523	5.388054	-0.706272
25	6	0	0.431145	5.005028	-0.705661
26	6	0	1.015944	3.041539	-3.966776
27	6	0	3.217050	3.040891	-2.456720
28	1	0	-1.159649	5.193571	-2.277908
29	1	0	0.793163	6.373750	-3.763076
30	1	0	3.053793	6.415013	-2.284727
31	1	0	2.502991	5.257551	0.117927
32	1	0	-0.093970	4.510772	0.108254
33	8	0	0.699776	2.629644	-5.002902
34	8	0	4.297041	2.622798	-2.530735
35	44	0	1.400344	-3.946786	-2.205255
36	6	0	3.315471	-3.274552	-3.257669
37	6	0	3.102622	-4.666394	-3.560727
38	6	0	3.169445	-5.400238	-2.342823
39	6	0	3.424865	-4.466208	-1.275528
40	6	0	3.529451	-3.162081	-1.848554
41	6	0	0.085353	-3.690901	-3.509591
42	6	0	0.220595	-4.944076	-1.154022
43	1	0	3.336340	-2.455101	-3.970471
44	1	0	2.919811	-5.083138	-4.547707
45	1	0	3.049836	-6.475055	-2.236330
46	1	0	3.541412	-4.710346	-0.223379
47	1	0	3.714991	-2.238221	-1.306770
48	8	0	-0.685758	-3.575837	-4.366934
49	8	0	-0.469476	-5.619699	-0.511821
50	44	0	-4.772599	0.074427	0.223235
51	6	0	-5.394346	-2.125832	0.266339
52	6	0	-6.579899	-1.320837	0.418598

53	*6*	*0*	*-6.456309*	*-0.581656*	*1.629206*
54	*6*	*0*	*-5.195094*	*-0.923727*	*2.235287*
55	*6*	*0*	*-4.554488*	*-1.888665*	*1.397390*
56	*6*	*0*	*-4.863104*	*0.468208*	*-1.602650*
57	*6*	*0*	*-4.710969*	*1.892042*	*0.651935*
58	*1*	*0*	*-5.182557*	*-2.812084*	*-0.548845*
59	*1*	*0*	*-7.420146*	*-1.285177*	*-0.269626*
60	*1*	*0*	*-7.186079*	*0.118571*	*2.027245*
61	*1*	*0*	*-4.805934*	*-0.540740*	*3.174444*
62	*1*	*0*	*-3.585133*	*-2.346263*	*1.578917*
63	*8*	*0*	*-4.988182*	*0.683888*	*-2.734557*
64	*8*	*0*	*-4.735802*	*3.012914*	*0.948864*
65	*16*	*0*	*1.409268*	*-1.909376*	*1.047967*
66	*16*	*0*	*1.591688*	*1.823425*	*0.919833*
67	*16*	*0*	*-1.495642*	*0.149378*	*2.171443*
68	*16*	*0*	*-1.537425*	*1.894284*	*-1.131992*
69	*16*	*0*	*-1.697801*	*-1.824527*	*-1.007588*
70	*16*	*0*	*1.397167*	*-0.135107*	*-2.245810*



T. E = –24782.229097

Figure S17. Optimized geometry of **2^{Se}.**

Cartesian coordinates for the calculated structure of **2^{Se}** (in Å).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.858364	1.819753	-1.257166
2	32	0	0.822561	-0.009220	2.168497
3	32	0	-2.406066	0.226071	0.056353
4	32	0	0.498531	-2.025187	-1.135523
5	44	0	1.897583	-0.043722	4.419995
6	6	0	3.718746	-1.417019	4.231647
7	6	0	3.678136	-0.908620	5.579013

8	*6*	*0*	*3.832957*	*0.505000*	*5.520891*
9	*6*	*0*	*3.970494*	*0.882042*	*4.137014*
10	*6*	*0*	*3.914965*	*-0.309425*	*3.350326*
11	*6*	*0*	*0.559018*	*-1.219371*	*4.983789*
12	*6*	*0*	*0.851951*	*1.432849*	*4.886916*
13	*1*	*0*	*3.640205*	*-2.459310*	*3.935488*
14	*1*	*0*	*3.550517*	*-1.500889*	*6.481209*
15	*1*	*0*	*3.844620*	*1.181924*	*6.371070*
16	*1*	*0*	*4.118166*	*1.888634*	*3.756241*
17	*1*	*0*	*3.983424*	*-0.361172*	*2.266332*
18	*8*	*0*	*-0.223428*	*-1.972034*	*5.391140*
19	*8*	*0*	*0.257674*	*2.366329*	*5.233259*
20	*44*	*0*	*1.748324*	*3.851103*	*-2.395904*
21	*6*	*0*	*0.186612*	*5.482205*	*-2.027502*
22	*6*	*0*	*1.255756*	*6.050082*	*-2.808536*
23	*6*	*0*	*2.445411*	*6.002966*	*-2.028664*
24	*6*	*0*	*2.120618*	*5.405441*	*-0.758104*
25	*6*	*0*	*0.724456*	*5.102901*	*-0.758843*
26	*6*	*0*	*1.202928*	*3.118695*	*-4.027652*
27	*6*	*0*	*3.403709*	*2.995038*	*-2.518587*
28	*1*	*0*	*-0.851524*	*5.384174*	*-2.332337*
29	*1*	*0*	*1.168510*	*6.445264*	*-3.817198*
30	*1*	*0*	*3.425947*	*6.356561*	*-2.336193*
31	*1*	*0*	*2.806336*	*5.238613*	*0.067812*
32	*1*	*0*	*0.170798*	*4.640292*	*0.054910*
33	*8*	*0*	*0.867240*	*2.738466*	*-5.069778*
34	*8*	*0*	*4.463809*	*2.530580*	*-2.599889*
35	*44*	*0*	*1.248285*	*-4.114271*	*-2.270581*
36	*6*	*0*	*3.198483*	*-3.559592*	*-3.330454*
37	*6*	*0*	*2.917920*	*-4.946253*	*-3.601597*
38	*6*	*0*	*2.945699*	*-5.652321*	*-2.365919*
39	*6*	*0*	*3.243666*	*-4.706671*	*-1.320016*
40	*6*	*0*	*3.413891*	*-3.423510*	*-1.924138*
41	*6*	*0*	*-0.041065*	*-3.801704*	*-3.588173*
42	*6*	*0*	*0.017792*	*-5.061876*	*-1.231535*
43	*1*	*0*	*3.263732*	*-2.760552*	*-4.063599*
44	*1*	*0*	*2.718649*	*-5.377316*	*-4.579170*
45	*1*	*0*	*2.772515*	*-6.717012*	*-2.233932*
46	*1*	*0*	*3.346093*	*-4.930079*	*-0.261745*
47	*1*	*0*	*3.641105*	*-2.496095*	*-1.403987*
48	*8*	*0*	*-0.796361*	*-3.656725*	*-4.455117*
49	*8*	*0*	*-0.703314*	*-5.713651*	*-0.598986*
50	*44*	*0*	*-4.888061*	*0.293932*	*0.258069*
51	*6*	*0*	*-5.602135*	*-1.880116*	*0.323083*
52	*6*	*0*	*-6.751543*	*-1.022405*	*0.464272*
53	*6*	*0*	*-6.598733*	*-0.277434*	*1.667719*
54	*6*	*0*	*-5.354480*	*-0.667923*	*2.280006*

55	*6*	*0*	*-4.755040*	*-1.668123*	*1.453574*
56	*6*	*0*	*-4.978179*	*0.677848*	*-1.569861*
57	*6*	*0*	*-4.759200*	*2.110445*	*0.676010*
58	*1*	*0*	*-5.421040*	*-2.585413*	*-0.483271*
59	*1*	*0*	*-7.587918*	*-0.956433*	*-0.226373*
60	*1*	*0*	*-7.298251*	*0.457692*	*2.056940*
61	*1*	*0*	*-4.951831*	*-0.293838*	*3.217112*
62	*1*	*0*	*-3.805981*	*-2.165049*	*1.640612*
63	*8*	*0*	*-5.109162*	*0.889733*	*-2.701833*
64	*8*	*0*	*-4.749332*	*3.232760*	*0.968098*
65	*34*	*0*	*1.398210*	*-2.109557*	*1.113291*
66	*34*	*0*	*1.802830*	*1.850716*	*0.973626*
67	*34*	*0*	*-1.565009*	*0.250739*	*2.323737*
68	*34*	*0*	*-1.539889*	*2.091069*	*-1.201225*
69	*34*	*0*	*-1.900644*	*-1.852169*	*-1.067660*
70	*34*	*0*	*1.465846*	*-0.209766*	*-2.404776*

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