Supporting Information for

Tuning π-Stacking of Oligomer Radical Cations through Multiple Effects

Xiaoyu Chen[1], Li Zhang,[3] Shengxin Yao[2], Gengwen Tan,[2] Xinping Wang[2]

[1] School of Safety, China University of Mining and Technology, Xuzhou 221008, P.R. China

[2] State Key Laboratory of Coordination Chemistry, Nanjing National Laboratory of Microstructures, Nanjing University, Nanjing 210093, P.R. China

[3] Center of Materials Science and Engineering, Guangxi University of Science and Technology, Liuzhou 545006, China

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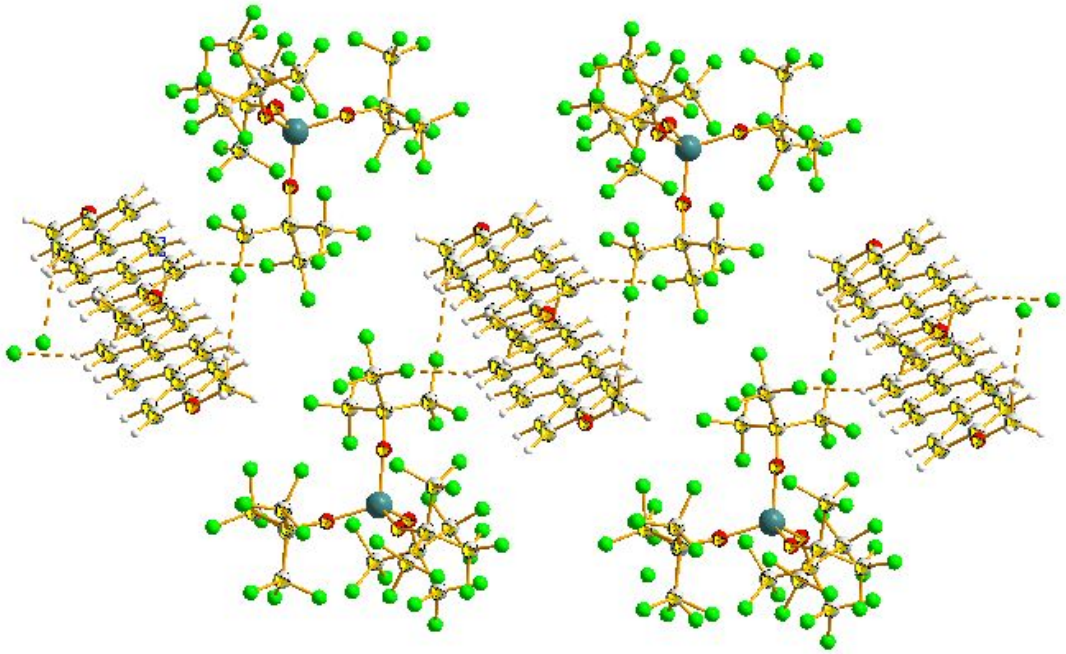


Figure S1. Crystal packing of **1a**$^{\bullet+}$[Al(OR$_F$)$_4$]$^-$•0.5CH_2Cl_2.

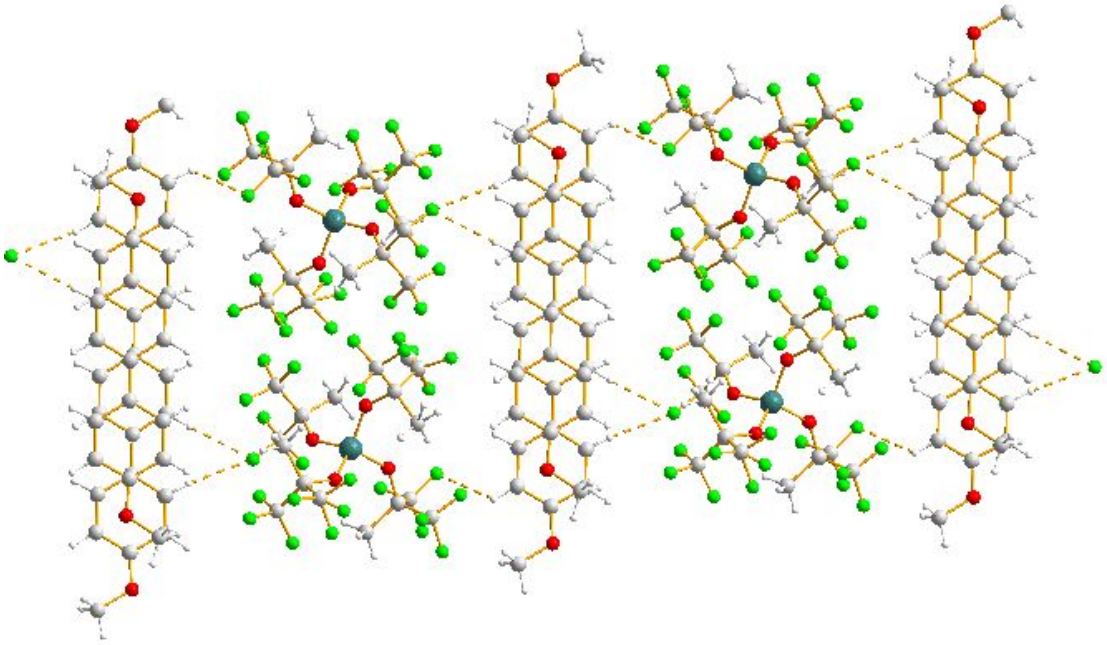


Figure S2. Crystal packing of **1b**$^{\bullet+}$[Al(OR$_{Me}$)$_4$]$^-$• CH_2Cl_2.

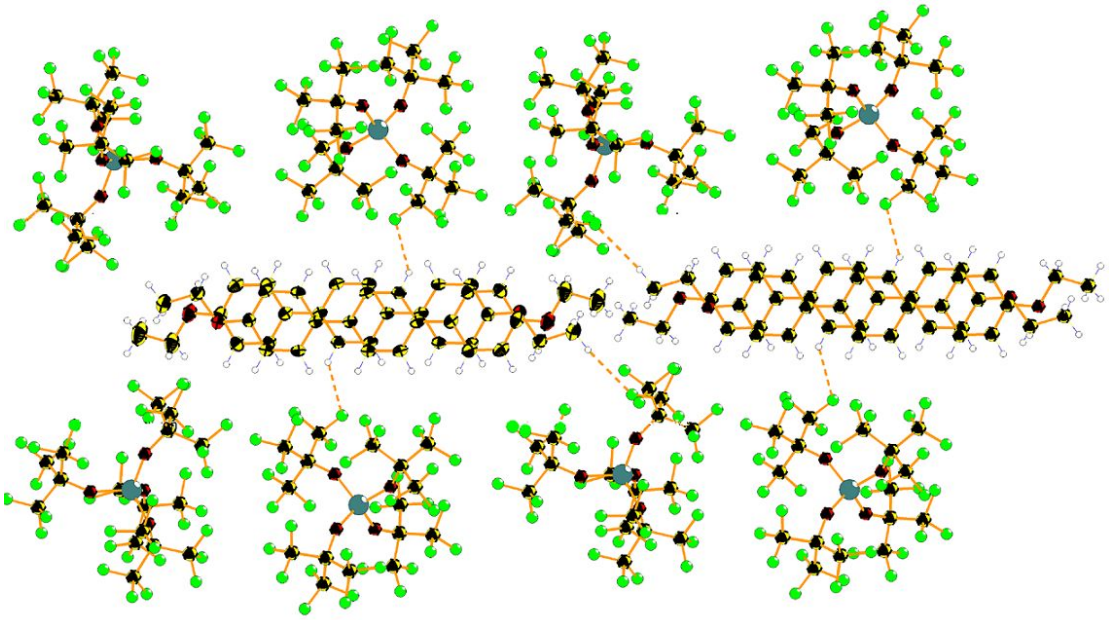


Figure S3. Crystal packing of $\mathbf{2}^{\bullet+}[Al(OR_F)_4]^-$.

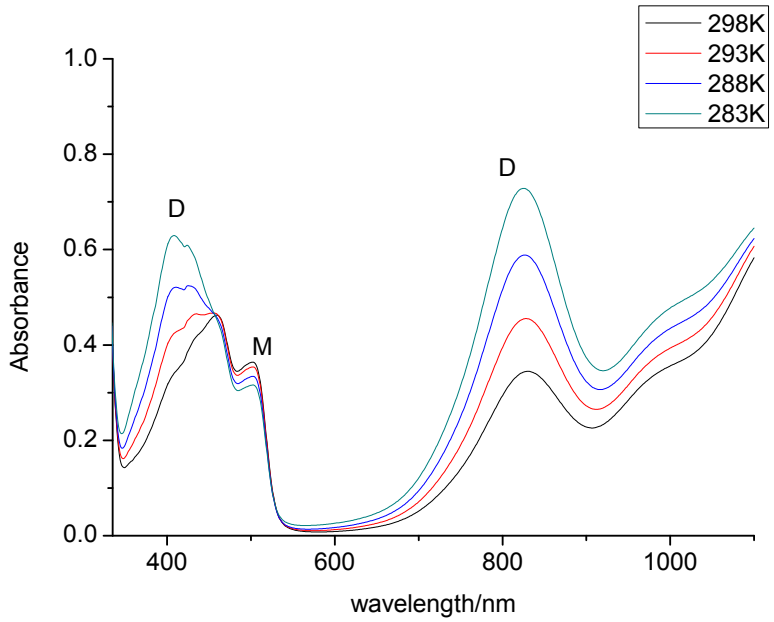


Figure S4. Absorption spectra of 1×10^{-4} M $\mathbf{1}^{\bullet+}[Al(OR_{Me})_4]^-$ in CH_3CN at a function of temperature: 10, 15, 20, 25 ^oC.

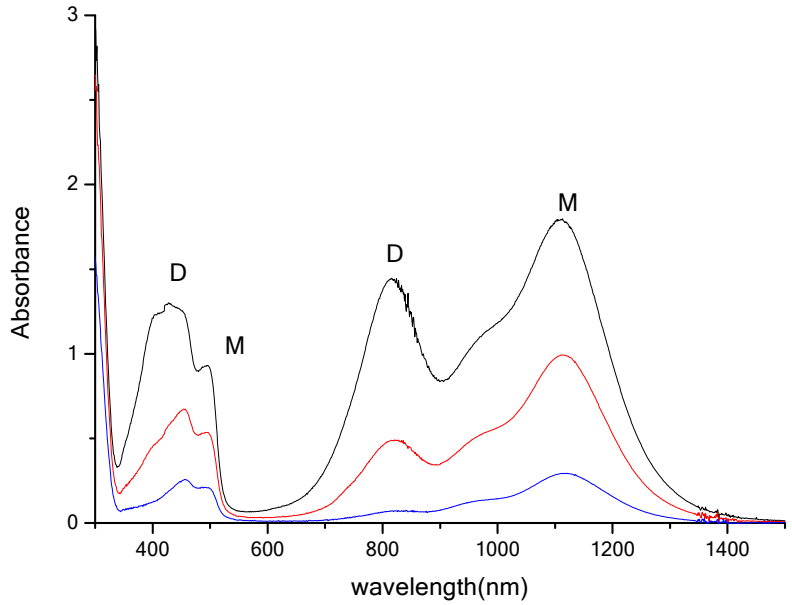


Figure S5. Absorption spectra of 1×10^{-4} $\mathbf{1}^{\bullet+}[Al(OR_F)_4]^-$ in CH_3CN at a function of concentrations at 25 ^oC: 5.0×10^{-4}, 2.5×10^{-4}, 1.2×10^{-4} M, 6.0×10^{-5} M.

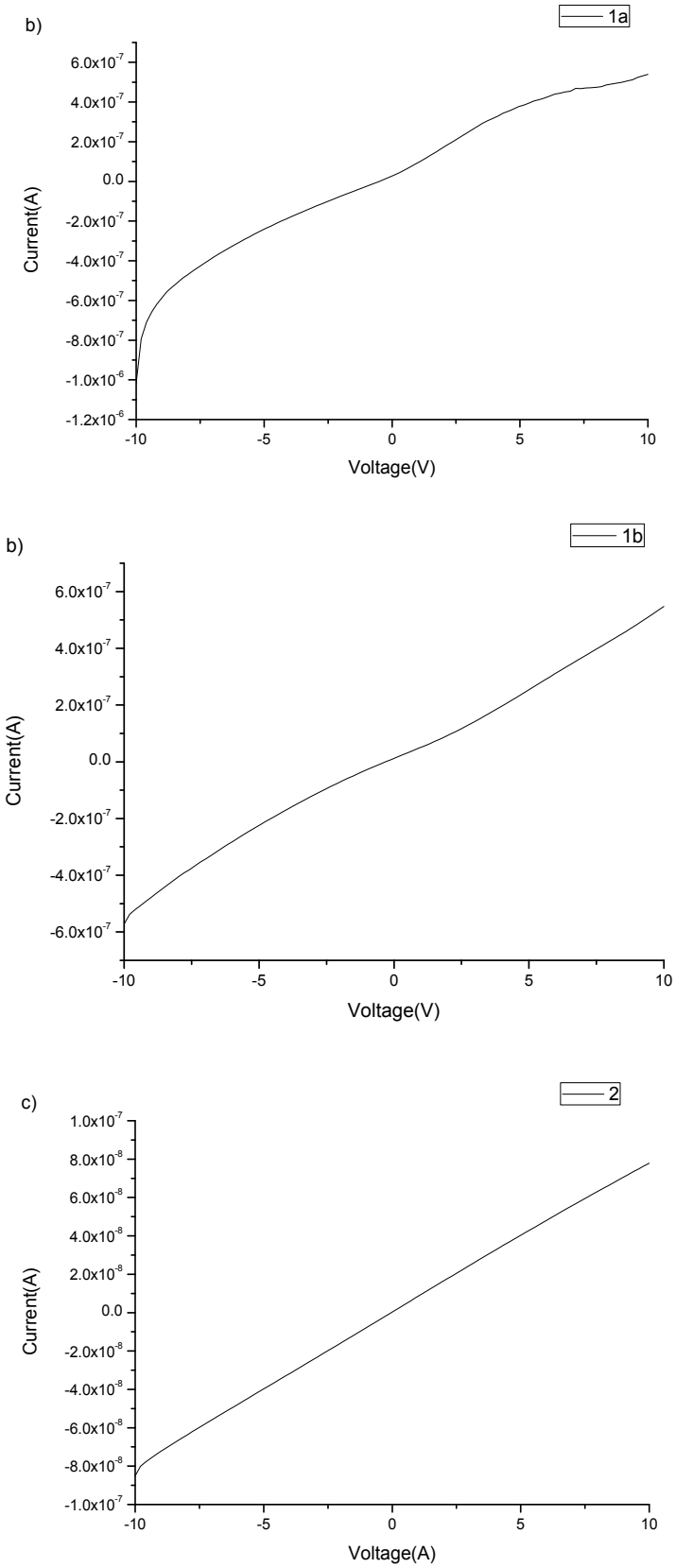


Figure S6. *I-V* curves for all compounds at room temperature.

Table 1. Crystal data and structure refinement for all compounds.

	1a$^{\bullet+}$[Al(OR$_F$)$_4$]$^-$•0.5CH$_2$Cl$_2$	**1b$^{\bullet+}$[Al(OR$_{Me}$)$_4$]$^-$•CH$_2$Cl$_2$**	**2$^{\bullet+}$[Al(OR$_F$)$_4$]$^-$**
formule	$C_{36.5}H_{19}AlF_{36}O_6Cl$	$C_{37}H_{32}AlF_{24}O_6Cl_2$	$C_{38}H_{22}AlF_{36}O_6$
***M*$_r$[g/mol]**	1299.95	1126.51	1285.54
crystal system	triclinic	triclinic	Monoclinic
space group	*P*-1	*P*-1	*P2(1)/c*
Z	2	2	4
***μ*[m/m]**	0.295	0.307	0.233
***a* [Å]**	9.587	11.0556	10.9939
***b* [Å]**	15.435	14.8388	16.930
***c* [Å]**	16.231	15.3013	25.148
***α* [°]**	104.002	64.018	90.00
***β* [°]**	98.381	87.977	91.162
***γ* [°]**	92.291	86.587	90.00
***V* [Å^3]**	2298.4	2252.4	4679.7
***R*$_1$(*I* > 2σ(*I*))**	0.0783 for 6073	0.0573 for 7549	0.0444 for 7225
***wR*$_2$(all data)**	0.2291	0.1753	0.1194

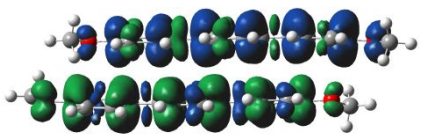
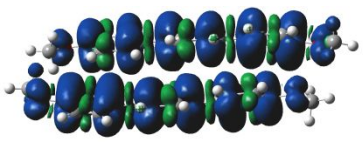
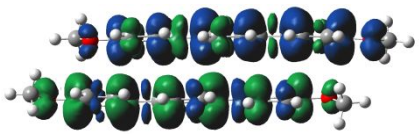
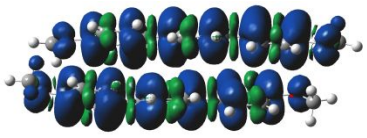
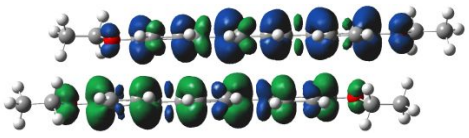
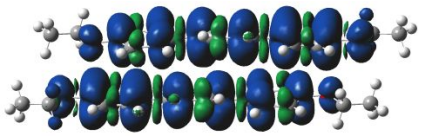
Theoretical calculations

All the calculations are performed at the Gaussian09 program.[S1] We have carried out density functional theory (DFT) calculations on the closed-shell singlet (CS), open-shell singlet (OS), and triplet (T) states of compounds **1a**$^{\bullet+}$-dimer, **1b**$^{\bullet+}$-dimer and **2**$^{\bullet+}$-dimer at the (U)M06-2X/6-31G(d) level of theory.[S2] Besides, the frequency calculations show that there is no imaginary frequency, which reveal that all the optimized structures reach to the stationary points. The symmetry-broken approach was used for open-shell singlet calculations and spin contamination errors were adjusted by approximate spin-projection method.[S3] The calculated results show that for each dimer, the OS state has the lowest energy (see Table S2), and the spin density contours of OS and T states for each dimer are shown in Table S3.

Table S2 The calculated energy of each ground state, spin contamination ($<S^2>$) and the energy gap ($\Delta E_{x\text{-}OS}$) of the studied compounds.

Compounds	Ground state	Energy/a.u.	$<S^2>$	$\Delta E_{x\text{-}OS}$/kcal•mol
1a$^{\bullet+}$-dimer	CS	-1844.829541		0.95
	OS	-1844.830071	0.2437	0
	T	-1844.822729	2.0517	5.23
1b$^{\bullet+}$-dimer	CS	-1844.829561		0.93
	OS	-1844.830056	0.2446	0
	T	-1844.822728	2.0518	5.22
2$^{\bullet+}$-dimer	CS	-2001.914068		0.63
	OS	-2001.914435	0.1383	0
	T	-2001.905725	2.0512	5.86

Table S3 Spin density contours of the studied compounds.

	Spin density (Isovalue=0.0004)	
Compounds	OS	T
1a$^{\bullet+}$-dimer		
1b$^{\bullet+}$-dimer		
2$^{\bullet+}$-dimer		

Coordinates of the studied molecules

1a$^{\bullet+}$-dimer, CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.265109	-1.529108	0.278722
2	6	0	0.509508	-1.733603	-0.900447
3	1	0	0.024581	-1.973797	-1.838294
4	6	0	1.876802	-1.660748	-0.894314
5	1	0	2.394795	-1.846723	-1.826661
6	6	0	2.614472	-1.367984	0.289748
7	6	0	1.841615	-1.174233	1.471528
8	1	0	2.331984	-0.970442	2.415225
9	6	0	0.473360	-1.251505	1.466067
10	1	0	-0.043290	-1.105404	2.406702
11	6	0	-4.534239	-1.793311	0.242275
12	6	0	-3.799107	-2.004896	-0.944912
13	1	0	-4.303686	-2.243289	-1.873450
14	6	0	-2.427189	-1.906609	-0.917767
15	1	0	-1.899850	-2.073481	-1.848877
16	6	0	-1.703779	-1.619881	0.273604
17	6	0	-2.475671	-1.443663	1.459119
18	1	0	-1.987469	-1.258753	2.408199
19	6	0	-3.843409	-1.524216	1.448833
20	1	0	-4.428646	-1.407292	2.354520
21	6	0	-6.615183	-2.331305	-0.784169
22	1	0	-6.462652	-1.703885	-1.665159
23	1	0	-7.655151	-2.276669	-0.469129
24	1	0	-6.339336	-3.367651	-0.996424
25	6	0	6.874511	-0.997187	0.258806
26	6	0	6.185193	-1.319733	-0.926529
27	1	0	6.718153	-1.457863	-1.859169
28	6	0	4.813654	-1.452032	-0.897178
29	1	0	4.321103	-1.699927	-1.829558
30	6	0	4.055474	-1.277163	0.289348
31	6	0	4.788663	-0.986812	1.475337
32	1	0	4.277907	-0.872696	2.423926
33	6	0	6.154209	-0.862616	1.466810
34	1	0	6.713351	-0.662620	2.374897
35	6	0	8.988426	-0.942725	-0.826675
36	1	0	8.918419	-1.961468	-1.217490
37	1	0	10.007369	-0.739826	-0.505034
38	1	0	8.684010	-0.218721	-1.588643

39	8	0	-5.853330	-1.842194	0.326283
40	8	0	8.180970	-0.800528	0.343882
41	6	0	0.263549	1.518041	-0.296787
42	6	0	-0.491635	1.703819	0.898415
43	1	0	0.010851	1.916248	1.833832
44	6	0	-1.859026	1.633132	0.914197
45	1	0	-2.361903	1.807217	1.857133
46	6	0	-2.615523	1.364191	-0.263078
47	6	0	-1.861900	1.188615	-1.460574
48	1	0	-2.368494	0.999406	-2.398791
49	6	0	-0.493398	1.261608	-1.476479
50	1	0	0.007388	1.139490	-2.429061
51	6	0	4.532725	1.779163	-0.322880
52	6	0	3.810368	2.058438	0.858713
53	1	0	4.325312	2.351611	1.765691
54	6	0	2.438279	1.960480	0.852658
55	1	0	1.920274	2.192646	1.775025
56	6	0	1.702398	1.607458	-0.312532
57	6	0	2.460948	1.365278	-1.495045
58	1	0	1.962333	1.115513	-2.423757
59	6	0	3.829076	1.444455	-1.504619
60	1	0	4.404448	1.271326	-2.407553
61	6	0	6.624851	2.372176	0.649727
62	1	0	6.485362	1.793642	1.565747
63	1	0	7.661056	2.302871	0.325325
64	1	0	6.348450	3.417968	0.807966
65	6	0	-6.877205	1.020309	-0.180372
66	6	0	-6.164826	1.261199	1.010706
67	1	0	-6.680482	1.340642	1.959803
68	6	0	-4.792921	1.384110	0.965629
69	1	0	-4.280641	1.558738	1.904026
70	6	0	-4.056728	1.280568	-0.243180
71	6	0	-4.812425	1.071814	-1.432078
72	1	0	-4.319602	1.022806	-2.395660
73	6	0	-6.178591	0.956702	-1.407131
74	1	0	-6.755056	0.820501	-2.316203
75	6	0	-8.973400	0.920021	0.935673
76	1	0	-8.883136	1.911376	1.387897
77	1	0	-9.999884	0.750630	0.618833
78	1	0	-8.667109	0.145909	1.645872
79	8	0	5.851172	1.820553	-0.422668
80	8	0	-8.186520	0.840730	-0.254588

1a$^{\bullet+}$-dimer, OS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.266888	-1.563317	0.258304
2	6	0	0.523836	-1.791386	-0.903871
3	1	0	0.053240	-2.061907	-1.840844
4	6	0	1.891021	-1.714788	-0.878313
5	1	0	2.423024	-1.917285	-1.799276
6	6	0	2.610060	-1.395393	0.310430
7	6	0	1.819924	-1.182270	1.476615
8	1	0	2.295008	-0.957337	2.423347
9	6	0	0.451711	-1.263413	1.451283
10	1	0	-0.081651	-1.089653	2.377819
11	6	0	-4.537909	-1.804689	0.158154
12	6	0	-3.790909	-1.956601	-1.028675
13	1	0	-4.285165	-2.137982	-1.975487
14	6	0	-2.417353	-1.868852	-0.980007
15	1	0	-1.879694	-1.977168	-1.914115
16	6	0	-1.708483	-1.648332	0.231664
17	6	0	-2.491570	-1.528234	1.414430
18	1	0	-2.013274	-1.403490	2.378462
19	6	0	-3.860425	-1.602608	1.383871
20	1	0	-4.454901	-1.531926	2.288349
21	6	0	-6.608578	-2.270013	-0.921051
22	1	0	-6.444439	-1.593064	-1.762919
23	1	0	-7.652722	-2.232236	-0.617169
24	1	0	-6.331759	-3.292772	-1.190699
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26	6	0	6.194983	-1.363716	-0.859151
27	1	0	6.742911	-1.535374	-1.777420
28	6	0	4.825973	-1.509994	-0.842467
29	1	0	4.348722	-1.804978	-1.768955
30	6	0	4.049105	-1.293245	0.326638
31	6	0	4.763120	-0.945808	1.510073
32	1	0	4.236921	-0.793115	2.444527
33	6	0	6.126199	-0.805531	1.514326
34	1	0	6.670783	-0.558567	2.419687
35	6	0	8.991304	-0.935423	-0.740218
36	1	0	8.943871	-1.969592	-1.091515
37	1	0	10.001898	-0.702125	-0.413121
38	1	0	8.683749	-0.246603	-1.532756
39	8	0	-5.860794	-1.846957	0.224328

40	8	0	8.165217	-0.762597	0.414037
41	6	0	0.262467	1.531586	-0.306103
42	6	0	-0.472947	1.698951	0.902770
43	1	0	0.046728	1.884391	1.834699
44	6	0	-1.840726	1.632416	0.938053
45	1	0	-2.330122	1.794047	1.890450
46	6	0	-2.613601	1.389631	-0.233420
47	6	0	-1.878300	1.231470	-1.444551
48	1	0	-2.399734	1.054693	-2.377229
49	6	0	-0.509258	1.298118	-1.478817
50	1	0	-0.020824	1.195379	-2.440239
51	6	0	4.533796	1.768413	-0.384267
52	6	0	3.824873	2.104263	0.789011
53	1	0	4.349283	2.438238	1.676271
54	6	0	2.450759	2.014695	0.800469
55	1	0	1.941470	2.300920	1.712731
56	6	0	1.704771	1.612692	-0.339049
57	6	0	2.448687	1.312355	-1.515148
58	1	0	1.938741	1.013689	-2.423279
59	6	0	3.818413	1.382873	-1.541185
60	1	0	4.383915	1.162057	-2.440004
61	6	0	6.635838	2.395501	0.542698
62	1	0	6.513400	1.851929	1.482782
63	1	0	7.668899	2.323629	0.208717
64	1	0	6.353288	3.444476	0.666065
65	6	0	-6.871296	1.040711	-0.103095
66	6	0	-6.139610	1.205697	1.090354
67	1	0	-6.639648	1.218328	2.050960
68	6	0	-4.769793	1.333715	1.030461
69	1	0	-4.239096	1.438462	1.969005
70	6	0	-4.053518	1.309206	-0.196047
71	6	0	-4.828875	1.180687	-1.384733
72	1	0	-4.351521	1.205202	-2.356999
73	6	0	-6.193291	1.061245	-1.344485
74	1	0	-6.785920	0.986179	-2.250230
75	6	0	-8.947971	0.849408	1.038279
76	1	0	-8.856441	1.806734	1.558248
77	1	0	-9.978176	0.695272	0.725890
78	1	0	-8.624204	0.028546	1.685189
79	8	0	5.854416	1.796981	-0.496950
80	8	0	-8.179587	0.861551	-0.167458

1a$^{\bullet+}$-dimer, T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.642435	-1.722266	0.062038
2	6	0	0.179969	-1.803464	-1.092289
3	1	0	-0.270875	-1.941400	-2.068346
4	6	0	1.548522	-1.762493	-1.004486
5	1	0	2.121159	-1.823962	-1.922303
6	6	0	2.216330	-1.621291	0.245152
7	6	0	1.389356	-1.542948	1.400068
8	1	0	1.835067	-1.467492	2.384724
9	6	0	0.021056	-1.596253	1.310294
10	1	0	-0.558567	-1.515726	2.222769
11	6	0	-4.911418	-1.793252	-0.193720
12	6	0	-4.143170	-1.525956	-1.338456
13	1	0	-4.617277	-1.316474	-2.289927
14	6	0	-2.762853	-1.515968	-1.243494
15	1	0	-2.194778	-1.271897	-2.134850
16	6	0	-2.093172	-1.764727	-0.026691
17	6	0	-2.893425	-2.057151	1.105204
18	1	0	-2.429272	-2.320840	2.049177
19	6	0	-4.266386	-2.075923	1.026163
20	1	0	-4.879726	-2.321512	1.886762
21	6	0	-6.966082	-1.718510	-1.392687
22	1	0	-6.791756	-0.761399	-1.894811
23	1	0	-8.018402	-1.806182	-1.128595
24	1	0	-6.676632	-2.546626	-2.045708
25	6	0	6.456328	-1.201545	0.431676
26	6	0	5.846907	-1.691910	-0.747139
27	1	0	6.443231	-1.942868	-1.615715
28	6	0	4.483402	-1.847300	-0.783551
29	1	0	4.045003	-2.245528	-1.690993
30	6	0	3.651264	-1.533355	0.329478
31	6	0	4.304385	-1.098088	1.520311
32	1	0	3.723861	-0.843656	2.398788
33	6	0	5.662106	-0.941343	1.576752
34	1	0	6.161250	-0.603854	2.479054
35	6	0	8.612976	-1.112825	-0.566548
36	1	0	8.638250	-2.159654	-0.879305
37	1	0	9.597486	-0.807908	-0.219306
38	1	0	8.280471	-0.469294	-1.386424
39	8	0	-6.249197	-1.783900	-0.160270

40	8	0	7.743211	-0.950177	0.559971
41	6	0	0.620953	1.754424	-0.200705
42	6	0	-0.041486	1.775789	1.054211
43	1	0	0.539876	1.796053	1.969119
44	6	0	-1.410260	1.735409	1.148401
45	1	0	-1.861908	1.774201	2.133089
46	6	0	-2.232797	1.689147	-0.010530
47	6	0	-1.567513	1.690527	-1.268494
48	1	0	-2.144770	1.648978	-2.185066
49	6	0	-0.198599	1.710227	-1.358890
50	1	0	0.256081	1.731466	-2.342762
51	6	0	4.888786	1.712261	-0.445334
52	6	0	4.255495	2.197602	0.711436
53	1	0	4.834393	2.563195	1.551117
54	6	0	2.874234	2.207118	0.778427
55	1	0	2.411320	2.610812	1.672437
56	6	0	2.071517	1.765795	-0.295092
57	6	0	2.736281	1.331238	-1.467837
58	1	0	2.163522	0.981566	-2.320075
59	6	0	4.108941	1.293547	-1.541925
60	1	0	4.621294	0.948224	-2.433484
61	6	0	7.062957	2.152574	0.411579
62	1	0	6.935733	1.622253	1.360901
63	1	0	8.079865	2.014160	0.049034
64	1	0	6.859361	3.219089	0.541987
65	6	0	-6.462657	1.234622	0.192806
66	6	0	-5.674566	1.018509	1.346208
67	1	0	-6.126386	0.671835	2.267590
68	6	0	-4.315365	1.206050	1.275694
69	1	0	-3.725532	0.980166	2.156378
70	6	0	-3.667605	1.608698	0.074511
71	6	0	-4.498536	1.885319	-1.052178
72	1	0	-4.062541	2.271293	-1.966348
73	6	0	-5.853732	1.714576	-0.997168
74	1	0	-6.495188	1.939168	-1.842997
75	6	0	-8.452330	0.468372	1.247807
76	1	0	-8.400006	1.159389	2.092860
77	1	0	-9.485084	0.356040	0.926065
78	1	0	-8.024857	-0.503990	1.509261
79	8	0	6.213072	1.602065	-0.593942
80	8	0	-7.758078	1.010881	0.117978

1b$^{\bullet+}$-dimer, CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.614191	-1.368231	0.286529
2	6	0	-1.874443	-1.658096	-0.896918
3	1	0	-2.390760	-1.842403	-1.830534
4	6	0	-0.507156	-1.730970	-0.900614
5	1	0	-0.020364	-1.967707	-1.838386
6	6	0	0.265392	-1.528915	0.280412
7	6	0	-0.475119	-1.254248	1.467089
8	1	0	0.039708	-1.111430	2.409204
9	6	0	-1.843397	-1.177210	1.470180
10	1	0	-2.335515	-0.975297	2.413365
11	6	0	-6.874366	-0.999364	0.250020
12	6	0	-6.182515	-1.312943	-0.936288
13	1	0	-6.713614	-1.443966	-1.871013
14	6	0	-4.810976	-1.444301	-0.905314
15	1	0	-4.316199	-1.683518	-1.838792
16	6	0	-4.055172	-1.278115	0.284046
17	6	0	-4.790859	-0.997176	1.470713
18	1	0	-4.282165	-0.890892	2.421311
19	6	0	-6.156435	-0.873424	1.460398
20	1	0	-6.717382	-0.680207	2.368838
21	6	0	-8.986390	-0.939156	-0.838943
22	1	0	-8.914373	-1.955127	-1.236511
23	1	0	-10.006089	-0.739785	-0.517555
24	1	0	-8.681677	-0.209564	-1.595449
25	6	0	4.534726	-1.790887	0.250495
26	6	0	3.800975	-2.010357	-0.936203
27	1	0	4.306813	-2.254226	-1.862647
28	6	0	2.428970	-1.913210	-0.911134
29	1	0	1.902646	-2.087991	-1.841357
30	6	0	1.704107	-1.619129	0.277538
31	6	0	2.474584	-1.434997	1.462749
32	1	0	1.985453	-1.242315	2.409816
33	6	0	3.842416	-1.515150	1.454571
34	1	0	4.426506	-1.391324	2.360058
35	6	0	6.617179	-2.333750	-0.770440
36	1	0	6.466937	-1.710652	-1.654886
37	1	0	7.656615	-2.278556	-0.453742
38	1	0	6.340647	-3.370892	-0.977785
39	8	0	-8.181005	-0.803793	0.333844

40	8	0	5.853799	-1.837957	0.336040
41	6	0	2.615003	1.365095	-0.265242
42	6	0	1.860421	1.636294	0.912784
43	1	0	2.364891	1.812289	1.854504
44	6	0	0.492976	1.706699	0.899391
45	1	0	-0.007489	1.922690	1.835044
46	6	0	-0.264308	1.518533	-0.294070
47	6	0	0.490794	1.259652	-1.474487
48	1	0	-0.011570	1.134560	-2.425847
49	6	0	1.859320	1.186841	-1.460954
50	1	0	2.364180	0.995722	-2.399707
51	6	0	6.876552	1.018776	-0.188877
52	6	0	6.166790	1.267021	1.002191
53	1	0	6.684271	1.351567	1.949841
54	6	0	4.794888	1.391333	0.959008
55	1	0	4.284834	1.572792	1.897306
56	6	0	4.056275	1.281479	-0.247679
57	6	0	4.809514	1.065921	-1.436968
58	1	0	4.314797	1.011917	-2.399309
59	6	0	6.175582	0.949608	-1.413974
60	1	0	6.750272	0.807945	-2.323334
61	6	0	8.974458	0.919099	0.923971
62	1	0	8.887988	1.912725	1.371945
63	1	0	9.999981	0.745094	0.606451
64	1	0	8.666766	0.149134	1.638060
65	6	0	-4.533582	1.780241	-0.313854
66	6	0	-3.810076	2.050987	0.868904
67	1	0	-4.324067	2.337471	1.778549
68	6	0	-2.437992	1.952583	0.860782
69	1	0	-1.919294	2.176508	1.784760
70	6	0	-1.703212	1.607856	-0.307600
71	6	0	-2.463060	1.373830	-1.490952
72	1	0	-1.965404	1.132210	-2.422280
73	6	0	-3.831138	1.453013	-1.498507
74	1	0	-4.407452	1.287009	-2.402199
75	6	0	-6.624455	2.367930	0.664540
76	1	0	-6.485741	1.781797	1.575812
77	1	0	-7.660868	2.303222	0.339877
78	1	0	-6.346093	3.411897	0.831179
79	8	0	8.185549	0.837052	-0.264776
80	8	0	-5.852053	1.823489	-0.412402

1b$^{\bullet+}$-dimer, OS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.609839	-1.395787	0.308830
2	6	0	-1.890505	-1.716202	-0.879448
3	1	0	-2.422293	-1.921218	-1.799967
4	6	0	-0.523279	-1.792272	-0.904703
5	1	0	-0.052387	-2.064521	-1.841037
6	6	0	0.267121	-1.562523	0.257340
7	6	0	-0.451697	-1.261230	1.449780
8	1	0	0.081669	-1.084925	2.375844
9	6	0	-1.819965	-1.180573	1.474805
10	1	0	-2.295250	-0.953262	2.420872
11	6	0	-6.864248	-0.983067	0.318737
12	6	0	-6.193916	-1.359305	-0.863109
13	1	0	-6.741030	-1.525896	-1.782798
14	6	0	-4.824923	-1.505588	-0.846021
15	1	0	-4.346811	-1.794658	-1.773915
16	6	0	-4.048948	-1.294461	0.324728
17	6	0	-4.763944	-0.953397	1.509430
18	1	0	-4.238665	-0.806717	2.445366
19	6	0	-6.127015	-0.813001	1.513187
20	1	0	-6.672374	-0.570839	2.419376
21	6	0	-8.990344	-0.932133	-0.744224
22	1	0	-8.942278	-1.964494	-1.100707
23	1	0	-10.001266	-0.700821	-0.416733
24	1	0	-8.682373	-0.239198	-1.533007
25	6	0	4.538156	-1.803684	0.158183
26	6	0	3.791607	-1.952727	-1.029254
27	1	0	4.286285	-2.131909	-1.976275
28	6	0	2.418016	-1.865043	-0.980897
29	1	0	1.880610	-1.970560	-1.915484
30	6	0	1.708782	-1.647211	0.231004
31	6	0	2.491401	-1.529546	1.414296
32	1	0	2.012626	-1.407621	2.378469
33	6	0	3.860304	-1.603771	1.384043
34	1	0	4.454459	-1.535402	2.288917
35	6	0	6.608725	-2.270779	-0.920442
36	1	0	6.447862	-1.591949	-1.761442
37	1	0	7.652644	-2.237039	-0.615328
38	1	0	6.328822	-3.292150	-1.192153
39	8	0	-8.165206	-0.764871	0.411541

40	8	0	5.861051	-1.847102	0.224756
41	6	0	2.613516	1.391398	-0.232955
42	6	0	1.840968	1.633334	0.938890
43	1	0	2.330629	1.794161	1.891284
44	6	0	0.473188	1.699748	0.904046
45	1	0	-0.046143	1.884615	1.836272
46	6	0	-0.262613	1.532962	-0.304685
47	6	0	0.508825	1.300433	-1.477790
48	1	0	0.020105	1.197894	-2.439083
49	6	0	1.877885	1.234054	-1.444002
50	1	0	2.399063	1.057794	-2.376925
51	6	0	6.870915	1.039970	-0.103636
52	6	0	6.139523	1.203966	1.090124
53	1	0	6.639687	1.214930	2.050684
54	6	0	4.769798	1.333047	1.030565
55	1	0	4.239277	1.436973	1.969289
56	6	0	4.053382	1.310635	-0.195910
57	6	0	4.828508	1.183430	-1.384896
58	1	0	4.351010	1.209507	-2.357050
59	6	0	6.192819	1.062938	-1.344959
60	1	0	6.785280	0.988660	-2.250875
61	6	0	8.947452	0.844603	1.037269
62	1	0	8.857324	1.801313	1.558614
63	1	0	9.977415	0.689423	0.724596
64	1	0	8.622510	0.023280	1.683010
65	6	0	-4.534130	1.768191	-0.380970
66	6	0	-3.824994	2.100772	0.793083
67	1	0	-4.349274	2.431885	1.681489
68	6	0	-2.450852	2.011795	0.803824
69	1	0	-1.941461	2.295467	1.716816
70	6	0	-1.704978	1.613341	-0.337045
71	6	0	-2.449147	1.315812	-1.513683
72	1	0	-1.939395	1.019949	-2.422842
73	6	0	-3.818923	1.385988	-1.539122
74	1	0	-4.384562	1.167718	-2.438481
75	6	0	-6.635987	2.391978	0.548624
76	1	0	-6.512871	1.845716	1.487074
77	1	0	-7.669183	2.320588	0.214957
78	1	0	-6.353921	3.440729	0.674948
79	8	0	8.179010	0.859595	-0.168405
80	8	0	-5.854806	1.796880	-0.493141

1b$^{\bullet+}$-dimer, T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.216022	-1.621624	0.244926
2	6	0	-1.548224	-1.761619	-1.004837
3	1	0	-2.120929	-1.821970	-1.922696
4	6	0	-0.179671	-1.802456	-1.092659
5	1	0	0.271112	-1.939194	-2.068906
6	6	0	0.642747	-1.722469	0.061755
7	6	0	-0.020794	-1.597676	1.310126
8	1	0	0.558739	-1.518126	2.222734
9	6	0	-1.389092	-1.544412	1.399931
10	1	0	-1.834876	-1.470007	2.384643
11	6	0	-6.455924	-1.201743	0.431475
12	6	0	-5.846559	-1.692264	-0.747308
13	1	0	-6.442899	-1.943359	-1.615836
14	6	0	-4.483057	-1.847724	-0.783706
15	1	0	-4.044595	-2.246191	-1.691024
16	6	0	-3.650942	-1.533716	0.329303
17	6	0	-4.303978	-1.098370	1.520146
18	1	0	-3.723367	-0.843799	2.398532
19	6	0	-5.661693	-0.941618	1.576582
20	1	0	-6.160911	-0.604092	2.478828
21	6	0	-8.612489	-1.112675	-0.566848
22	1	0	-8.637950	-2.159502	-0.879594
23	1	0	-9.596969	-0.807581	-0.219677
24	1	0	-8.279763	-0.469210	-1.386684
25	6	0	4.911814	-1.792956	-0.193790
26	6	0	4.143583	-1.525444	-1.338497
27	1	0	4.617716	-1.315671	-2.289891
28	6	0	2.763265	-1.515640	-1.243628
29	1	0	2.195310	-1.271475	-2.135027
30	6	0	2.093481	-1.764828	-0.026958
31	6	0	2.893742	-2.057530	1.104875
32	1	0	2.429621	-2.321612	2.048749
33	6	0	4.266704	-2.076113	1.025944
34	1	0	4.879996	-2.321947	1.886506
35	6	0	6.966558	-1.718144	-1.392647
36	1	0	6.792512	-0.760932	-1.894690
37	1	0	8.018845	-1.806062	-1.128504
38	1	0	6.676916	-2.546162	-2.045696
39	8	0	-7.742773	-0.950181	0.559747

40	8	0	6.249576	-1.783514	-0.160242
41	6	0	2.232414	1.689036	-0.010321
42	6	0	1.409871	1.735085	1.148616
43	1	0	1.861507	1.773618	2.133317
44	6	0	0.041100	1.775571	1.054432
45	1	0	-0.540270	1.795618	1.969340
46	6	0	-0.621346	1.754505	-0.200482
47	6	0	0.198214	1.710385	-1.358672
48	1	0	-0.256454	1.731763	-2.342549
49	6	0	1.567125	1.690598	-1.268280
50	1	0	2.144386	1.649128	-2.184854
51	6	0	6.462324	1.234916	0.192873
52	6	0	5.674279	1.018429	1.346238
53	1	0	6.126144	0.671648	2.267558
54	6	0	4.315058	1.205837	1.275780
55	1	0	3.725257	0.979749	2.156431
56	6	0	3.667234	1.608657	0.074693
57	6	0	4.498101	1.885606	-1.051960
58	1	0	4.062066	2.271737	-1.966044
59	6	0	5.853329	1.715096	-0.996977
60	1	0	6.494764	1.940003	-1.842723
61	6	0	8.452055	0.468496	1.247622
62	1	0	8.399867	1.159311	2.092852
63	1	0	9.484777	0.356137	0.925783
64	1	0	8.024482	-0.503880	1.508860
65	6	0	-4.889188	1.712330	-0.445049
66	6	0	-4.255873	2.197906	0.711613
67	1	0	-4.834742	2.563674	1.551237
68	6	0	-2.874613	2.207429	0.778577
69	1	0	-2.411687	2.611230	1.672535
70	6	0	-2.071886	1.766001	-0.294892
71	6	0	-2.736682	1.331376	-1.467598
72	1	0	-2.163948	0.981707	-2.319857
73	6	0	-4.109336	1.293585	-1.541634
74	1	0	-4.621698	0.948141	-2.433142
75	6	0	-7.063313	2.152338	0.412085
76	1	0	-6.935667	1.622133	1.361417
77	1	0	-8.080257	2.013505	0.049812
78	1	0	-6.859999	3.218931	0.542268
79	8	0	7.757786	1.011384	0.117980
80	8	0	-6.213456	1.602032	-0.593621

$2^{\bullet+}$-dimer, CS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.270416	-1.500671	-0.370743
2	6	0	0.496592	-1.761759	0.802432
3	1	0	0.004959	-2.036699	1.727065
4	6	0	1.863756	-1.693541	0.808541
5	1	0	2.374191	-1.924083	1.734932
6	6	0	2.610176	-1.350425	-0.355830
7	6	0	1.845369	-1.101362	-1.532815
8	1	0	2.343680	-0.860178	-2.463652
9	6	0	0.476350	-1.173044	-1.539759
10	1	0	-0.034108	-0.988450	-2.477155
11	6	0	-4.542806	-1.745211	-0.352714
12	6	0	-3.804318	-2.055404	0.812295
13	1	0	-4.308431	-2.364601	1.719644
14	6	0	-2.432883	-1.962128	0.791034
15	1	0	-1.905664	-2.211690	1.703413
16	6	0	-1.709078	-1.584008	-0.374168
17	6	0	-2.482236	-1.305886	-1.539648
18	1	0	-1.993630	-1.038613	-2.468951
19	6	0	-3.850560	-1.378864	-1.533487
20	1	0	-4.436623	-1.180495	-2.424311
21	6	0	-6.619319	-2.402909	0.632283
22	1	0	-6.236208	-3.418447	0.780024
23	1	0	-6.467883	-1.824441	1.549469
24	6	0	-8.069395	-2.404948	0.208546
25	1	0	-8.192342	-2.936081	-0.737637
26	1	0	-8.669745	-2.908476	0.969979
27	1	0	-8.438012	-1.382024	0.102362
28	6	0	6.884366	-1.137796	-0.298478
29	6	0	6.173714	-1.450630	0.877517
30	1	0	6.695893	-1.646288	1.805643
31	6	0	4.797923	-1.516804	0.841117
32	1	0	4.291764	-1.769412	1.764832
33	6	0	4.052433	-1.277366	-0.342306
34	6	0	4.801428	-0.958809	-1.510747
35	1	0	4.298699	-0.778002	-2.453406
36	6	0	6.171847	-0.897150	-1.495095
37	1	0	6.741634	-0.682518	-2.393191
38	6	0	9.013130	-1.310405	0.780881
39	1	0	8.734203	-0.593209	1.562364

40	1	0	8.802671	-2.325383	1.135391
41	6	0	10.456940	-1.152473	0.363546
42	1	0	10.648691	-0.137987	0.005821
43	1	0	11.108495	-1.347030	1.218441
44	1	0	10.705346	-1.858852	-0.431090
45	8	0	-5.859982	-1.790519	-0.434581
46	8	0	8.202407	-1.054818	-0.383204
47	6	0	0.270416	1.500662	0.370771
48	6	0	-0.496592	1.761751	-0.802404
49	1	0	-0.004957	2.036691	-1.727037
50	6	0	-1.863756	1.693535	-0.808515
51	1	0	-2.374193	1.924077	-1.734905
52	6	0	-2.610175	1.350418	0.355856
53	6	0	-1.845371	1.101353	1.532841
54	1	0	-2.343683	0.860168	2.463676
55	6	0	-0.476351	1.173034	1.539787
56	1	0	0.034106	0.988439	2.477183
57	6	0	4.542806	1.745211	0.352714
58	6	0	3.804309	2.055398	-0.812289
59	1	0	4.308416	2.364594	-1.719642
60	6	0	2.432875	1.962119	-0.791017
61	1	0	1.905649	2.211676	-1.703393
62	6	0	1.709078	1.584000	0.374190
63	6	0	2.482246	1.305883	1.539666
64	1	0	1.993649	1.038612	2.468975
65	6	0	3.850571	1.378866	1.533495
66	1	0	4.436642	1.180502	2.424314
67	6	0	6.619301	2.402912	-0.632310
68	1	0	6.236185	3.418449	-0.780046
69	1	0	6.467853	1.824443	-1.549492
70	6	0	8.069383	2.404956	-0.208593
71	1	0	8.192342	2.936089	0.737587
72	1	0	8.669720	2.908485	-0.970035
73	1	0	8.438004	1.382032	-0.102414
74	6	0	-6.884365	1.137801	0.298467
75	6	0	-6.173700	1.450638	-0.877519
76	1	0	-6.695869	1.646301	-1.805650
77	6	0	-4.797909	1.516807	-0.841106
78	1	0	-4.291740	1.769418	-1.764815
79	6	0	-4.052432	1.277361	0.342323
80	6	0	-4.801440	0.958801	1.510756
81	1	0	-4.298722	0.777989	2.453419
82	6	0	-6.171859	0.897147	1.495090
83	1	0	-6.741655	0.682513	2.393180

84	6	0	-9.013115	1.310420	-0.780914
85	1	0	-8.734183	0.593228	-1.562398
86	1	0	-8.802649	2.325400	-1.135417
87	6	0	-10.456931	1.152492	-0.363595
88	1	0	-10.648690	0.138005	-0.005878
89	1	0	-11.108476	1.347056	-1.218497
90	1	0	-10.705343	1.858868	0.431041
91	8	0	5.859982	1.790524	0.434567
92	8	0	-8.202407	1.054826	0.383179

$2^{\bullet+}$-dimer, OS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.271880	-1.529946	0.348538
2	6	0	-0.515564	-1.810737	-0.805138
3	1	0	-0.042108	-2.116589	-1.729524
4	6	0	-1.882412	-1.736560	-0.787791
5	1	0	-2.409879	-1.979095	-1.701513
6	6	0	-2.607112	-1.366913	0.382608
7	6	0	-1.821472	-1.101647	1.541471
8	1	0	-2.302111	-0.843018	2.476933
9	6	0	-0.452753	-1.180834	1.525099
10	1	0	0.076418	-0.971936	2.446911
11	6	0	4.544666	-1.764562	0.253334
12	6	0	3.790483	-2.001371	-0.917371
13	1	0	4.281374	-2.246385	-1.851182
14	6	0	2.418567	-1.913618	-0.869733
15	1	0	1.878664	-2.090574	-1.791709
16	6	0	1.711786	-1.611788	0.326803
17	6	0	2.500358	-1.405560	1.495469
18	1	0	2.024806	-1.210904	2.449355
19	6	0	3.868961	-1.476338	1.464666
20	1	0	4.466843	-1.338536	2.359100
21	6	0	6.606844	-2.350900	-0.801746
22	1	0	6.227750	-3.358898	-1.002390
23	1	0	6.434096	-1.721030	-1.680599
24	6	0	8.065147	-2.366189	-0.407265
25	1	0	8.210088	-2.949111	0.504724
26	1	0	8.653624	-2.821544	-1.207314
27	1	0	8.429573	-1.348202	-0.250368
28	6	0	-6.878428	-1.112507	0.385435

29	6	0	-6.191554	-1.504940	-0.781683
30	1	0	-6.732313	-1.753033	-1.686340
31	6	0	-4.816759	-1.583633	-0.764844
32	1	0	-4.329805	-1.903059	-1.678022
33	6	0	-4.048040	-1.281162	0.389717
34	6	0	-4.773352	-0.884515	1.549896
35	1	0	-4.251121	-0.645901	2.468734
36	6	0	-6.142535	-0.807578	1.553592
37	1	0	-6.694295	-0.530599	2.445835
38	6	0	-9.028210	-1.336037	-0.642586
39	1	0	-8.758727	-0.675723	-1.475725
40	1	0	-8.831670	-2.374403	-0.931015
41	6	0	-10.462441	-1.137864	-0.209863
42	1	0	-10.640387	-0.099850	0.081268
43	1	0	-11.131593	-1.384863	-1.037164
44	1	0	-10.700411	-1.786459	0.635605
45	8	0	5.864421	-1.808491	0.312888
46	8	0	-8.193043	-1.009865	0.486826
47	6	0	-0.266529	1.500133	-0.385211
48	6	0	0.477672	1.735350	0.807389
49	1	0	-0.034295	1.973906	1.731299
50	6	0	1.845147	1.671222	0.837034
51	1	0	2.338938	1.883033	1.776952
52	6	0	2.612041	1.362303	-0.322845
53	6	0	1.868823	1.138014	-1.518805
54	1	0	2.384631	0.916461	-2.445051
55	6	0	0.499501	1.202560	-1.548111
56	1	0	0.005466	1.046721	-2.499568
57	6	0	-4.539804	1.726479	-0.436045
58	6	0	-3.818168	2.105084	0.718550
59	1	0	-4.335189	2.466381	1.599023
60	6	0	-2.445350	2.017611	0.720902
61	1	0	-1.929469	2.332776	1.619628
62	6	0	-1.707071	1.577682	-0.411004
63	6	0	-2.462350	1.232887	-1.568977
64	1	0	-1.959467	0.906005	-2.471357
65	6	0	-3.831815	1.298191	-1.584594
66	1	0	-4.405115	1.044065	-2.469571
67	6	0	-6.630404	2.439314	0.477725
68	1	0	-6.244414	3.460359	0.570016
69	1	0	-6.498475	1.918665	1.431872
70	6	0	-8.073481	2.423452	0.030774
71	1	0	-8.177775	2.895307	-0.948451
72	1	0	-8.682877	2.976254	0.749670

73	1	0	-8.446998	1.398016	-0.017696
74	6	0	6.884716	1.166933	-0.200152
75	6	0	6.150213	1.385111	0.983125
76	1	0	6.653950	1.507787	1.933733
77	6	0	4.775595	1.447419	0.925154
78	1	0	4.248529	1.615680	1.856335
79	6	0	4.053652	1.295830	-0.288073
80	6	0	4.826430	1.072484	-1.463672
81	1	0	4.342729	0.971867	-2.428004
82	6	0	6.196095	1.015639	-1.426169
83	1	0	6.784570	0.875444	-2.326921
84	6	0	8.992561	1.256522	0.930359
85	1	0	8.699960	0.477175	1.644259
86	1	0	8.773681	2.239031	1.362578
87	6	0	10.443951	1.133481	0.528029
88	1	0	10.644012	0.151251	0.093204
89	1	0	11.079327	1.258579	1.407715
90	1	0	10.705537	1.901980	-0.202128
91	8	0	-5.857846	1.758950	-0.535937
92	8	0	8.203596	1.097150	-0.265913

$2^{\bullet+}$-dimer, T

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.574566	1.753867	-0.227434
2	6	0	-0.155433	1.570207	0.974387
3	1	0	0.373662	1.441578	1.911688
4	6	0	-1.526152	1.499037	0.979290
5	1	0	-2.029688	1.320510	1.922396
6	6	0	-2.282947	1.584518	-0.222543
7	6	0	-1.548090	1.775999	-1.425670
8	1	0	-2.072519	1.917237	-2.363605
9	6	0	-0.178189	1.866759	-1.424790
10	1	0	0.326773	2.076215	-2.360926
11	6	0	4.852886	1.801197	-0.225789
12	6	0	4.144648	2.082071	0.954985
13	1	0	4.667941	2.308984	1.875952
14	6	0	2.760954	2.068948	0.941083
15	1	0	2.240806	2.315733	1.860455
16	6	0	2.029155	1.801205	-0.233365
17	6	0	2.766233	1.557386	-1.416547

18	1	0	2.249710	1.344402	-2.346622
19	6	0	4.141914	1.546164	-1.415538
20	1	0	4.709436	1.352026	-2.319405
21	6	0	6.975027	2.201515	0.794424
22	1	0	6.619436	3.191245	1.101871
23	1	0	6.841429	1.503297	1.630556
24	6	0	8.414162	2.252087	0.336975
25	1	0	8.524605	2.934720	-0.508106
26	1	0	9.049752	2.601657	1.153911
27	1	0	8.752058	1.257245	0.039212
28	6	0	-6.541030	1.288273	-0.213003
29	6	0	-5.845645	1.548586	0.993069
30	1	0	-6.383308	1.682133	1.923411
31	6	0	-4.475745	1.636588	0.974926
32	1	0	-3.969640	1.867537	1.905269
33	6	0	-3.719068	1.485724	-0.222588
34	6	0	-4.449254	1.233004	-1.422418
35	1	0	-3.920635	1.083109	-2.356546
36	6	0	-5.812565	1.133882	-1.422740
37	1	0	-6.372692	0.947604	-2.332958
38	6	0	-8.688921	1.384817	0.844654
39	1	0	-8.467133	0.587698	1.563628
40	1	0	-8.436985	2.353510	1.288130
41	6	0	-10.124028	1.351623	0.373054
42	1	0	-10.368137	0.390150	-0.084271
43	1	0	-10.788319	1.506285	1.226401
44	1	0	-10.305465	2.144000	-0.355877
45	8	0	6.184683	1.751236	-0.317594
46	8	0	-7.847673	1.183985	-0.315604
47	6	0	-0.574570	-1.753867	0.227422
48	6	0	0.155439	-1.570197	-0.974394
49	1	0	-0.373646	-1.441563	-1.911699
50	6	0	1.526159	-1.499024	-0.979285
51	1	0	2.029707	-1.320489	-1.922384
52	6	0	2.282942	-1.584511	0.222554
53	6	0	1.548077	-1.776002	1.425674
54	1	0	2.072499	-1.917241	2.363613
55	6	0	0.178176	-1.866762	1.424782
56	1	0	-0.326793	-2.076219	2.360915
57	6	0	-4.852888	-1.801195	0.225779
58	6	0	-4.144662	-2.082055	-0.954999
59	1	0	-4.667968	-2.308960	-1.875964
60	6	0	-2.760969	-2.068934	-0.941101
61	1	0	-2.240831	-2.315718	-1.860477

62	6	0	-2.029161	-1.801202	0.233349
63	6	0	-2.766236	-1.557394	1.416537
64	1	0	-2.249711	-1.344418	2.346613
65	6	0	-4.141918	-1.546172	1.415529
66	1	0	-4.709440	-1.352042	2.319397
67	6	0	-6.974996	-2.201498	-0.794461
68	1	0	-6.619389	-3.191222	-1.101912
69	1	0	-6.841393	-1.503271	-1.630583
70	6	0	-8.414131	-2.252080	-0.337021
71	1	0	-8.524582	-2.934730	0.508045
72	1	0	-9.049707	-2.601636	-1.153973
73	1	0	-8.752032	-1.257243	-0.039242
74	6	0	6.541026	-1.288280	0.213025
75	6	0	5.845640	-1.548601	-0.993045
76	1	0	6.383302	-1.682161	-1.923386
77	6	0	4.475742	-1.636598	-0.974903
78	1	0	3.969636	-1.867560	-1.905243
79	6	0	3.719063	-1.485720	0.222607
80	6	0	4.449249	-1.232987	1.422437
81	1	0	3.920629	-1.083080	2.356562
82	6	0	5.812562	-1.133872	1.422759
83	1	0	6.372689	-0.947588	2.332976
84	6	0	8.688924	-1.384833	-0.844630
85	1	0	8.467146	-0.587710	-1.563600
86	1	0	8.436980	-2.353522	-1.288111
87	6	0	10.124032	-1.351656	-0.373029
88	1	0	10.368147	-0.390188	0.084304
89	1	0	10.788327	-1.506315	-1.226375
90	1	0	10.305461	-2.144040	0.355896
91	8	0	-6.184681	-1.751231	0.317578
92	8	0	7.847671	-1.183997	0.315625

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