Isolable cyclic radical cations of heavy main-group elements

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Content

Experimental section

General considerations: All operations were carried out under an atmosphere of dry argon or nitrogen by using modified Schlenck line and a glovebox. All solvents were freshly distilled from Na/benzophenone or CaH_2 and degassed prior to use. UV-Vis spectra were recorded on the Lambda 750 spectrometer. Element analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences and Center of Mordern Analysis, Nanjing University. The ^{1}H NMR and ^{13}C NMR spectroscopic data were recorded on a Bruker DRX 400 and 500 MHz NMR spectrometers. EPR spectra were obtained using Bruker plus-6/1 X-band variable-temperature apparatus. The X-ray single crystal diffraction data were collected on Bruker D8 CMOS detectors at 173 K. Compounds L^HGeCl (L^H = CH[CHNDipp]$_2$, Dipp=2,6-*i*Pr$_2$C$_6$H$_3$),[S1] $[L^HGeP]_2$,[S1] NaAsCO•(18-c-6)[S2] and Ag[Al(OR$_F$)$_4$] (R$_F$ = C(CF$_3$)$_3$)[S3] were prepared by the published procedures.

Synthesis of 2: Cold toluene (60 ml) was added to the mixture of L^HGeCl (1.32 g, 2.65 mmol) and NaAsCO•(18-c-6) (1.33 g, 3.41 mmol) at -78 °C. The mixture was allowed to warm to room temperature in 2 h and a dark mixture was formed. After filtration, the black filtrate was stored in dark place at room temperature for 2 d and dark brown crystals were formed (0.31 g, 21.8 %); m.p.: 259.6-261.3 °C; ^{1}H NMR (500 MHz, d^8-THF): δ = 7.23 – 7.16 (m, 8H, Ar-*H* and beta-*H*), 7.07 (d, *J*=7.7, 8H, Ar-*H*), 4.99 (t, *J*=6.6, 2H, gamma-*H*), 3.44 (m, 8H, C*H*(CH$_3$)$_2$), 1.03 (dd, *J*=6.6, 3.5, 48H, CH(C*H*$_3$)$_2$); ^{13}C NMR (101 MHz, d^8-THF): δ = 163.59, 155.60 (beta-*C*), 145.78, 144.51, 128.00, 124.66 (Ar-*C*), 92.47 (gamma-*C*H), 29.72 (*C*H(CH$_3$)$_2$), 26.23, 23.78 (CH(*C*H$_3$)$_2$). Elemental analysis calcd (%) for C$_{54}$H$_{74}$As$_2$Ge$_2$N$_4$: C, 60.37; H, 6.94; N, 5.22; Found: C, 60.59; H, 6.84; N, 5.55.

Synthesis of $1^{\bullet+}$•[Al(OR$_F$)$_4$]$^-$: Fluorobenzene (30 ml) was added to the mixture of **1** (105 mg, 0.11 mmol) and Ag[Al(OR$_F$)$_4$] (116 mg, 0.11 mmol) under dark. In 30 min, the light green suspension changed into orange red solution and gray precipitate (Ag

metal) was formed. The mixture was stirred overnight. After filtration, the filtrate was concentrated to ca. 3 mL and stored at 4 °C for 1 d to afford orange crystals of $\mathbf{1}^{\bullet+}\bullet[Al(OR_F)_4]^-$ (68 mg, 32.7%); m.p.: 240.5-241.3 °C; elemental analysis calcd (%) for $C_{70}H_{74}AlF_{36}Ge_2N_4O_4P_2$: C, 43.04; H, 3.82; N, 2.87; Found: C, 43.02; H, 3.93; N, 2.79.

Synthesis of $\mathbf{2}^{\bullet+}\bullet[Al(OR_F)_4]^-$: Fluorobenzene (30 ml) was added to the mixture of **2** (174 mg, 0.16 mmol) and $Ag[Al(OR_F)_4]$ (176 mg, 0.16 mmol). The mixture was stirred overnight. Brown precipitate (Ag metal) was formed. After filtration, the orange filtrate was concentrated to ca. 3 mL and stored at 4 °C for 1 d to afford orange crystals of $\mathbf{2}^{\bullet+}\bullet[Al(OR_F)_4]^-$ (230 mg, 75.4%); m.p. 192.1-194.5 °C; Elemental analysis calcd (%) for $C_{70}H_{74}AlAs_2F_{36}Ge_2N_4O_4\bullet C_6H_5F$: C, 42.70; H, 3.73; N, 2.62; found: C, 42.79; H, 3.76; N, 2.62.

Table S1. Crystal data and structure refinement

	2	$\mathbf{1}^{\bullet+}\bullet[Al(OR_F)_4]^-$	$\mathbf{2}^{\bullet+}\bullet[Al(OR_F)_4]^-$
CCDC No.	1889601	1889602	1889603
Formula	$C_{54}H_{74}As_2Ge_2N_4$	$C_{70}H_{74}AlF_{36}Ge_2N_4O_4P_2$	$C_{70}H_{74}AlAs_2F_{36}Ge_2N_4O_4$
Formula weight	1074.32	1953.51	2041.41
Temp. (K)	123(2)	123(2)	123(2)
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	$P2_1/c$	$C2/c$	$Cmc2_1$
a (Å)	21.3357(6)	29.5048(15)	19.7185(18)
b (Å)	15.3136(4)	16.5238(7)	19.794(2)
c (Å)	16.1347(5)	19.4551(9)	22.651(2)
β (°)	93.7100(10)	118.250(2)	90
V [Å^3]	5260.6(3)	8355.2(7)	8841.0(15)
Z	4	4	4
ρ_{calcd} (g·cm^{-3})	1.356	1.553	1.606
μ (mm^{-1})	2.039	0.896	1.559
F(000)	2224	3940	4284
Collected data	92072	30017	36382
Unique data	9471 [R(int) = 0.0755]	7363 [R(int) = 0.0678]	9935 [R(int) = 0.0553]
GOF on F^2	1.053	1.203	1.050
Final R indexes [I > 2σ(I)]	R_1 = 0.0425 ωR_2 = 0.1103	R_1 = 0.0956 ωR_2 = 0.1998	R_1 = 0.0536 ωR_2 = 0.1455
R indexes (all data)	R_1 = 0.0512 ωR_2 = 0.1176	R_1 = 0.1309 ωR_2 = 0.2098	R_1 = 0.0596 ωR_2 = 0.1518
Completeness	0.999	0.999	0.996

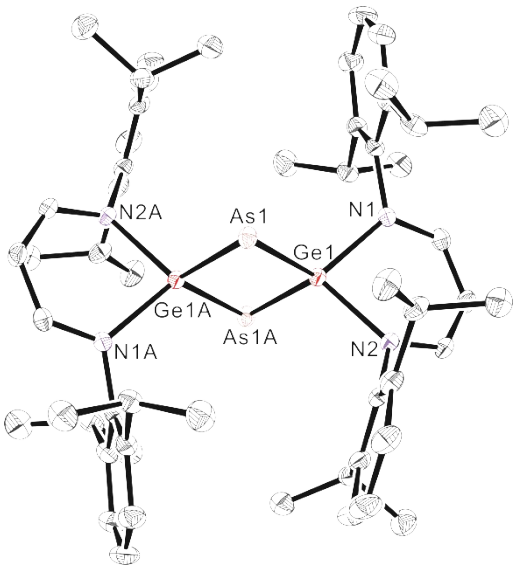


Fig. S1 Molecular structure of **2** drawn at 50% probability. Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): Ge1–N1 1.988(2), Ge1–N2 1.988(2), Ge1–As1 2.3668(4), Ge1–As1A 2.3733(4); N1–Ge1–N2 88.76(9), As1–Ge1–As1A 106.603(14), Ge1–As1–Ge1A 73.398(14).

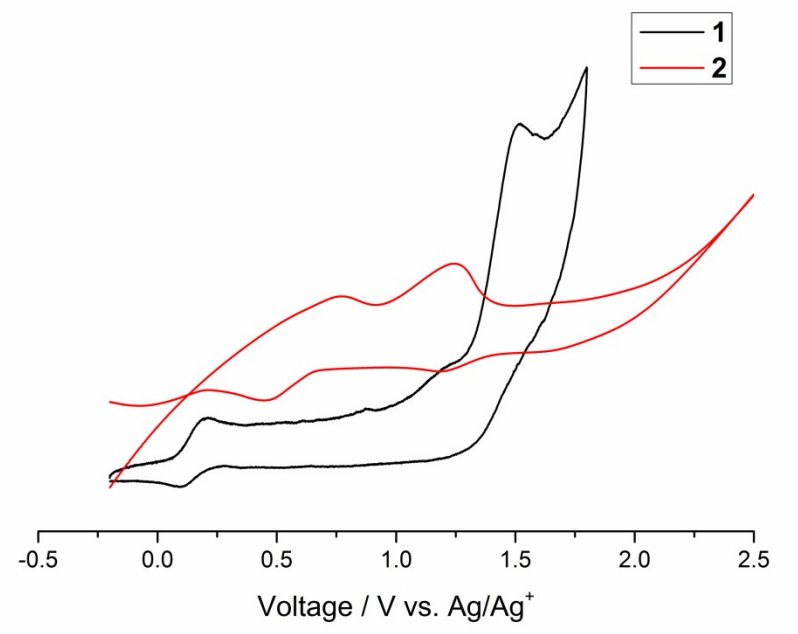


Fig. S2 Cyclic voltammograms of **1** and **2** measured in fluorobenzene solutions at room temperature, containing 0.05 M $^{n}Bu_4PF_6$, measured at 100 mV/s.

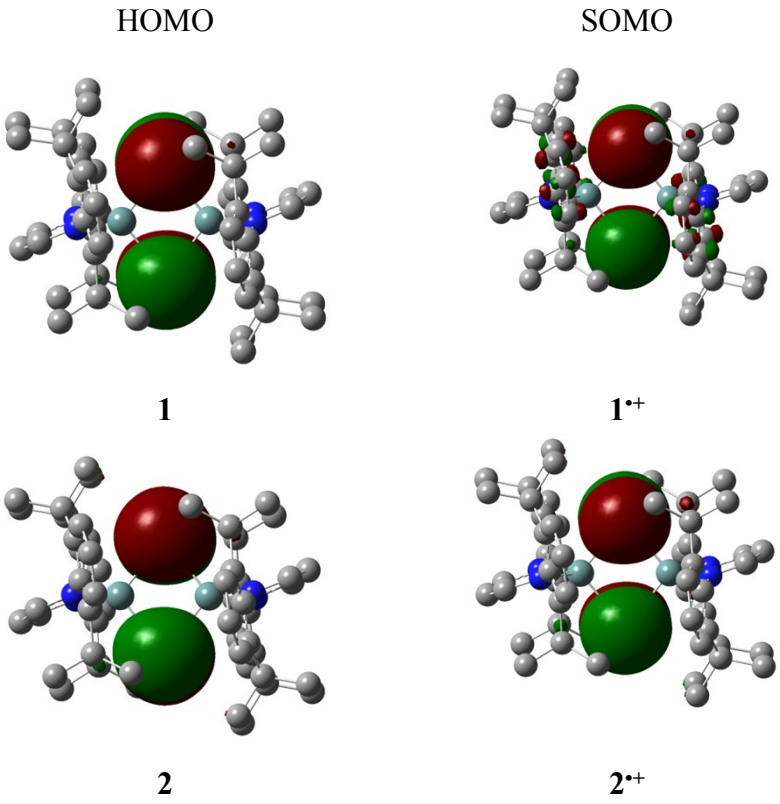


Fig. S3 Comparison of selected molecular orbitals of neutral and radical cation of **1** and **2**.

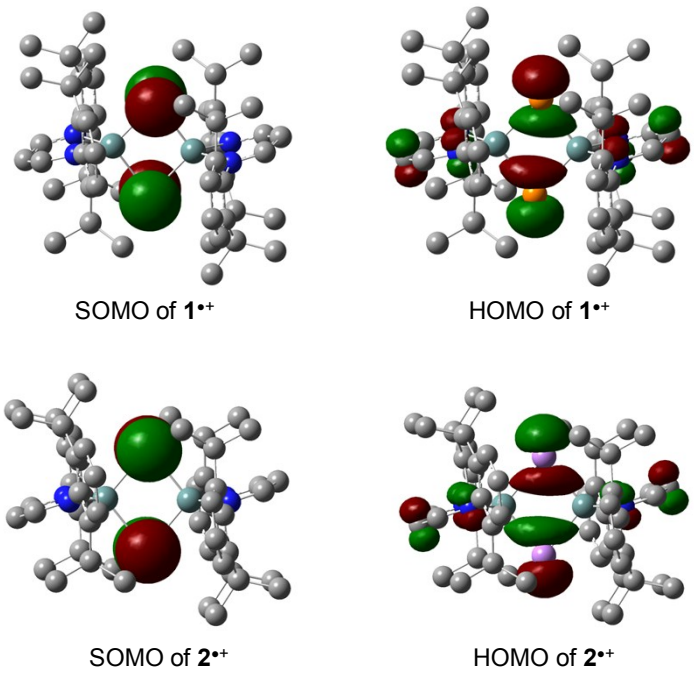


Fig. S4 Selected molecular orbitals of $\mathbf{1}^{\bullet+}$ and $\mathbf{2}^{\bullet+}$.

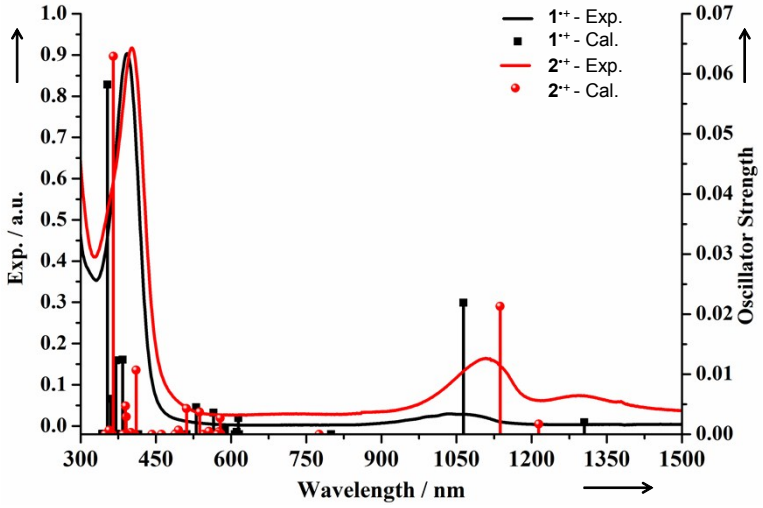


Fig. S5 UV/Vis spectra of $\mathbf{1}^{\bullet+}$ and $\mathbf{2}^{\bullet+}$ in fluorobenzene solution at room temperature, together with transitions calculated at the UB3LYP/6-31G(d) level of theory.

Calculation details for the electron occupation of 3s and 3p orbitals in $\mathbf{1}^{\bullet+}$.

$\rho(^{31}\mathrm{P(3s)}) = a_{iso}/\mathrm{A} = 43.7 \times 2.8 / 13306 = 0.9\%$

$$\rho(^{31}\mathrm{P(3p)}) = \frac{\frac{1}{3}(a\perp - a\parallel)}{\frac{2}{5}P} = \frac{\frac{1}{3}(153-19)\times 2.8}{\frac{2}{5}\times 917} = 34.1\%$$

A (in MHz) is the isotropic hyperfine interaction for unit spin density in the corresponding s orbital.

P (in MHz) is the anisotropic hyperfine parameter including the angular factor.

A and *P* values could be obtained from Table 1 in the reference.[S4]

DFT calculations

All the calculations were performed at Gaussian 09 program suite.[S5] The calculations were carried out with Becke's three-parameter hybrid exchange functional and the Lee–Yang–Parr correlation functional (B3LYP)[S6] combined with the SDD[S7] basis set, which was used for Ge. The ground-state structures of the studied compounds were optimized at the (U)B3LYP/6-31G(d)+SDD level of approximation, including two neutral compounds **1** and **2**, as well as their corresponding oxidation states ($\mathbf{1}^{\bullet+}$ and $\mathbf{2}^{\bullet+}$), and no imaginary frequency was found, which confirmed the local minimum of the optimized structures. Besides, we also carried out the calculation on the UV/Vis absorption spectra of $\mathbf{1}^{\bullet+}$ and $\mathbf{2}^{\bullet+}$ according to the time-dependent DFT (TD-DFT) method at the UB3LYP/6-31(d)+SDD level,[S8] and the calculated results are in good agreement with the experimental value. In addition, considering the solvent effects, the Polarizable Continuum Model (PCM) model was used in the TD-DFT calculations.[S9]

Table S2. Calculated *g* values and hyperfine coupling constants (G) of $\mathbf{1}^{\bullet+}$ and $\mathbf{2}^{\bullet+}$ at the UB3LYP/def2TZVP level in comparison with the experimental results.

		g_x	g_y	g_z	a_x	a_y	a_z
$\mathbf{1}^{\bullet+}$	Exp.	2.0145	2.0145	2.0036	19	19	153
	Calculated	2.0036	2.0123	2.0194	66.3	62.7	129.0
$\mathbf{2}^{\bullet+}$	Exp.	2.0393	2.0793	2.0031	44	44	126
	Calculated	2.0049	2.0363	2.0694	55.4	53.2	108.6

Table S3. Calculated Ge–E distances, Ge–E Wiberg bond indices, NBO charges at the (U)B3LYP/6-31G(d)+SDD level of theory.

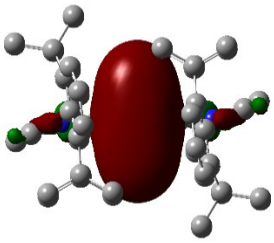
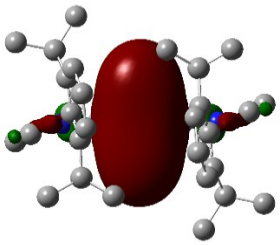
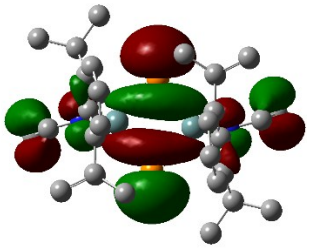
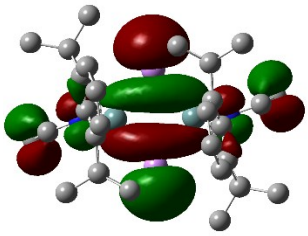
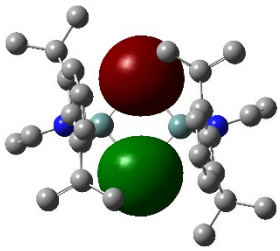
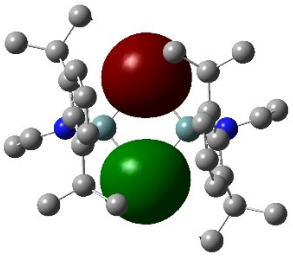
	Ge–E/Å	WBI(Ge–E)	q(Ge)	q(E)
1	2.33853/2.33950	1.15/1.17	1.15	-0.76
	(2.2658(5)/ 2.2717(5)/) [a]			
2	2.44096/2.44022	1.16/1.15	1.05	-0.65
	2.44093/2.44021			
	(2.3668(4)/ 2.3733(4)) [a]			
1$^{\bullet+}$	2.34915/2.35942	1.12/1.14	0.56	0.07
	2.34907/2.35940			
	(2.278(2)/2.3110(19))[a]			
2$^{\bullet+}$	2.46043/2.45187	1.14/1.12	0.51	0.13
	(2.3825(13)/2.4085(12)) [a]			

[a] Experimental bond lengths.

Table S4. Calculated excited wavelengths (λ) and oscillator strengths (*f*) of selected transitions of **1**$^{\bullet+}$ and **2**$^{\bullet+}$.

Compound	Excited state	Wavelength/nm	*f*	Transition nature	
1$^{\bullet+}$	S_1	1305.1	0.002	HOMO-1(*β*)→LUMO(*β*)	91.9%
	S_2	1064.0	0.022	HOMO(*β*)→LUMO(*β*)	96.6%
2$^{\bullet+}$	S_1	1214.0	0.002	HOMO-1(*β*)→LUMO(*β*)	95.1%
	S_2	1137.0	0.021	HOMO(*β*)→LUMO(*β*)	96.7%

Table S5. Main frontier molecular orbitals related to UV/vis absorption transitions of **1**$^{\bullet+}$ and **2**$^{\bullet+}$.

	1$^{\bullet+}$	**2**$^{\bullet+}$
HOMO(β)		
HOMO-1(β)		
LUMO(β)		

Coordinates of the studied molecules

1$^{\bullet+}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.000131	1.418884	0.508892
2	32	0	-0.000196	-1.418910	-0.508842
3	15	0	0.000052	-0.618077	1.699503
4	15	0	-0.000235	0.618035	-1.699530
5	7	0	1.449153	2.724329	1.014096
6	7	0	-1.448562	2.724685	1.014150
7	7	0	-1.449128	-2.724426	-1.014110
8	7	0	1.448583	-2.724630	-1.014120
9	6	0	-1.225407	3.750535	1.835872
10	6	0	0.000491	4.201352	2.312587
11	6	0	1.226260	3.750246	1.835814
12	6	0	2.817509	2.587348	0.539316
13	6	0	3.768655	1.944850	1.363074
14	6	0	5.096679	1.917072	0.917190
15	6	0	5.469337	2.514162	-0.282989
16	6	0	4.516147	3.157730	-1.067581
17	6	0	3.171867	3.210790	-0.679053
18	6	0	3.419945	1.372449	2.735497
19	6	0	3.870761	2.326306	3.863225
20	6	0	4.009601	-0.028773	2.963152
21	6	0	2.172420	4.007891	-1.515090
22	6	0	2.264148	3.711628	-3.022663

23	6	0	2.332180	5.520270	-1.249360
24	6	0	-2.816965	2.587920	0.539483
25	6	0	-3.768054	1.945382	1.363284
26	6	0	-5.096111	1.917651	0.917509
27	6	0	-5.468865	2.514889	-0.282575
28	6	0	-4.515744	3.158536	-1.067174
29	6	0	-3.171415	3.211508	-0.678781
30	6	0	-3.419216	1.372934	2.735651
31	6	0	-4.009027	-0.028204	2.963453
32	6	0	-3.869720	2.326900	3.863418
33	6	0	-2.172031	4.008575	-1.514908
34	6	0	-2.331794	5.520968	-1.249217
35	6	0	-2.263870	3.712160	-3.022450
36	6	0	-1.226183	-3.749972	-1.836264
37	6	0	-0.000379	-4.200800	-2.313223
38	6	0	1.225491	-3.750159	-1.836261
39	6	0	-2.817480	-2.587544	-0.539344
40	6	0	-3.768665	-1.945043	-1.363076
41	6	0	-5.096700	-1.917392	-0.917207
42	6	0	-5.469316	-2.514529	0.282965
43	6	0	-4.516080	-3.158035	1.067549
44	6	0	-3.171808	-3.211025	0.679012
45	6	0	-3.420010	-1.372411	-2.735417
46	6	0	-4.009773	0.028813	-2.962810
47	6	0	-3.870761	-2.326031	-3.863335
48	6	0	-2.172296	-4.008103	1.514991
49	6	0	-2.331919	-5.520473	1.249075
50	6	0	-2.264066	-3.711971	3.022578
51	6	0	2.816967	-2.587895	-0.539431
52	6	0	3.171298	-3.211314	0.678953

53	6	0	4.515620	-3.158540	1.067367
54	6	0	5.468878	-2.515171	0.282702
55	6	0	5.096243	-1.917998	-0.917446
56	6	0	3.768186	-1.945548	-1.363245
57	6	0	2.171726	-4.008098	1.515142
58	6	0	2.263796	-3.711809	3.022686
59	6	0	2.330947	-5.520521	1.249335
60	6	0	3.419524	-1.372987	-2.735622
61	6	0	4.009434	0.028150	-2.963139
62	6	0	3.870173	-2.326788	-3.863442
63	1	0	2.330981	1.275433	2.796316
64	1	0	3.595310	1.915750	4.841296
65	1	0	4.958464	2.460502	3.848566
66	1	0	3.416087	3.319281	3.776784
67	1	0	3.634763	-0.440526	3.907021
68	1	0	5.103061	-0.005923	3.031557
69	1	0	3.737781	-0.713958	2.156769
70	1	0	1.163581	3.727744	-1.193798
71	1	0	2.149430	2.643111	-3.229710
72	1	0	1.470517	4.247592	-3.555477
73	1	0	3.218033	4.041869	-3.448388
74	1	0	2.194489	5.765243	-0.190218
75	1	0	1.595533	6.091215	-1.826346
76	1	0	3.330354	5.865549	-1.542004
77	1	0	-2.330259	1.275767	2.796328
78	1	0	-3.633632	-0.440208	3.906989
79	1	0	-3.737907	-0.713300	2.156758
80	1	0	-5.102435	-0.005125	3.032617
81	1	0	-3.594323	1.916275	4.841475
82	1	0	-3.414784	3.319751	3.776939

83	1	0	-4.957388	2.461383	3.848814
84	1	0	-1.163167	3.728476	-1.193670
85	1	0	-3.330026	5.866248	-1.541667
86	1	0	-2.193928	5.765962	-0.190101
87	1	0	-1.595267	6.091931	-1.826337
88	1	0	-3.217846	4.042225	-3.448092
89	1	0	-2.149039	2.643620	-3.229344
90	1	0	-1.470366	4.248157	-3.555428
91	1	0	-2.331056	-1.275272	-2.796225
92	1	0	-3.737895	0.713936	-2.156396
93	1	0	-3.635116	0.440709	-3.906690
94	1	0	-5.103250	0.005892	-3.031045
95	1	0	-3.416081	-3.319023	-3.777127
96	1	0	-3.595345	-1.915220	-4.841308
97	1	0	-4.958470	-2.460275	-3.848717
98	1	0	-1.163484	-3.727821	1.193735
99	1	0	-1.595201	-6.091438	1.825950
100	1	0	-3.330048	-5.865890	1.541708
101	1	0	-2.194249	-5.765286	0.189896
102	1	0	-1.470505	-4.248040	3.555393
103	1	0	-3.217992	-4.042147	3.448259
104	1	0	-2.149260	-2.643472	3.229702
105	1	0	1.162929	-3.727622	1.194003
106	1	0	1.470225	-4.247648	3.555717
107	1	0	3.217732	-4.042117	3.448237
108	1	0	2.149251	-2.643256	3.229678
109	1	0	1.594199	-6.091257	1.826397
110	1	0	3.329043	-5.866182	1.541793
111	1	0	2.193008	-5.765373	0.190199
112	1	0	2.330578	-1.275758	-2.796409

113	1	0	3.737816	0.713270	-2.156641
114	1	0	5.102888	0.005079	-3.031639
115	1	0	3.634631	0.440098	-3.906941
116	1	0	3.415150	-3.319624	-3.777243
117	1	0	3.594969	-1.915974	-4.841477
118	1	0	4.957825	-2.461339	-3.848673
119	1	0	-5.852073	1.437096	1.530335
120	1	0	-6.507327	2.491832	-0.601067
121	1	0	-4.822811	3.638851	-1.990921
122	1	0	-2.113862	4.310674	2.123804
123	1	0	0.000608	5.045417	2.990388
124	1	0	2.114850	4.310193	2.123695
125	1	0	5.852680	1.436553	1.529997
126	1	0	6.507774	2.491080	-0.601559
127	1	0	4.823121	3.637944	-1.991408
128	1	0	-4.823025	-3.638269	1.991376
129	1	0	-6.507753	-2.491512	0.601541
130	1	0	-5.852750	-1.436959	-1.530025
131	1	0	-2.114731	-4.309890	-2.124340
132	1	0	-0.000447	-5.044624	-2.991325
133	1	0	2.113961	-4.310200	-2.124327
134	1	0	4.822580	-3.638827	1.991164
135	1	0	6.507340	-2.492278	0.601204
136	1	0	5.852287	-1.437586	-1.530280

2$^{\bullet+}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	0.000205	-1.457900	-0.541317
2	7	0	-1.449505	-2.766914	-1.059979
3	7	0	1.450359	-2.766449	-1.060016
4	33	0	0.000060	-0.668050	1.779848
5	6	0	-1.226639	-3.791478	-1.882185
6	6	0	0.000658	-4.242057	-2.357741
7	6	0	1.227831	-3.791083	-1.882216
8	6	0	-2.813560	-2.618838	-0.580916
9	6	0	-3.169039	-3.240317	0.637958
10	6	0	-4.508611	-3.163740	1.038618
11	6	0	-5.455959	-2.498561	0.264946
12	6	0	-5.082111	-1.901759	-0.935253
13	6	0	-3.758531	-1.951538	-1.392013
14	6	0	-2.175898	-4.057185	1.462328
15	6	0	-2.230468	-3.744695	2.968364
16	6	0	-2.380448	-5.566795	1.212601
17	6	0	-3.406294	-1.374269	-2.761631
18	6	0	-3.985039	0.032402	-2.984791
19	6	0	-3.862523	-2.320302	-3.893609
20	6	0	2.814357	-2.617874	-0.580998
21	6	0	3.170139	-3.239294	0.637830
22	6	0	4.509703	-3.162242	1.038424
23	6	0	5.456730	-2.496561	0.264789

24	6	0	5.082590	-1.899795	-0.935339
25	6	0	3.759032	-1.950152	-1.392094
26	6	0	2.177332	-4.056608	1.462163
27	6	0	2.382501	-5.566134	1.212451
28	6	0	2.231671	-3.744159	2.968220
29	6	0	3.406529	-1.373106	-2.761732
30	6	0	3.862789	-2.319262	-3.893610
31	6	0	3.985016	0.033604	-2.985296
32	32	0	-0.000243	1.457909	0.541289
33	7	0	1.449525	2.766864	1.060023
34	7	0	-1.450321	2.766574	1.059864
35	33	0	-0.000195	0.668062	-1.779871
36	6	0	1.226692	3.791307	1.882390
37	6	0	-0.000613	4.241886	2.357934
38	6	0	-1.227780	3.791053	1.882261
39	6	0	2.813592	2.618703	0.581051
40	6	0	3.169246	3.240204	-0.637764
41	6	0	4.508836	3.163435	-1.038333
42	6	0	5.456020	2.498012	-0.264660
43	6	0	5.081999	1.901207	0.935479
44	6	0	3.758403	1.951216	1.392169
45	6	0	2.176300	4.057357	-1.462109
46	6	0	2.230393	3.744551	-2.968096
47	6	0	2.381548	5.566919	-1.212697
48	6	0	3.406002	1.374031	2.761767
49	6	0	3.984335	-0.032797	2.984949
50	6	0	3.862514	2.319931	3.893757
51	6	0	-2.814326	2.618076	0.580833
52	6	0	-3.170031	3.239460	-0.638031
53	6	0	-4.509606	3.162581	-1.038616

54	6	0	-5.456751	2.497177	-0.264896
55	6	0	-5.082701	1.900482	0.935293
56	6	0	-3.759112	1.950584	1.391995
57	6	0	-2.177149	4.056630	-1.462420
58	6	0	-2.382131	5.566187	-1.212750
59	6	0	-2.231613	3.744075	-2.968446
60	6	0	-3.406743	1.373494	2.761661
61	6	0	-3.863450	2.319420	3.893526
62	6	0	-3.984913	-0.033410	2.984901
63	1	0	-1.166460	-3.806434	1.119352
64	1	0	-1.454007	-4.311828	3.494362
65	1	0	-2.062151	-2.680484	3.162094
66	1	0	-3.191854	-4.025186	3.412034
67	1	0	-1.646324	-6.152499	1.777891
68	1	0	-2.272170	-5.822243	0.152505
69	1	0	-3.380569	-5.884503	1.528915
70	1	0	-2.316395	-1.283846	-2.820475
71	1	0	-3.607795	0.443231	-3.928174
72	1	0	-3.706622	0.714175	-2.177563
73	1	0	-5.078661	0.018957	-3.052590
74	1	0	-3.584182	-1.907860	-4.870111
75	1	0	-3.414311	-3.316426	-3.810483
76	1	0	-4.951126	-2.447371	-3.879580
77	1	0	1.167797	-3.806291	1.119162
78	1	0	3.382787	-5.883394	1.528703
79	1	0	1.648672	-6.152119	1.777834
80	1	0	2.274242	-5.821696	0.152381
81	1	0	2.062894	-2.680031	3.162018
82	1	0	3.193146	-4.024278	3.411946
83	1	0	1.455425	-4.311677	3.494118

84	1	0	2.316607	-1.282865	-2.820448
85	1	0	3.584331	-1.907012	-4.870161
86	1	0	4.951409	-2.446183	-3.879627
87	1	0	3.414729	-3.315442	-3.810320
88	1	0	3.607570	0.444113	-3.928738
89	1	0	5.078633	0.020311	-3.053256
90	1	0	3.706599	0.715554	-2.178227
91	1	0	1.166818	3.807128	-1.118883
92	1	0	3.191792	4.024554	-3.412045
93	1	0	1.454048	4.311914	-3.494018
94	1	0	2.061586	2.680374	-3.161590
95	1	0	3.381704	5.884160	-1.529367
96	1	0	1.647490	6.152826	-1.777864
97	1	0	2.273694	5.822592	-0.152611
98	1	0	2.316080	1.283933	2.820649
99	1	0	3.705663	-0.714524	2.177782
100	1	0	5.077972	-0.019676	3.052659
101	1	0	3.607028	-0.443454	3.928379
102	1	0	4.951184	2.446452	3.879898
103	1	0	3.583804	1.907687	4.870238
104	1	0	3.414811	3.316270	3.810462
105	1	0	-1.167631	3.806219	-1.119419
106	1	0	-1.648263	6.152079	-1.778178
107	1	0	-2.273770	5.821739	-0.152689
108	1	0	-3.382393	5.883570	-1.528943
109	1	0	-1.455149	4.311229	-3.494417
110	1	0	-2.063253	2.679864	-3.162149
111	1	0	-3.192986	4.024526	-3.412176
112	1	0	-2.316815	1.283527	2.820619
113	1	0	-4.952067	2.446308	3.879222

114	1	0	-3.415394	3.315626	3.810501
115	1	0	-3.585261	1.907029	4.870097
116	1	0	-3.706158	-0.715139	2.177769
117	1	0	-3.607513	-0.443981	3.928332
118	1	0	-5.078540	-0.020430	3.052667
119	1	0	2.116148	-4.350662	-2.172568
120	1	0	0.000773	-5.085712	-3.036100
121	1	0	-2.114786	-4.351332	-2.172540
122	1	0	2.114859	4.351048	2.172901
123	1	0	-0.000735	5.085435	3.036424
124	1	0	-2.116083	4.350647	2.172635
125	1	0	5.833689	1.401818	1.538370
126	1	0	6.491159	2.456675	-0.592037
127	1	0	4.817313	3.642583	-1.962353
128	1	0	4.818264	-3.641278	1.962471
129	1	0	6.491850	-2.454957	0.592193
130	1	0	-4.816943	-3.642841	1.962711
131	1	0	-6.491085	-2.457387	0.592382
132	1	0	-5.833934	-1.402555	-1.538130
133	1	0	-5.834386	1.401137	1.538223
134	1	0	-6.491889	2.455779	-0.592269
135	1	0	-4.818101	3.641623	-1.962685
136	1	0	5.834177	-1.400164	-1.538156

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Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	32	0	-0.000040	1.346673	-0.480469
2	32	0	0.000104	-1.346650	0.480381
3	15	0	-0.000294	-0.622742	-1.743278
4	15	0	0.000397	0.622760	1.743194
5	7	0	-1.454306	2.728233	-1.014701
6	7	0	1.453916	2.728462	-1.014634
7	7	0	1.454269	-2.728230	1.014652
8	7	0	-1.453972	-2.728369	1.014609
9	6	0	1.228881	3.713764	-1.877037
10	6	0	-0.000286	4.142100	-2.372736
11	6	0	-1.229418	3.713597	-1.877041
12	6	0	-2.821000	2.616583	-0.547687
13	6	0	-3.786194	1.980112	-1.360774
14	6	0	-5.115136	1.977771	-0.915310
15	6	0	-5.479756	2.586588	0.280941
16	6	0	-4.513966	3.215690	1.061850
17	6	0	-3.170392	3.244183	0.669979
18	6	0	-3.446620	1.373247	-2.720513
19	6	0	-3.901585	2.298523	-3.869812
20	6	0	-4.040285	-0.032033	-2.907797
21	6	0	-2.152581	4.018922	1.503337
22	6	0	-2.240774	3.715037	3.008687
23	6	0	-2.281919	5.534243	1.240574
24	6	0	2.820678	2.616977	-0.547764
25	6	0	3.785867	1.980531	-1.360884
26	6	0	5.114838	1.978309	-0.915516

27	6	0	5.479519	2.587289	0.280637
28	6	0	4.513750	3.216383	1.061562
29	6	0	3.170132	3.244711	0.669807
30	6	0	3.446267	1.373487	-2.720533
31	6	0	4.040010	-0.031782	-2.907654
32	6	0	3.901130	2.298652	-3.869961
33	6	0	2.152337	4.019456	1.503171
34	6	0	2.281922	5.534812	1.240665
35	6	0	2.240353	3.715303	3.008475
36	6	0	1.229332	-3.713624	1.876958
37	6	0	0.000197	-4.142114	2.372631
38	6	0	-1.228972	-3.713678	1.877009
39	6	0	2.820992	-2.616665	0.547677
40	6	0	3.786169	-1.980202	1.360777
41	6	0	5.115131	-1.977928	0.915380
42	6	0	5.479804	-2.586894	-0.280786
43	6	0	4.514040	-3.216044	-1.061679
44	6	0	3.170432	-3.244408	-0.669907
45	6	0	3.446555	-1.373276	2.720483
46	6	0	4.040279	0.031984	2.907703
47	6	0	3.901412	-2.298514	3.869840
48	6	0	2.152675	-4.019234	-1.503258
49	6	0	2.282125	-5.534542	-1.240446
50	6	0	2.240871	-3.715355	-3.008615
51	6	0	-2.820736	-2.616797	0.547751
52	6	0	-3.170200	-3.244388	-0.669915
53	6	0	-4.513825	-3.216055	-1.061619
54	6	0	-5.479592	-2.587050	-0.280602
55	6	0	-5.114894	-1.978187	0.915599
56	6	0	-3.785910	-1.980446	1.360950

57	6	0	-2.152389	-4.019009	-1.503398
58	6	0	-2.240868	-3.715201	-3.008748
59	6	0	-2.281431	-5.534334	-1.240512
60	6	0	-3.446288	-1.373570	2.720691
61	6	0	-4.039882	0.031733	2.907914
62	6	0	-3.901280	-2.298781	3.870003
63	1	0	-2.360358	1.264385	-2.779468
64	1	0	-3.629216	1.863291	-4.838800
65	1	0	-4.989899	2.435321	-3.856622
66	1	0	-3.444017	3.292301	-3.809056
67	1	0	-3.683952	-0.460044	-3.851998
68	1	0	-5.136200	-0.014351	-2.948625
69	1	0	-3.738782	-0.700179	-2.098581
70	1	0	-1.154813	3.714631	1.175024
71	1	0	-2.119617	2.644588	3.198394
72	1	0	-1.443345	4.246318	3.541941
73	1	0	-3.193939	4.042707	3.440525
74	1	0	-2.145476	5.774286	0.179964
75	1	0	-1.528042	6.089639	1.811848
76	1	0	-3.270785	5.902070	1.540372
77	1	0	2.360017	1.264522	-2.779420
78	1	0	3.683914	-0.459817	-3.851933
79	1	0	3.738298	-0.699919	-2.098498
80	1	0	5.135935	-0.014100	-2.948208
81	1	0	3.628720	1.863302	-4.838885
82	1	0	3.443541	3.292425	-3.809299
83	1	0	4.989442	2.435471	-3.856834
84	1	0	1.154554	3.715365	1.174719
85	1	0	3.270735	5.902482	1.540833
86	1	0	2.145851	5.775028	0.180048

87	1	0	1.527935	6.090234	1.811769
88	1	0	3.193498	4.042832	3.440470
89	1	0	2.119109	2.644822	3.197966
90	1	0	1.442906	4.246530	3.541752
91	1	0	2.360295	-1.264343	2.779356
92	1	0	3.738706	0.700136	2.098514
93	1	0	3.684049	0.460007	3.851934
94	1	0	5.136197	0.014280	2.948430
95	1	0	3.443814	-3.292278	3.809103
96	1	0	3.629001	-1.863222	4.838789
97	1	0	4.989723	-2.435341	3.856717
98	1	0	1.154876	-3.715030	-1.174959
99	1	0	1.528240	-6.090016	-1.811635
100	1	0	3.270991	-5.902330	-1.540296
101	1	0	2.145783	-5.774550	-0.179814
102	1	0	1.443557	-4.246775	-3.541904
103	1	0	3.194112	-4.042867	-3.440407
104	1	0	2.119534	-2.644922	-3.198326
105	1	0	-1.154620	-3.714522	-1.175274
106	1	0	-1.443454	-4.246382	-3.542123
107	1	0	-3.194054	-4.043004	-3.440444
108	1	0	-2.119884	-2.644731	-3.198493
109	1	0	-1.527464	-6.089642	-1.811752
110	1	0	-3.270238	-5.902356	-1.540274
111	1	0	-2.144935	-5.774269	-0.179885
112	1	0	-2.360020	-1.264741	2.779639
113	1	0	-3.738204	0.699863	2.098743
114	1	0	-5.135799	0.014142	2.948595
115	1	0	-3.683639	0.459700	3.852163
116	1	0	-3.443790	-3.292594	3.809228

117	1	0	-3.628828	-1.863547	4.838963
118	1	0	-4.989607	-2.435498	3.856873
119	1	0	5.876367	1.499739	-1.523910
120	1	0	6.517924	2.578498	0.602014
121	1	0	4.808889	3.700803	1.987628
122	1	0	2.111663	4.270847	-2.193143
123	1	0	-0.000337	4.958355	-3.084474
124	1	0	-2.112269	4.270594	-2.193117
125	1	0	-5.876677	1.499186	-1.523683
126	1	0	-6.518135	2.577695	0.602397
127	1	0	-4.809065	3.699974	1.987999
128	1	0	4.809173	-3.700457	-1.987752
129	1	0	6.518206	-2.578091	-0.602171
130	1	0	5.876657	-1.499335	1.523760
131	1	0	2.112165	-4.270651	2.193024
132	1	0	0.000239	-4.958421	3.084310
133	1	0	-2.111776	-4.270691	2.193174
134	1	0	-4.808983	-3.700363	-1.987737
135	1	0	-6.518005	-2.578253	-0.601948
136	1	0	-5.876415	-1.499664	1.524042

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2

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

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1	32	0	-0.000044	1.381602	-0.508030
2	7	0	1.455297	2.765176	-1.058048
3	7	0	-1.455675	2.764983	-1.058135
4	33	0	0.000061	0.671110	1.827206
5	6	0	1.230169	3.742658	-1.928543
6	6	0	-0.000266	4.166686	-2.426632
7	6	0	-1.230674	3.742527	-1.928552
8	6	0	2.819274	2.646633	-0.588431
9	6	0	3.169345	3.275159	0.628578
10	6	0	4.509566	3.229586	1.029865
11	6	0	5.471414	2.583128	0.258121
12	6	0	5.106043	1.972542	-0.937109
13	6	0	3.779976	1.989862	-1.390647
14	6	0	2.155391	4.067608	1.450055
15	6	0	2.225745	3.769688	2.957474
16	6	0	2.306887	5.579605	1.180768
17	6	0	3.437879	1.374936	-2.746226
18	6	0	4.018815	-0.037205	-2.923017
19	6	0	3.901351	2.288059	-3.901680
20	6	0	-2.819592	2.646259	-0.588419
21	6	0	-3.169704	3.274900	0.628526
22	6	0	-4.509906	3.229242	1.029844
23	6	0	-5.471719	2.582644	0.258165
24	6	0	-5.106323	1.972010	-0.937033
25	6	0	-3.780263	1.989367	-1.390570
26	6	0	-2.155855	4.067636	1.449849
27	6	0	-2.307725	5.579581	1.180413
28	6	0	-2.226005	3.769881	2.957318

29	6	0	-3.438113	1.374411	-2.746114
30	6	0	-3.901511	2.287486	-3.901612
31	6	0	-4.019132	-0.037721	-2.922859
32	32	0	0.000098	-1.381703	0.507890
33	7	0	-1.455336	-2.765190	1.058003
34	7	0	1.455698	-2.765087	1.058012
35	33	0	-0.000017	-0.671196	-1.827377
36	6	0	-1.230216	-3.742935	1.928204
37	6	0	0.000228	-4.167213	2.426059
38	6	0	1.230637	-3.742937	1.928081
39	6	0	-2.819348	-2.646520	0.588499
40	6	0	-3.169607	-3.275124	-0.628437
41	6	0	-4.509894	-3.229580	-1.029502
42	6	0	-5.471621	-2.583094	-0.257635
43	6	0	-5.106078	-1.972477	0.937522
44	6	0	-3.779948	-1.989742	1.390841
45	6	0	-2.155818	-4.067697	-1.449996
46	6	0	-2.225967	-3.769491	-2.957382
47	6	0	-2.307740	-5.579706	-1.181016
48	6	0	-3.437641	-1.374777	2.746330
49	6	0	-4.018924	0.037205	2.923255
50	6	0	-3.900584	-2.288041	3.901897
51	6	0	2.819670	-2.646254	0.588444
52	6	0	3.169982	-3.274710	-0.628526
53	6	0	4.510246	-3.228883	-1.029656
54	6	0	5.471883	-2.582208	-0.257824
55	6	0	5.106268	-1.971707	0.937381
56	6	0	3.780171	-1.989352	1.390785
57	6	0	2.156292	-4.067357	-1.450145
58	6	0	2.308369	-5.579368	-1.181227

59	6	0	2.226477	-3.769087	-2.957509
60	6	0	3.437798	-1.374628	2.746390
61	6	0	3.901013	-2.287932	3.901778
62	6	0	4.018877	0.037412	2.923564
63	1	0	1.156552	3.774464	1.114233
64	1	0	1.438027	4.323249	3.482638
65	1	0	2.076054	2.703138	3.150032
66	1	0	3.183554	4.074772	3.395104
67	1	0	1.555694	6.148016	1.742692
68	1	0	2.182569	5.815470	0.117747
69	1	0	3.298034	5.936050	1.486740
70	1	0	2.350595	1.273465	-2.804655
71	1	0	3.663794	-0.465675	-3.867587
72	1	0	3.704274	-0.699001	-2.113371
73	1	0	5.115036	-0.031184	-2.957261
74	1	0	3.626087	1.848754	-4.868048
75	1	0	3.452289	3.286068	-3.847677
76	1	0	4.990801	2.415643	-3.888525
77	1	0	-1.156970	3.774686	1.113977
78	1	0	-3.298935	5.935815	1.486414
79	1	0	-1.556619	6.148224	1.742221
80	1	0	-2.183540	5.815366	0.117356
81	1	0	-2.076082	2.703390	3.150000
82	1	0	-3.183842	4.074846	3.394986
83	1	0	-1.438333	4.323628	3.482358
84	1	0	-2.350824	1.272914	-2.804506
85	1	0	-3.626251	1.848122	-4.867950
86	1	0	-4.990959	2.415100	-3.888471
87	1	0	-3.452406	3.285482	-3.847636
88	1	0	-3.663980	-0.466332	-3.867320

89	1	0	-5.115350	-0.031586	-2.957297
90	1	0	-3.704831	-0.699477	-2.113079
91	1	0	-1.156918	-3.774905	-1.114068
92	1	0	-3.183749	-4.074421	-3.395188
93	1	0	-1.438226	-4.323014	-3.482552
94	1	0	-2.076174	-2.702911	-3.149731
95	1	0	-3.298958	-5.935805	-1.487167
96	1	0	-1.556646	-6.148187	-1.743000
97	1	0	-2.183590	-5.815844	-0.118036
98	1	0	-2.350372	-1.273021	2.804456
99	1	0	-3.704751	0.699038	2.113499
100	1	0	-5.115140	0.030924	2.957786
101	1	0	-3.663787	0.465837	3.867719
102	1	0	-4.989992	-2.415956	3.888944
103	1	0	-3.625280	-1.848598	4.868190
104	1	0	-3.451223	-3.285914	3.847861
105	1	0	1.157343	-3.774677	-1.114237
106	1	0	1.557404	-6.147930	-1.743305
107	1	0	2.184131	-5.815567	-0.118269
108	1	0	3.299659	-5.935355	-1.487268
109	1	0	1.438918	-4.322784	-3.482773
110	1	0	2.076424	-2.702551	-3.149829
111	1	0	3.184381	-4.073764	-3.395223
112	1	0	2.350496	-1.273119	2.804639
113	1	0	4.990473	-2.415497	3.888839
114	1	0	3.451949	-3.285923	3.847501
115	1	0	3.625544	-1.848753	4.868144
116	1	0	3.704816	0.699393	2.113861
117	1	0	3.663507	0.465800	3.868034
118	1	0	5.115078	0.031174	2.958295

119	1	0	-2.113218	4.296648	-2.251155
120	1	0	-0.000315	4.977054	-3.145132
121	1	0	2.112649	4.296830	-2.251202
122	1	0	-2.112722	-4.297108	2.250796
123	1	0	0.000270	-4.977803	3.144308
124	1	0	2.113157	-4.297181	2.250519
125	1	0	-5.864666	-1.479108	1.537691
126	1	0	-6.507743	-2.561323	-0.585708
127	1	0	-4.806117	-3.714374	-1.955069
128	1	0	-4.805986	3.714048	1.955453
129	1	0	-6.507784	2.560808	0.586410
130	1	0	4.805643	3.714334	1.955502
131	1	0	6.507479	2.561323	0.586367
132	1	0	5.864715	1.479204	-1.537185
133	1	0	5.864752	-1.478155	1.537517
134	1	0	6.507980	-2.560175	-0.585957
135	1	0	4.806500	-3.713597	-1.955258
136	1	0	-5.864965	1.478598	-1.537091

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