Electronic Supplementary Information (ESI)

Table ESI-1. Vertical Ionization Energy (*VIE*) and Vertical Electron Affinities (*VEA*), for [metal-pterins] complexes in gas phase.

WT/B3LYP/LAN2DZ/6-311G(d,p)	*VIE*(KJ)	*VEA*(KJ)
Ptr-Cu	509.77	-15.65
Ptr-Ag	535.08	67.42
Ptr-Au	653.71	85.33
Ptr-Zn	750.80	5.50
Ptr-Cd	699.36	43.58
Ptr-Hg	745.03	24.41
7-Xap-Cu	496.09	20.89
7-Xap-Ag	547.02	52.15
7-Xap-Au	653.03	76.95
7-Xap-Zn	736.52	0.62
7-Xap-Cd	698.46	27.32
7-Xap-Hg	740.05	19.16
Sep-Cu	508.80	7.01
Sep-Ag	491.74	21.53
Sep-Au	590.08	91.25
Sep-Zn	672.79	23.22
Sep-Cd	621.41	61.53
Sep-Hg	665.42	43.57

Table ESI-2. Vertical Ionization Energy (*VIE*) and Vertical Electron Affinities (*VEA*), for [metal-pterins]$^{+1}$ complexes in water. Pterin, isoxanthropterin and sepiapterin are neutrals.

WT/B3LYP/LAN2DZ/6-311G(d,p)	*VIE*(KJ)	*VEA*(KJ)
Ptr-Cu	545.77	279.99
Ptr-Ag	644.10	276.73
Ptr-Au	654.37	340.36
Ptr-Zn	273.43	223.19
Ptr-Cd	236.29	214.93
Ptr-Hg	275.41	227.01
7-Xap-Cu	537.60	253.28
7-Xap-Ag	625.86	224.76
7-Xap-Au	638.91	340.77
7-Xap-Zn	272.34	221.95
7-Xap-Cd	235.34	195.25
7-Xap-Hg	274.08	225.74
Sep-Cu	473.92	280.53
Sep-Ag	566.36	283.70

Sep-Au	582.91	304.10
Sep-Zn	270.18	246.60
Sep-Cd	306.89	172.05
Sep-Hg	278.51	231.48
OH	1183.07	401.22
Pterin	636.78	220.24
isoxanthropterin	609.64	195.90
sepiapterin	552.28	222.83
Cu	779.53	370.57
Ag	936.80	343.58
Au	893.97	513.19
Zn	446.36	380.82
Cd	359.73	321.82
Hg	389.79	344.24

Table ESI-3. Vertical Ionization Energy (*VIE*) and Vertical Electron Affinities (*VEA*), for [metal-pterins]$^{+2}$ complexes in water

WT/B3LYP/LAN2DZ/6-311G(d,p)	*VIE*(KJ)	*VEA*(KJ)
Ptr-Cu	818.66	497.08
Ptr-Ag	785.22	613.71
Ptr-Au	779.00	627.18
Ptr-Zn	685.05	226.88
Ptr-Cd	666.00	205.71
Ptr-Hg	653.56	243.84
7-Xap-Cu	803.79	486.62
7-Xap-Ag	768.07	589.88
7-Xap-Au	778.06	607.63
7-Xap-Zn	669.24	226.15
7-Xap-Cd	650.93	206.47
7-Xap-Hg	641.77	238.31
Sep-Cu	764.53	415.58
Sep-Ag	699.87	520.30
Sep-Au	709.78	536.63
Sep-Zn	617.38	348.43
Sep-Cd	595.51	330.07
Sep-Hg	589.40	318.05

OPTIMIZED GEOMETRIES

[Ptr-Cu]

Input orientation:

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.033448	-0.055398	0.028420
2	6	0	0.032615	-0.023388	2.328882
3	6	0	1.462114	0.006859	2.343973
4	6	0	2.196114	-0.005010	1.126226
5	8	0	3.458036	-0.004788	0.989392
6	6	0	0.025662	0.000592	4.610935
7	6	0	1.398505	0.031309	4.673075
8	1	0	-0.555551	-0.001300	5.526865
9	7	0	2.160459	0.035579	3.552052
10	7	0	-0.687210	-0.027295	3.443550
11	7	0	-0.651382	-0.037192	1.126978
12	7	0	1.404764	-0.032686	-0.028029
13	7	0	-0.618048	-0.149054	-1.184314
14	1	0	-1.614276	-0.013433	-1.087334
15	1	0	-0.211044	0.346763	-1.964172
16	1	0	1.901534	-0.151966	-0.899406
17	1	0	1.922375	0.054218	5.621269
18	29	0	3.957226	0.023142	3.020190

$[Ptr\text{-}Cu]^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.012535	-0.000313	0.028902
2	6	0	0.028781	-0.000006	2.309961
3	6	0	1.440191	-0.000099	2.348313
4	6	0	2.200104	-0.000292	1.099627
5	8	0	3.430142	-0.000467	1.026803
6	6	0	0.017399	0.000042	4.590891
7	6	0	1.431384	0.000101	4.639656
8	1	0	-0.545755	0.000231	5.519521
9	7	0	2.131353	0.000012	3.512486
10	7	0	-0.673940	0.000026	3.472276
11	7	0	-0.663279	-0.000158	1.149657
12	7	0	1.402248	-0.000334	-0.022763
13	7	0	-0.640126	-0.000380	-1.142127
14	1	0	-1.648422	-0.000325	-1.109685
15	1	0	-0.182286	-0.000386	-2.038181
16	1	0	1.893798	-0.000444	-0.909913
17	1	0	1.968412	0.000220	5.578747
18	29	0	4.012803	-0.000478	3.174382

$[Ptr\text{-}Cu]^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029571	-0.010753	0.015936
2	6	0	-0.001455	0.040231	2.314379
3	6	0	1.413338	0.071816	2.347943
4	6	0	2.164690	0.005902	1.123507

5	8	0	3.423335	0.000122	1.124481
6	6	0	-0.002545	-0.042699	4.596778
7	6	0	1.438337	0.008847	4.639955
8	1	0	-0.549547	-0.077439	5.535891
9	7	0	2.114559	0.036492	3.507989
10	7	0	-0.690015	-0.009064	3.489585
11	7	0	-0.653927	-0.013868	1.152877
12	7	0	1.430798	-0.043979	-0.014658
13	7	0	-0.622336	0.012823	-1.133759
14	1	0	-1.636547	0.035894	-1.101996
15	1	0	-0.176843	0.029334	-2.042130
16	1	0	1.939438	-0.085920	-0.896658
17	1	0	1.967949	0.061762	5.584192
18	29	0	4.026542	-0.022549	2.984241

Ptr-Ag

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.043338	-0.866132	-0.112942
2	6	0	1.835605	1.071464	-0.039596
3	6	0	0.630913	0.374687	0.239160
4	6	0	0.647869	-1.080515	0.353516
5	8	0	-0.310307	-1.810284	0.560344
6	6	0	0.663935	3.019405	0.018690
7	6	0	-0.531073	2.333743	0.253091
8	1	0	0.663825	4.104297	-0.039422
9	7	0	-0.554189	1.005754	0.371306
10	7	0	1.839424	2.413807	-0.138603
11	7	0	3.033157	0.427673	-0.220987
12	7	0	1.925731	-1.622980	0.158144
13	7	0	4.224563	-1.546404	-0.224772
14	1	0	4.988591	-0.979581	-0.560972
15	1	0	4.213807	-2.501576	-0.546662
16	1	0	1.988813	-2.625799	0.278073
17	1	0	-1.474225	2.859701	0.350367
18	47	0	-2.530270	-0.430545	-0.167048

$[Ptr\text{-}Ag]^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.003083	-0.000216	0.028775
2	6	0	0.010766	0.000706	2.308302
3	6	0	1.426509	0.000343	2.358610
4	6	0	2.182354	0.000240	1.108657
5	8	0	3.412292	-0.000632	1.006818
6	6	0	-0.022340	0.000165	4.588410
7	6	0	1.392758	-0.000080	4.643856
8	1	0	-0.593626	-0.000139	5.512212
9	7	0	2.100634	-0.000069	3.526571

10	7	0	-0.701672	0.000398	3.463902
11	7	0	-0.680408	0.000270	1.146905
12	7	0	1.385648	-0.000226	-0.014747
13	7	0	-0.650857	-0.000642	-1.145584
14	1	0	-1.659200	-0.000676	-1.117040
15	1	0	-0.189410	-0.000870	-2.039668
16	1	0	1.881846	-0.000687	-0.899393
17	1	0	1.917862	-0.000587	5.590582
18	47	0	4.405269	-0.000348	3.161386

[Ptr-Ag]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.044185	-0.000314	-0.009284
2	6	0	0.004225	-0.000043	2.308962
3	6	0	1.433403	-0.000192	2.358758
4	6	0	2.204131	-0.000325	1.091186
5	8	0	3.415813	-0.000354	1.027876
6	6	0	-0.065957	0.000154	4.578167
7	6	0	1.368201	-0.000007	4.627151
8	1	0	-0.633495	0.000383	5.504708
9	7	0	2.104174	-0.000179	3.514828
10	7	0	-0.733569	0.000145	3.453608
11	7	0	-0.660001	-0.000106	1.151733
12	7	0	1.411145	-0.000418	-0.053664
13	7	0	-0.672135	-0.000370	-1.113589
14	1	0	-1.685867	-0.000247	-1.019058
15	1	0	-0.280419	-0.000508	-2.050465
16	1	0	1.914527	-0.000449	-0.939691
17	1	0	1.884569	0.000001	5.580932
18	47	0	4.562412	-0.000219	3.216398

[Ptr-Au]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.041858	-0.035337	0.008650
2	6	0	0.019179	-0.018275	2.287599
3	6	0	1.439006	-0.014788	2.318446
4	6	0	2.189950	-0.036565	1.046828
5	8	0	3.389499	-0.053309	0.897570
6	6	0	0.013662	-0.003139	4.563507
7	6	0	1.418093	0.006819	4.596739
8	1	0	-0.550790	-0.001574	5.492155
9	7	0	2.118482	-0.000830	3.472039
10	7	0	-0.683169	-0.014241	3.441565
11	7	0	-0.703976	-0.016445	1.127558
12	7	0	1.331656	-0.045570	-0.067008
13	7	0	-0.718264	-0.090085	-1.173080
14	1	0	-1.713802	0.049719	-1.092585

15	1	0	-0.283970	0.241303	-2.019336
16	1	0	1.804794	-0.111349	-0.959654
17	1	0	1.968955	0.021093	5.529589
18	79	0	4.617895	0.119525	3.757973

$[Ptr\text{-}Au]^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.004075	-0.000199	0.016417
2	6	0	0.028788	0.000186	2.297320
3	6	0	1.448490	0.000037	2.332194
4	6	0	2.198732	-0.000051	1.070978
5	8	0	3.417971	-0.000444	0.963604
6	6	0	0.007097	0.000199	4.580119
7	6	0	1.419889	-0.000054	4.636430
8	1	0	-0.557558	0.000141	5.507793
9	7	0	2.112402	-0.000102	3.504153
10	7	0	-0.674328	0.000226	3.458604
11	7	0	-0.669144	0.000020	1.145074
12	7	0	1.380492	-0.000270	-0.042891
13	7	0	-0.670262	-0.000486	-1.145037
14	1	0	-1.678371	-0.000471	-1.100509
15	1	0	-0.223353	-0.000711	-2.046874
16	1	0	1.866447	-0.000500	-0.933242
17	1	0	1.954155	-0.000176	5.575224
18	79	0	4.257970	-0.000394	3.409197

$[Ptr\text{-}Au]^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.043340	-0.000227	-0.026598
2	6	0	0.038445	0.000271	2.298917
3	6	0	1.467509	0.000076	2.327862
4	6	0	2.223951	-0.000197	1.045821
5	8	0	3.426753	-0.000705	0.963780
6	6	0	-0.023445	0.000168	4.570371
7	6	0	1.406212	-0.000200	4.618079
8	1	0	-0.585594	0.000145	5.500293
9	7	0	2.131826	-0.000143	3.494044
10	7	0	-0.692270	0.000408	3.447069
11	7	0	-0.641894	0.000025	1.149777
12	7	0	1.404093	-0.000361	-0.088214
13	7	0	-0.697523	-0.000447	-1.114028
14	1	0	-1.709326	-0.000397	-0.998495
15	1	0	-0.325679	-0.000687	-2.059438
16	1	0	1.897353	-0.000494	-0.980280
17	1	0	1.929347	-0.000403	5.566568
18	79	0	4.322242	0.000119	3.513028

[Ptr-Zn]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.128408	-0.005270	-0.014027
2	6	0	-0.131212	-0.015245	2.265393
3	6	0	1.278072	0.137500	2.339044
4	6	0	2.061657	0.240665	1.090011
5	8	0	3.255180	0.388356	0.974085
6	6	0	-0.193273	-0.030927	4.538254
7	6	0	1.202613	0.116854	4.600192
8	1	0	-0.779053	-0.096255	5.451988
9	7	0	1.936499	0.202116	3.501470
10	7	0	-0.860665	-0.097537	3.398358
11	7	0	-0.818657	-0.098657	1.081819
12	7	0	1.236888	0.156596	-0.051188
13	7	0	-0.771600	-0.020602	-1.221644
14	1	0	-1.744195	-0.281755	-1.159697
15	1	0	-0.279536	-0.356640	-2.034636
16	1	0	1.721589	0.281467	-0.930936
17	1	0	1.719258	0.166259	5.553583
18	30	0	6.910186	-0.689975	3.846484

[Ptr-Zn]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.004337	-0.000270	0.030448
2	6	0	0.003210	-0.000154	2.310600
3	6	0	1.414004	-0.000206	2.356680
4	6	0	2.176113	-0.000368	1.120446
5	8	0	3.411629	-0.000397	1.069854
6	6	0	-0.007112	0.000168	4.591911
7	6	0	1.410876	0.000058	4.637338
8	1	0	-0.570943	0.000323	5.520193
9	7	0	2.105090	-0.000115	3.512776
10	7	0	-0.698216	0.000070	3.473295
11	7	0	-0.680515	-0.000167	1.145627
12	7	0	1.397667	-0.000371	-0.009216
13	7	0	-0.636026	-0.000353	-1.146398
14	1	0	-1.644788	-0.000273	-1.124086
15	1	0	-0.169855	-0.000410	-2.038316
16	1	0	1.897225	-0.000434	-0.892289
17	1	0	1.948010	0.000118	5.577956
18	30	0	4.254633	-0.000268	3.091736

[Ptr-Zn]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.021884	-0.000315	0.022500
2	6	0	0.010946	-0.000050	2.308441
3	6	0	1.428221	-0.000151	2.354775
4	6	0	2.166417	-0.000315	1.123137
5	8	0	3.440860	-0.000408	1.082953
6	6	0	-0.008724	0.000144	4.598643
7	6	0	1.427875	0.000049	4.662711
8	1	0	-0.568371	0.000263	5.530733
9	7	0	2.112863	-0.000096	3.535512
10	7	0	-0.685273	0.000089	3.484001
11	7	0	-0.654322	-0.000140	1.156364
12	7	0	1.427475	-0.000390	-0.005436
13	7	0	-0.617691	-0.000350	-1.136156
14	1	0	-1.631105	-0.000262	-1.112446
15	1	0	-0.165267	-0.000432	-2.039467
16	1	0	1.935333	-0.000508	-0.888257
17	1	0	1.951125	0.000093	5.610509
18	30	0	4.023095	-0.000270	2.940037

[Ptr-Cd]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.055540	0.046040	0.019815
2	6	0	-0.055439	0.031843	2.299112
3	6	0	1.361178	0.071628	2.369063
4	6	0	2.145003	0.115692	1.119921
5	8	0	3.349685	0.167967	1.003288
6	6	0	-0.111871	0.012955	4.572386
7	6	0	1.292572	0.045049	4.631772
8	1	0	-0.698080	-0.006810	5.487779
9	7	0	2.025552	0.076810	3.530351
10	7	0	-0.785498	0.005345	3.434837
11	7	0	-0.748604	0.006867	1.117511
12	7	0	1.319679	0.098612	-0.018659
13	7	0	-0.698185	0.082869	-1.185406
14	1	0	-1.689498	-0.094875	-1.126905
15	1	0	-0.233539	-0.273787	-2.005457
16	1	0	1.812921	0.182485	-0.898710
17	1	0	1.815075	0.045421	5.582974
18	48	0	5.569929	-0.617161	3.294881

$[Ptr\text{-}Cd]^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.009270	-0.000199	0.029478
2	6	0	-0.007826	0.000018	2.309078

3	6	0	1.405789	-0.000082	2.361641
4	6	0	2.162992	-0.000196	1.122690
5	8	0	3.401015	-0.000310	1.042741
6	6	0	-0.035681	0.000236	4.589110
7	6	0	1.382418	-0.000089	4.642018
8	1	0	-0.605089	0.000235	5.514033
9	7	0	2.086770	-0.000151	3.524723
10	7	0	-0.718240	0.000270	3.466386
11	7	0	-0.692550	-0.000032	1.144177
12	7	0	1.383166	-0.000393	-0.006146
13	7	0	-0.647944	-0.000437	-1.148915
14	1	0	-1.656677	-0.000341	-1.128015
15	1	0	-0.180544	-0.000602	-2.040082
16	1	0	1.884967	-0.000569	-0.887986
17	1	0	1.911307	-0.000154	5.587431
18	48	0	4.550736	-0.000255	3.106194

$[Ptr\text{-}Cd]^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.007528	-0.000354	0.019826
2	6	0	0.003580	0.000028	2.304621
3	6	0	1.426528	-0.000101	2.356184
4	6	0	2.161374	-0.000284	1.118942
5	8	0	3.426790	-0.000466	1.041132
6	6	0	-0.032082	0.000094	4.593218
7	6	0	1.401447	0.000078	4.660453
8	1	0	-0.597444	0.000185	5.521911
9	7	0	2.096974	-0.000050	3.539520
10	7	0	-0.699539	0.000064	3.473934
11	7	0	-0.665377	-0.000119	1.153381
12	7	0	1.408209	-0.000415	-0.007256
13	7	0	-0.635814	-0.000353	-1.138906
14	1	0	-1.648635	-0.000238	-1.112500
15	1	0	-0.184901	-0.000399	-2.042446
16	1	0	1.914835	-0.000578	-0.890066
17	1	0	1.915719	0.000153	5.612877
18	48	0	4.316148	-0.000293	3.023730

[Ptr-Hg]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.077634	-0.000245	0.012340
2	6	0	-0.062724	0.000145	2.291769
3	6	0	1.356122	-0.000886	2.354163
4	6	0	2.133674	-0.001407	1.099410
5	8	0	3.337192	-0.002426	0.970898
6	6	0	-0.105753	0.000385	4.566303
7	6	0	1.299055	-0.000746	4.617554
8	1	0	-0.686923	0.000652	5.485293

9	7	0	2.026096	-0.001361	3.511652
10	7	0	-0.786125	0.000739	3.432907
11	7	0	-0.764319	0.000466	1.117027
12	7	0	1.298818	-0.001197	-0.034835
13	7	0	-0.729479	-0.000335	-1.177362
14	1	0	-1.734928	0.001070	-1.148757
15	1	0	-0.257914	0.000448	-2.063572
16	1	0	1.793965	-0.001845	-0.917605
17	1	0	1.826949	-0.001188	5.565889
18	80	0	5.749268	0.004681	3.545479

$[Ptr\text{-}Hg]^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.015371	-0.000271	0.026196
2	6	0	-0.006108	-0.000422	2.305264
3	6	0	1.411976	-0.000370	2.359374
4	6	0	2.167798	-0.000641	1.111142
5	8	0	3.398421	-0.000429	1.006873
6	6	0	-0.041812	0.000173	4.586573
7	6	0	1.374711	0.000114	4.643655
8	1	0	-0.615256	0.000443	5.509123
9	7	0	2.077800	-0.000110	3.526519
10	7	0	-0.717807	-0.000024	3.460565
11	7	0	-0.694735	-0.000277	1.143216
12	7	0	1.373501	-0.000472	-0.013191
13	7	0	-0.660028	-0.000212	-1.149402
14	1	0	-1.668543	-0.000079	-1.123299
15	1	0	-0.196452	-0.000244	-2.042486
16	1	0	1.871730	-0.000439	-0.896779
17	1	0	1.901680	0.000312	5.589872
18	80	0	4.653836	-0.000100	3.185337

$[Ptr\text{-}Hg]^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003283	-0.000111	0.009819
2	6	0	-0.004509	-0.000198	2.297656
3	6	0	1.430802	-0.000233	2.355985
4	6	0	2.166119	-0.000438	1.104711
5	8	0	3.415642	-0.000467	1.014403
6	6	0	-0.038891	0.000172	4.592991
7	6	0	1.398480	0.000051	4.663896
8	1	0	-0.605063	0.000307	5.522590
9	7	0	2.072682	-0.000115	3.536372
10	7	0	-0.691267	0.000078	3.471855
11	7	0	-0.665792	-0.000125	1.148194
12	7	0	1.397468	-0.000346	-0.018149
13	7	0	-0.648381	-0.000285	-1.142284

14	1	0	-1.661398	-0.000324	-1.110551
15	1	0	-0.202811	-0.000450	-2.048984
16	1	0	1.901006	-0.000516	-0.902514
17	1	0	1.911615	0.000145	5.616376
18	80	0	4.436356	-0.000194	3.116188

[7-Xap-Cu]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.005981	-0.047879	0.013613
2	6	0	0.042172	-0.049799	2.284533
3	6	0	1.431971	0.034148	2.356139
4	6	0	2.184773	0.065892	1.132394
5	8	0	3.406202	0.089823	1.010409
6	6	0	-0.056428	0.009852	4.740592
7	6	0	1.373131	0.110426	4.699177
8	7	0	2.103962	0.121932	3.564121
9	7	0	-0.657018	-0.103292	3.451095
10	7	0	-0.675487	-0.067866	1.129012
11	7	0	1.367669	0.000368	-0.020422
12	7	0	-0.655731	-0.127002	-1.184307
13	1	0	-1.653703	-0.002125	-1.103618
14	1	0	-0.235300	0.303409	-1.993536
15	1	0	1.874264	-0.042540	-0.894841
16	1	0	1.891025	0.210738	5.642354
17	8	0	-0.767056	0.024729	5.735995
18	1	0	-1.666344	-0.148286	3.415096
19	29	0	3.850257	-0.560231	3.469133

[7-Xap-Cu]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.010675	0.001042	0.025081
2	6	0	-0.001026	-0.002407	2.294886
3	6	0	1.396617	-0.017205	2.375660
4	6	0	2.164307	-0.023235	1.162119
5	8	0	3.399147	-0.037032	1.090364
6	6	0	-0.096630	-0.005601	4.740753
7	6	0	1.381553	-0.020679	4.695015
8	7	0	2.061046	-0.025997	3.587454
9	7	0	-0.694299	0.002826	3.464060
10	7	0	-0.689229	0.006606	1.144988
11	7	0	1.386155	-0.013111	0.007454
12	7	0	-0.634912	0.009629	-1.146427
13	1	0	-1.643373	0.020040	-1.127431
14	1	0	-0.166834	0.005802	-2.037694
15	1	0	1.902318	-0.017916	-0.864937
16	1	0	1.896470	-0.027224	5.647157
17	8	0	-0.742343	-0.000971	5.757835

18	1	0	-1.709248	0.013514	3.426697
19	29	0	3.943944	-0.045784	3.203909

[7-Xap-Cu]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.758875	-0.323364	-0.013159
2	6	0	0.992753	1.125194	0.056124
3	6	0	0.071319	0.052449	0.093121
4	6	0	0.554289	-1.276473	0.016120
5	8	0	-0.231929	-2.270439	-0.005667
6	6	0	-0.904957	2.655476	-0.027435
7	6	0	-1.786002	1.436997	0.023543
8	7	0	-1.295826	0.237375	0.055325
9	7	0	0.476775	2.377812	0.018868
10	7	0	2.300679	0.927545	0.011096
11	7	0	1.907576	-1.426669	-0.041166
12	7	0	4.062202	-0.533313	-0.015236
13	1	0	4.675970	0.273491	0.009431
14	1	0	4.489038	-1.450192	-0.033561
15	1	0	2.271534	-2.376139	-0.084065
16	1	0	-2.855033	1.613595	0.073252
17	8	0	-1.357644	3.761154	-0.068549
18	1	0	1.110706	3.176056	-0.020057
19	29	0	-2.043191	-1.595292	-0.014928

[7-Xap-Ag]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.025148	0.031502	0.021985
2	6	0	-0.009607	0.021028	2.285008
3	6	0	1.382597	0.097771	2.382731
4	6	0	2.157040	0.149276	1.161681
5	8	0	3.364834	0.209645	1.031768
6	6	0	-0.137305	0.002995	4.731932
7	6	0	1.328707	0.075402	4.685129
8	7	0	2.026046	0.119191	3.591502
9	7	0	-0.715659	-0.027718	3.448511
10	7	0	-0.721838	-0.016006	1.133678
11	7	0	1.335180	0.106143	0.001126
12	7	0	-0.681472	0.042764	-1.166645
13	1	0	-1.670818	-0.143200	-1.121049
14	1	0	-0.205302	-0.200811	-2.019327
15	1	0	1.844488	0.172069	-0.871034
16	1	0	1.842589	0.088563	5.640313
17	8	0	-0.820668	-0.026003	5.735148
18	1	0	-1.726135	-0.082483	3.395331
19	47	0	4.596811	-0.797832	3.379150

[7-Xap-Ag]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.006779	0.002080	0.026389
2	6	0	-0.018023	-0.000030	2.294620
3	6	0	1.383596	-0.019085	2.386249
4	6	0	2.144464	-0.028144	1.172211
5	8	0	3.378366	-0.044625	1.068660
6	6	0	-0.134505	-0.001135	4.738529
7	6	0	1.346160	-0.020910	4.698342
8	7	0	2.032364	-0.029021	3.599953
9	7	0	-0.720109	0.008229	3.458209
10	7	0	-0.706844	0.010437	1.144968
11	7	0	1.366689	-0.016468	0.015905
12	7	0	-0.648334	0.011989	-1.147762
13	1	0	-1.656697	0.025750	-1.132813
14	1	0	-0.176759	0.006753	-2.037143
15	1	0	1.887870	-0.022566	-0.853499
16	1	0	1.849362	-0.028565	5.657716
17	8	0	-0.787445	0.006361	5.751009
18	1	0	-1.734626	0.021902	3.410104
19	47	0	4.365588	-0.060655	3.195292

[7-Xap-Ag]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.007044	0.002101	0.008631
2	6	0	-0.078176	0.001805	2.297571
3	6	0	1.368163	-0.017290	2.406321
4	6	0	2.149026	-0.028269	1.152213
5	8	0	3.366644	-0.044475	1.116265
6	6	0	-0.154242	-0.001735	4.727616
7	6	0	1.331811	-0.017577	4.688165
8	7	0	2.034851	-0.026344	3.576377
9	7	0	-0.769059	0.009286	3.454677
10	7	0	-0.709025	0.011277	1.144462
11	7	0	1.384614	-0.018600	-0.001109
12	7	0	-0.647958	0.013333	-1.132884
13	1	0	-1.662819	0.028218	-1.103467
14	1	0	-0.201405	0.008363	-2.042408
15	1	0	1.905664	-0.024436	-0.875754
16	1	0	1.835883	-0.021714	5.649487
17	8	0	-0.779107	0.000419	5.751847
18	1	0	-1.789503	0.021538	3.426535
19	47	0	4.571933	-0.073602	3.202393

[7-Xap-Au]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.051453	0.036343	0.004846
2	6	0	0.006854	0.015769	2.266605
3	6	0	1.403582	-0.019071	2.341371
4	6	0	2.162461	-0.022248	1.103266
5	8	0	3.361104	-0.042327	0.941433
6	6	0	-0.098304	-0.001972	4.714169
7	6	0	1.370826	-0.038346	4.651972
8	7	0	2.048840	-0.045353	3.548359
9	7	0	-0.686607	0.023572	3.439714
10	7	0	-0.728130	0.036684	1.131321
11	7	0	1.308119	0.007166	-0.041288
12	7	0	-0.730485	0.098442	-1.166255
13	1	0	-1.731499	0.002856	-1.105262
14	1	0	-0.288856	-0.136514	-2.039161
15	1	0	1.805227	0.038557	-0.922433
16	1	0	1.899812	-0.060426	5.597862
17	8	0	-0.765285	0.006097	5.727225
18	1	0	-1.698901	0.049249	3.394316
19	79	0	4.577035	-0.126181	3.858878

[7-Xap-Au]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.008924	0.002112	0.014903
2	6	0	0.000662	-0.000532	2.284545
3	6	0	1.403853	-0.019252	2.359308
4	6	0	2.162033	-0.027919	1.134360
5	8	0	3.385171	-0.043971	1.025439
6	6	0	-0.107865	-0.001758	4.729162
7	6	0	1.371725	-0.021404	4.689462
8	7	0	2.042720	-0.029091	3.576519
9	7	0	-0.695040	0.007402	3.453077
10	7	0	-0.696941	0.009998	1.143736
11	7	0	1.362219	-0.016055	-0.011913
12	7	0	-0.668261	0.012182	-1.147226
13	1	0	-1.676616	0.025580	-1.116560
14	1	0	-0.210935	0.007208	-2.044379
15	1	0	1.872143	-0.021795	-0.888147
16	1	0	1.884127	-0.029276	5.641286
17	8	0	-0.749539	0.005690	5.747816
18	1	0	-1.709941	0.020939	3.407443
19	79	0	4.203747	-0.057761	3.448109

[7-Xap-Au] $^{+2}$

Input orientation:

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

1	6	0	0.007924	0.002345	-0.008210
2	6	0	-0.047420	0.000541	2.287460
3	6	0	1.400418	-0.019605	2.373760
4	6	0	2.168248	-0.028763	1.105884
5	8	0	3.378460	-0.045388	1.055854
6	6	0	-0.116170	-0.001181	4.716890
7	6	0	1.370216	-0.021705	4.674748
8	7	0	2.063752	-0.030119	3.553843
9	7	0	-0.732934	0.008731	3.450343
10	7	0	-0.690019	0.010704	1.143894
11	7	0	1.379570	-0.016577	-0.037361
12	7	0	-0.673376	0.013019	-1.132893
13	1	0	-1.687709	0.026983	-1.080917
14	1	0	-0.247472	0.008163	-2.052877
15	1	0	1.890183	-0.022592	-0.918489
16	1	0	1.879292	-0.029767	5.632327
17	8	0	-0.724810	0.006096	5.749636
18	1	0	-1.753629	0.022868	3.424337
19	79	0	4.299817	-0.061456	3.508711

[7-Xap-Zn]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.869670	-1.765974	-0.303366
2	6	0	2.176198	0.380057	-0.138641
3	6	0	0.934539	0.058342	0.417547
4	6	0	0.622234	-1.342470	0.646914
5	8	0	-0.373074	-1.839670	1.119807
6	6	0	1.569186	2.750909	-0.022481
7	6	0	0.306005	2.263416	0.553091
8	7	0	0.019891	1.018075	0.753459
9	7	0	2.447960	1.701203	-0.337411
10	7	0	3.140385	-0.498420	-0.509109
11	7	0	1.696739	-2.196460	0.234069
12	7	0	3.814375	-2.697161	-0.604564
13	1	0	4.606543	-2.355890	-1.125715
14	1	0	3.552946	-3.658679	-0.747672
15	1	0	1.533112	-3.178307	0.416565
16	1	0	-0.421581	3.024069	0.819953
17	8	0	1.867029	3.911672	-0.222850
18	1	0	3.344552	1.949159	-0.739415
19	30	0	-5.108989	-0.257090	-0.315762

[7-Xap-Zn]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.002400	0.001203	0.025542
2	6	0	-0.028489	-0.000563	2.294549

3	6	0	1.369798	-0.018972	2.382081
4	6	0	2.138860	-0.027801	1.181931
5	8	0	3.378890	-0.043888	1.131628
6	6	0	-0.117286	-0.001550	4.741848
7	6	0	1.364832	-0.020871	4.690512
8	7	0	2.035192	-0.028706	3.583307
9	7	0	-0.718829	0.007452	3.464391
10	7	0	-0.707117	0.009451	1.139966
11	7	0	1.380103	-0.016634	0.019529
12	7	0	-0.631914	0.010867	-1.151052
13	1	0	-1.640655	0.024223	-1.141358
14	1	0	-0.156326	0.005844	-2.038542
15	1	0	1.903968	-0.022489	-0.848512
16	1	0	1.883248	-0.028471	5.642497
17	8	0	-0.760816	0.006110	5.758983
18	1	0	-1.734112	0.020835	3.431748
19	30	0	4.202593	-0.053745	3.137891

[7-Xap-Zn]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.019268	0.000226	0.019902
2	6	0	-0.033199	-0.000622	2.300248
3	6	0	1.379371	-0.018244	2.380723
4	6	0	2.124359	-0.025492	1.182370
5	8	0	3.407192	-0.041310	1.145593
6	6	0	-0.116109	-0.002266	4.745618
7	6	0	1.382495	-0.019955	4.714633
8	7	0	2.045517	-0.027117	3.600635
9	7	0	-0.719009	0.006352	3.469050
10	7	0	-0.684407	0.008066	1.147345
11	7	0	1.411464	-0.016131	0.022175
12	7	0	-0.609018	0.008787	-1.142903
13	1	0	-1.622173	0.020924	-1.136307
14	1	0	-0.142581	0.004092	-2.039442
15	1	0	1.942961	-0.022319	-0.845071
16	1	0	1.888423	-0.026667	5.673190
17	8	0	-0.728606	0.004433	5.771418
18	1	0	-1.738069	0.018726	3.440329
19	30	0	3.956463	-0.049186	2.997435

[7-Xap-Cd]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.071378	0.060405	0.014279
2	6	0	-0.063001	0.036969	2.275612
3	6	0	1.329430	-0.031258	2.382943
4	6	0	2.114857	-0.051645	1.163247
5	8	0	3.318141	-0.099561	1.027171

6	6	0	-0.210760	0.019012	4.721345
7	6	0	1.259049	-0.051517	4.679864
8	7	0	1.961907	-0.073839	3.594728
9	7	0	-0.777595	0.060251	3.435978
10	7	0	-0.774144	0.075222	1.122932
11	7	0	1.288449	-0.001166	-0.001443
12	7	0	-0.719842	0.145078	-1.176392
13	1	0	-1.722753	0.056936	-1.134200
14	1	0	-0.267273	-0.141001	-2.028655
15	1	0	1.804699	0.025459	-0.871543
16	1	0	1.764618	-0.086170	5.640073
17	8	0	-0.899142	0.041509	5.721190
18	1	0	-1.788006	0.109933	3.374540
19	48	0	5.617084	-0.272320	3.505271

[7-Xap-Cd]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.011450	0.002374	0.025861
2	6	0	-0.037591	0.000711	2.294244
3	6	0	1.363493	-0.019202	2.387445
4	6	0	2.126163	-0.028660	1.184169
5	8	0	3.368625	-0.046379	1.103499
6	6	0	-0.143784	-0.000255	4.739819
7	6	0	1.338546	-0.021169	4.695703
8	7	0	2.019272	-0.029712	3.595393
9	7	0	-0.735653	0.009339	3.459179
10	7	0	-0.718381	0.011389	1.140580
11	7	0	1.365047	-0.016923	0.022566
12	7	0	-0.645056	0.012366	-1.151636
13	1	0	-1.653718	0.026809	-1.142713
14	1	0	-0.168785	0.007065	-2.038685
15	1	0	1.890779	-0.023711	-0.844309
16	1	0	1.848911	-0.029238	5.652063
17	8	0	-0.794346	0.007738	5.752620
18	1	0	-1.750577	0.023670	3.417598
19	48	0	4.502844	-0.063915	3.153545

[7-Xap-Cd]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.003871	0.001355	0.019939
2	6	0	-0.035426	-0.000023	2.297715
3	6	0	1.379581	-0.018644	2.382570
4	6	0	2.119872	-0.027068	1.179528
5	8	0	3.393715	-0.043845	1.103628
6	6	0	-0.139339	-0.001105	4.739704
7	6	0	1.357135	-0.020418	4.711854
8	7	0	2.031933	-0.028208	3.605562

9	7	0	-0.730761	0.007921	3.462080
10	7	0	-0.695122	0.009551	1.148348
11	7	0	1.391501	-0.016639	0.021919
12	7	0	-0.628673	0.010608	-1.142673
13	1	0	-1.641219	0.023765	-1.133003
14	1	0	-0.163915	0.005540	-2.039527
15	1	0	1.921389	-0.023093	-0.845615
16	1	0	1.852689	-0.027604	5.675452
17	8	0	-0.759066	0.005876	5.762918
18	1	0	-1.748991	0.021162	3.421509
19	48	0	4.255166	-0.056834	3.075031

[7-Xap-Hg]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075963	0.054169	0.011772
2	6	0	-0.073499	0.029274	2.273083
3	6	0	1.319227	-0.025332	2.385454
4	6	0	2.109326	-0.037164	1.167589
5	8	0	3.312188	-0.072920	1.033234
6	6	0	-0.230834	0.008382	4.718029
7	6	0	1.239466	-0.047621	4.681679
8	7	0	1.947461	-0.062430	3.599656
9	7	0	-0.792821	0.044837	3.430762
10	7	0	-0.782074	0.061153	1.118201
11	7	0	1.283962	0.005973	0.000072
12	7	0	-0.722043	0.134193	-1.181264
13	1	0	-1.723832	0.032946	-1.140748
14	1	0	-0.265068	-0.154088	-2.030510
15	1	0	1.802492	0.039194	-0.868409
16	1	0	1.740994	-0.077834	5.644134
17	8	0	-0.923645	0.023454	5.715326
18	1	0	-1.803367	0.084623	3.365058
19	80	0	5.802369	-0.218513	3.523822

[7-Xap-Hg]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.018587	0.003346	0.023582
2	6	0	-0.033012	0.000845	2.290892
3	6	0	1.369958	-0.019683	2.384240
4	6	0	2.131266	-0.029348	1.173127
5	8	0	3.366709	-0.047257	1.068066
6	6	0	-0.150402	-0.000182	4.737433
7	6	0	1.331395	-0.021715	4.696713
8	7	0	2.010061	-0.030365	3.596602
9	7	0	-0.733918	0.009749	3.454972
10	7	0	-0.720364	0.012193	1.141304
11	7	0	1.355493	-0.016780	0.015808

12	7	0	-0.658523	0.013338	-1.150904
13	1	0	-1.667044	0.028063	-1.136579
14	1	0	-0.186718	0.007702	-2.040243
15	1	0	1.877246	-0.023643	-0.853271
16	1	0	1.840282	-0.030124	5.653733
17	8	0	-0.804904	0.008246	5.748102
18	1	0	-1.748482	0.024577	3.407243
19	80	0	4.603882	-0.066665	3.236122

[7-Xap-Hg]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.001093	-0.002290	0.017027
2	6	0	-0.031926	-0.006108	2.293965
3	6	0	1.385249	-0.011487	2.379612
4	6	0	2.126564	-0.012502	1.167959
5	8	0	3.389275	-0.022829	1.072958
6	6	0	-0.148804	0.011788	4.735158
7	6	0	1.353342	-0.022668	4.715219
8	7	0	2.010009	-0.029115	3.604006
9	7	0	-0.729907	0.004934	3.459181
10	7	0	-0.696221	0.001384	1.149419
11	7	0	1.384027	-0.011479	0.015446
12	7	0	-0.639741	0.006014	-1.141167
13	1	0	-1.652486	0.018338	-1.126383
14	1	0	-0.179866	0.000026	-2.040846
15	1	0	1.909160	-0.011743	-0.855068
16	1	0	1.848735	-0.051550	5.677903
17	8	0	-0.766685	0.029650	5.759275
18	1	0	-1.748013	0.017471	3.412406
19	80	0	4.352722	-0.085539	3.150871

[Sep-Cu]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.146649	0.098093	0.062371
2	6	0	-0.016194	0.453817	2.303574
3	6	0	1.356438	0.280303	2.476600
4	6	0	2.107510	-0.290773	1.424791
5	8	0	3.231359	-0.855594	1.563604
6	6	0	-0.239523	0.533251	4.803434
7	6	0	1.199351	0.034324	4.804621
8	7	0	1.951745	0.247920	3.702935
9	7	0	-0.765366	0.626429	3.414018
10	7	0	-0.614136	0.417151	1.077673
11	7	0	1.464323	-0.270463	0.185140
12	7	0	-0.363901	0.164212	-1.215501
13	1	0	-1.368973	0.257774	-1.227099
14	1	0	-0.003085	-0.486056	-1.898351

15	1	0	1.990702	-0.612269	-0.607519
16	1	0	-1.761487	0.708814	3.283357
17	1	0	-0.304824	1.525087	5.266775
18	1	0	-0.888157	-0.126748	5.377628
19	6	0	1.895592	-0.710522	5.784841
20	6	0	1.468418	-0.891124	7.226647
21	6	0	2.552314	-0.378051	8.178524
22	1	0	2.286586	-0.594104	9.219580
23	1	0	2.664614	0.702943	8.062695
24	1	0	3.503124	-0.859928	7.950791
25	8	0	0.223559	-0.216603	7.452750
26	8	0	3.008831	-1.318369	5.488260
27	1	0	0.025991	-0.284694	8.391256
28	1	0	1.336456	-1.970924	7.394551
29	29	0	3.406468	-1.132767	3.580880

[Sep-Cu]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.165841	0.249224	0.037861
2	6	0	-0.091081	0.227744	2.297250
3	6	0	1.197222	-0.310410	2.448187
4	6	0	2.032355	-0.601172	1.337376
5	8	0	3.174121	-1.087776	1.416339
6	6	0	-0.320497	0.170610	4.804318
7	6	0	1.088814	-0.414560	4.779968
8	7	0	1.702556	-0.595712	3.659983
9	7	0	-0.792752	0.449309	3.415025
10	7	0	-0.602716	0.508577	1.085303
11	7	0	1.436606	-0.284338	0.115086
12	7	0	-0.314100	0.519131	-1.183783
13	1	0	-1.242431	0.907287	-1.246174
14	1	0	0.202113	0.352587	-2.031466
15	1	0	1.980153	-0.467889	-0.719422
16	1	0	-1.720870	0.834990	3.305139
17	1	0	-0.343236	1.095480	5.383594
18	1	0	-1.014610	-0.519094	5.287718
19	6	0	1.971463	-0.862328	5.911031
20	6	0	1.559859	-0.790917	7.367402
21	6	0	2.573338	0.012933	8.188085
22	1	0	2.301231	-0.018424	9.245902
23	1	0	2.585321	1.056235	7.864921
24	1	0	3.572394	-0.409509	8.077747
25	8	0	0.248497	-0.242875	7.428886
26	8	0	3.087729	-1.323990	5.643504
27	1	0	-0.027714	-0.201476	8.349917
28	1	0	1.557957	-1.833117	7.719263
29	29	0	3.526819	-1.369388	3.539863

[Sep-Cu]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.202747	0.235339	0.037673
2	6	0	-0.166198	0.260759	2.294960
3	6	0	1.107078	-0.333959	2.462278
4	6	0	1.974654	-0.642707	1.400249
5	8	0	3.118615	-1.153088	1.620981
6	6	0	-0.394961	0.198461	4.813063
7	6	0	1.010616	-0.397897	4.817215
8	7	0	1.591429	-0.600336	3.672221
9	7	0	-0.847041	0.514583	3.411522
10	7	0	-0.594592	0.534449	1.064329
11	7	0	1.477712	-0.343377	0.164559
12	7	0	-0.219269	0.496096	-1.188783
13	1	0	-1.135581	0.913628	-1.296581
14	1	0	0.315026	0.301596	-2.024021
15	1	0	2.048867	-0.542128	-0.651995
16	1	0	-1.759982	0.947635	3.318196
17	1	0	-0.417784	1.112401	5.407617
18	1	0	-1.098049	-0.501943	5.267503
19	6	0	1.937057	-0.849850	5.887731
20	6	0	1.613207	-0.791450	7.350158
21	6	0	2.659261	0.026647	8.128010
22	1	0	2.413209	-0.008560	9.190848
23	1	0	2.652069	1.068767	7.803755
24	1	0	3.656397	-0.394801	7.996077
25	8	0	0.301907	-0.265448	7.432296
26	8	0	3.051902	-1.314222	5.517369
27	1	0	0.017248	-0.237341	8.353244
28	1	0	1.650147	-1.836804	7.697856
29	29	0	3.328692	-1.345320	3.580495

[Sep-Ag]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037762	0.094123	0.040093
2	6	0	-0.019153	-0.015489	2.308096
3	6	0	1.371854	-0.107954	2.414511
4	6	0	2.165047	-0.139458	1.226989
5	8	0	3.394162	-0.277528	1.145828
6	6	0	-0.117046	0.226786	4.756396
7	6	0	1.327470	-0.250715	4.766921
8	7	0	1.990553	-0.299524	3.611783
9	7	0	-0.743043	-0.084345	3.458942
10	7	0	-0.688402	0.077881	1.125474
11	7	0	1.402057	-0.001711	0.049772
12	7	0	-0.567773	0.271400	-1.187867
13	1	0	-1.572088	0.180610	-1.133396
14	1	0	-0.161097	-0.218210	-1.972292
15	1	0	1.934619	0.059514	-0.807487
16	1	0	-1.730294	0.099629	3.358388
17	1	0	-0.151089	1.307094	4.953569

18	1	0	-0.699970	-0.252701	5.543516
19	6	0	2.070569	-0.548434	5.950207
20	6	0	1.369411	-0.495836	7.310528
21	6	0	2.316105	-0.778014	8.468409
22	1	0	1.768934	-0.748250	9.417083
23	1	0	3.110784	-0.031471	8.492560
24	1	0	2.776993	-1.761357	8.363742
25	8	0	0.768315	0.808216	7.434227
26	8	0	3.299130	-0.874892	5.929167
27	1	0	0.305095	0.832168	8.278560
28	1	0	0.568428	-1.254908	7.310469
29	47	0	4.189026	-0.694374	3.691403

[Sep-Ag]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.066701	0.082828	0.033484
2	6	0	-0.061510	0.069443	2.302083
3	6	0	1.338662	-0.087497	2.430743
4	6	0	2.151490	-0.223589	1.263453
5	8	0	3.364697	-0.451340	1.222881
6	6	0	-0.193469	0.246816	4.770861
7	6	0	1.252221	-0.233750	4.753755
8	7	0	1.903574	-0.314502	3.642654
9	7	0	-0.785010	0.081975	3.428743
10	7	0	-0.688663	0.148507	1.116603
11	7	0	1.427451	-0.086244	0.068390
12	7	0	-0.523103	0.183939	-1.165861
13	1	0	-1.522442	0.314210	-1.186531
14	1	0	-0.016331	0.163157	-2.034969
15	1	0	1.970670	-0.165013	-0.782702
16	1	0	-1.786199	0.176070	3.325889
17	1	0	-0.228985	1.295524	5.085058
18	1	0	-0.791079	-0.314001	5.488331
19	6	0	2.057125	-0.604774	5.969315
20	6	0	1.404265	-0.579044	7.350347
21	6	0	2.419436	-0.621473	8.483258
22	1	0	1.899459	-0.651587	9.444258
23	1	0	3.055350	0.264913	8.456073
24	1	0	3.050629	-1.507262	8.409111
25	8	0	0.589063	0.591014	7.384078
26	8	0	3.223769	-0.958964	5.856690
27	1	0	0.185474	0.658223	8.255801
28	1	0	0.771687	-1.483948	7.393166
29	47	0	4.181426	-0.871380	3.540628

[Sep-Ag]$^{+2}$

Input orientation:

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

1	6	0	0.126174	0.278738	0.042604
2	6	0	-0.058888	0.195150	2.316134
3	6	0	1.290137	-0.312939	2.454101
4	6	0	2.090997	-0.528487	1.236838
5	8	0	3.232344	-0.952098	1.242383
6	6	0	-0.206371	0.078903	4.786859
7	6	0	1.196889	-0.441850	4.756788
8	7	0	1.849537	-0.601644	3.631990
9	7	0	-0.732000	0.367939	3.451572
10	7	0	-0.602224	0.475662	1.144933
11	7	0	1.420901	-0.203302	0.066054
12	7	0	-0.420085	0.559188	-1.126662
13	1	0	-1.369697	0.911839	-1.137634
14	1	0	0.053630	0.442028	-2.012172
15	1	0	1.943446	-0.340958	-0.795085
16	1	0	-1.681190	0.725110	3.379462
17	1	0	-0.254942	0.977804	5.414905
18	1	0	-0.857126	-0.638927	5.302854
19	6	0	2.026248	-0.849023	5.999608
20	6	0	1.489715	-0.775028	7.418451
21	6	0	2.427731	0.040157	8.319248
22	1	0	2.068044	-0.009357	9.348915
23	1	0	2.450041	1.086724	8.008995
24	1	0	3.437404	-0.370409	8.293442
25	8	0	0.170683	-0.254565	7.372900
26	8	0	3.153825	-1.258041	5.802584
27	1	0	-0.188008	-0.212337	8.267185
28	1	0	1.481394	-1.820524	7.763191
29	47	0	4.177746	-1.447501	3.555150

[Sep-Au]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.001717	0.093912	0.044894
2	6	0	0.013749	-0.028520	2.309147
3	6	0	1.416549	0.033648	2.398374
4	6	0	2.186083	0.171230	1.186838
5	8	0	3.388173	0.243945	1.040688
6	6	0	-0.067662	0.245656	4.721874
7	6	0	1.394430	-0.184400	4.706841
8	7	0	2.056364	-0.215491	3.591386
9	7	0	-0.678429	-0.166686	3.459030
10	7	0	-0.695520	-0.031352	1.153698
11	7	0	1.348590	0.220074	0.023625
12	7	0	-0.669498	0.149428	-1.140580
13	1	0	-1.646090	-0.095008	-1.092525
14	1	0	-0.189335	-0.068008	-1.998580
15	1	0	1.854021	0.349001	-0.843178
16	1	0	-1.683802	-0.186722	3.375289
17	1	0	-0.132633	1.334367	4.863025
18	1	0	-0.615399	-0.212157	5.542633
19	6	0	2.126956	-0.547285	5.954730
20	6	0	1.368124	-0.491659	7.292874

21	6	0	2.284951	-0.734880	8.481006
22	1	0	1.707120	-0.718042	9.410771
23	1	0	3.053858	0.037765	8.526438
24	1	0	2.779383	-1.703372	8.398297
25	8	0	0.737231	0.794043	7.355121
26	8	0	3.286862	-0.913768	5.938407
27	1	0	0.298214	0.865641	8.208518
28	1	0	0.598355	-1.282528	7.258690
29	79	0	3.975456	-1.907704	3.361492

[Sep-Au]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029094	0.081751	0.012665
2	6	0	-0.066180	0.063425	2.283252
3	6	0	1.338210	-0.085521	2.393649
4	6	0	2.133388	-0.209492	1.210452
5	8	0	3.347330	-0.424998	1.141669
6	6	0	-0.167545	0.254640	4.749581
7	6	0	1.273153	-0.237980	4.723878
8	7	0	1.907576	-0.315112	3.603417
9	7	0	-0.775076	0.072935	3.418596
10	7	0	-0.709631	0.139318	1.108121
11	7	0	1.391125	-0.075116	0.028784
12	7	0	-0.578451	0.181100	-1.176485
13	1	0	-1.579497	0.300926	-1.182794
14	1	0	-0.085260	0.158728	-2.053607
15	1	0	1.924716	-0.144191	-0.829384
16	1	0	-1.778074	0.161434	3.327904
17	1	0	-0.189798	1.308092	5.048839
18	1	0	-0.758885	-0.291502	5.482556
19	6	0	2.071396	-0.616719	5.943929
20	6	0	1.407679	-0.582993	7.320874
21	6	0	2.413605	-0.648572	8.460618
22	1	0	1.884412	-0.666421	9.416874
23	1	0	3.070297	0.222516	8.438249
24	1	0	3.024177	-1.549201	8.393051
25	8	0	0.615536	0.602219	7.350857
26	8	0	3.234188	-0.981271	5.846413
27	1	0	0.230342	0.691324	8.229038
28	1	0	0.758146	-1.476180	7.354608
29	79	0	4.128413	-0.882008	3.483220

[Sep-Au]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.099446	0.293774	0.022617
2	6	0	-0.064336	0.198217	2.297446
3	6	0	1.279554	-0.328772	2.420115

4	6	0	2.064973	-0.549878	1.190971
5	8	0	3.200178	-0.989885	1.173805
6	6	0	-0.197739	0.070323	4.770197
7	6	0	1.201285	-0.459730	4.729814
8	7	0	1.836118	-0.622512	3.597390
9	7	0	-0.725510	0.373961	3.440164
10	7	0	-0.614525	0.493385	1.134497
11	7	0	1.386567	-0.208009	0.030927
12	7	0	-0.454326	0.590736	-1.138139
13	1	0	-1.398814	0.957713	-1.136603
14	1	0	0.008192	0.473440	-2.029806
15	1	0	1.898956	-0.348615	-0.836074
16	1	0	-1.670573	0.743885	3.376345
17	1	0	-0.238933	0.963431	5.407109
18	1	0	-0.850286	-0.649192	5.282373
19	6	0	2.031843	-0.869533	5.970556
20	6	0	1.503858	-0.784851	7.392572
21	6	0	2.440628	0.053279	8.274863
22	1	0	2.085639	0.014707	9.306605
23	1	0	2.451855	1.095348	7.949603
24	1	0	3.453712	-0.348916	8.249860
25	8	0	0.179223	-0.281786	7.350402
26	8	0	3.158144	-1.288088	5.782881
27	1	0	-0.176069	-0.239492	8.246270
28	1	0	1.512944	-1.826347	7.748625
29	79	0	4.092379	-1.475465	3.523441

[Sep-Zn]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.059507	0.214509	0.083492
2	6	0	-0.069090	0.033616	2.342751
3	6	0	1.330887	0.113116	2.456465
4	6	0	2.117744	0.295903	1.259866
5	8	0	3.317203	0.398131	1.124088
6	6	0	-0.187638	0.225380	4.764079
7	6	0	1.277049	-0.206115	4.737716
8	7	0	1.957636	-0.176235	3.644862
9	7	0	-0.777668	-0.146719	3.478120
10	7	0	-0.765821	0.039800	1.175851
11	7	0	1.287352	0.372401	0.085733
12	7	0	-0.711632	0.292917	-1.113352
13	1	0	-1.680947	0.017888	-1.083254
14	1	0	-0.213323	0.085461	-1.963708
15	1	0	1.799900	0.542772	-0.769472
16	1	0	-1.780728	-0.183663	3.377042
17	1	0	-0.254048	1.308106	4.941902
18	1	0	-0.745920	-0.264267	5.560479
19	6	0	2.002162	-0.664733	5.971810
20	6	0	1.320994	-0.453566	7.338365
21	6	0	2.292821	-0.637352	8.493759
22	1	0	1.770391	-0.535632	9.450386
23	1	0	3.082245	0.114408	8.440251

24	1	0	2.757853	-1.622700	8.452367
25	8	0	0.743065	0.857355	7.325747
26	8	0	3.081441	-1.209677	5.913771
27	1	0	0.325555	1.004219	8.179979
28	1	0	0.521422	-1.211641	7.411732
29	30	0	5.754988	-3.552551	2.448000

[Sep-Zn]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.067140	0.116907	0.009789
2	6	0	-0.094283	0.082730	2.278240
3	6	0	1.295704	-0.128464	2.414781
4	6	0	2.119488	-0.271518	1.260409
5	8	0	3.323592	-0.536833	1.269004
6	6	0	-0.224028	0.245132	4.745605
7	6	0	1.197310	-0.299631	4.734076
8	7	0	1.853919	-0.396299	3.622231
9	7	0	-0.821627	0.110896	3.401452
10	7	0	-0.700338	0.194347	1.085328
11	7	0	1.424070	-0.088926	0.057194
12	7	0	-0.505937	0.243626	-1.194094
13	1	0	-1.501500	0.399397	-1.225324
14	1	0	0.010134	0.216830	-2.057772
15	1	0	1.975138	-0.174722	-0.788336
16	1	0	-1.819647	0.235423	3.300286
17	1	0	-0.212196	1.293913	5.062436
18	1	0	-0.844836	-0.289691	5.462029
19	6	0	2.006392	-0.706853	5.932355
20	6	0	1.429029	-0.628132	7.340563
21	6	0	2.511940	-0.523361	8.407175
22	1	0	2.056864	-0.549853	9.400351
23	1	0	3.060831	0.413895	8.298200
24	1	0	3.213830	-1.353417	8.329148
25	8	0	0.525922	0.474044	7.360382
26	8	0	3.141736	-1.132643	5.757093
27	1	0	0.176504	0.570188	8.252444
28	1	0	0.876687	-1.575057	7.476203
29	30	0	3.952544	-0.890799	3.537575

[Sep-Zn]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.193716	0.246612	0.039976
2	6	0	-0.156579	0.263627	2.294552
3	6	0	1.114888	-0.335373	2.461742
4	6	0	1.975369	-0.645178	1.388692
5	8	0	3.125730	-1.162468	1.570814
6	6	0	-0.379243	0.198139	4.818760

7	6	0	1.022528	-0.405284	4.807495
8	7	0	1.594824	-0.606140	3.668150
9	7	0	-0.832120	0.515526	3.415627
10	7	0	-0.598299	0.546037	1.069259
11	7	0	1.465619	-0.336720	0.158814
12	7	0	-0.232191	0.512726	-1.185419
13	1	0	-1.147238	0.933910	-1.286820
14	1	0	0.297621	0.319045	-2.023237
15	1	0	2.030248	-0.534700	-0.661822
16	1	0	-1.744107	0.950428	3.324206
17	1	0	-0.399714	1.113483	5.410657
18	1	0	-1.088045	-0.495519	5.273583
19	6	0	1.955087	-0.864202	5.891416
20	6	0	1.607093	-0.798247	7.351750
21	6	0	2.633984	0.036011	8.136998
22	1	0	2.373400	0.007920	9.196677
23	1	0	2.621511	1.075711	7.804967
24	1	0	3.636822	-0.376700	8.022946
25	8	0	0.290569	-0.285558	7.418889
26	8	0	3.074434	-1.334303	5.557937
27	1	0	-0.002576	-0.256769	8.337055
28	1	0	1.650685	-1.840810	7.705591
29	30	0	3.410367	-1.390072	3.559573

[Sep-Cd]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.008685	0.106111	0.044331
2	6	0	-0.012570	0.030930	2.310611
3	6	0	1.390870	0.090017	2.409986
4	6	0	2.172730	0.171104	1.201472
5	8	0	3.377944	0.200130	1.061580
6	6	0	-0.115192	0.281211	4.737381
7	6	0	1.357098	-0.122236	4.710388
8	7	0	2.024740	-0.135304	3.605115
9	7	0	-0.714488	-0.092119	3.455171
10	7	0	-0.713399	0.007520	1.148907
11	7	0	1.343681	0.213335	0.029949
12	7	0	-0.666672	0.147857	-1.147794
13	1	0	-1.645967	-0.085981	-1.103078
14	1	0	-0.182004	-0.090837	-1.997545
15	1	0	1.857075	0.307750	-0.836587
16	1	0	-1.718693	-0.125651	3.363236
17	1	0	-0.199695	1.362057	4.919868
18	1	0	-0.660614	-0.216067	5.537354
19	6	0	2.111487	-0.499551	5.946359
20	6	0	1.363815	-0.496559	7.292594
21	6	0	2.297917	-0.733347	8.468362
22	1	0	1.728914	-0.757155	9.403438
23	1	0	3.039776	0.064770	8.524219
24	1	0	2.825545	-1.681551	8.359517
25	8	0	0.691432	0.766192	7.386072
26	8	0	3.278134	-0.836659	5.903761

27	1	0	0.248926	0.801928	8.239796
28	1	0	0.619696	-1.311206	7.247028
29	48	0	4.402582	-2.315560	3.307335

[Sep-Cd]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.939482	0.867401	-0.040340
2	6	0	1.805006	1.650424	-0.061465
3	6	0	1.273100	0.348710	0.097837
4	6	0	2.149251	-0.773716	0.137694
5	8	0	1.813570	-1.963356	0.183067
6	6	0	-0.500110	2.525220	0.120189
7	6	0	-0.930702	1.073566	-0.045477
8	7	0	-0.063258	0.116249	0.005404
9	7	0	0.933521	2.656459	-0.199401
10	7	0	3.122104	1.902136	-0.137177
11	7	0	3.506225	-0.426846	0.105733
12	7	0	5.260167	1.085944	-0.088912
13	1	0	5.574082	2.038520	-0.190895
14	1	0	5.945581	0.354026	-0.002790
15	1	0	4.157765	-1.201536	0.142567
16	1	0	1.318749	3.581054	-0.335971
17	1	0	-0.703227	2.852532	1.145795
18	1	0	-1.067912	3.183812	-0.535008
19	6	0	-2.347839	0.607691	-0.229094
20	6	0	-3.492294	1.616244	-0.289772
21	6	0	-4.851424	0.975170	-0.046162
22	1	0	-5.638815	1.724567	-0.160010
23	1	0	-4.901052	0.564855	0.963912
24	1	0	-5.037591	0.172613	-0.759882
25	8	0	-3.185075	2.636066	0.658223
26	8	0	-2.579236	-0.586895	-0.360887
27	1	0	-3.911046	3.268493	0.674693
28	1	0	-3.462322	2.027922	-1.314757
29	48	0	-0.671762	-2.290490	0.019495

[Sep-Cd]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.159633	0.308273	0.054775
2	6	0	-0.087371	0.247026	2.319844
3	6	0	1.176145	-0.396848	2.442338
4	6	0	1.977794	-0.668359	1.308374
5	8	0	3.129731	-1.194519	1.356384
6	6	0	-0.299141	0.098210	4.821811
7	6	0	1.112442	-0.479225	4.785238
8	7	0	1.689309	-0.683883	3.644894
9	7	0	-0.735485	0.505658	3.452897

10	7	0	-0.573355	0.588830	1.126842
11	7	0	1.411577	-0.302963	0.111677
12	7	0	-0.312689	0.624402	-1.143408
13	1	0	-1.220565	1.068618	-1.191485
14	1	0	0.175738	0.443531	-2.008200
15	1	0	1.946487	-0.484340	-0.731801
16	1	0	-1.629365	0.978466	3.376639
17	1	0	-0.344025	0.964835	5.480393
18	1	0	-0.995256	-0.641025	5.223720
19	6	0	1.993212	-0.907592	5.924441
20	6	0	1.579150	-0.806063	7.373999
21	6	0	2.493198	0.173727	8.132060
22	1	0	2.206749	0.177949	9.185626
23	1	0	2.384741	1.187579	7.741871
24	1	0	3.536176	-0.137812	8.065645
25	8	0	0.216613	-0.431997	7.399386
26	8	0	3.128009	-1.373975	5.684922
27	1	0	-0.101570	-0.424908	8.309564
28	1	0	1.723642	-1.816945	7.783154
29	48	0	3.752862	-1.565522	3.497227

[Sep-Hg]

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.021727	0.133596	0.058108
2	6	0	-0.044675	-0.015815	2.319676
3	6	0	1.356654	0.052028	2.437075
4	6	0	2.149331	0.202859	1.240734
5	8	0	3.352721	0.280967	1.109954
6	6	0	-0.168092	0.201251	4.739730
7	6	0	1.294031	-0.239487	4.723132
8	7	0	1.975402	-0.228022	3.630115
9	7	0	-0.757146	-0.176435	3.454750
10	7	0	-0.734997	-0.016619	1.150015
11	7	0	1.328044	0.270834	0.063242
12	7	0	-0.667239	0.203442	-1.141498
13	1	0	-1.641006	-0.055509	-1.112880
14	1	0	-0.168628	-0.017805	-1.988152
15	1	0	1.845719	0.421427	-0.792625
16	1	0	-1.760284	-0.209865	3.352640
17	1	0	-0.227878	1.285817	4.907237
18	1	0	-0.732338	-0.276741	5.538604
19	6	0	2.015702	-0.687305	5.962147
20	6	0	1.328746	-0.480269	7.325177
21	6	0	2.299929	-0.646396	8.484092
22	1	0	1.771827	-0.550883	9.438189
23	1	0	3.077972	0.117284	8.432344
24	1	0	2.779597	-1.624672	8.447288
25	8	0	0.730620	0.820804	7.306027
26	8	0	3.100845	-1.223192	5.911659
27	1	0	0.333402	0.976731	8.168189
28	1	0	0.540922	-1.250910	7.398284
29	80	0	5.136930	-2.215988	2.965573

[Sep-Hg]$^{+1}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.009169	0.077213	0.019781
2	6	0	-0.071457	0.046138	2.290565
3	6	0	1.337020	-0.078101	2.399228
4	6	0	2.125365	-0.169929	1.210869
5	8	0	3.343286	-0.353984	1.133738
6	6	0	-0.163684	0.252259	4.747725
7	6	0	1.276191	-0.244557	4.718321
8	7	0	1.922447	-0.317300	3.603033
9	7	0	-0.778608	0.039410	3.427259
10	7	0	-0.724123	0.110726	1.118697
11	7	0	1.374165	-0.040809	0.031323
12	7	0	-0.606516	0.162429	-1.167281
13	1	0	-1.610290	0.255045	-1.169319
14	1	0	-0.115774	0.159480	-2.045865
15	1	0	1.907653	-0.089533	-0.828217
16	1	0	-1.783196	0.109231	3.339324
17	1	0	-0.180571	1.312715	5.023169
18	1	0	-0.750940	-0.275291	5.497388
19	6	0	2.058045	-0.631827	5.942762
20	6	0	1.387457	-0.563382	7.316771
21	6	0	2.381707	-0.680263	8.461878
22	1	0	1.848373	-0.670930	9.416034
23	1	0	3.082686	0.155703	8.442839
24	1	0	2.946125	-1.610803	8.396452
25	8	0	0.661242	0.664254	7.338686
26	8	0	3.210958	-1.023182	5.846425
27	1	0	0.269337	0.773540	8.211602
28	1	0	0.689633	-1.419398	7.349317
29	80	0	4.448684	-0.897725	3.456321

[Sep-Hg]$^{+2}$

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.081290	0.162530	0.003616
2	6	0	-0.121483	0.155962	2.272953
3	6	0	1.270698	-0.134498	2.414706
4	6	0	2.081296	-0.346702	1.266782
5	8	0	3.291552	-0.701299	1.282049
6	6	0	-0.263721	0.240342	4.772414
7	6	0	1.157485	-0.315741	4.753573
8	7	0	1.778631	-0.401694	3.624854
9	7	0	-0.829313	0.240011	3.396864
10	7	0	-0.688312	0.300193	1.077334
11	7	0	1.431782	-0.160051	0.067837
12	7	0	-0.455081	0.336263	-1.196300

13	1	0	-1.437941	0.571810	-1.245681
14	1	0	0.059833	0.256163	-2.061036
15	1	0	1.982125	-0.287348	-0.775600
16	1	0	-1.822035	0.424294	3.302911
17	1	0	-0.263699	1.254974	5.179305
18	1	0	-0.904849	-0.359266	5.415496
19	6	0	1.995702	-0.754541	5.927021
20	6	0	1.470819	-0.707490	7.355912
21	6	0	2.552498	-0.333119	8.370461
22	1	0	2.132682	-0.395380	9.376582
23	1	0	2.898753	0.688088	8.200733
24	1	0	3.397628	-1.018831	8.316049
25	8	0	0.365988	0.172679	7.362862
26	8	0	3.142281	-1.196634	5.753267
27	1	0	0.064009	0.303987	8.269385
28	1	0	1.146452	-1.747800	7.544645
29	80	0	3.979313	-1.195772	3.499833