Ten-Vertex Clusters of Germanium, Tin, and Lead Containing Interstitial Nickel, Palladium, and Platinum Atoms with 26 Skeletal Electrons: Isovalent Analogues of the Known $Pd@Bi_{10}^{4+}$

R. B. King,[1] I. Silaghi-Dumitrescu[2,3] and M. M. Uţă[2]

[1]*Department of Chemistry, University of Georgia, Athens, Georgia, 30602*

[2]*Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, Cluj-Napoca, Roumania*

Supporting Information

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[1] University of Georgia

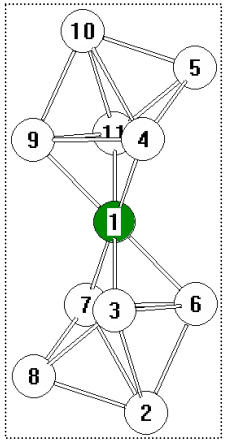
[2] Babeş-Bolyai University

[3] This paper is dedicated to the memory of Prof. Ioan Silaghi-Dumitrescu (1950–2009) in recognition of his contributions to diverse areas of inorganic and computational chemistry as well as his leadership in Romanian science

Table S1. $Ni@Ge_{10}^{6-}$ optimized structures

Charge 6-

		1	2	3	4	5	6	7	8	9	10	11
1	Ni	0.000000										
2	Ge	4.345487	0.000000									
3	Ge	2.580704	3.099595	0.000000								
4	Ge	2.585933	6.444738	3.887404	0.000000							
5	Ge	3.902014	7.808559	6.022187	2.739338	0.000000						
6	Ge	2.621485	2.677023	2.762606	4.413520	5.301135	0.000000					
7	Ge	2.585933	3.099350	3.403270	5.171865	6.026736	2.763930	0.000000				
8	Ge	3.902014	2.691534	2.739480	6.026736	7.804028	4.011703	2.739338	0.000000			
9	Ge	2.621485	6.659162	4.408225	2.763930	4.011703	5.242971	4.413520	5.301135	0.000000		
10	Ge	4.345487	8.690974	6.440427	3.099350	2.691534	6.659162	6.444738	7.808559	2.677023	0.000000	
11	Ge	2.580704	6.440427	5.161408	3.403270	2.739480	4.408225	3.887404	6.022187	2.762606	3.099595	0.000000

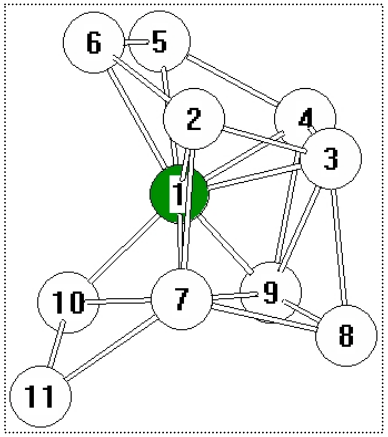


1-1-5 APP – D_{5d} → C_i [1] [1]

- 205.8743300 (+0.00 kcal/mol)

Charge 6-

		1	2	3	4	5	6	7	8	9	10	11
1	Ni	0.000000										
2	Ge	2.662888	0.000000									
3	Ge	2.675388	2.690542	0.000000								
4	Ge	2.846995	4.358524	2.675746	0.000000							
5	Ge	2.944432	4.193962	4.193354	2.636495	0.000000						
6	Ge	2.889671	2.625094	4.248995	4.283020	2.534433	0.000000					
7	Ge	2.477551	2.959666	3.407575	4.898612	5.379044	4.513824	0.000000				
8	Ge	3.747266	4.409381	2.887140	4.570054	6.294319	6.260932	2.769461	0.000000			
9	Ge	2.419282	4.598106	3.119876	2.915327	4.461085	5.249858	3.202336	2.707826	0.000000		
10	Ge	2.601357	4.718748	5.095298	4.897875	4.546372	4.451341	3.104914	4.913052	3.270575	0.000000	
11	Ge	4.155616	5.230908	6.051358	6.801692	6.681962	5.815082	2.815911	5.011433	4.664932	2.521961	0.000000

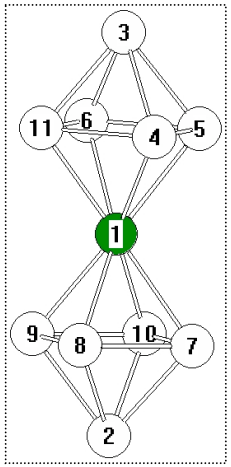


1-1-9 PP – D_{5h} → C_s → C_1 [2] [3]

- 205.8419238 (+20.33 kcal/mol)

Charge 6-

		1	2	3	4	5	6	7	8	9	10	11
1	Ni	0.000000										
2	Ge	4.480455	0.000000									
3	Ge	4.480455	8.960910	0.000000								
4	Ge	3.022872	7.087670	2.861713	0.000000							
5	Ge	3.022872	7.087670	2.861713	2.695833	0.000000						
6	Ge	3.022872	7.087670	2.861713	3.812483	2.695833	0.000000					
7	Ge	3.022872	2.861713	7.087670	4.913715	4.913715	5.867062	0.000000				
8	Ge	3.022872	2.861713	7.087670	4.913715	5.867062	5.867062	2.695833	0.000000			
9	Ge	3.022872	2.861713	7.087670	5.867062	5.867062	4.913715	3.812483	2.695833	0.000000		
10	Ge	3.022872	2.861713	7.087670	5.867062	4.913715	4.913715	2.695833	3.812483	2.695833	0.000000	
11	Ge	3.022872	7.087670	2.861713	2.695833	3.812483	2.695833	5.867062	4.913715	4.913715	5.867062	0.000000

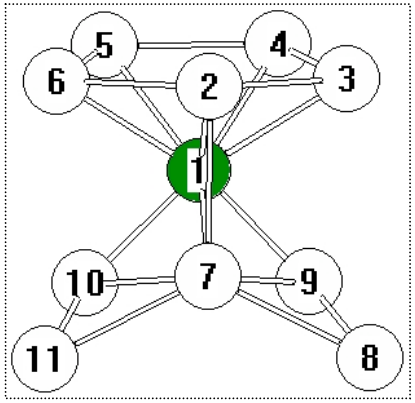


1-1-4 APT – D_{4d} [1b] [2]

- 205.8613559 (+8.14 kcal/mol) ** i -16 **

Charge 6-

		1	2	3	4	5	6	7	8	9	10	11
1	Ni	0.000000										
2	Ge	2.666860	0.000000									
3	Ge	2.607994	2.658897	0.000000								
4	Ge	2.793502	4.292274	2.641662	0.000000							
5	Ge	2.793502	4.292274	4.206206	2.531958	0.000000						
6	Ge	2.607994	2.658897	4.231427	4.206206	2.641662	0.000000					
7	Ge	2.523492	2.798798	3.771920	5.154363	5.154363	3.771920	0.000000				
8	Ge	3.933465	4.704025	4.147325	5.697846	6.668122	6.103451	2.698149	0.000000			
9	Ge	2.432962	4.531135	3.354084	3.622105	4.627365	5.010886	3.181421	2.612401	0.000000		
10	Ge	2.432962	4.531135	5.010886	4.627365	3.622105	3.354084	3.181421	4.727099	3.275278	0.000000	
11	Ge	3.933465	4.704025	6.103451	6.668122	5.697846	4.147325	2.698149	4.738782	4.727099	2.612401	0.000000



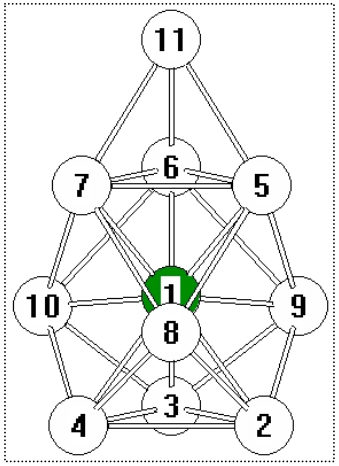
1-1-9 PP – D_{5h} → C_s [2b] [4]

- 205.8265882 (+29.96 kcal/mol) ** i -44 **

Charge 6-

		1	2	3	4	5	
1	Ni	0.000000					
2	Ge	2.690941	0.000000				
3	Ge	2.690941	3.054994	0.000000			
4	Ge	2.690941	3.054994	3.054994	0.000000		
5	Ge	2.577592	3.960429	4.973800	4.973800	0.000000	
6	Ge	2.577592	4.973800	3.960429	4.973800	2.963571	
7	Ge	2.577592	4.973800	4.973800	3.960429	2.963571	
8	Ge	2.449883	2.778105	4.536593	2.778105	3.108151	
9	Ge	2.449883	2.778105	2.778105	4.536593	3.108151	
10	Ge	2.449883	4.536593	2.778105	2.778105	4.705154	
11	Ge	4.253322	6.528385	6.528385	6.528385	2.887154	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.963571	0.000000				
8	Ge	4.705154	3.108151	0.000000			
9	Ge	3.108151	4.705154	4.210419	0.000000		
10	Ge	3.108151	3.108151	4.210419	4.210419	0.000000	
11	Ge	2.887154	2.887154	5.165546	5.165546	5.165546	0.000000



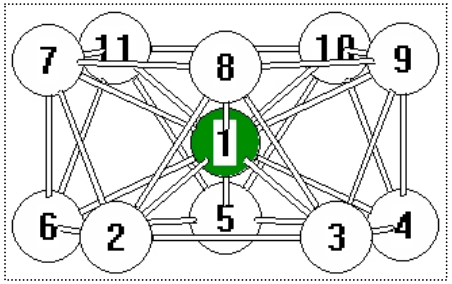
1-1-3 PTT – C_{3v} [3b] [5]

- 205.8146599 (+37.44 kcal/mol) ** i -51 **

Charge 6-

		1	2	3	4	5	
1	Ni	0.000000					
2	Ge	2.768182	0.000000				
3	Ge	2.768182	2.953265	0.000000			
4	Ge	2.768182	4.778484	2.953265	0.000000		
5	Ge	2.768182	4.778484	4.778484	2.953265	0.000000	
6	Ge	2.768182	2.953265	4.778484	4.778484	2.953265	
7	Ge	2.768182	2.795964	4.682899	5.536363	4.682899	
8	Ge	2.768182	2.795964	2.795964	4.682899	5.536363	
9	Ge	2.768182	4.682899	2.795964	2.795964	4.682899	
10	Ge	2.768182	5.536363	4.682899	2.795964	2.795964	
11	Ge	2.768182	4.682899	5.536363	4.682899	2.795964	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.795964	0.000000				
8	Ge	4.682899	2.953265	0.000000			
9	Ge	5.536363	4.778484	2.953265	0.000000		
10	Ge	4.682899	4.778484	4.778484	2.953265	0.000000	
11	Ge	2.795964	2.953265	4.778484	4.778484	2.953265	0.000000



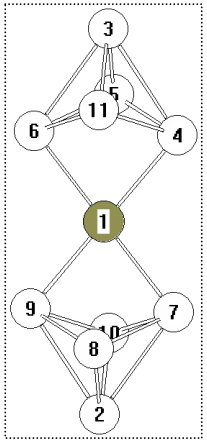
1-1-5 APP – D_{5d} [4b] [6]

- 205.7771992 (+60.95 kcal/mol) ** i -36 **

Table S2. $Pd@Ge_{10}^{6-}$ optimized structures

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pd	0.000000										
2 Ge	4.728523	0.000000									
3 Ge	4.729840	9.458363	0.000000								
4 Ge	2.792880	7.122537	3.097484	0.000000							
5 Ge	3.533222	7.907032	2.677454	2.748334	0.000000						
6 Ge	2.792880	7.122537	3.097484	3.503410	2.747461	0.000000					
7 Ge	2.796514	3.095595	7.127013	4.353172	5.749992	5.589393	0.000000				
8 Ge	3.528807	2.679036	7.903527	5.742399	7.062028	5.740654	2.747289	0.000000			
9 Ge	2.796514	3.095595	7.127013	5.589393	5.748301	4.353172	3.508359	2.746298	0.000000		
10 Ge	3.528807	2.679036	7.903527	5.740654	5.848841	5.742399	2.746298	3.956751	2.747289	0.000000	
11 Ge	3.533222	7.907032	2.677454	2.747461	3.958631	2.748334	5.748301	5.848841	5.749992	7.062028	0.000000

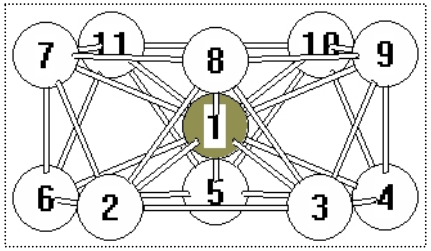


1-2-4 APT – D_{4d} [T] → C_2 [1b] [1]

- 163.3432283 (+0.00 kcal/mol) ** i -43 **

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pd	0.000000										
2 Ge	2.888264	0.000000									
3 Ge	2.888264	3.134025	0.000000								
4 Ge	2.888264	5.070959	3.134025	0.000000							
5 Ge	2.888264	5.070959	5.070959	3.134025	0.000000						
6 Ge	2.888264	3.134025	5.070959	5.070959	3.134025	0.000000					
7 Ge	2.888264	2.766524	4.852439	5.776528	4.852439	2.766524	0.000000				
8 Ge	2.888264	2.766524	2.766524	4.852439	5.776528	2.766524	3.134025	0.000000			
9 Ge	2.888264	4.852439	2.766524	2.766524	4.852439	4.852439	5.776528	3.134025	0.000000		
10 Ge	2.888264	5.776528	4.852439	2.766524	2.766524	5.776528	4.852439	2.766524	3.134025	0.000000	
11 Ge	2.888264	4.852439	5.776528	4.852439	2.766524	4.852439	5.776528	4.852439	2.766524	3.134025	0.000000



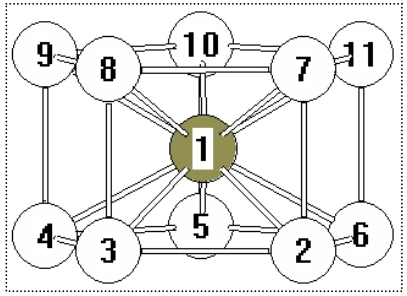
1-2-5 APP – D_{5d} [2b] [2]

- 163.2529932 (+56.62 kcal/mol) ** i -32 **

Charge 6-

		1	2	3	4	5	
1	Pd	0.000000					
2	Ge	2.817096	0.000000				
3	Ge	2.817096	2.906792	0.000000			
4	Ge	2.817096	4.703288	2.906792	0.000000		
5	Ge	2.817096	4.703288	4.703288	2.906792	0.000000	
6	Ge	2.817096	2.906792	4.703288	4.703288	2.906792	
7	Ge	2.817096	2.699601	3.967025	5.422985	5.422985	
8	Ge	2.817096	3.967025	2.699601	3.967025	5.422985	
9	Ge	2.817096	5.422985	3.967025	2.699601	3.967025	
10	Ge	2.817096	5.422985	5.422985	3.967025	2.699601	
11	Ge	2.817096	3.967025	5.422985	5.422985	3.967025	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.967025	0.000000				
8	Ge	5.422985	2.906792	0.000000			
9	Ge	5.422985	4.703288	2.906792	0.000000		
10	Ge	3.967025	4.703288	4.703288	2.906792	0.000000	
11	Ge	2.699601	2.906792	4.703288	4.703288	2.906792	0.000000



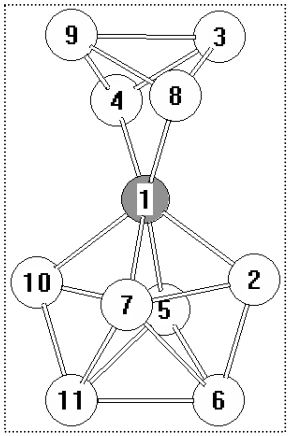
1-2-9 PP – D_{5h} [3b] [3]

- 163.2454313 (+61.37 kcal/mol) ** i -49 **

Table S3. $Pt@Ge_{10}^{6-}$ optimized structures

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Ge	2.870895	0.000000									
3 Ge	3.458544	5.021784	0.000000								
4 Ge	2.713385	5.333096	2.664390	0.000000							
5 Ge	2.861095	3.658387	5.499041	4.108617	0.000000						
6 Ge	4.084281	2.675996	6.976155	6.367089	2.844678	0.000000					
7 Ge	2.861095	2.579638	5.984488	5.498005	3.969815	3.166849	0.000000				
8 Ge	2.713385	3.853712	2.695220	3.788659	5.498005	6.111636	4.108617	0.000000			
9 Ge	3.458544	5.884590	2.962962	2.695220	5.984488	7.520986	5.499041	2.664390	0.000000		
10 Ge	2.870895	4.826497	5.884590	3.853712	2.579638	4.339119	3.658387	5.333096	5.021784	0.000000	
11 Ge	4.084281	4.339119	7.520986	6.111636	3.166849	2.807461	2.844678	6.367089	6.976155	2.675996	0.000000

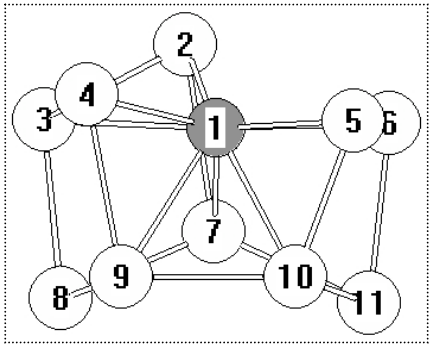


1-3-5 APP – D_{5d} → C_2 [1] [4]

- 155.7167174 (+25.53 kcal/mol)

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Ge	2.550154	0.000000									
3 Ge	2.815043	2.740746	0.000000								
4 Ge	2.630491	4.178723	2.731983	0.000000							
5 Ge	2.824989	4.926459	5.536432	4.115918	0.000000						
6 Ge	2.762305	3.637732	5.307224	5.241367	2.672333	0.000000					
7 Ge	2.991965	2.927900	3.494326	5.074076	5.184238	3.633851	0.000000				
8 Ge	3.797925	4.393616	2.767635	4.378372	6.185936	5.745130	2.797861	0.000000			
9 Ge	2.934929	4.954897	3.409793	2.873346	4.344843	5.096601	4.005297	2.738285	0.000000		
10 Ge	2.760479	5.025812	4.940599	4.294958	2.697173	3.239012	3.780469	4.328753	2.679291	0.000000	
11 Ge	3.844214	4.905479	5.741490	6.203034	4.336077	2.850189	2.831684	4.734472	4.620001	2.694671	0.000000

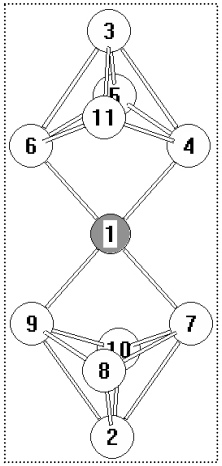


1-3-9 PP – D_{5h} → C_s → C_1 [2] [5]

- 155.6765588 (+50.73 kcal/mol)

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Ge	4.591378	0.000000									
3 Ge	4.607546	9.198923	0.000000								
4 Ge	2.676161	6.832496	3.144195	0.000000							
5 Ge	3.516200	7.747886	2.629488	2.807478	0.000000						
6 Ge	2.676161	6.832496	3.144195	3.537876	2.813098	0.000000					
7 Ge	2.703528	3.125911	6.871870	4.036018	5.619804	5.379490	0.000000				
8 Ge	3.475389	2.641170	7.719022	5.554438	6.991448	5.525617	2.793151	0.000000			
9 Ge	2.703528	3.125911	6.871870	5.379490	5.589578	4.036018	3.576649	2.801434	0.000000		
10 Ge	3.475389	2.641170	7.719022	5.525617	5.746642	5.554438	2.801434	3.973966	2.793151	0.000000	
11 Ge	3.516200	7.747886	2.629488	2.813098	3.990919	2.807478	5.589578	5.746642	5.619804	6.991448	0.000000

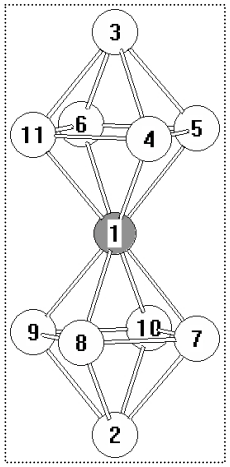


1-3-4 APT – D_{4d} ^{T} → C_2 [1b] [1]

- 155.7574007 (+0.00 kcal/mol) ** i -54 **

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Ge	4.392438	0.000000									
3 Ge	4.392438	8.784876	0.000000								
4 Ge	2.932627	6.886088	2.892995	0.000000							
5 Ge	2.932627	6.886088	2.892995	2.705842	0.000000						
6 Ge	2.932627	6.886088	2.892995	3.826638	2.705842	0.000000					
7 Ge	2.932627	2.892995	6.886088	4.680008	4.680008	5.679503	0.000000				
8 Ge	2.932627	2.892995	6.886088	4.680008	5.679503	4.680008	2.705842	0.000000			
9 Ge	2.932627	2.892995	6.886088	5.679503	5.679503	4.680008	3.826638	2.705842	0.000000		
10 Ge	2.932627	2.892995	6.886088	5.679503	4.680008	4.680008	2.705842	3.826638	2.705842	0.000000	
11 Ge	2.932627	6.886088	2.892995	2.705842	3.826638	2.705842	5.679503	4.680008	4.680008	5.679503	0.000000



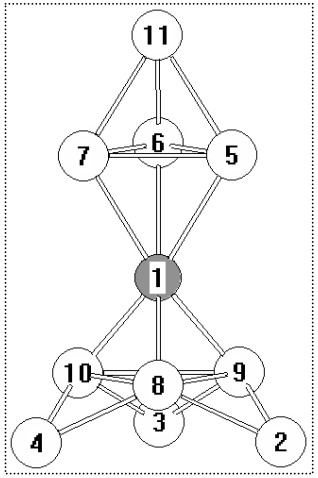
1-3-4 APT – D_{4d} ^{T} [2b] [2]

- 155.7338603 (+14.77 kcal/mol) ** i -52 **

Charge 6-

		1	2	3	4	5	
1	Pt	0.000000					
2	Ge	4.098145	0.000000				
3	Ge	4.098145	4.723846	0.000000			
4	Ge	4.098145	4.723846	4.723846	0.000000		
5	Ge	2.953023	5.615191	6.708391	6.708391	0.000000	
6	Ge	2.953023	6.708391	5.615191	6.708391	2.851942	
7	Ge	2.953023	6.708391	6.708391	5.615191	2.851942	
8	Ge	2.624594	2.659617	4.664773	2.659617	4.694785	
9	Ge	2.624594	2.659617	2.659617	4.664773	4.694785	
10	Ge	2.624594	4.664773	2.659617	2.659617	5.559475	
11	Ge	4.693168	8.217785	8.217785	8.217785	2.781529	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	2.851942	0.000000				
8	Ge	5.559475	4.694785	0.000000			
9	Ge	4.694785	5.559475	3.109023	0.000000		
10	Ge	4.694785	4.694785	3.109023	3.109023	0.000000	
11	Ge	2.781529	2.781529	6.847433	6.847433	6.847433	0.000000



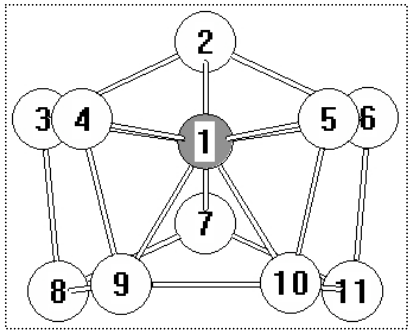
1-3-3 PTT – C_{3v} [3b] [3]

- 155.7308698 (+16.65 kcal/mol) ** i -67 **

Charge 6-

		1	2	3	4	5	
1	Pt	0.000000					
2	Ge	2.529299	0.000000				
3	Ge	2.775023	3.031120	0.000000			
4	Ge	2.642596	4.364251	2.747434	0.000000		
5	Ge	2.642596	4.364251	5.277615	3.933029	0.000000	
6	Ge	2.775023	3.031120	5.162642	5.277615	2.747434	
7	Ge	2.989825	2.961195	3.529411	5.116640	5.116640	
8	Ge	3.715360	4.606522	2.833181	4.355897	6.115484	
9	Ge	2.779208	4.982048	3.437463	2.812134	4.305912	
10	Ge	2.779208	4.982048	5.076725	4.305912	2.812134	
11	Ge	3.715360	4.606522	5.675620	6.115484	4.355897	

		6	7	8	9	10	11
6	Ge	0.000000					
7	Ge	3.529411	0.000000				
8	Ge	5.675620	2.787414	0.000000			
9	Ge	5.076725	3.966036	2.734833	0.000000		
10	Ge	3.437463	3.966036	4.488248	2.703458	0.000000	
11	Ge	2.833181	2.787414	4.684762	4.488248	2.734833	0.000000



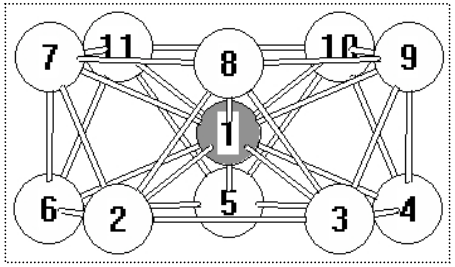
1-3-9 PP – D_{5h} → C_s [4b] [6]

- 155.6760924 (+51.02 kcal/mol) ** i -17 **

Charge 6-

	1	2	3	4	5	
1 Pt	0.000000					
2 Ge	2.897246	0.000000				
3 Ge	2.897246	3.146797	0.000000			
4 Ge	2.897246	5.091625	3.146797	0.000000		
5 Ge	2.897246	5.091625	5.091625	3.146797	0.000000	
6 Ge	2.897246	3.146797	5.091625	5.091625	3.146797	
7 Ge	2.897246	2.766135	4.865574	5.794492	4.865574	
8 Ge	2.897246	2.766135	2.766135	4.865574	5.794492	
9 Ge	2.897246	4.865574	2.766135	2.766135	4.865574	
10 Ge	2.897246	5.794492	4.865574	2.766135	2.766135	
11 Ge	2.897246	4.865574	5.794492	4.865574	2.766135	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	2.766135	0.000000				
8 Ge	4.865574	3.146797	0.000000			
9 Ge	5.794492	5.091625	3.146797	0.000000		
10 Ge	4.865574	5.091625	5.091625	3.146797	0.000000	
11 Ge	2.766135	3.146797	5.091625	5.091625	3.146797	0.000000



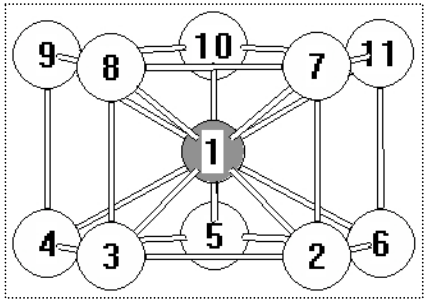
1-3-5 APP – D_{5d} [5b] [7]

- 155.6674295 (+56.46 kcal/mol) ** i -30 **

Charge 6-

	1	2	3	4	5	
1 Pt	0.000000					
2 Ge	2.830235	0.000000				
3 Ge	2.830235	2.922972	0.000000			
4 Ge	2.830235	4.729468	2.922972	0.000000		
5 Ge	2.830235	4.729468	4.729468	2.922972	0.000000	
6 Ge	2.830235	2.922972	4.729468	4.729468	2.922972	
7 Ge	2.830235	2.704000	3.981881	5.447888	5.447888	
8 Ge	2.830235	3.981881	2.704000	3.981881	5.447888	
9 Ge	2.830235	5.447888	3.981881	2.704000	3.981881	
10 Ge	2.830235	5.447888	5.447888	3.981881	2.704000	
11 Ge	2.830235	3.981881	5.447888	5.447888	3.981881	

	6	7	8	9	10	11
6 Ge	0.000000					
7 Ge	3.981881	0.000000				
8 Ge	5.447888	2.922972	0.000000			
9 Ge	5.447888	4.729468	2.922972	0.000000		
10 Ge	3.981881	4.729468	4.729468	2.922972	0.000000	
11 Ge	2.704000	2.922972	4.729468	4.729468	2.922972	0.000000



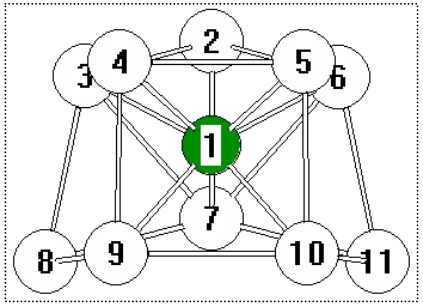
1-3-9 PP – D_{5h} [6b] [8]

- 155.6612189 (+60.35 kcal/mol) ** i -42 **

Table S4. $Ni@Sn_{10}^{6-}$ optimized structures

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Ni	0.000000										
2 Sn	4.034569	0.000000									
3 Sn	2.772850	3.173668	0.000000								
4 Sn	2.675429	5.553201	3.111423	0.000000							
5 Sn	2.675429	5.553201	4.774542	3.082544	0.000000						
6 Sn	2.772850	3.173668	4.254698	4.774542	3.111423	0.000000					
7 Sn	2.969113	3.110226	3.456342	5.338711	5.338711	3.456342	0.000000				
8 Sn	3.713426	5.090761	3.165856	4.783527	6.326134	5.803210	3.113826	0.000000			
9 Sn	2.763224	6.325968	4.042578	3.222520	4.497145	5.470257	4.393428	3.089307	0.000000		
10 Sn	2.763224	6.325968	5.470257	4.497145	3.222520	4.042578	4.393428	5.224037	3.192066	0.000000	
11 Sn	3.713426	5.090761	5.803210	6.326134	4.783527	3.165856	3.113826	5.559643	5.224037	3.089307	0.000000

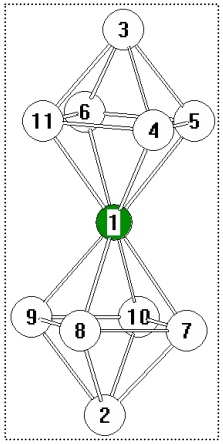


2-1-9 PP – D_{5h} → C_s [1] [3]

- 202.1644044 (+29.07 kcal/mol)

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Ni	0.000000										
2 Sn	5.052381	0.000000									
3 Sn	5.052381	10.104761	0.000000								
4 Sn	3.417559	8.001684	3.222666	0.000000							
5 Sn	3.417559	8.001684	3.222666	3.044537	0.000000						
6 Sn	3.417559	8.001684	3.222666	4.305626	3.044537	0.000000					
7 Sn	3.417559	3.222666	8.001684	5.558356	5.558356	6.633548	0.000000				
8 Sn	3.417559	3.222666	8.001684	5.558356	6.633548	6.633548	3.044537	0.000000			
9 Sn	3.417559	3.222666	8.001684	6.633548	6.633548	5.558356	5.558356	3.044537	0.000000		
10 Sn	3.417559	3.222666	8.001684	6.633548	5.558356	5.558356	6.633548	4.305626	3.044537	0.000000	
11 Sn	3.417559	8.001684	3.222666	3.044537	4.305626	6.633548	5.558356	5.558356	6.633548	3.044537	0.000000



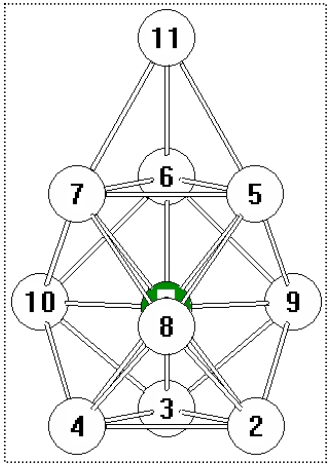
2-1-4 APT – D_{4d} [1b] [1]

- 202.2107385 (+0.00 kcal/mol) ** i -63 **

Charge 6-

		1	2	3	4	5	
1	Ni	0.000000					
2	Sn	2.826228	0.000000				
3	Sn	2.826228	3.290469	0.000000			
4	Sn	2.826228	3.290469	3.290469	0.000000		
5	Sn	2.894206	4.286763	5.397424	5.397424	0.000000	
6	Sn	2.894206	5.397424	4.286763	5.397424	3.268790	
7	Sn	2.894206	5.397424	5.397424	4.286763	3.268790	
8	Sn	2.687492	3.140791	5.017745	3.140791	3.283476	
9	Sn	2.687492	3.140791	3.140791	5.017745	3.283476	
10	Sn	2.687492	5.017745	3.140791	3.140791	5.098384	
11	Sn	4.972516	7.315963	7.315963	7.315963	3.358628	

		6	7	8	9	10	11
6	Sn	0.000000					
7	Sn	3.268790	0.000000				
8	Sn	5.098384	3.283476	0.000000			
9	Sn	3.283476	5.098384	4.653802	0.000000		
10	Sn	3.283476	3.283476	4.653802	4.653802	0.000000	
11	Sn	3.358628	3.358628	5.702782	5.702782	5.702782	0.000000



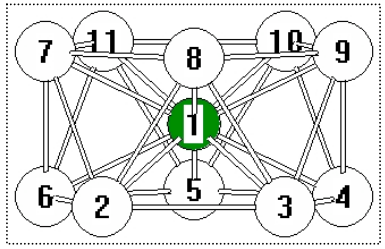
2-1-3 PTT – C_{3v} [2b] [2]

- 202.1901700 (+12.91 kcal/mol) ** i -8 **

Charge 6-

		1	2	3	4	5	
1	Ni	0.000000					
2	Sn	3.055812	0.000000				
3	Sn	3.055812	3.232385	0.000000			
4	Sn	3.055812	5.230109	3.232385	0.000000		
5	Sn	3.055812	5.230109	5.230109	3.232385	0.000000	
6	Sn	3.055812	3.232385	5.230109	5.230109	3.232385	
7	Sn	3.055812	3.161946	5.186871	6.111624	5.186871	
8	Sn	3.055812	3.161946	3.161946	5.186871	6.111624	
9	Sn	3.055812	5.186871	3.161946	3.161946	5.186871	
10	Sn	3.055812	6.111624	5.186871	3.161946	3.161946	
11	Sn	3.055812	5.186871	6.111624	5.186871	3.161946	

		6	7	8	9	10	11
6	Sn	0.000000					
7	Sn	3.161946	0.000000				
8	Sn	5.186871	3.232385	0.000000			
9	Sn	6.111624	5.230109	3.232385	0.000000		
10	Sn	5.186871	5.230109	5.230109	3.232385	0.000000	
11	Sn	3.161946	3.232385	5.230109	5.230109	3.232385	0.000000

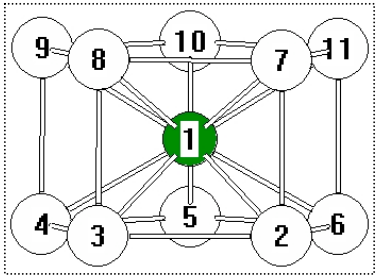


2-1-5 APP – D_{5d} [3b] [4]

- 202.1406861 (+43.96 kcal/mol) ** i -72 **

Charge 6-

		1	2	3	4	5	6	7	8	9	10	11
1	Ni	0.000000										
2	Sn	3.060308	0.000000									
3	Sn	3.060308	3.131625	0.000000								
4	Sn	3.060308	5.067076	3.131625	0.000000							
5	Sn	3.060308	5.067076	5.067076	3.131625	0.000000						
6	Sn	3.060308	3.131625	5.067076	5.067076	3.131625	0.000000					
7	Sn	3.060308	3.012653	4.345475	5.895026	5.895026	4.345475	0.000000				
8	Sn	3.060308	4.345475	3.012653	4.345475	5.895026	5.895026	3.131625	0.000000			
9	Sn	3.060308	5.895026	4.345475	3.012653	4.345475	5.067076	5.067076	3.131625	0.000000		
10	Sn	3.060308	5.895026	5.895026	4.345475	3.012653	5.067076	3.131625	5.067076	3.131625	0.000000	
11	Sn	3.060308	4.345475	5.895026	5.895026	4.345475	3.131625	5.067076	5.067076	3.131625	3.131625	0.000000

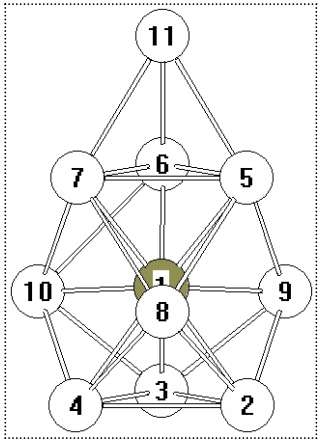


2-1-9 PP – D_{5h} [4b] [5]

- 202.1383091 (+45.45 kcal/mol) ** i -96 **

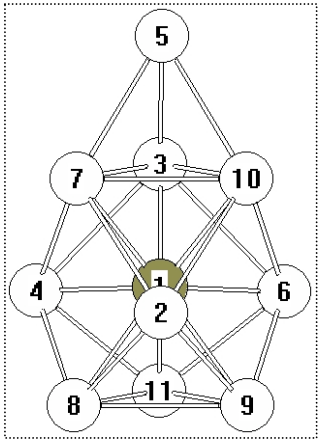
Table S5. $Pd@Sn_{10}^{6-}$ optimized structures

Charge 6-		1	2	3	4	5		
	1 Pd	0.000000						
	2 Sn	2.964180	0.000000					
	3 Sn	2.964180	3.365901	0.000000				
	4 Sn	2.964180	3.365901	3.365901	0.000000			
	5 Sn	2.929333	4.461367	5.570086	5.570086	0.000000		
	6 Sn	2.929333	5.570086	4.461367	5.570086	3.304335		
	7 Sn	2.929333	5.570086	5.570086	4.461367	3.304335		
	8 Sn	2.797000	3.188227	5.139653	3.188227	3.479491		
	9 Sn	2.797000	3.188227	3.188227	5.139653	3.479491		
	10 Sn	2.797000	5.139653	3.188227	3.188227	5.297249		
	11 Sn	4.921435	7.418765	7.418765	7.418765	3.304760		
		6	7	8	9	10	11	
	6 Sn	0.000000						
	7 Sn	3.304335	0.000000					
	8 Sn	5.297249	3.479491	0.000000				
	9 Sn	3.479491	5.297249	4.828200	0.000000			
	10 Sn	3.479491	3.479491	4.828200	4.828200	0.000000		
	11 Sn	3.304760	3.304760	5.856910	5.856910	5.856910	0.000000	
Charge 6-		1	2	3	4	5		
	1 Pd	0.000000						
	2 Sn	2.795120	0.000000					
	3 Sn	2.930507	5.299193	0.000000				
	4 Sn	2.797372	4.823135	3.481109	0.000000			
	5 Sn	4.919136	5.860361	3.301480	5.856435	0.000000		
	6 Sn	2.795299	4.829025	3.477540	4.825933	5.851721		
	7 Sn	2.926094	3.477059	3.305604	3.475582	3.310110		
	8 Sn	2.968376	3.186087	5.574432	3.188142	7.422780		
	9 Sn	2.963716	3.188235	5.570606	5.137695	7.417237		
	10 Sn	2.929302	3.485433	3.304758	5.297499	3.301094		
	11 Sn	2.965759	5.139231	4.459109	3.185657	7.414550		
		6	7	8	9	10	11	
	6 Sn	0.000000						
	7 Sn	5.294098	0.000000					
	8 Sn	5.140675	4.461421	0.000000				
	9 Sn	3.188354	5.567408	3.366460	0.000000			
	10 Sn	3.480132	3.305062	5.575578	4.463868	0.000000		
	11 Sn	3.186989	5.566103	3.368199	3.368594	5.571613	0.000000	



2-2-3 PTT – C_{3v} [1] [1]

- 159.6662295 (**+0.00 kcal/mol**)



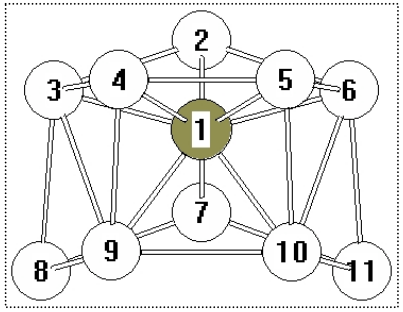
2-2-4 APT – $D_{4d}{}^{T}$ → C_1 [1] [1]

- 159.6662295 (**+0.00 kcal/mol**)

Charge 6-

		1	2	3	4	5	
1	Pd	0.000000					
2	Sn	2.862098	0.000000				
3	Sn	2.819741	3.209631	0.000000			
4	Sn	2.934269	5.023984	3.341156	0.000000		
5	Sn	2.936420	5.027039	5.166118	2.954908	0.000000	
6	Sn	2.821123	3.208303	5.247547	5.161992	3.340605	
7	Sn	2.914416	3.045771	3.829706	5.631311	5.629864	
8	Sn	4.216695	5.018179	3.389251	5.585268	6.931474	
9	Sn	2.855000	5.276990	3.496196	3.358374	4.551167	
10	Sn	2.853623	5.276406	5.383419	4.547578	3.351431	
11	Sn	4.216510	5.018075	6.439316	6.928858	5.576018	

		6	7	8	9	10	11
6	Sn	0.000000					
7	Sn	3.826688	0.000000				
8	Sn	6.437711	3.119868	0.000000			
9	Sn	5.386783	3.916232	3.102165	0.000000		
10	Sn	3.498803	3.914617	5.278479	3.195172	0.000000	
11	Sn	3.384576	3.120638	5.713772	5.282218	3.102866	0.000000



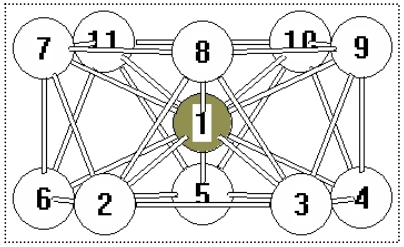
2-2-9 PP – D_{5h} → C_1 [2] [2]

- 159.6594439 (+4.26 kcal/mol)

Charge 6-

		1	2	3	4	5	
1	Pd	0.000000					
2	Sn	3.125061	0.000000				
3	Sn	3.125061	3.340238	0.000000			
4	Sn	3.125061	5.404619	3.340238	0.000000		
5	Sn	3.125061	5.404619	5.404619	3.340238	0.000000	
6	Sn	3.125061	3.340238	5.404619	5.404619	3.340238	
7	Sn	3.125061	3.139128	5.282692	6.250122	5.282692	
8	Sn	3.125061	3.139128	3.139128	5.282692	6.250122	
9	Sn	3.125061	5.282692	3.139128	3.139128	5.282692	
10	Sn	3.125061	6.250122	5.282692	3.139128	3.139128	
11	Sn	3.125061	5.282692	6.250122	5.282692	3.139128	

		6	7	8	9	10	11
6	Sn	0.000000					
7	Sn	3.139128	0.000000				
8	Sn	5.282692	3.340238	0.000000			
9	Sn	6.250122	5.404619	3.340238	0.000000		
10	Sn	5.282692	5.404619	5.404619	3.340238	0.000000	
11	Sn	3.139128	3.340238	5.404619	5.404619	3.340238	0.000000

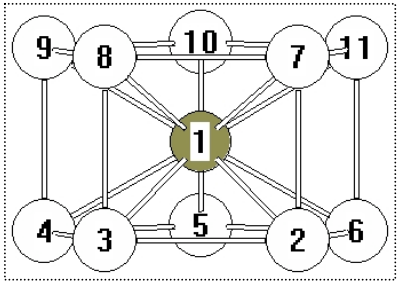


2-2-5 APP – D_{5d} [3] [3]

- 159.6387043 (+17.27 kcal/mol)

Charge 6-

		1	2	3	4	5	6	7	8	9	10	11
1	Pd	0.000000										
2	Sn	3.100974	0.000000									
3	Sn	3.100974	3.183950	0.000000								
4	Sn	3.100974	5.151739	3.183950	0.000000							
5	Sn	3.100974	5.151739	5.151739	3.183950	0.000000						
6	Sn	3.100974	3.183950	5.151739	5.151739	3.183950	0.000000					
7	Sn	3.100974	3.020231	4.388545	5.971784	5.971784	4.388545	0.000000				
8	Sn	3.100974	4.388545	3.020231	4.388545	5.971784	5.971784	3.183950	0.000000			
9	Sn	3.100974	5.971784	4.388545	3.020231	4.388545	5.151739	3.183950	3.183950	0.000000		
10	Sn	3.100974	5.971784	5.971784	4.388545	3.020231	5.151739	5.151739	3.183950	3.183950	0.000000	
11	Sn	3.100974	4.388545	5.971784	5.971784	4.388545	5.151739	5.151739	3.183950	3.183950	3.183950	0.000000

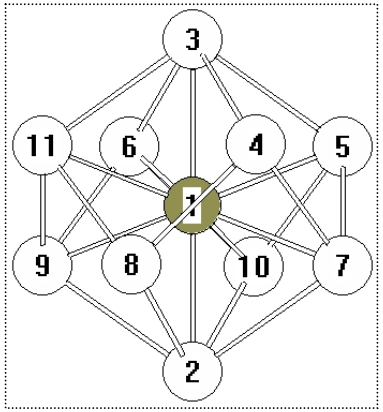


2-2-9 PP – D_{5h} [1b] [4]

- 159.6277983 (+24.12 kcal/mol) ** i -64 **

Charge 6-

		1	2	3	4	5	6	7	8	9	10	11
1	Pd	0.000000										
2	Sn	2.930396	0.000000									
3	Sn	2.930396	5.860792	0.000000								
4	Sn	3.048236	4.905843	3.419156	0.000000							
5	Sn	3.048236	4.905843	3.419156	4.043969	0.000000						
6	Sn	3.048236	4.905843	3.419156	5.719037	4.043969	0.000000					
7	Sn	3.048236	3.419156	4.905843	3.041296	3.041296	5.690087	0.000000				
8	Sn	3.048236	3.419156	4.905843	3.041296	5.690087	5.690087	4.043969	0.000000			
9	Sn	3.048236	3.419156	4.905843	5.690087	5.690087	3.041296	3.041296	4.043969	0.000000		
10	Sn	3.048236	3.419156	4.905843	5.690087	3.041296	5.690087	4.043969	3.041296	4.043969	0.000000	
11	Sn	3.048236	4.905843	3.419156	4.043969	5.719037	4.043969	5.690087	3.041296	3.041296	5.690087	0.000000



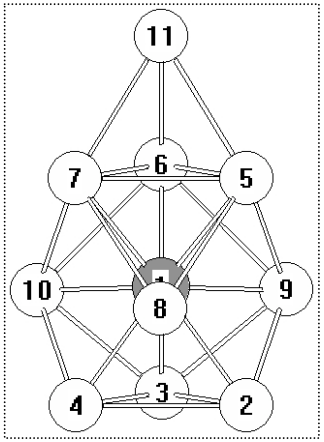
2-2-4 APT – D_{4d} [2b] [5]

- 159.6061848 (+37.68 kcal/mol) ** i -47 **

Table S6. $Pt@Sn_{10}^{6-}$ optimized structures

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Sn	2.961671	0.000000									
3 Sn	2.961671	3.337256	0.000000								
4 Sn	2.961671	3.337256	3.337256	0.000000							
5 Sn	2.935490	4.460690	5.572814	5.572814	0.000000						
6 Sn	2.935490	5.572814	4.460690	5.572814	3.343614	0.000000					
7 Sn	2.935490	5.572814	5.572814	4.460690	3.343614	3.343614	0.000000				
8 Sn	2.809127	3.224778	5.157404	3.224778	3.456479	5.308270	3.456479	0.000000			
9 Sn	2.809127	3.224778	3.224778	5.157404	3.456479	3.456479	5.308270	3.456479	0.000000		
10 Sn	2.809127	5.157404	3.224778	3.224778	5.308270	3.456479	3.456479	4.854175	4.854175	0.000000	
11 Sn	4.898304	7.402688	7.402688	7.402688	3.308439	3.308439	3.308439	5.810796	5.810796	5.810796	0.000000

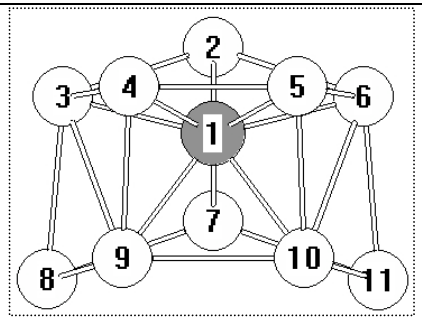


2-3-3 PTT – C_{3v} [1] [3]

- 152.0905820 (+22.91 kcal/mol)

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Sn	2.883436	0.000000									
3 Sn	2.822745	3.225082	0.000000								
4 Sn	2.953890	5.127452	3.416822	0.000000							
5 Sn	2.952732	5.126212	5.214279	2.952490	0.000000						
6 Sn	2.822492	3.224875	5.257395	5.216178	3.417270	0.000000					
7 Sn	2.884823	3.053194	3.792355	5.607200	5.606859	3.792365	0.000000				
8 Sn	4.256975	5.040893	3.364631	5.592482	6.954999	6.462541	3.138029	0.000000			
9 Sn	2.868429	5.298220	3.497688	3.318119	4.519037	5.384443	3.857885	3.119096	0.000000		
10 Sn	2.868217	5.298711	5.384077	4.518750	3.318834	3.498757	3.858542	5.308841	3.186501	0.000000	
11 Sn	4.255792	5.040602	6.461916	6.954707	5.592184	3.363970	3.137984	5.790298	5.308012	3.119045	0.000000



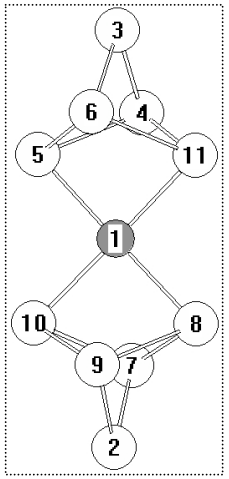
2-3-9 PP – D_{5h} → C_1 [2] [4]

- 152.0871609 (+25.05 kcal/mol)

Charge 6-

		1	2	3	4	5	
1	Pt	0.000000					
2	Sn	4.993346	0.000000				
3	Sn	5.011576	10.004922	0.000000			
4	Sn	3.787650	8.347258	2.992374	0.000000		
5	Sn	2.805679	7.275624	3.575595	3.144389	0.000000	
6	Sn	3.787650	8.347258	2.992374	4.508627	3.163699	
7	Sn	3.760027	2.997106	8.333799	6.059887	5.772323	
8	Sn	2.817451	3.565002	7.299988	5.807317	5.619513	
9	Sn	3.760027	2.997106	8.333799	7.545040	5.915303	
10	Sn	2.817451	3.565002	7.299988	5.951803	4.039587	
11	Sn	2.805679	7.275624	3.575595	3.163699	3.903394	

		6	7	8	9	10	11
6	Sn	0.000000					
7	Sn	7.545040	0.000000				
8	Sn	5.951803	3.137314	0.000000			
9	Sn	6.059887	4.499058	3.158790	0.000000		
10	Sn	5.807317	3.158790	3.930398	3.137314	0.000000	
11	Sn	3.144389	5.915303	4.039587	5.772323	5.619513	0.000000



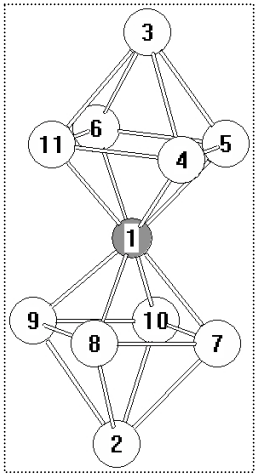
2-3-4 APT – D_{4d} ^{T} → C_2 [1b] [1]

- 152.1270877 (+0.00 kcal/mol) ** i -39 **

Charge 6-

		1	2	3	4	5	
1	Pt	0.000000					
2	Sn	4.623185	0.000000				
3	Sn	4.623185	9.246370	0.000000			
4	Sn	3.015162	7.072605	3.302777	0.000000		
5	Sn	3.015162	7.072605	3.302777	3.038976	0.000000	
6	Sn	3.015162	7.072605	3.302777	4.297761	3.038976	
7	Sn	3.015162	3.302777	7.072605	4.538615	4.538615	
8	Sn	3.015162	3.302777	7.072605	4.538615	5.801709	
9	Sn	3.015162	3.302777	7.072605	5.801709	5.801709	
10	Sn	3.015162	3.302777	7.072605	5.801709	4.538615	
11	Sn	3.015162	7.072605	3.302777	3.038976	4.297761	

		6	7	8	9	10	11
6	Sn	0.000000					
7	Sn	5.801709	0.000000				
8	Sn	5.801709	3.038976	0.000000			
9	Sn	4.538615	4.297761	3.038976	0.000000		
10	Sn	4.538615	3.038976	4.297761	3.038976	0.000000	
11	Sn	3.038976	5.801709	4.538615	4.538615	5.801709	0.000000



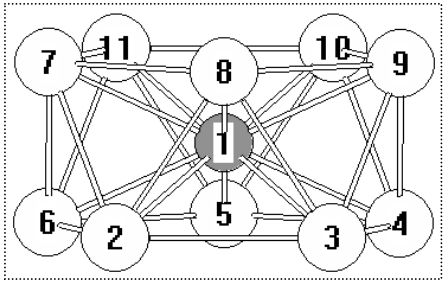
2-3-4 APT – D_{4d} ^{T} [2b] [2]

- 152.1035906 (+14.74 kcal/mol) ** i -28 **

Charge 6-

	1	2	3	4	5	
1 Pt	0.000000					
2 Sn	3.121396	0.000000				
3 Sn	3.121396	3.336691	0.000000			
4 Sn	3.121396	5.398879	3.336691	0.000000		
5 Sn	3.121396	5.398879	5.398879	3.336691	0.000000	
6 Sn	3.121396	3.336691	5.398879	5.398879	3.336691	
7 Sn	3.121396	3.134417	5.276264	6.242793	5.276264	
8 Sn	3.121396	3.134417	3.134417	5.276264	6.242793	
9 Sn	3.121396	5.276264	3.134417	3.134417	5.276264	
10 Sn	3.121396	6.242793	5.276264	3.134417	3.134417	
11 Sn	3.121396	5.276264	6.242793	5.276264	3.134417	

	6	7	8	9	10	11
6 Sn	0.000000					
7 Sn	3.134417	0.000000				
8 Sn	5.276264	3.336691	0.000000			
9 Sn	6.242793	5.398879	3.336691	0.000000		
10 Sn	5.276264	5.398879	5.398879	3.336691	0.000000	
11 Sn	3.134417	3.336691	5.398879	5.398879	3.336691	0.000000



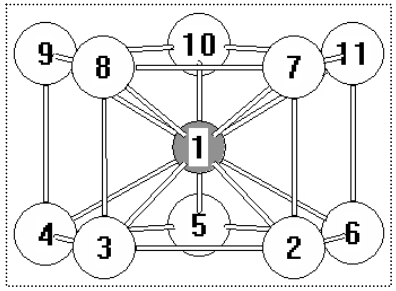
2-3-5 APP – D_{5d} [3b] [5]

- 152.0557673 (+44.75 kcal/mol) ** i -10 **

Charge 6-

	1	2	3	4	5	
1 Pt	0.000000					
2 Sn	3.097934	0.000000				
3 Sn	3.097934	3.180000	0.000000			
4 Sn	3.097934	5.145349	3.180000	0.000000		
5 Sn	3.097934	5.145349	5.145349	3.180000	0.000000	
6 Sn	3.097934	3.180000	5.145349	5.145349	3.180000	
7 Sn	3.097934	3.019797	4.385382	5.966053	5.966053	
8 Sn	3.097934	4.385382	3.019797	4.385382	5.966053	
9 Sn	3.097934	5.966053	4.385382	3.019797	4.385382	
10 Sn	3.097934	5.966053	5.966053	4.385382	3.019797	
11 Sn	3.097934	4.385382	5.966053	5.966053	4.385382	

	6	7	8	9	10	11
6 Sn	0.000000					
7 Sn	4.385382	0.000000				
8 Sn	5.966053	3.180000	0.000000			
9 Sn	5.966053	5.145349	3.180000	0.000000		
10 Sn	4.385382	5.145349	5.145349	3.180000	0.000000	
11 Sn	3.019797	3.180000	5.145349	5.145349	3.180000	0.000000



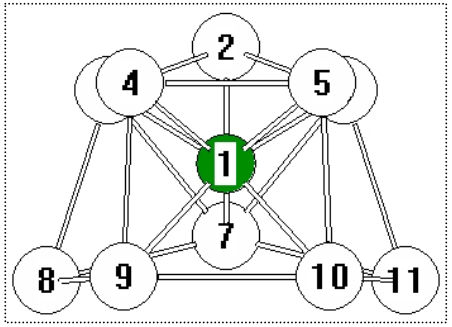
2-3-9 PP – D_{5h} [4b] [6]

- 152.0486673 (+49.21 kcal/mol) ** i -57 **

Table S7. $Ni@Pb_{10}^{6-}$ optimized structures

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Ni	0.000000										
2 Pb	4.525648	0.000000									
3 Pb	2.693349	3.374654	0.000000								
4 Pb	2.812339	6.241954	3.365195	0.000000							
5 Pb	2.813748	6.244508	4.859259	3.162466	0.000000						
6 Pb	2.692521	3.373382	3.877745	4.855008	3.366380	0.000000					
7 Pb	3.083508	3.353521	3.383175	5.606078	5.610816	3.390307	0.000000				
8 Pb	3.826582	5.528483	3.289877	4.883857	6.529245	5.817630	3.351827	0.000000			
9 Pb	2.882901	6.884061	4.173925	3.228286	4.603365	5.534762	4.618278	3.124740	0.000000		
10 Pb	2.880621	6.885305	5.532385	4.598312	3.227423	4.178477	4.622732	5.470750	3.398828	0.000000	
11 Pb	3.813915	5.522538	5.805738	6.516216	4.878327	3.289019	3.349739	5.919743	5.460699	3.121533	0.000000

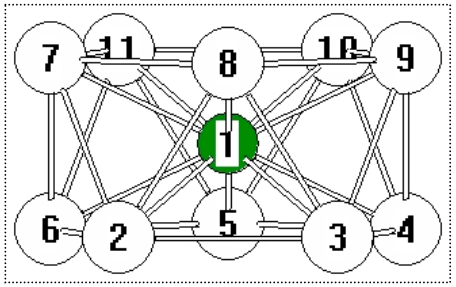


3-1-9 PP – D_{5h} → C_1 [1] [1]

- 203.1386880 (+0.00 kcal/mol)

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Ni	0.000000										
2 Pb	3.169365	0.000000									
3 Pb	3.169365	3.372612	0.000000								
4 Pb	3.169365	5.457001	3.372612	0.000000							
5 Pb	3.169365	5.457001	5.457001	3.372612	0.000000						
6 Pb	3.169365	3.372612	5.457001	5.457001	3.372612	0.000000					
7 Pb	3.169365	3.225000	5.367027	6.338729	5.367027	3.225000	0.000000				
8 Pb	3.169365	3.225000	3.225000	5.367027	6.338729	5.367027	3.372612	0.000000			
9 Pb	3.169365	5.367027	3.225000	3.225000	5.367027	6.338729	5.457001	3.372612	0.000000		
10 Pb	3.169365	6.338729	5.367027	3.225000	3.225000	5.367027	5.457001	5.457001	3.372612	0.000000	
11 Pb	3.169365	5.367027	6.338729	5.367027	3.225000	3.225000	3.372612	5.457001	5.457001	3.372612	0.000000



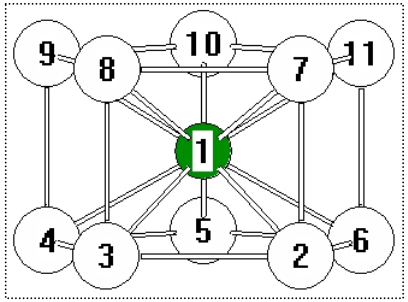
3-1-5 APP – D_{5d} [1b] [2]

- 203.1254879 (+8.28 kcal/mol) ** i -73 **

Charge 6-

		1	2	3	4	5	
1	Ni	0.000000					
2	Pb	3.157050	0.000000				
3	Pb	3.157050	3.231911	0.000000			
4	Pb	3.157050	5.229342	3.231911	0.000000		
5	Pb	3.157050	5.229342	5.229342	3.231911	0.000000	
6	Pb	3.157050	3.231911	5.229342	5.229342	3.231911	
7	Pb	3.157050	3.104007	4.481084	6.081190	6.081190	
8	Pb	3.157050	4.481084	3.104007	4.481084	6.081190	
9	Pb	3.157050	6.081190	4.481084	3.104007	4.481084	
10	Pb	3.157050	6.081190	6.081190	4.481084	3.104007	
11	Pb	3.157050	4.481084	6.081190	6.081190	4.481084	

		6	7	8	9	10	11
6	Pb	0.000000					
7	Pb	4.481084	0.000000				
8	Pb	6.081190	3.231911	0.000000			
9	Pb	6.081190	5.229342	3.231911	0.000000		
10	Pb	4.481084	5.229342	5.229342	3.231911	0.000000	
11	Pb	3.104007	3.231911	5.229342	5.229342	3.231911	0.000000



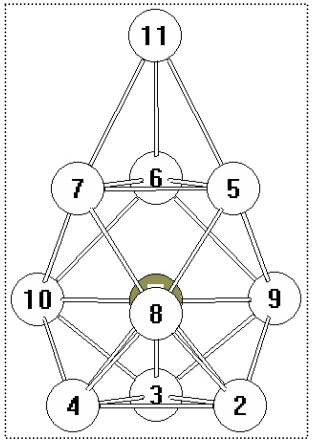
3-1-9 PP – D_{5h} [2b] [3]

- 203.1054890 (+20.83 kcal/mol) ** i -74 **

Table S8. $Pd@Pb_{10}^{6-}$ optimized structures

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pd	0.000000										
2 Pb	2.936341	0.000000									
3 Pb	2.936341	3.499803	0.000000								
4 Pb	2.936341	3.499803	3.499803	0.000000							
5 Pb	3.075051	4.559943	5.677671	5.677671	0.000000						
6 Pb	3.075051	5.677671	4.559943	5.677671	3.269575	0.000000					
7 Pb	3.075051	5.677671	5.677671	4.559943	3.269575	3.269575	0.000000				
8 Pb	2.859663	3.273354	5.295668	3.273354	3.548054	5.364510	3.548054	0.000000			
9 Pb	2.859663	3.273354	3.273354	5.295668	3.548054	3.548054	5.364510	4.951495	0.000000		
10 Pb	2.859663	5.295668	3.273354	3.273354	5.364510	3.548054	3.548054	4.951495	4.951495	0.000000	
11 Pb	5.557695	7.949334	7.949334	7.949334	3.655372	3.655372	3.655372	6.314302	6.314302	6.314302	0.000000

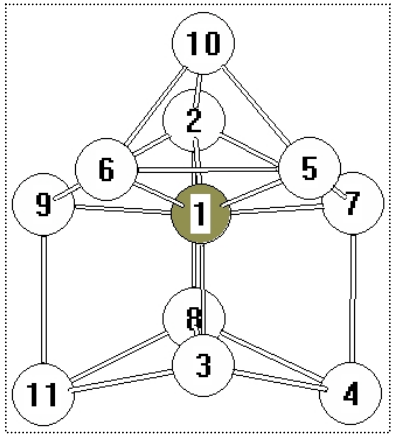


3-2-3 PTT – C_{3v} [1b] [1]

- 160.6605700 (+0.00 kcal/mol) ** i -29 **

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pd	0.000000										
2 Pb	2.826407	0.000000									
3 Pb	2.771227	5.244236	0.000000								
4 Pb	4.465607	5.683318	3.453297	0.000000							
5 Pb	2.923793	4.862352	4.234542	5.452019	0.000000						
6 Pb	2.923793	4.862352	4.234542	7.049169	3.627509	0.000000					
7 Pb	2.883521	3.476536	4.231037	3.448528	3.161100	5.624897	0.000000				
8 Pb	3.088614	3.553502	3.175395	3.237424	5.624897	3.161100	5.530301	3.817777	0.000000		
9 Pb	2.883521	3.476536	4.231037	6.506292	5.482132	5.482132	3.161100	3.817777	0.000000		
10 Pb	3.136672	3.346208	5.744056	7.180171	3.190003	3.190003	4.283891	5.881533	4.283891	0.000000	
11 Pb	4.465607	5.683318	3.453297	5.504128	7.049169	5.452019	6.506292	3.237424	3.448528	7.180171	0.000000



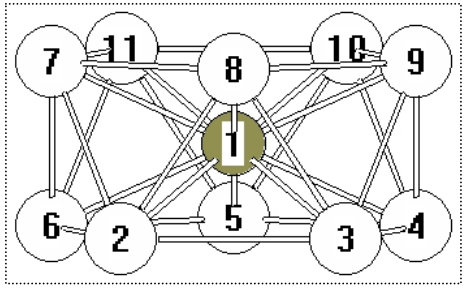
3-2-4 APT – D_{4d} [T] → C_s [2b] [2]

- 160.6284769 (+20.14 kcal/mol) ** i -12 **

Charge 6-

		1	2	3	4	5	
1	Pd	0.000000					
2	Pb	3.224212	0.000000				
3	Pb	3.224212	3.457374	0.000000			
4	Pb	3.224212	5.594149	3.457374	0.000000		
5	Pb	3.224212	5.594149	5.594149	3.457374	0.000000	
6	Pb	3.224212	3.457374	5.594149	5.594149	3.457374	
7	Pb	3.224212	3.207440	5.443229	6.448424	5.443229	
8	Pb	3.224212	3.207440	3.207440	5.443229	6.448424	
9	Pb	3.224212	5.443229	3.207440	3.207440	5.443229	
10	Pb	3.224212	6.448424	5.443229	3.207440	3.207440	
11	Pb	3.224212	5.443229	6.448424	5.443229	3.207440	

		6	7	8	9	10	11
6	Pb	0.000000					
7	Pb	3.207440	0.000000				
8	Pb	5.443229	3.457374	0.000000			
9	Pb	6.448424	5.594149	3.457374	0.000000		
10	Pb	5.443229	5.594149	5.594149	3.457374	0.000000	
11	Pb	3.207440	3.457374	5.594149	5.594149	3.457374	0.000000



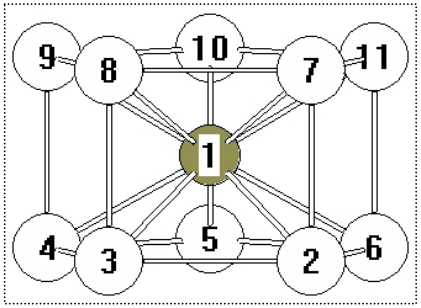
3-2-5 APP – D_{5d} [3b] [3]

- 160.6262286 (+21.55 kcal/mol) ** i -6 **

Charge 6-

		1	2	3	4	5	
1	Pd	0.000000					
2	Pb	3.193959	0.000000				
3	Pb	3.193959	3.280434	0.000000			
4	Pb	3.193959	5.307854	3.280434	0.000000		
5	Pb	3.193959	5.307854	5.307854	3.280434	0.000000	
6	Pb	3.193959	3.280434	5.307854	5.307854	3.280434	
7	Pb	3.193959	3.107706	4.518749	6.150704	6.150704	
8	Pb	3.193959	4.518749	3.107706	4.518749	6.150704	
9	Pb	3.193959	6.150704	4.518749	3.107706	4.518749	
10	Pb	3.193959	6.150704	6.150704	4.518749	3.107706	
11	Pb	3.193959	4.518749	6.150704	6.150704	4.518749	

		6	7	8	9	10	11
6	Pb	0.000000					
7	Pb	4.518749	0.000000				
8	Pb	6.150704	3.280434	0.000000			
9	Pb	6.150704	5.307854	3.280434	0.000000		
10	Pb	4.518749	5.307854	5.307854	3.280434	0.000000	
11	Pb	3.107706	3.280434	5.307854	5.307854	3.280434	0.000000



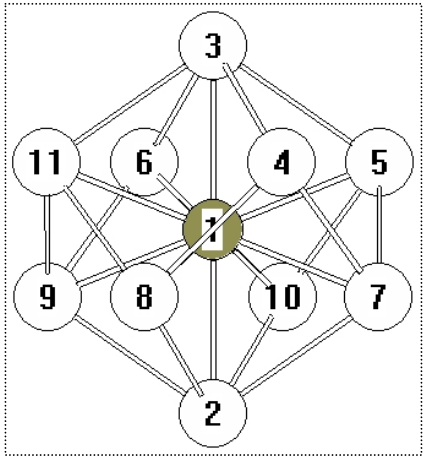
3-2-9 PP – D_{5h} [4b] [4]

- 160.5983030 (+39.07 kcal/mol) ** i -50 **

Charge 6-

		1	2	3	4	5	
1	Pd	0.000000					
2	Pb	3.005175	0.000000				
3	Pb	3.005175	6.010350	0.000000			
4	Pb	3.133347	5.045828	3.498214	0.000000		
5	Pb	3.133347	5.045828	3.498214	4.149179	0.000000	
6	Pb	3.133347	5.045828	3.498214	5.867826	4.149179	
7	Pb	3.133347	3.498214	5.045828	3.143635	3.143635	
8	Pb	3.133347	3.498214	5.045828	3.143635	5.850564	
9	Pb	3.133347	3.498214	5.045828	5.850564	5.850564	
10	Pb	3.133347	3.498214	5.045828	5.850564	3.143635	
11	Pb	3.133347	5.045828	3.498214	4.149179	5.867826	

		6	7	8	9	10	11
6	Pb	0.000000					
7	Pb	5.850564	0.000000				
8	Pb	5.850564	4.149179	0.000000			
9	Pb	3.143635	5.867826	4.149179	0.000000		
10	Pb	3.143635	4.149179	5.867826	4.149179	0.000000	
11	Pb	4.149179	5.850564	3.143635	3.143635	5.850564	0.000000



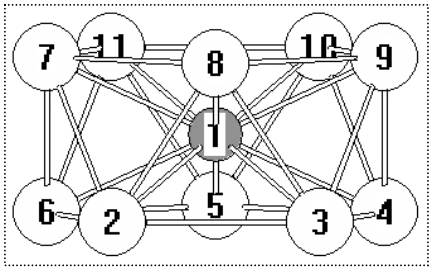
3-2-4 APT – D_{4d} ^{T} [5b] [5]

- 160.5790380 (+51.16 kcal/mol) ** i -53 **

Table S9. $Pt@Pb_{10}^{6-}$ optimized structures

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Pb	3.214636	0.000000									
3 Pb	3.214636	3.443561	0.000000								
4 Pb	3.214636	5.571799	3.443561	0.000000							
5 Pb	3.214636	5.571799	5.571799	3.443561	0.000000						
6 Pb	3.214636	3.443561	5.571799	5.571799	3.443561	0.000000					
7 Pb	3.214636	3.207894	5.429311	6.429272	5.429311	3.207894	0.000000				
8 Pb	3.214636	3.207894	3.207894	5.429311	6.429272	5.429311	3.443561	0.000000			
9 Pb	3.214636	5.429311	3.207894	3.207894	5.429311	5.429311	5.571799	3.443561	0.000000		
10 Pb	3.214636	6.429272	5.429311	3.207894	3.207894	5.429311	5.571799	5.571799	3.443561	0.000000	
11 Pb	3.214636	5.429311	6.429272	5.429311	3.207894	5.429311	5.571799	5.571799	3.443561	3.443561	0.000000

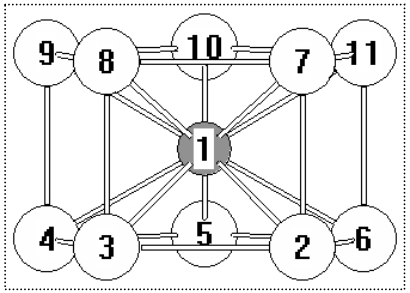


3-3-5 APP – D_{5d} [1b] [1]

- 153.0387003 (+0.00 kcal/mol) ** i -9 **

Charge 6-

	1	2	3	4	5	6	7	8	9	10	11
1 Pt	0.000000										
2 Pb	3.191855	0.000000									
3 Pb	3.191855	3.276903	0.000000								
4 Pb	3.191855	5.302141	3.276903	0.000000							
5 Pb	3.191855	5.302141	5.302141	3.276903	0.000000						
6 Pb	3.191855	3.276903	5.302141	5.302141	3.276903	0.000000					
7 Pb	3.191855	3.109842	4.517656	6.146854	6.146854	4.517656	0.000000				
8 Pb	3.191855	4.517656	3.109842	4.517656	6.146854	6.146854	3.276903	0.000000			
9 Pb	3.191855	6.146854	4.517656	3.109842	4.517656	6.146854	5.302141	3.276903	0.000000		
10 Pb	3.191855	6.146854	6.146854	4.517656	3.109842	4.517656	5.302141	5.302141	3.276903	0.000000	
11 Pb	3.191855	4.517656	6.146854	6.146854	4.517656	3.109842	5.302141	5.302141	3.276903	3.276903	0.000000



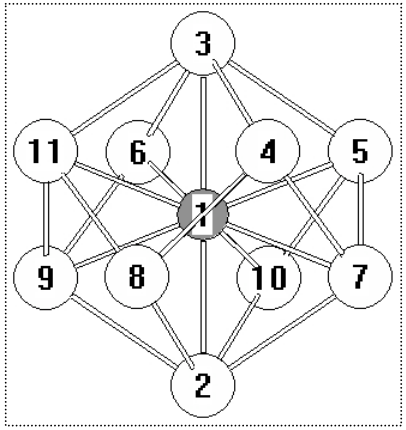
3-3-9 PP – D_{5h} [2b] [2]

- 153.0143746 (+15.26 kcal/mol) ** i -46 **

Charge 6-

		1	2	3	4	5	
1	Pt	0.000000					
2	Pb	2.972451	0.000000				
3	Pb	2.972451	5.944902	0.000000			
4	Pb	3.150462	5.028083	3.498591	0.000000		
5	Pb	3.150462	5.028083	3.498591	4.176674	0.000000	
6	Pb	3.150462	5.028083	3.498591	5.906709	4.176674	
7	Pb	3.150462	3.498591	5.028083	3.149895	3.149895	
8	Pb	3.150462	3.498591	5.028083	3.149895	5.881517	
9	Pb	3.150462	3.498591	5.028083	5.881517	5.881517	
10	Pb	3.150462	3.498591	5.028083	5.881517	3.149895	
11	Pb	3.150462	5.028083	3.498591	4.176674	5.906709	

		6	7	8	9	10	11
6	Pb	0.000000					
7	Pb	5.881517	0.000000				
8	Pb	5.881517	4.176674	0.000000			
9	Pb	3.149895	5.906709	4.176674	0.000000		
10	Pb	3.149895	4.176674	5.906709	4.176674	0.000000	
11	Pb	4.176674	5.881517	3.149895	3.149895	5.881517	0.000000



3-3-4 APT – D_{4d} ^{T} [3b] [3]

- 152.9973368 (+25.96 kcal/mol) ** i -50 **

Complete Gaussian03 reference (reference 40)

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian 03, Revision C.02; Gaussian, Inc., Wallingford CT, **2004**.