Insights into the nature of M≡E bonds in $[(PMe_3)_4M{\equiv}E(Mes)]^+$ (M = Mo, W) and $[(PMe_3)_5W{\equiv}E(Mes)]^+$: A dispersion-corrected DFT study

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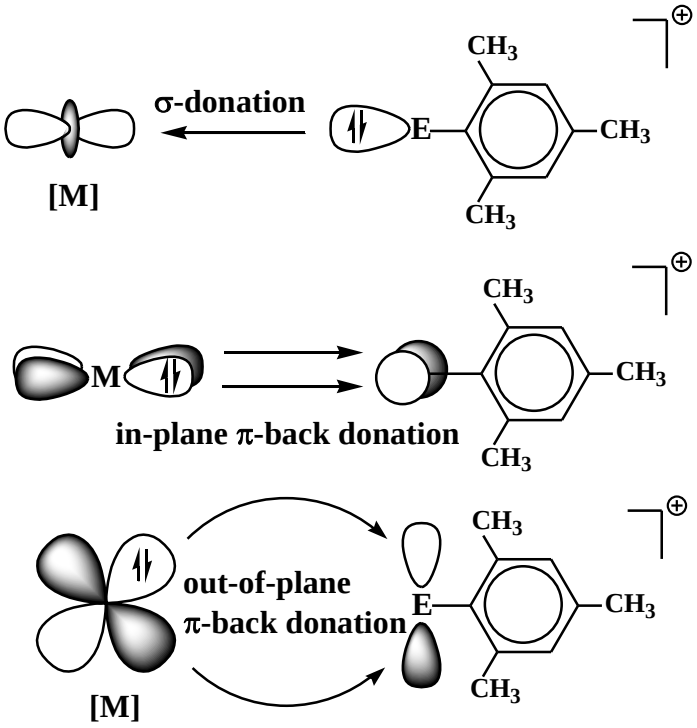
Supporting Information



donor-acceptor interactions

Fig.S1. Schematic representation of the orbital interaction between closed shell metal fragments [M] and group 14 ligand fragments $[E(Mes)]^+$.

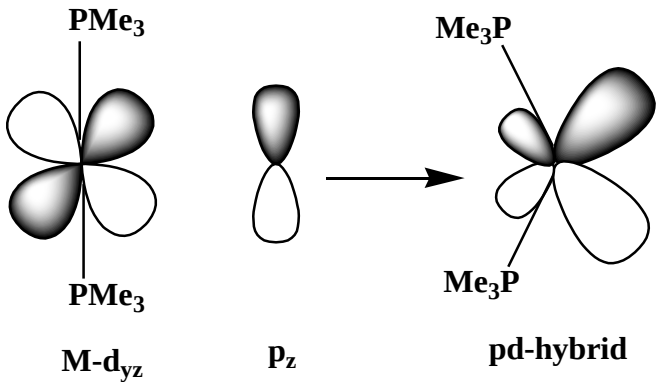


Fig.S2. Schematic presentation of the formation of pd hybrid orbital due to the mixing of pure atomic orbitals.

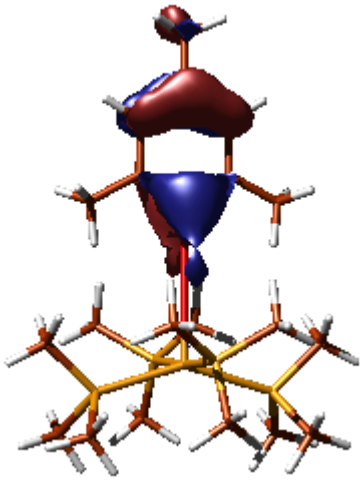


Fig. S3 Plot of E-C π bonding orbital (HOMO-4) of the cationic molybdenum germylidyne complex, **II**.

Table S1 Selected optimized structural parameters for cationic transition metal-ylidyne complexes $[(PMe_3)_4M{\equiv}E(Mes)]^+$ (M = Mo, W) and $[(PMe_3)_5W{\equiv}E(Mes)]^+$ using PBE and PW91 functionals.

Complexes	Bond distances				Bond angles	
	M-E		E-C		M-E-C	
	PBE	PW91	PBE	PW91	PBE	PW91
$[(PMe_3)_4Mo{\equiv}Si(Mes)]^+$ (**I**)	2.207	2.208	1.882	1.880	178.8	180.0
$[(PMe_3)_4Mo{\equiv}Ge(Mes)]^+$ (**II**)	2.255	2.254	1.959	1.957	178.9	179.9
$[(PMe_3)_4Mo{\equiv}Sn(Mes)]^+$ (**III**)	2.450	2.449	2.154	2.150	178.6	179.8
$[(PMe_3)_4Mo{\equiv}Pb(Mes)]^+$ (**IV**)	2.507	2.504	2.229	2.230	179.5	179.6
$[(PMe_3)_4W{\equiv}Si(Mes)]^+$ (**V**)	2.224	2.224	1.880	1.876	179.4	180.0
$[(PMe_3)_4W{\equiv}Ge(Mes)]^+$ (**VI**)	2.268	2.266	1.955	1.952	179.3	179.9
$[(PMe_3)_4W{\equiv}Sn(Mes)]^+$ (**VII**)	2.463	2.461	2.148	2.146	179.6	179.2
$[(PMe_3)_4W{\equiv}Pb(Mes)]^+$ (**VIII**)	2.516	2.516	2.225	2.224	179.6	179.5
$[(PMe_3)_5W{\equiv}Si(Mes)]^+$ (**IX**)	2.283	2.283	1.903	1.895	171.4	171.8
$[(PMe_3)_5W{\equiv}Ge(Mes)]^+$ (**X**)	2.329	2.326	1.981	1.976	171.5	171.6
$[(PMe_3)_5W{\equiv}Sn(Mes)]^+$ (**XI**)	2.527	2.525	2.173	2.169	172.8	172.8
$[(PMe_3)_5W{\equiv}Pb(Mes)]^+$ (**XII**)	2.586	2.585	2.252	2.248	173.6	174.6

Table S2 Results of NBO analysis in cationic transition metal-ylidyne complexes $[(PMe_3)_4M{\equiv}E(Mes)]^+$ and $[(PMe_3)_5M{\equiv}E(Mes)]^+$ (M = Mo, W; E = Si, Ge, Sn, Pb).

		M					E			
Complexes	Occup.	%	%s	%p	%d	%f	%	%s	%p	%d
M≡E σ-bond										
$[(PMe_3)_4Mo{\equiv}Si(Mes)]^+$ **(I)**	1.841	51.4	32.8	17.9	49.3	0.0	48.6	60.0	40.0	0.0
$[(PMe_3)_4Mo{\equiv}Ge(Mes)]^+$ **(II)**	1.825	50.3	31.5	20.1	48.3	0.1	49.7	60.3	39.7	0.0
$[(PMe_3)_4Mo{\equiv}Sn(Mes)]^+$ **(III)**	1.787	51.5	31.4	23.5	45.1	0.0	48.5	60.0	39.9	0.1
$[(PMe_3)_4Mo{\equiv}Pb(Mes)]^+$ **(IV)**	1.739	46.0	28.2	26.8	44.9	0.1	54.0	59.3	40.5	0.2
$[(PMe_3)_4W{\equiv}Si(Mes)]^+$ **(V)**	1.887	52.3	31.6	16.9	51.5	0.0	47.7	59.2	40.8	0.0
$[(PMe_3)_4W{\equiv}Ge(Mes)]^+$ **(VI)**	1.871	51.5	30.4	18.8	50.8	0.0	48.5	59.5	49.5	0.0
$[(PMe_3)_4W{\equiv}Sn(Mes)]^+$ **(VII)**	1.833	53.6	29.8	21.9	48.3	0.0	46.4	59.2	40.8	0.0
$[(PMe_3)_4W{\equiv}Pb(Mes)]^+$ **(VIII)**	1.784	48.5	26.6	24.8	48.6	0.0	51.5	58.9	40.9	0.2
$[(PMe_3)_5W{\equiv}Si(Mes)]^+$ **(IX)**	1.791	47.7	24.3	48.2	24.5	0.0	52.3	62.8	37.2	0.0
$[(PMe_3)_5W{\equiv}Ge(Mes)]^+$ **(X)**	1.779	47.3	22.8	49.5	27.7	0.0	52.7	63.1	36.9	0.0
$[(PMe_3)_5W{\equiv}Sn(Mes)]^+$ **(XI)**	1.728	49.8	20.9	52.8	26.3	0.0	50.2	61.9	38.0	0.1
$[(PMe_3)_5W{\equiv}Pb(Mes)]^+$ **(XII)**	1.691	44.9	18.4	53.7	27.9	0.0	55.1	61.3	38.5	0.2
M≡E π-bond (1)										
$[(PMe_3)_4Mo{\equiv}Si(Mes)]^+$ **(I)**	1.759	68.9	0.0	26.1	73.8	0.0	31.1	0.0	99.7	0.3
$[(PMe_3)_4Mo{\equiv}Ge(Mes)]^+$ **(II)**	1.750	71.2	0.0	26.5	73.5	0.0	28.8	0.0	99.9	0.1
$[(PMe_3)_4Mo{\equiv}Sn(Mes)]^+$ **(III)**	1.738	74.1	0.0	26.7	73.3	0.0	25.9	0.0	100.0	0.0
$[(PMe_3)_4Mo{\equiv}Pb(Mes)]^+$ **(IV)**	1.729	75.7	0.0	26.4	73.6	0.0	24.3	0.0	99.8	0.2
$[(PMe_3)_4W{\equiv}Si(Mes)]^+$ **(V)**	1.764	66.8	0.0	26.8	73.2	0.0	33.1	0.0	99.8	0.2
$[(PMe_3)_4W{\equiv}Ge(Mes)]^+$ **(VI)**	1.755	69.3	0.0	27.1	72.8	0.0	30.6	0.0	99.9	0.1
$[(PMe_3)_4W{\equiv}Sn(Mes)]^+$ **(VII)**	1.736	72.5	0.0	27.7	72.3	0.0	27.5	0.0	100.0	0.0
$[(PMe_3)_4W{\equiv}Pb(Mes)]^+$ **(VIII)**	1.726	74.3	0.0	27.3	72.7	0.0	25.6	0.0	99.8	0.2
$[(PMe_3)_5W{\equiv}Si(Mes)]^+$ **(IX)**	1.835	75.0	0.0	12.3	87.7	0.0	25.0	0.0	99.8	0.2
$[(PMe_3)_5W{\equiv}Ge(Mes)]^+$ **(X)**	1.824	77.2	0.0	12.1	87.9	0.0	22.8	0.0	99.9	0.1
$[(PMe_3)_5W{\equiv}Sn(Mes)]^+$ **(XI)**	1.812	80.6	0.0	10.6	89.4	0.0	19.4	0.0	99.9	0.1
$[(PMe_3)_5W{\equiv}Pb(Mes)]^+$ **(XII)**	1.805	82.3	0.0	9.5	90.5	0.0	17.7	0.0	99.7	0.3
M≡E π-bond (2)										
$[(PMe_3)_4Mo{\equiv}Si(Mes)]^+$ **(I)**	1.834	77.1	0.0	7.0	93.0	0.0	22.9	0.0	99.6	0.4
$[(PMe_3)_4Mo{\equiv}Ge(Mes)]^+$ **(II)**	1.831	78.6	0.0	7.2	92.8	0.0	21.4	0.0	99.8	0.2
$[(PMe_3)_4Mo{\equiv}Sn(Mes)]^+$ **(III)**	1.827	80.7	0.0	7.1	92.9	0.0	19.3	0.0	100.0	0.0
$[(PMe_3)_4Mo{\equiv}Pb(Mes)]^+$ **(IV)**	1.825	82.0	0.0	7.1	92.9	0.0	18.0	0.0	99.8	0.2
$[(PMe_3)_4W{\equiv}Si(Mes)]^+$ **(V)**	1.826	75.9	0.0	5.8	94.2	0.0	24.1	0.0	99.6	0.4
$[(PMe_3)_4W{\equiv}Ge(Mes)]^+$ **(VI)**	1.823	77.6	0.0	5.9	94.1	0.0	22.4	0.0	99.8	0.2
$[(PMe_3)_4W{\equiv}Sn(Mes)]^+$ **(VII)**	1.816	80.0	0.0	5.8	94.2	0.0	20.0	0.0	100.0	0.0
$[(PMe_3)_4W{\equiv}Pb(Mes)]^+$ **(VIII)**	1.814	81.4	0.0	5.8	94.2	0.0	18.6	0.0	99.8	0.2
$[(PMe_3)_5W{\equiv}Si(Mes)]^+$ **(IX)**	1.879	77.2	0.3	2.7	97.0	0.0	22.8	0.1	99.6	0.3
$[(PMe_3)_5W{\equiv}Ge(Mes)]^+$ **(X)**	1.814	79.0	0.3	2.5	97.2	0.0	21.0	0.1	99.8	0.1
$[(PMe_3)_5W{\equiv}Sn(Mes)]^+$ **(XI)**	1.806	81.2	0.2	1.7	98.1	0.0	18.8	0.1	99.9	0.0
$[(PMe_3)_5W{\equiv}Pb(Mes)]^+$ **(XII)**	1.806	82.5	0.1	1.4	98.5	0.0	17.5	0.1	99.7	0.2

Table S3 Important frontier orbitals, their energies and percentage contribution of major atomic orbitals of transition metal and heavier carbyne element E of the complexes $[(PMe_3)_4M{\equiv}E(Mes)]^+$ (M = Mo, W; E = Si, Ge, Sn, Pb).

Complex	M.O.	Energy (eV)	Type of M.O.	Contribution of transition metal	Contribution of E
$[(PMe_3)_4Mo{\equiv}Si(Mes)]^+$ (**I**)	π (a')	-7.255	(HOMO-1); AA	Mo: 54.2% (d_{xy})	Si:15.9% (p_x)
	π (a")	-7.298	(HOMO-2); AAA	Mo: 45.6% (d_{yz}), 4.3% (p_z)	Si: 29.4% (p_z)
$[(PMe_3)_4Mo{\equiv}Ge(Mes)]^+$ (**II**)	π (a')	-7.236	(HOMO-1); AA	Mo: 53.1% (d_{xy}),	Ge: 16.3% (p_x)
	π (a")	-7.299	(HOMO-2); AAA	Mo: 45.7% (d_{yz}), 2.8% (p_z)	Ge: 31.2% (p_z)
$[(PMe_3)_4Mo{\equiv}Sn(Mes)]^+$ (**III**)	π (a')	-7.133	(HOMO-1); AA	Mo: 56.4% (d_{xy}),	Sn:17.3% (p_x)
	π (a")	-7.135	(HOMO-2); AAA	Mo: 48.6% (d_{yz}), 3.8% (p_z)	Sn: 29.1% (p_z)
$[(PMe_3)_4Mo{\equiv}Pb(Mes)]^+$ (**IV**)	π (a")	-7.064	(HOMO-1); AAA	Mo: 51.6% (d_{yz}), 4.4% (p_z),	Pb:26.5% (p_z)
	π (a')	-7.082	(HOMO-2); AA	Mo: 58.4% (d_{xy}),	Pb: 16.1% (p_x)
$[(PMe_3)_4W{\equiv}Si(Mes)]^+$ (**V**)	π (a')	-7.144	(HOMO-1); AA	W: 51.9% (d_{xy}),	Si: 17.4% (p_x)
	π (a")	-7.146	(HOMO-2); AAA	W: 42.5% (d_{yz}), 2.7% (p_z)	Si:32.0% (p_z)
$[(PMe_3)_4W{\equiv}Ge(Mes)]^+$ (**VI**)	π (a')	-7.135	(HOMO-1); AA	W: 50.7% (d_{xy}),	Ge: 17.8% (p_x)
	π (a")	-7.154	(HOMO-2); AAA	W: 42.3% (d_{yz}), 3.3% (p_z)	Ge:34.0% (p_z)
$[(PMe_3)_4W{\equiv}Sn(Mes)]^+$ (**VII**)	π (a")	-7.010	(HOMO-1); AAA	W: 44.5% (d_{yz}), 2.9% (p_z)	Sn: 32.0% (p_z)
	π (a')	-7.050	(HOMO-2); AA	W: 53.4% (d_{xy}),	Sn: 18.8% (p_x)
$[(PMe_3)_4W{\equiv}Pb(Mes)]^+$ (**VIII**)	π (a")	-6.937	(HOMO-1); AAA	W: 48.6% (d_{yz}), 2.7% (p_z)	Pb:29.4% (p_z)
	π (a')	-6.987	(HOMO-2); AA	W: 55.2% (d_{xy}),	Pb: 17.5% (p_x)

Cartesian coordinates of all optimized geometries of the five-coordinated cationic metal ylidyne complexes $[(PMe_3)_4M{\equiv}E(Mes)]^+$ (M = Mo: E = Si, **I**; E = Ge, **II**; E = Sn, **III**; E = Pb, **IV**; M = W: E = Si, **V**; E = Ge, **VI**; E = Sn, **VII**; E = Pb, **VIII**) and in the six-coordinated cationic transition metal-ylidyne complexes having PMe_3 as a trans ligand $[(PMe_3)_5W{\equiv}E(Mes)]^+$ (E = Si, **IX**; E = Ge, **X**; E = Sn, **XI**; E = Pb, **XII**)

$[(PMe_3)_4Mo{\equiv}Si(Mes)]^+$ (I)
BP86/TZ2P

C	-0.002272	2.971940	0.000000
C	0.003055	3.685825	1.226282
C	0.014380	5.081013	1.200112
C	0.018197	5.801036	0.000000
C	0.014380	5.081013	-1.200112
C	0.003055	3.685825	-1.226282
C	-0.000487	2.987005	2.562838
C	0.000920	7.307236	0.000000
C	-0.000487	2.987005	-2.562838
Si	-0.003515	1.089565	0.000000
Mo	-0.001497	-1.123039	0.000000
P	-0.000501	-1.832115	2.430044
C	1.385555	-2.945809	2.980417
P	-0.000501	-1.832115	-2.430044
C	1.385555	-2.945809	-2.980417
P	-2.498272	-1.017269	0.000000
C	-3.518600	-2.579684	0.000000
P	2.495161	-1.015219	0.000000
C	3.515551	-2.577600	0.000000
C	-1.384836	-2.948122	-2.979314
C	-0.001257	-0.608871	-3.814881
C	-3.335671	-0.113002	1.392740
C	-3.335671	-0.113002	-1.392740
C	3.332144	-0.110482	1.392576
C	3.332144	-0.110482	-1.392576
C	-1.384836	-2.948122	2.979314
C	-0.001257	-0.608871	3.814881
H	0.023742	5.625404	2.147133
H	0.023742	5.625404	-2.147133
H	1.220191	-3.266897	4.018516
H	1.421357	-3.840131	2.342715
H	2.353948	-2.436578	2.918655
H	-1.218608	-3.271261	4.016636
H	-1.420214	-3.841077	2.339651
H	-0.893205	0.026875	3.751470
H	-2.353731	-2.439621	2.919127
H	0.889805	0.028069	3.751020
H	-0.000562	-1.136793	4.779126
H	1.220191	-3.266897	-4.018516
H	1.421357	-3.840131	-2.342715
H	2.353948	-2.436578	-2.918655
H	-1.218608	-3.271261	-4.016636

H	-1.420214	-3.841077	-2.339651
H	-0.893205	0.026875	-3.751470
H	-2.353731	-2.439621	-2.919127
H	0.889805	0.028069	-3.751020
H	-0.000562	-1.136793	-4.779126
H	-4.590452	-2.335332	0.000000
H	-3.296755	-3.183621	0.888719
H	-3.296755	-3.183621	-0.888719
H	4.587418	-2.333279	0.000000
H	3.293706	-3.181554	0.888705
H	3.293706	-3.181554	-0.888705
H	-4.428346	-0.153992	1.280601
H	-3.064216	-0.540677	2.365462
H	-3.015006	0.937629	-1.379928
H	-3.015006	0.937629	1.379928
H	-3.064216	-0.540677	-2.365462
H	-4.428346	-0.153992	-1.280601
H	4.424824	-0.151224	1.280460
H	4.424824	-0.151224	-1.280460
H	3.060782	-0.537838	2.365447
H	3.011254	0.940061	-1.379291
H	3.011254	0.940061	1.379291
H	3.060782	-0.537838	-2.365447
H	-0.000418	1.894272	-2.447265
H	-0.886694	3.261928	-3.151381
H	0.882062	3.262042	-3.156627
H	-1.034755	7.679777	0.000000
H	0.494147	7.715345	-0.890304
H	0.494147	7.715345	0.890304
H	-0.000418	1.894272	2.447265
H	0.882062	3.262042	3.156627
H	-0.886694	3.261928	3.151381

PBE/TZ2P

C	0.001000	2.947358	0.000000
C	0.019104	3.660176	1.226101
C	0.061138	5.054536	1.200110
C	0.081800	5.774310	0.000000
C	0.061138	5.054536	-1.200110
C	0.019104	3.660176	-1.226101
C	-0.004204	2.958405	2.559404
C	0.099230	7.279302	0.000000
C	-0.004204	2.958405	-2.559404
Si	-0.024911	1.065003	0.000000
H	0.081239	5.599123	2.147855
H	0.081239	5.599123	-2.147855
H	-0.023314	1.865987	-2.439334
H	-0.889204	3.247292	-3.144260
H	0.880003	3.215749	-3.159807
H	-0.928012	7.675679	0.000000
H	0.601518	7.676457	-0.890846

H	0.601518	7.676457	0.890846
H	-0.023314	1.865987	2.439334
H	0.880003	3.215749	3.159807
H	-0.889204	3.247292	3.144260
Mo	-0.008543	-1.142365	0.000000
P	-0.000925	-1.827578	2.428014
C	1.402810	-2.913050	2.983751
P	-0.000925	-1.827578	-2.428014
C	1.402810	-2.913050	-2.983751
P	-2.501563	-1.015828	0.000000
C	-3.543740	-2.561560	0.000000
P	2.480588	-0.951449	0.000000
C	3.561273	-2.470868	0.000000
C	-1.373609	-2.952546	-2.981719
C	-0.018155	-0.593720	-3.801447
C	-3.322723	-0.099375	1.392976
C	-3.322723	-0.099375	-1.392976
C	3.279314	-0.014789	1.392782
C	3.279314	-0.014789	-1.392782
C	-1.373609	-2.952546	2.981719
C	-0.018155	-0.593720	3.801447
H	1.241828	-3.235733	4.022562
H	1.458606	-3.806590	2.345465
H	2.360228	-2.382064	2.921745
H	-1.203335	-3.272430	4.019900
H	-1.403948	-3.846163	2.341802
H	-0.917511	0.032028	3.730913
H	-2.345770	-2.448943	2.920821
H	0.866971	0.052238	3.733654
H	-0.013428	-1.115558	4.769535
H	1.241828	-3.235733	-4.022562
H	1.458606	-3.806590	-2.345465
H	2.360228	-2.382064	-2.921745
H	-1.203335	-3.272430	-4.019900
H	-1.403948	-3.846163	-2.341802
H	-0.917511	0.032028	-3.730913
H	-2.345770	-2.448943	-2.920821
H	0.866971	0.052238	-3.733654
H	-0.013428	-1.115558	-4.769535
H	-4.612892	-2.303382	0.000000
H	-3.327591	-3.167830	0.889405
H	-3.327591	-3.167830	-0.889405
H	4.623510	-2.185552	0.000000
H	3.360597	-3.082356	0.889479
H	3.360597	-3.082356	-0.889479
H	-4.416426	-0.122304	1.280753
H	-3.056857	-0.532772	2.365324
H	-2.983755	0.946384	-1.380091
H	-2.983755	0.946384	1.380091
H	-3.056857	-0.532772	-2.365324
H	-4.416426	-0.122304	-1.280753
H	4.373351	-0.013215	1.281497

H	4.373351	-0.013215	-1.281497
H	3.022396	-0.452622	2.365549
H	2.917427	1.023275	-1.378027
H	2.917427	1.023275	1.378027
H	3.022396	-0.452622	-2.365549

PW91/TZ2P

C	0.001037	2.944807	0.000000
C	0.004449	3.656928	1.224905
C	0.012206	5.050404	1.198504
C	0.014071	5.769036	0.000000
C	0.012206	5.050404	-1.198504
C	0.004449	3.656928	-1.224905
C	0.001456	2.956805	2.557176
C	-0.006165	7.271786	0.000000
C	0.001456	2.956805	-2.557176
Si	-0.000355	1.064828	0.000000
Mo	-0.000894	-1.143000	0.000000
P	-0.001506	-1.826588	2.427596
C	1.386010	-2.929074	2.984125
P	-0.001506	-1.826588	-2.427596
C	1.386010	-2.929074	-2.984125
P	-2.488699	-0.997752	0.000000
C	-3.536841	-2.537869	0.000000
P	2.487101	-0.998796	0.000000
C	3.534061	-2.539719	0.000000
C	-1.385876	-2.933373	-2.980724
C	-0.005139	-0.593030	-3.798718
C	-3.303634	-0.076078	1.390506
C	-3.303634	-0.076078	-1.390506
C	3.302877	-0.077700	1.390378
C	3.302877	-0.077700	-1.390378
C	-1.385876	-2.933373	2.980724
C	-0.005139	-0.593030	3.798718
H	0.019964	5.594642	2.144366
H	0.019964	5.594642	-2.144366
H	1.221244	-3.247026	4.022130
H	1.428494	-3.822883	2.348910
H	2.349474	-2.413228	2.921230
H	-1.221414	-3.252563	4.018395
H	-1.424924	-3.826313	2.344059
H	-0.897005	0.039716	3.728728
H	-2.350911	-2.420428	2.917528
H	0.884460	0.043904	3.729984
H	-0.004646	-1.112730	4.765792
H	1.221244	-3.247026	-4.022130
H	1.428494	-3.822883	-2.348910
H	2.349474	-2.413228	-2.921230
H	-1.221414	-3.252563	-4.018395
H	-1.424924	-3.826313	-2.344059
H	-0.897005	0.039716	-3.728728

H	-2.350911	-2.420428	-2.917528
H	0.884460	0.043904	-3.729984
H	-0.004646	-1.112730	-4.765792
H	-4.602964	-2.275646	0.000000
H	-3.323507	-3.143580	0.887798
H	-3.323507	-3.143580	-0.887798
H	4.600374	-2.278267	0.000000
H	3.320321	-3.145286	0.887806
H	3.320321	-3.145286	-0.887806
H	-4.395780	-0.092195	1.278100
H	-3.041672	-0.508584	2.362055
H	-2.959228	0.965881	-1.376420
H	-2.959228	0.965881	1.376420
H	-3.041672	-0.508584	-2.362055
H	-4.395780	-0.092195	-1.278100
H	4.395011	-0.095150	1.278030
H	4.395011	-0.095150	-1.278030
H	3.040375	-0.509530	2.362078
H	2.959832	0.964684	-1.375860
H	2.959832	0.964684	1.375860
H	3.040375	-0.509530	-2.362078
H	0.004765	1.865698	-2.439069
H	-0.884914	3.227399	-3.145289
H	0.881744	3.232584	-3.151840
H	-1.041080	7.642155	0.000000
H	0.485612	7.680831	-0.889567
H	0.485612	7.680831	0.889567
H	0.004765	1.865698	2.439069
H	0.881744	3.232584	3.151840
H	-0.884914	3.227399	3.145289

$[(PMe_3)_4Mo{\equiv}Ge(Mes)]^+$ (II)
BP86/TZ2P

C	0.000312	3.052636	0.000000
C	0.006234	3.758299	1.226770
C	0.018037	5.155472	1.199248
C	0.021784	5.875820	0.000000
C	0.018037	5.155472	-1.199248
C	0.006234	3.758299	-1.226770
C	0.002756	3.065082	2.567333
C	0.004632	7.382825	0.000000
C	0.002756	3.065082	-2.567333
Ge	-0.003793	1.089679	0.000000
Mo	-0.002239	-1.165305	0.000000
P	-0.001022	-1.836379	2.436297
C	1.386905	-2.936825	3.005861
P	-0.001022	-1.836379	-2.436297
C	1.386905	-2.936825	-3.005861
P	-2.503078	-1.051088	0.000000
C	-3.528849	-2.608290	0.000000
P	2.498296	-1.044998	0.000000

C	3.527217	-2.600112	0.000000
C	-1.383866	-2.944586	-3.002450
C	-0.005259	-0.585158	-3.796458
C	-3.334554	-0.137076	1.390303
C	-3.334554	-0.137076	-1.390303
C	3.327795	-0.128728	1.389952
C	3.327795	-0.128728	-1.389952
C	-1.383866	-2.944586	3.002450
C	-0.005259	-0.585158	3.796458
H	0.027827	5.699486	2.146698
H	0.027827	5.699486	-2.146698
H	1.224824	-3.236718	4.050810
H	1.421038	-3.843674	2.385999
H	2.355046	-2.428834	2.930851
H	-1.220750	-3.246973	4.046514
H	-1.414010	-3.849625	2.379732
H	-0.897251	0.048807	3.717273
H	-2.354134	-2.440431	2.928726
H	0.885116	0.051425	3.719602
H	-0.005551	-1.091617	4.772213
H	1.224824	-3.236718	-4.050810
H	1.421038	-3.843674	-2.385999
H	2.355046	-2.428834	-2.930851
H	-1.220750	-3.246973	-4.046514
H	-1.414010	-3.849625	-2.379732
H	-0.897251	0.048807	-3.717273
H	-2.354134	-2.440431	-2.928726
H	0.885116	0.051425	-3.719602
H	-0.005551	-1.091617	-4.772213
H	-4.599959	-2.360836	0.000000
H	-3.308031	-3.212521	0.888963
H	-3.308031	-3.212521	-0.888963
H	4.597852	-2.350614	0.000000
H	3.307553	-3.204762	0.888973
H	3.307553	-3.204762	-0.888973
H	-4.427457	-0.175288	1.279555
H	-3.063495	-0.557828	2.365935
H	-3.011240	0.912605	-1.369233
H	-3.011240	0.912605	1.369233
H	-3.063495	-0.557828	-2.365935
H	-4.427457	-0.175288	-1.279555
H	4.420784	-0.165596	1.279696
H	4.420784	-0.165596	-1.279696
H	3.056881	-0.548611	2.365966
H	3.003201	0.920518	-1.367483
H	3.003201	0.920518	1.367483
H	3.056881	-0.548611	-2.365966
H	0.008163	1.972571	-2.460085
H	-0.885928	3.340004	-3.152272
H	0.882369	3.348531	-3.161611
H	-1.030345	7.757117	0.000000
H	0.498749	7.790890	-0.889932

H	0.498749	7.790890	0.889932
H	0.008163	1.972571	2.460085
H	0.882369	3.348531	3.161611
H	-0.885928	3.340004	3.152272

PBE/TZ2P

C	0.000750	3.039662	0.000000
C	0.019476	3.743107	1.227125
C	0.057596	5.139405	1.199643
C	0.075614	5.858737	0.000000
C	0.057596	5.139405	-1.199643
C	0.019476	3.743107	-1.227125
C	0.002580	3.046288	2.564446
C	0.088785	7.364316	0.000000
C	0.002580	3.046288	-2.564446
Ge	-0.023682	1.080332	0.000000
H	0.077644	5.684130	2.147439
H	0.077644	5.684130	-2.147439
H	-0.012830	1.953837	-2.453446
H	-0.881499	3.335924	-3.150355
H	0.887530	3.310950	-3.160599
H	-0.938946	7.759104	0.000000
H	0.590837	7.762591	-0.890514
H	0.590837	7.762591	0.890514
H	-0.012830	1.953837	2.453446
H	0.887530	3.310950	3.160599
H	-0.881499	3.335924	3.150355
Mo	-0.008898	-1.174654	0.000000
P	-0.002560	-1.838753	2.431989
C	1.397191	-2.921399	3.002180
P	-0.002560	-1.838753	-2.431989
C	1.397191	-2.921399	-3.002180
P	-2.506389	-1.061922	0.000000
C	-3.531787	-2.617606	0.000000
P	2.485244	-1.000160	0.000000
C	3.548997	-2.530166	0.000000
C	-1.374112	-2.957236	-3.000540
C	-0.017451	-0.582445	-3.785373
C	-3.334336	-0.147961	1.390695
C	-3.334336	-0.147961	-1.390695
C	3.291316	-0.065845	1.390273
C	3.291316	-0.065845	-1.390273
C	-1.374112	-2.957236	3.000540
C	-0.017451	-0.582445	3.785373
H	1.235871	-3.225475	4.046578
H	1.444651	-3.825969	2.378933
H	2.358276	-2.398777	2.929507
H	-1.204342	-3.259453	4.044124
H	-1.398587	-3.861320	2.375227
H	-0.915575	0.043481	3.701964
H	-2.348367	-2.459340	2.929618

H	0.868460	0.060940	3.703957
H	-0.013333	-1.085860	4.763302
H	1.235871	-3.225475	-4.046578
H	1.444651	-3.825969	-2.378933
H	2.358276	-2.398777	-2.929507
H	-1.204342	-3.259453	-4.044124
H	-1.398587	-3.861320	-2.375227
H	-0.915575	0.043481	-3.701964
H	-2.348367	-2.459340	-2.929618
H	0.868460	0.060940	-3.703957
H	-0.013333	-1.085860	-4.763302
H	-4.603588	-2.370513	0.000000
H	-3.308757	-3.221102	0.889662
H	-3.308757	-3.221102	-0.889662
H	4.614292	-2.256314	0.000000
H	3.341147	-3.138986	0.889714
H	3.341147	-3.138986	-0.889714
H	-4.427801	-0.184657	1.279814
H	-3.062088	-0.571099	2.365476
H	-3.007971	0.901528	-1.369733
H	-3.007971	0.901528	1.369733
H	-3.062088	-0.571099	-2.365476
H	-4.427801	-0.184657	-1.279814
H	4.385396	-0.078088	1.280111
H	4.385396	-0.078088	-1.280111
H	3.027997	-0.493490	2.365531
H	2.941960	0.976241	-1.367549
H	2.941960	0.976241	1.367549
H	3.027997	-0.493490	-2.365531

PW91/TZ2P

C	0.000687	3.038228	0.000000
C	0.005738	3.741029	1.225690
C	0.015659	5.135647	1.198003
C	0.018665	5.853876	0.000000
C	0.015659	5.135647	-1.198003
C	0.005738	3.741029	-1.225690
C	0.004050	3.045524	2.561658
C	0.001425	7.357122	0.000000
C	0.004050	3.045524	-2.561658
Ge	-0.002179	1.080605	0.000000
Mo	-0.001112	-1.173406	0.000000
P	-0.002140	-1.830723	2.434171
C	1.384318	-2.924831	3.008978
P	-0.002140	-1.830723	-2.434171
C	1.384318	-2.924831	-3.008978
P	-2.495956	-1.040641	0.000000
C	-3.532151	-2.587525	0.000000
P	2.493542	-1.035514	0.000000
C	3.531319	-2.581332	0.000000
C	-1.385107	-2.932200	-3.001157

C	-0.008947	-0.571025	-3.782303
C	-3.315442	-0.119198	1.388303
C	-3.315442	-0.119198	-1.388303
C	3.311914	-0.112352	1.387889
C	3.311914	-0.112352	-1.387889
C	-1.385107	-2.932200	3.001157
C	-0.008947	-0.571025	3.782303
H	0.025246	5.679980	2.143816
H	0.025246	5.679980	-2.143816
H	1.220406	-3.221387	4.053353
H	1.420681	-3.830937	2.391395
H	2.349574	-2.414755	2.933556
H	-1.222986	-3.231643	4.044975
H	-1.416234	-3.836365	2.380379
H	-0.899223	0.061408	3.695055
H	-2.352181	-2.425621	2.924754
H	0.881272	0.063431	3.701671
H	-0.011748	-1.070187	4.760067
H	1.220406	-3.221387	-4.053353
H	1.420681	-3.830937	-2.391395
H	2.349574	-2.414755	-2.933556
H	-1.222986	-3.231643	-4.044975
H	-1.416234	-3.836365	-2.380379
H	-0.899223	0.061408	-3.695055
H	-2.352181	-2.425621	-2.924754
H	0.881272	0.063431	-3.701671
H	-0.011748	-1.070187	-4.760067
H	-4.600082	-2.333269	0.000000
H	-3.313707	-3.191048	0.887892
H	-3.313707	-3.191048	-0.887892
H	4.599032	-2.326162	0.000000
H	3.313376	-3.185024	0.887930
H	3.313376	-3.185024	-0.887930
H	-4.407321	-0.145493	1.277072
H	-3.048468	-0.543048	2.362353
H	-2.980037	0.925331	-1.366649
H	-2.980037	0.925331	1.366649
H	-3.048468	-0.543048	-2.362353
H	-4.407321	-0.145493	-1.277072
H	4.403868	-0.138576	1.277291
H	4.403868	-0.138576	-1.277291
H	3.044441	-0.534938	2.362315
H	2.976537	0.932175	-1.364753
H	2.976537	0.932175	1.364753
H	3.044441	-0.534938	-2.362315
H	0.011275	1.954653	-2.451724
H	-0.883685	3.316851	-3.147168
H	0.882445	3.328409	-3.155506
H	-1.031946	7.730888	0.000000
H	0.495005	7.764587	-0.889161
H	0.495005	7.764587	0.889161
H	0.011275	1.954653	2.451724

H	0.882445	3.328409	3.155506
H	-0.883685	3.316851	3.147168

$[(PMe_3)_4Mo{\equiv}Sn(Mes)]^+$ (III)
BP86/TZ2P

C	0.000331	3.343919	0.000000
C	0.004818	4.043618	1.226502
C	0.015144	5.441984	1.199832
C	0.018237	6.161454	0.000000
C	0.015144	5.441984	-1.199832
C	0.004818	4.043618	-1.226502
C	0.000813	3.354181	2.570680
C	0.000023	7.668728	0.000000
C	0.000813	3.354181	-2.570680
Sn	-0.001692	1.187721	0.000000
Mo	-0.001809	-1.264404	0.000000
P	-0.001351	-1.906764	2.439824
C	1.377974	-3.007742	3.030638
P	-0.001351	-1.906764	-2.439824
C	1.377974	-3.007742	-3.030638
P	-2.503002	-1.193166	0.000000
C	-3.469552	-2.788084	0.000000
P	2.499723	-1.190647	0.000000
C	3.468053	-2.784416	0.000000
C	-1.380536	-3.007516	-3.031474
C	-0.000116	-0.626714	-3.774698
C	-3.374982	-0.308436	1.386593
C	-3.374982	-0.308436	-1.386593
C	3.370735	-0.305402	1.386697
C	3.370735	-0.305402	-1.386697
C	-1.380536	-3.007516	3.031474
C	-0.000116	-0.626714	3.774698
H	0.024647	5.986734	2.147052
H	0.024647	5.986734	-2.147052
H	1.214117	-3.280682	4.082649
H	1.395555	-3.929893	2.432972
H	2.353818	-2.518023	2.941758
H	-1.219017	-3.275706	4.085065
H	-1.394343	-3.932216	2.437640
H	-0.890258	0.007841	3.677810
H	-2.357141	-2.520361	2.937687
H	0.891606	0.005518	3.677440
H	-0.000415	-1.107189	4.763872
H	1.214117	-3.280682	-4.082649
H	1.395555	-3.929893	-2.432972
H	2.353818	-2.518023	-2.941758
H	-1.219017	-3.275706	-4.085065
H	-1.394343	-3.932216	-2.437640
H	-0.890258	0.007841	-3.677810
H	-2.357141	-2.520361	-2.937687
H	0.891606	0.005518	-3.677440

H	-0.000415	-1.107189	-4.763872
H	-4.549241	-2.582561	0.000000
H	-3.225338	-3.383187	0.888734
H	-3.225338	-3.383187	-0.888734
H	4.547521	-2.577698	0.000000
H	3.224523	-3.379716	0.888804
H	3.224523	-3.379716	-0.888804
H	-4.464751	-0.411001	1.285316
H	-3.072990	-0.694650	2.367021
H	-3.113773	0.757970	-1.346650
H	-3.113773	0.757970	1.346650
H	-3.072990	-0.694650	-2.367021
H	-4.464751	-0.411001	-1.285316
H	4.460664	-0.405160	1.284354
H	4.460664	-0.405160	-1.284354
H	3.070572	-0.693859	2.366760
H	3.106951	0.760428	-1.348519
H	3.106951	0.760428	1.348519
H	3.070572	-0.693859	-2.366760
H	0.018751	2.258613	-2.475695
H	-0.894811	3.618939	-3.149570
H	0.874135	3.646828	-3.169434
H	-1.035135	8.042392	0.000000
H	0.494265	8.076775	-0.889904
H	0.494265	8.076775	0.889904
H	0.018751	2.258613	2.475695
H	0.874135	3.646828	3.169434
H	-0.894811	3.618939	3.149570

PBE/TZ2P

C	0.003238	3.323591	0.000000
C	0.023850	4.021505	1.226848
C	0.067758	5.418769	1.199949
C	0.088669	6.137425	0.000000
C	0.067758	5.418769	-1.199949
C	0.023850	4.021505	-1.226848
C	0.002855	3.330877	2.569262
C	0.109379	7.643282	0.000000
C	0.002855	3.330877	-2.569262
Sn	-0.030987	1.169720	0.000000
H	0.090594	5.964076	2.147558
H	0.090594	5.964076	-2.147558
H	-0.009144	2.234515	-2.475029
H	-0.884976	3.619627	-3.149654
H	0.884515	3.599763	-3.168022
H	-0.916205	8.043480	0.000000
H	0.613947	8.038597	-0.890442
H	0.613947	8.038597	0.890442
H	-0.009144	2.234515	2.475029
H	0.884515	3.599763	3.168022
H	-0.884976	3.619627	3.149654

Mo	-0.010110	-1.280856	0.000000
P	-0.003405	-1.909217	2.438001
C	1.392879	-2.981702	3.036665
P	-0.003405	-1.909217	-2.438001
C	1.392879	-2.981702	-3.036665
P	-2.508814	-1.214563	0.000000
C	-3.472215	-2.809259	0.000000
P	2.485543	-1.143301	0.000000
C	3.492017	-2.711523	0.000000
C	-1.365664	-3.025118	-3.035072
C	-0.023883	-0.615864	-3.757891
C	-3.377480	-0.330169	1.386587
C	-3.377480	-0.330169	-1.386587
C	3.330983	-0.235865	1.386436
C	3.330983	-0.235865	-1.386436
C	-1.365664	-3.025118	3.035072
C	-0.023883	-0.615864	3.757891
H	1.234918	-3.247369	4.091934
H	1.422802	-3.908715	2.445908
H	2.361009	-2.477225	2.939803
H	-1.198208	-3.288290	4.089508
H	-1.368168	-3.951214	2.442157
H	-0.923730	0.004320	3.650016
H	-2.348771	-2.549978	2.940824
H	0.859420	0.028261	3.653353
H	-0.019133	-1.085713	4.752751
H	1.234918	-3.247369	-4.091934
H	1.422802	-3.908715	-2.445908
H	2.361009	-2.477225	-2.939803
H	-1.198208	-3.288290	-4.089508
H	-1.368168	-3.951214	-2.442157
H	-0.923730	0.004320	-3.650016
H	-2.348771	-2.549978	-2.940824
H	0.859420	0.028261	-3.653353
H	-0.019133	-1.085713	-4.752751
H	-4.553377	-2.608745	0.000000
H	-3.223394	-3.402977	0.889187
H	-3.223394	-3.402977	-0.889187
H	4.567340	-2.481631	0.000000
H	3.259511	-3.311741	0.889252
H	3.259511	-3.311741	-0.889252
H	-4.467965	-0.431630	1.285851
H	-3.073698	-0.717741	2.366470
H	-3.113959	0.736467	-1.346218
H	-3.113959	0.736467	1.346218
H	-3.073698	-0.717741	-2.366470
H	-4.467965	-0.431630	-1.285851
H	4.423714	-0.311978	1.287649
H	4.423714	-0.311978	-1.287649
H	3.034647	-0.628044	2.366779
H	3.043343	0.824494	-1.343255
H	3.043343	0.824494	1.343255

H	3.034647	-0.628044	-2.366779

PW91/TZ2P

C	0.001578	3.326528	0.000000
C	0.006685	4.022926	1.225614
C	0.016872	5.418553	1.199126
C	0.019725	6.136661	0.000000
C	0.016872	5.418553	-1.199126
C	0.006685	4.022926	-1.225614
C	0.003452	3.331573	2.565805
C	0.002993	7.640141	0.000000
C	0.003452	3.331573	-2.565805
Sn	-0.002998	1.176722	0.000000
H	0.027382	5.963539	2.144759
H	0.027382	5.963539	-2.144759
H	0.026974	2.237338	-2.470053
H	-0.893422	3.590691	-3.142956
H	0.873109	3.627242	-3.166097
H	-1.030314	8.014309	0.000000
H	0.497023	8.047285	-0.889152
H	0.497023	8.047285	0.889152
H	0.026974	2.237338	2.470053
H	0.873109	3.627242	3.166097
H	-0.893422	3.590691	3.142956
Mo	-0.001782	-1.272239	0.000000
P	-0.001906	-1.898628	2.436625
C	1.377517	-2.989169	3.034655
P	-0.001906	-1.898628	-2.436625
C	1.377517	-2.989169	-3.034655
P	-2.495712	-1.182925	0.000000
C	-3.471776	-2.768597	0.000000
P	2.492441	-1.177767	0.000000
C	3.471612	-2.761537	0.000000
C	-1.378654	-2.993616	-3.034657
C	-0.003953	-0.603878	-3.752159
C	-3.355945	-0.289947	1.384103
C	-3.355945	-0.289947	-1.384103
C	3.351311	-0.283528	1.384181
C	3.351311	-0.283528	-1.384181
C	-1.378654	-2.993616	3.034657
C	-0.003953	-0.603878	3.752159
H	1.213612	-3.255093	4.087288
H	1.397004	-3.913167	2.442893
H	2.350455	-2.497733	2.942237
H	-1.215799	-3.255983	4.088343
H	-1.392734	-3.919259	2.445314
H	-0.894057	0.026325	3.644084
H	-2.353471	-2.506637	2.938804
H	0.885687	0.027222	3.645160
H	-0.004100	-1.070536	4.746372
H	1.213612	-3.255093	-4.087288

H	1.397004	-3.913167	-2.442893
H	2.350455	-2.497733	-2.942237
H	-1.215799	-3.255983	-4.088343
H	-1.392734	-3.919259	-2.445314
H	-0.894057	0.026325	-3.644084
H	-2.353471	-2.506637	-2.938804
H	0.885687	0.027222	-3.645160
H	-0.004100	-1.070536	-4.746372
H	-4.548936	-2.557207	0.000000
H	-3.229468	-3.362952	0.887745
H	-3.229468	-3.362952	-0.887745
H	4.548352	-2.547950	0.000000
H	3.230571	-3.356375	0.887787
H	3.230571	-3.356375	-0.887787
H	-4.445547	-0.380314	1.282696
H	-3.057525	-0.678353	2.363438
H	-3.082045	0.772030	-1.342294
H	-3.082045	0.772030	1.342294
H	-3.057525	-0.678353	-2.363438
H	-4.445547	-0.380314	-1.282696
H	4.441080	-0.371470	1.282233
H	4.441080	-0.371470	-1.282233
H	3.054258	-0.673288	2.363406
H	3.075302	0.777961	-1.343268
H	3.075302	0.777961	1.343268
H	3.054258	-0.673288	-2.363406

$[(PMe_3)_4Mo{\equiv}Pb(Mes)]^+$ (IV)
BP86/TZ2P

C	-0.003448	3.451493	0.000000
C	0.003746	4.143730	1.226803
C	0.020171	5.543490	1.199624
C	0.027132	6.262791	0.000000
C	0.020171	5.543490	-1.199624
C	0.003746	4.143730	-1.226803
C	-0.003619	3.457610	2.573717
C	0.016738	7.770605	0.000000
C	-0.003619	3.457610	-2.573717
Pb	-0.004421	1.213784	0.000000
Mo	-0.000679	-1.296776	0.000000
P	0.000216	-1.926049	2.440777
C	1.379231	-3.025167	3.037448
P	0.000216	-1.926049	-2.440777
C	1.379231	-3.025167	-3.037448
P	-2.501566	-1.239930	0.000000
C	-3.451003	-2.844697	0.000000
P	2.500569	-1.234683	0.000000
C	3.451552	-2.838564	0.000000
C	-1.375409	-3.029584	-3.036818
C	-0.001476	-0.642988	-3.773920

C	-3.383302	-0.361333	1.384838
C	-3.383302	-0.361333	-1.384838
C	3.381314	-0.355059	1.384799
C	3.381314	-0.355059	-1.384799
C	-1.375409	-3.029584	3.036818
C	-0.001476	-0.642988	3.773920
H	0.031398	6.087675	2.147299
H	0.031398	6.087675	-2.147299
H	1.217467	-3.289782	4.091850
H	1.391572	-3.951938	2.446904
H	2.356723	-2.540491	2.942339
H	-1.212648	-3.294716	4.090918
H	-1.385415	-3.955827	2.445402
H	-0.893142	-0.011013	3.674770
H	-2.354233	-2.547443	2.942401
H	0.888119	-0.008233	3.673940
H	-0.000187	-1.118782	4.765344
H	1.217467	-3.289782	-4.091850
H	1.391572	-3.951938	-2.446904
H	2.356723	-2.540491	-2.942339
H	-1.212648	-3.294716	-4.090918
H	-1.385415	-3.955827	-2.445402
H	-0.893142	-0.011013	-3.674770
H	-2.354233	-2.547443	-2.942401
H	0.888119	-0.008233	-3.673940
H	-0.000187	-1.118782	-4.765344
H	-4.532991	-2.652008	0.000000
H	-3.199690	-3.436846	0.888528
H	-3.199690	-3.436846	-0.888528
H	4.533381	-2.645006	0.000000
H	3.200707	-3.430899	0.888549
H	3.200707	-3.430899	-0.888549
H	-4.471882	-0.477171	1.285525
H	-3.075446	-0.738780	2.366602
H	-3.136361	0.708325	-1.340057
H	-3.136361	0.708325	1.340057
H	-3.075446	-0.738780	-2.366602
H	-4.471882	-0.477171	-1.285525
H	4.470006	-0.469891	1.285467
H	4.470006	-0.469891	-1.285467
H	3.073886	-0.732531	2.366683
H	3.133395	0.714340	-1.339702
H	3.133395	0.714340	1.339702
H	3.073886	-0.732531	-2.366683
H	0.000097	2.361745	-2.486455
H	-0.893638	3.736329	-3.154621
H	0.875547	3.742038	-3.167988
H	-1.016040	8.150451	0.000000
H	0.513739	8.175795	-0.889639
H	0.513739	8.175795	0.889639
H	0.000097	2.361745	2.486455
H	0.875547	3.742038	3.167988

H -0.893638 3.736329 3.154621

PBE/TZ2P

C	3.424193	-0.432884	0.000000
C	4.111366	-0.507381	-1.227081
C	5.502781	-0.656623	-1.199757
C	6.217378	-0.734788	0.000000
C	5.502781	-0.656623	1.199757
C	4.111366	-0.507381	1.227081
C	3.429203	-0.431005	-2.573173
C	3.429203	-0.431005	2.573173
C	7.711926	-0.923891	0.000000
Pb	1.211563	-0.163928	0.000000
H	6.045326	-0.710691	-2.147871
H	6.045326	-0.710691	2.147871
H	2.337051	-0.329555	2.489437
H	3.628302	-1.333297	3.168503
H	3.793899	0.428536	3.153422
H	2.337051	-0.329555	-2.489437
H	3.793899	0.428536	-3.153422
H	3.628302	-1.333297	-3.168503
H	7.966248	-1.994954	0.000000
H	8.173464	-0.478705	-0.890250
H	8.173464	-0.478705	0.890250
Mo	-1.274743	0.159441	0.000000
P	-1.884242	0.239512	-2.436631
C	-2.791124	1.745963	-3.043646
P	-1.884242	0.239512	2.436631
C	-2.791124	1.745963	3.043646
P	-1.523227	-2.325281	0.000000
C	-3.231326	-3.069597	0.000000
P	-0.871360	2.623314	0.000000
C	-2.328704	3.784184	0.000000
C	-3.148595	-0.983792	3.041480
C	-0.596645	0.068953	3.752760
C	-0.758580	-3.306748	-1.384092
C	-0.758580	-3.306748	1.384092
C	0.121650	3.373160	-1.383927
C	0.121650	3.373160	1.383927
C	-3.148595	-0.983792	-3.041480
C	-0.596645	0.068953	-3.752760
H	-3.066355	1.615774	-4.100212
H	-3.713237	1.877540	-2.459245
H	-2.185845	2.653974	-2.945561
H	-3.381096	-0.789420	-4.098460
H	-4.073488	-0.872579	-2.457244
H	-0.086051	-0.896888	-3.640777
H	-2.797226	-2.016753	-2.941246
H	0.145944	0.870641	-3.643483
H	-1.055279	0.127475	-4.751075
H	-3.066355	1.615774	4.100212

H	-3.713237	1.877540	2.459245
H	-2.185845	2.653974	2.945561
H	-3.381096	-0.789420	4.098460
H	-4.073488	-0.872579	2.457244
H	-0.086051	-0.896888	3.640777
H	-2.797226	-2.016753	2.941246
H	0.145944	0.870641	3.643483
H	-1.055279	0.127475	4.751075
H	-3.174623	-4.167707	0.000000
H	-3.787132	-2.745186	-0.889057
H	-3.787132	-2.745186	0.889057
H	-1.989971	4.830271	0.000000
H	-2.949482	3.614507	-0.889061
H	-2.949482	3.614507	0.889061
H	-1.006194	-4.373543	-1.283605
H	-1.095402	-2.954937	-2.366433
H	0.333809	-3.191086	1.338177
H	0.333809	-3.191086	-1.338177
H	-1.095402	-2.954937	2.366433
H	-1.006194	-4.373543	1.283605
H	0.158103	4.467765	-1.284133
H	0.158103	4.467765	1.284133
H	-0.293992	3.119591	-2.366338
H	1.147065	2.979216	1.337124
H	1.147065	2.979216	-1.337124
H	-0.293992	3.119591	2.366338

PW91/TZ2P

C	0.008877	3.431960	0.000000
C	0.016199	4.121397	1.225786
C	0.029364	5.518776	1.198339
C	0.032900	6.236177	0.000000
C	0.029364	5.518776	-1.198339
C	0.016199	4.121397	-1.225786
C	0.011310	3.434840	2.569589
C	0.015166	7.740234	0.000000
C	0.011310	3.434840	-2.569589
Pb	-0.005924	1.202017	0.000000
Mo	-0.003858	-1.302379	0.000000
P	-0.000750	-1.910787	2.438616
C	1.381000	-2.995541	3.045383
P	-0.000750	-1.910787	-2.438616
C	1.381000	-2.995541	-3.045383
P	-2.498707	-1.236040	0.000000
C	-3.449737	-2.836642	0.000000
P	2.490472	-1.217612	0.000000
C	3.453602	-2.810847	0.000000
C	-1.369774	-3.009834	-3.046574
C	-0.006439	-0.607866	-3.747546
C	-3.374392	-0.352071	1.381068
C	-3.374392	-0.352071	-1.381068

C	3.359209	-0.327373	1.381467
C	3.359209	-0.327373	-1.381467
C	-1.369774	-3.009834	3.046574
C	-0.006439	-0.607866	3.747546
H	0.039556	6.063398	2.144394
H	0.039556	6.063398	-2.144394
H	1.220485	-3.249727	4.101341
H	1.396280	-3.926002	2.463854
H	2.354639	-2.507826	2.944180
H	-1.205071	-3.263174	4.102096
H	-1.376175	-3.940058	2.464478
H	-0.899065	0.017981	3.635056
H	-2.348718	-2.532541	2.947255
H	0.879975	0.026614	3.634351
H	-0.003769	-1.065278	4.745994
H	1.220485	-3.249727	-4.101341
H	1.396280	-3.926002	-2.463854
H	2.354639	-2.507826	-2.944180
H	-1.205071	-3.263174	-4.102096
H	-1.376175	-3.940058	-2.464478
H	-0.899065	0.017981	-3.635056
H	-2.348718	-2.532541	-2.947255
H	0.879975	0.026614	-3.634351
H	-0.003769	-1.065278	-4.745994
H	-4.530188	-2.643404	0.000000
H	-3.197408	-3.426833	0.887550
H	-3.197408	-3.426833	-0.887550
H	4.532559	-2.609422	0.000000
H	3.205670	-3.402892	0.887561
H	3.205670	-3.402892	-0.887561
H	-4.462187	-0.463193	1.281478
H	-3.068042	-0.727359	2.362741
H	-3.122193	0.714889	-1.332198
H	-3.122193	0.714889	1.332198
H	-3.068042	-0.727359	-2.362741
H	-4.462187	-0.463193	-1.281478
H	4.447849	-0.430475	1.282491
H	4.447849	-0.430475	-1.282491
H	3.055013	-0.704917	2.362994
H	3.099414	0.737813	-1.332502
H	3.099414	0.737813	1.332502
H	3.055013	-0.704917	-2.362994
H	0.023172	2.340076	-2.484060
H	-0.880301	3.707288	-3.148673
H	0.886379	3.725519	-3.164476
H	-1.018071	8.114272	0.000000
H	0.509380	8.147572	-0.888935
H	0.509380	8.147572	0.888935
H	0.023172	2.340076	2.484060
H	0.886379	3.725519	3.164476
H	-0.880301	3.707288	3.148673

Non-relativistic at BP86

C	0.005751	3.502389	0.000000
C	0.025854	4.203364	1.225837
C	0.069026	5.602338	1.199462
C	0.090002	6.322027	0.000000
C	0.069026	5.602338	-1.199462
C	0.025854	4.203364	-1.225837
C	0.004144	3.520773	2.574119
C	0.109023	7.829698	0.000000
C	0.004144	3.520773	-2.574119
Pb	-0.023801	1.239856	0.000000
Mo	-0.003598	-1.331075	0.000000
P	0.003231	-1.974412	2.440548
C	1.398389	-3.066165	3.007090
P	0.003231	-1.974412	-2.440548
C	1.398389	-3.066165	-3.007090
P	-2.521498	-1.280136	0.000000
C	-3.487916	-2.876443	0.000000
P	2.512143	-1.218334	0.000000
C	3.514091	-2.792702	0.000000
C	-1.362554	-3.104926	-3.001914
C	-0.016516	-0.710423	-3.789774
C	-3.391731	-0.400881	1.390490
C	-3.391731	-0.400881	-1.390490
C	3.362517	-0.318696	1.390055
C	3.362517	-0.318696	-1.390055
C	-1.362554	-3.104926	3.001914
C	-0.016516	-0.710423	3.789774
H	0.090474	6.146650	2.146898
H	0.090474	6.146650	-2.146898
H	1.244215	-3.361116	4.054901
H	1.425931	-3.976093	2.391952
H	2.367037	-2.562102	2.921284
H	-1.201884	-3.398971	4.048998
H	-1.365204	-4.013284	2.383825
H	-0.915328	-0.087176	3.695184
H	-2.344104	-2.626412	2.916502
H	0.865716	-0.063458	3.698433
H	-0.011640	-1.198082	4.776132
H	1.244215	-3.361116	-4.054901
H	1.425931	-3.976093	-2.391952
H	2.367037	-2.562102	-2.921284
H	-1.201884	-3.398971	-4.048998
H	-1.365204	-4.013284	-2.383825
H	-0.915328	-0.087176	-3.695184
H	-2.344104	-2.626412	-2.916502
H	0.865716	-0.063458	-3.698433
H	-0.011640	-1.198082	-4.776132
H	-4.567342	-2.666238	0.000000
H	-3.246892	-3.473062	0.889225
H	-3.246892	-3.473062	-0.889225

H	4.588644	-2.558809	0.000000
H	3.286157	-3.394407	0.889292
H	3.286157	-3.394407	-0.889292
H	-4.481872	-0.513638	1.298315
H	-3.077489	-0.783378	2.368799
H	-3.140502	0.668308	-1.349263
H	-3.140502	0.668308	1.349263
H	-3.077489	-0.783378	-2.368799
H	-4.481872	-0.513638	-1.298315
H	4.454862	-0.408947	1.299353
H	4.454862	-0.408947	-1.299353
H	3.054991	-0.705081	2.368954
H	3.089692	0.745093	-1.346044
H	3.089692	0.745093	1.346044
H	3.054991	-0.705081	-2.368954
H	-0.008376	2.422934	-2.488010
H	-0.884165	3.812091	-3.151925
H	0.885624	3.791650	-3.171674
H	-0.916411	8.229466	0.000000
H	0.613416	8.225461	-0.889868
H	0.613416	8.225461	0.889868
H	-0.008376	2.422934	2.488010
H	0.885624	3.791650	3.171674
H	-0.884165	3.812091	3.151925

$[(PMe_3)_4W{\equiv}Si(Mes)]^+$ (V)
BP86/TZ2P

C	-0.003427	2.987233	0.000000
C	0.001867	3.702129	1.226034
C	0.014295	5.097605	1.199470
C	0.019452	5.818156	0.000000
C	0.014295	5.097605	-1.199470
C	0.001867	3.702129	-1.226034
C	-0.002981	3.006517	2.564206
C	0.005033	7.324690	0.000000
C	-0.002981	3.006517	-2.564206
Si	-0.003734	1.107475	0.000000
W	-0.001430	-1.122148	0.000000
P	-0.000436	-1.858739	2.409987
C	1.384733	-2.971973	2.968621
P	-0.000436	-1.858739	-2.409987
C	1.384733	-2.971973	-2.968621
P	-2.495446	-1.021973	0.000000
C	-3.525306	-2.579386	0.000000
P	2.492701	-1.019995	0.000000
C	3.522626	-2.577371	0.000000
C	-1.383679	-2.974415	-2.967842
C	-0.001139	-0.623894	-3.784007
C	-3.335235	-0.115707	1.391323
C	-3.335235	-0.115707	-1.391323
C	3.332161	-0.113465	1.391299

C	3.332161	-0.113465	-1.391299
C	-1.383679	-2.974415	2.967842
C	-0.001139	-0.623894	3.784007
H	0.023725	5.641423	2.146842
H	0.023725	5.641423	-2.146842
H	1.216995	-3.289843	4.007196
H	1.421476	-3.868215	2.333903
H	2.353335	-2.462896	2.907394
H	-1.214679	-3.294370	4.005569
H	-1.420172	-3.869269	2.331138
H	-0.892919	0.010543	3.713729
H	-2.352813	-2.466103	2.908566
H	0.889438	0.012136	3.712879
H	-0.000141	-1.144515	4.751972
H	1.216995	-3.289843	-4.007196
H	1.421476	-3.868215	-2.333903
H	2.353335	-2.462896	-2.907394
H	-1.214679	-3.294370	-4.005569
H	-1.420172	-3.869269	-2.331138
H	-0.892919	0.010543	-3.713729
H	-2.352813	-2.466103	-2.908566
H	0.889438	0.012136	-3.712879
H	-0.000141	-1.144515	-4.751972
H	-4.595252	-2.328060	0.000000
H	-3.308198	-3.184864	0.888692
H	-3.308198	-3.184864	-0.888692
H	4.592582	-2.326067	0.000000
H	3.305523	-3.182879	0.888667
H	3.305523	-3.182879	-0.888667
H	-4.427430	-0.149898	1.272178
H	-3.072922	-0.547696	2.364841
H	-3.007987	0.932814	-1.382530
H	-3.007987	0.932814	1.382530
H	-3.072922	-0.547696	-2.364841
H	-4.427430	-0.149898	-1.272178
H	4.424369	-0.147639	1.272239
H	4.424369	-0.147639	-1.272239
H	3.069813	-0.545212	2.364910
H	3.004895	0.935031	-1.382157
H	3.004895	0.935031	1.382157
H	3.069813	-0.545212	-2.364910
H	-0.004151	1.913804	-2.450202
H	-0.889141	3.284894	-3.151341
H	0.879620	3.282961	-3.157420
H	-1.029684	7.699841	0.000000
H	0.499357	7.731892	-0.890220
H	0.499357	7.731892	0.890220
H	-0.004151	1.913804	2.450202
H	0.879620	3.282961	3.157420
H	-0.889141	3.284894	3.151341

PBE/TZ2P

C	3.116860	0.309497	0.000000
C	3.825849	0.390975	-1.225961
C	5.211708	0.552379	-1.199514
C	5.927394	0.634064	0.000000
C	5.211708	0.552379	1.199514
C	3.825849	0.390975	1.225961
C	3.131321	0.310643	-2.560698
C	3.131321	0.310643	2.560698
C	7.425166	0.780718	0.000000
Si	1.246648	0.111413	0.000000
H	5.752267	0.619905	-2.147515
H	5.752267	0.619905	2.147515
H	2.046131	0.184324	2.441704
H	3.507010	-0.536479	3.152311
H	3.302591	1.221389	3.152295
H	2.046131	0.184324	-2.441704
H	3.302591	1.221389	-3.152295
H	3.507010	-0.536479	-3.152311
H	7.909781	-0.208118	0.000000
H	7.779266	1.314712	-0.890561
H	7.779266	1.314712	0.890561
W	-0.967671	-0.101401	0.000000
P	-1.680615	-0.168013	-2.407333
C	-2.911408	1.108777	-2.971097
P	-1.680615	-0.168013	2.407333
C	-2.911408	1.108777	2.971097
P	-0.583725	-2.564293	0.000000
C	-2.004904	-3.773615	0.000000
P	-1.050012	2.389874	0.000000
C	-2.671717	3.313160	0.000000
C	-2.650581	-1.652454	2.972521
C	-0.439862	-0.051015	3.769434
C	0.416477	-3.288180	-1.391212
C	0.416477	-3.288180	1.391212
C	-0.202233	3.287476	-1.391243
C	-0.202233	3.287476	1.391243
C	-2.650581	-1.652454	-2.972521
C	-0.439862	-0.051015	-3.769434
H	-3.212375	0.909702	-4.009748
H	-3.807241	1.068804	-2.334994
H	-2.487618	2.118438	-2.911673
H	-2.982126	-1.513195	-4.011606
H	-3.538855	-1.781137	-2.337594
H	0.275607	-0.879564	-3.692181
H	-2.045232	-2.564870	-2.912438
H	0.108104	0.896683	-3.692750
H	-0.951871	-0.099722	-4.741381
H	-3.212375	0.909702	4.009748
H	-3.807241	1.068804	2.334994
H	-2.487618	2.118438	2.911673

H	-2.982126	-1.513195	4.011606
H	-3.538855	-1.781137	2.337594
H	0.275607	-0.879564	3.692181
H	-2.045232	-2.564870	2.912438
H	0.108104	0.896683	3.692750
H	-0.951871	-0.099722	4.741381
H	-1.626678	-4.806155	0.000000
H	-2.631730	-3.628771	-0.889483
H	-2.631730	-3.628771	0.889483
H	-2.492409	4.398068	0.000000
H	-3.260603	3.054089	-0.889454
H	-3.260603	3.054089	0.889454
H	0.513287	-4.377006	-1.270735
H	-0.045142	-3.079169	-2.364654
H	1.418700	-2.836665	1.382256
H	1.418700	-2.836665	-1.382256
H	-0.045142	-3.079169	2.364654
H	0.513287	-4.377006	1.270735
H	-0.310554	4.375247	-1.271079
H	-0.310554	4.375247	1.271079
H	-0.616332	2.995623	-2.364757
H	0.866741	3.031287	1.381808
H	0.866741	3.031287	-1.381808
H	-0.616332	2.995623	2.364757

PW91/TZ2P

C	-0.000945	2.966959	0.000000
C	0.002599	3.679152	1.224731
C	0.010137	5.072484	1.197961
C	0.012216	5.790889	0.000000
C	0.010137	5.072484	-1.197961
C	0.002599	3.679152	-1.224731
C	0.002544	2.981347	2.558232
C	-0.007795	7.293683	0.000000
C	0.002544	2.981347	-2.558232
Si	-0.000321	1.090642	0.000000
W	-0.000449	-1.133405	0.000000
P	-0.001609	-1.850740	2.409339
C	1.381223	-2.958523	2.973788
P	-0.001609	-1.850740	-2.409339
C	1.381223	-2.958523	-2.973788
P	-2.487302	-1.005680	0.000000
C	-3.536870	-2.546779	0.000000
P	2.486786	-1.007247	0.000000
C	3.535087	-2.549189	0.000000
C	-1.387849	-2.954318	-2.971478
C	-0.000385	-0.604738	-3.769297
C	-3.310047	-0.087751	1.389980
C	-3.310047	-0.087751	-1.389980
C	3.310253	-0.089416	1.389564
C	3.310253	-0.089416	-1.389564

C	-1.387849	-2.954318	2.971478
C	-0.000385	-0.604738	3.769297
H	0.018614	5.616473	2.143780
H	0.018614	5.616473	-2.143780
H	1.213032	-3.269899	4.013085
H	1.418350	-3.856013	2.343833
H	2.347332	-2.448305	2.908992
H	-1.220910	-3.268525	4.010119
H	-1.428057	-3.850300	2.339539
H	-0.889711	0.029893	3.691458
H	-2.352210	-2.440555	2.907611
H	0.890928	0.027162	3.692081
H	-0.001454	-1.116909	4.740070
H	1.213032	-3.269899	-4.013085
H	1.418350	-3.856013	-2.343833
H	2.347332	-2.448305	-2.908992
H	-1.220910	-3.268525	-4.010119
H	-1.428057	-3.850300	-2.339539
H	-0.889711	0.029893	-3.691458
H	-2.352210	-2.440555	-2.907611
H	0.890928	0.027162	-3.692081
H	-0.001454	-1.116909	-4.740070
H	-4.601953	-2.281720	0.000000
H	-3.326039	-3.152918	0.887728
H	-3.326039	-3.152918	-0.887728
H	4.600394	-2.285016	0.000000
H	3.323777	-3.155162	0.887714
H	3.323777	-3.155162	-0.887714
H	-4.401424	-0.105243	1.271054
H	-3.053079	-0.523508	2.361245
H	-2.966237	0.954178	-1.379883
H	-2.966237	0.954178	1.379883
H	-3.053079	-0.523508	-2.361245
H	-4.401424	-0.105243	-1.271054
H	4.401617	-0.108047	1.270676
H	4.401617	-0.108047	-1.270676
H	3.052851	-0.524338	2.361057
H	2.967542	0.952859	-1.378817
H	2.967542	0.952859	1.378817
H	3.052851	-0.524338	-2.361057
H	0.006326	1.890398	-2.440523
H	-0.883010	3.253362	-3.146815
H	0.883790	3.259552	-3.150221
H	-1.042367	7.664428	0.000000
H	0.484387	7.702168	-0.889467
H	0.484387	7.702168	0.889467
H	0.006326	1.890398	2.440523
H	0.883790	3.259552	3.150221
H	-0.883010	3.253362	3.146815

$[(PMe_3)_4W{\equiv}Ge(Mes)]^+$ (VI)

BP86/TZ2P

C	-0.002810	3.062465	0.000000
C	0.002857	3.768708	1.226421
C	0.015488	5.166064	1.198533
C	0.020770	5.887053	0.000000
C	0.015488	5.166064	-1.198533
C	0.002857	3.768708	-1.226421
C	-0.002152	3.078337	2.568192
C	0.006792	7.394312	0.000000
C	-0.002152	3.078337	-2.568192
Ge	-0.003944	1.103362	0.000000
W	-0.001241	-1.165198	0.000000
P	-0.000365	-1.863153	2.418055
C	1.385138	-2.963095	2.998704
P	-0.000365	-1.863153	-2.418055
C	1.385138	-2.963095	-2.998704
P	-2.497845	-1.055000	0.000000
C	-3.529979	-2.608829	0.000000
P	2.495254	-1.051687	0.000000
C	3.528746	-2.604574	0.000000
C	-1.384696	-2.965032	-2.997139
C	-0.001365	-0.596453	-3.763151
C	-3.332884	-0.139968	1.388847
C	-3.332884	-0.139968	-1.388847
C	3.329195	-0.135644	1.388744
C	3.329195	-0.135644	-1.388744
C	-1.384696	-2.965032	2.997139
C	-0.001365	-0.596453	3.763151
H	0.024952	5.709411	2.146346
H	0.024952	5.709411	-2.146346
H	1.220121	-3.255754	4.045078
H	1.419036	-3.874123	2.385164
H	2.354111	-2.456734	2.922453
H	-1.218936	-3.260318	4.042649
H	-1.418727	-3.874441	2.381209
H	-0.892307	0.037023	3.675529
H	-2.353877	-2.458740	2.922767
H	0.889422	0.037312	3.676055
H	-0.001446	-1.092372	4.744093
H	1.220121	-3.255754	-4.045078
H	1.419036	-3.874123	-2.385164
H	2.354111	-2.456734	-2.922453
H	-1.218936	-3.260318	-4.042649
H	-1.418727	-3.874441	-2.381209
H	-0.892307	0.037023	-3.675529
H	-2.353877	-2.458740	-2.922767
H	0.889422	0.037312	-3.676055
H	-0.001446	-1.092372	-4.744093
H	-4.599761	-2.356812	0.000000
H	-3.312306	-3.214012	0.888976
H	-3.312306	-3.214012	-0.888976

H	4.598317	-2.351683	0.000000
H	3.311573	-3.209953	0.888955
H	3.311573	-3.209953	-0.888955
H	-4.425197	-0.173337	1.271258
H	-3.070099	-0.564171	2.365396
H	-3.004633	0.908100	-1.371319
H	-3.004633	0.908100	1.371319
H	-3.070099	-0.564171	-2.365396
H	-4.425197	-0.173337	-1.271258
H	4.421545	-0.168439	1.271461
H	4.421545	-0.168439	-1.271461
H	3.066408	-0.559346	2.365499
H	3.000352	0.912207	-1.370399
H	3.000352	0.912207	1.370399
H	3.066408	-0.559346	-2.365499
H	0.001308	1.986016	-2.461778
H	-0.890574	3.357005	-3.151813
H	0.877712	3.362424	-3.161851
H	-1.027150	7.771403	0.000000
H	0.502098	7.801301	-0.889838
H	0.502098	7.801301	0.889838
H	0.001308	1.986016	2.461778
H	0.877712	3.362424	3.161851
H	-0.890574	3.357005	3.151813

PBE/TZ2P

C	3.033580	-0.382483	0.000000
C	3.734085	-0.457341	-1.226729
C	5.123402	-0.603164	-1.198973
C	5.839540	-0.680191	0.000000
C	5.123402	-0.603164	1.198973
C	3.734085	-0.457341	1.226729
C	3.043616	-0.383474	-2.565443
C	3.043616	-0.383474	2.565443
C	7.333714	-0.867243	0.000000
Ge	1.092147	-0.152844	0.000000
H	5.665213	-0.656080	-2.147193
H	5.665213	-0.656080	2.147193
H	1.956698	-0.271865	2.455975
H	3.230986	-1.291051	3.157052
H	3.412198	0.468768	3.154270
H	1.956698	-0.271865	-2.455975
H	3.412198	0.468768	-3.154270
H	3.230986	-1.291051	-3.157052
H	7.588898	-1.938247	0.000000
H	7.795215	-0.422387	-0.890452
H	7.795215	-0.422387	0.890452
W	-1.157204	0.141524	0.000000
P	-1.846428	0.234109	-2.414067
C	-2.750917	1.752513	-2.994510
P	-1.846428	0.234109	2.414067

C	-2.750917	1.752513	2.994510
P	-1.352284	-2.345718	0.000000
C	-3.018039	-3.182376	0.000000
P	-0.689782	2.591818	0.000000
C	-2.075537	3.838585	0.000000
C	-3.118629	-0.992971	2.994859
C	-0.587488	0.064379	3.753664
C	-0.545578	-3.283003	-1.389171
C	-0.545578	-3.283003	1.389171
C	0.335771	3.282682	-1.389253
C	0.335771	3.282682	1.389253
C	-3.118629	-0.992971	-2.994859
C	-0.587488	0.064379	-3.753664
H	-3.065136	1.625977	-4.040603
H	-3.648075	1.908239	-2.378193
H	-2.118466	2.645157	-2.919765
H	-3.386719	-0.789572	-4.041683
H	-4.026154	-0.906028	-2.380194
H	-0.078379	-0.903592	-3.662393
H	-2.743885	-2.020607	-2.918144
H	0.158947	0.863884	-3.663903
H	-1.077616	0.129229	-4.736003
H	-3.065136	1.625977	4.040603
H	-3.648075	1.908239	2.378193
H	-2.118466	2.645157	2.919765
H	-3.386719	-0.789572	4.041683
H	-4.026154	-0.906028	2.380194
H	-0.078379	-0.903592	3.662393
H	-2.743885	-2.020607	2.918144
H	0.158947	0.863884	3.663903
H	-1.077616	0.129229	4.736003
H	-2.897282	-4.275395	0.000000
H	-3.592163	-2.891742	-0.889454
H	-3.592163	-2.891742	0.889454
H	-1.670458	4.860924	0.000000
H	-2.705996	3.709826	-0.889478
H	-2.705996	3.709826	0.889478
H	-0.712427	-4.363722	-1.272865
H	-0.934408	-2.967514	-2.365449
H	0.535312	-3.084075	1.369976
H	0.535312	-3.084075	-1.369976
H	-0.934408	-2.967514	2.365449
H	-0.712427	-4.363722	1.272865
H	0.459920	4.369171	-1.273397
H	0.459920	4.369171	1.273397
H	-0.122433	3.080435	-2.365475
H	1.326002	2.805841	1.369786
H	1.326002	2.805841	-1.369786
H	-0.122433	3.080435	2.365475

PW91/TZ2P

C	-0.000092	3.050041	0.000000
C	0.003704	3.752656	1.225507
C	0.011148	5.147256	1.197575
C	0.013301	5.865756	0.000000
C	0.011148	5.147256	-1.197575
C	0.003704	3.752656	-1.225507
C	0.003486	3.058663	2.562036
C	-0.005142	7.368980	0.000000
C	0.003486	3.058663	-2.562036
Ge	-0.002221	1.097682	0.000000
W	-0.001168	-1.168179	0.000000
P	-0.000983	-1.856445	2.414515
C	1.381108	-2.955074	2.995876
P	-0.000983	-1.856445	-2.414515
C	1.381108	-2.955074	-2.995876
P	-2.490513	-1.045050	0.000000
C	-3.529140	-2.591399	0.000000
P	2.488204	-1.044486	0.000000
C	3.525480	-2.591717	0.000000
C	-1.384463	-2.951604	-2.996975
C	0.003089	-0.583492	-3.749264
C	-3.316507	-0.125058	1.386383
C	-3.316507	-0.125058	-1.386383
C	3.314775	-0.125311	1.386627
C	3.314775	-0.125311	-1.386627
C	-1.384463	-2.951604	2.996975
C	0.003089	-0.583492	3.749264
H	0.020219	5.691021	2.143631
H	0.020219	5.691021	-2.143631
H	1.215389	-3.244498	4.041855
H	1.412304	-3.865405	2.384402
H	2.349059	-2.450540	2.917475
H	-1.216990	-3.244180	4.041794
H	-1.420097	-3.860306	2.383295
H	-0.884851	0.051146	3.656793
H	-2.351119	-2.443942	2.922371
H	0.894948	0.045093	3.656615
H	0.001705	-1.073976	4.731221
H	1.215389	-3.244498	-4.041855
H	1.412304	-3.865405	-2.384402
H	2.349059	-2.450540	-2.917475
H	-1.216990	-3.244180	-4.041794
H	-1.420097	-3.860306	-2.383295
H	-0.884851	0.051146	-3.656793
H	-2.351119	-2.443942	-2.922371
H	0.894948	0.045093	-3.656615
H	0.001705	-1.073976	-4.731221
H	-4.596055	-2.334040	0.000000
H	-3.313238	-3.195562	0.887879
H	-3.313238	-3.195562	-0.887879
H	4.592663	-2.335485	0.000000
H	3.308898	-3.195689	0.887859

H	3.308898	-3.195689	-0.887859
H	-4.407635	-0.150026	1.267748
H	-3.056901	-0.551444	2.361418
H	-2.979088	0.918658	-1.368106
H	-2.979088	0.918658	1.368106
H	-3.056901	-0.551444	-2.361418
H	-4.407635	-0.150026	-1.267748
H	4.405916	-0.151634	1.268376
H	4.405916	-0.151634	-1.268376
H	3.054313	-0.551446	2.361557
H	2.978817	0.918923	-1.368294
H	2.978817	0.918923	1.368294
H	3.054313	-0.551446	-2.361557
H	0.012487	1.968035	-2.451730
H	-0.884652	3.329774	-3.147088
H	0.881482	3.344268	-3.155233
H	-1.038643	7.742224	0.000000
H	0.488284	7.776791	-0.889076
H	0.488284	7.776791	0.889076
H	0.012487	1.968035	2.451730
H	0.881482	3.344268	3.155233
H	-0.884652	3.329774	3.147088

Non-relativistic at BP86

C	-0.002375	3.032365	0.000000
C	0.011472	3.735150	1.229928
C	0.043144	5.131462	1.200730
C	0.058390	5.851387	0.000000
C	0.043144	5.131462	-1.200730
C	0.011472	3.735150	-1.229928
C	-0.005813	3.037444	2.565855
C	0.064812	7.357732	0.000000
C	-0.005813	3.037444	-2.565855
Ge	-0.017629	1.075777	0.000000
H	0.059444	5.675886	2.147630
H	0.059444	5.675886	-2.147630
H	-0.017792	1.944969	-2.450602
H	-0.892118	3.321376	-3.149884
H	0.876874	3.301743	-3.164156
H	-0.965109	7.746177	0.000000
H	0.563809	7.759031	-0.890213
H	0.563809	7.759031	0.890213
H	-0.017792	1.944969	2.450602
H	0.876874	3.301743	3.164156
H	-0.892118	3.321376	3.149884
W	-0.004743	-1.184188	0.000000
P	-0.000083	-1.810478	2.388202
C	1.387885	-2.875086	2.978561
P	-0.000083	-1.810478	-2.388202
C	1.387885	-2.875086	-2.978561
P	-2.449871	-1.079701	0.000000

C	-3.452729	-2.626150	0.000000
P	2.438491	-1.040398	0.000000
C	3.465807	-2.570727	0.000000
C	-1.370261	-2.898186	-2.977616
C	-0.011330	-0.516118	-3.682346
C	-3.286479	-0.172246	1.368924
C	-3.286479	-0.172246	-1.368924
C	3.260324	-0.119222	1.368686
C	3.260324	-0.119222	-1.368686
C	-1.370261	-2.898186	2.977616
C	-0.011330	-0.516118	3.682346
H	1.220732	-3.116753	4.038482
H	1.414724	-3.812323	2.406130
H	2.357793	-2.378326	2.875158
H	-1.198324	-3.139368	4.036871
H	-1.382907	-3.834558	2.403277
H	-0.905235	0.108866	3.572127
H	-2.347999	-2.416584	2.876054
H	0.873226	0.122242	3.573813
H	-0.008650	-0.983887	4.677743
H	1.220732	-3.116753	-4.038482
H	1.414724	-3.812323	-2.406130
H	2.357793	-2.378326	-2.875158
H	-1.198324	-3.139368	-4.036871
H	-1.382907	-3.834558	-2.403277
H	-0.905235	0.108866	-3.572127
H	-2.347999	-2.416584	-2.876054
H	0.873226	0.122242	-3.573813
H	-0.008650	-0.983887	-4.677743
H	-4.520405	-2.359808	0.000000
H	-3.236308	-3.233718	0.886011
H	-3.236308	-3.233718	-0.886011
H	4.529058	-2.287201	0.000000
H	3.259229	-3.181710	0.886016
H	3.259229	-3.181710	-0.886016
H	-4.375637	-0.249246	1.237451
H	-3.012493	-0.558056	2.356278
H	-2.992418	0.885219	-1.326473
H	-2.992418	0.885219	1.326473
H	-3.012493	-0.558056	-2.356278
H	-4.375637	-0.249246	-1.237451
H	4.350592	-0.178706	1.237245
H	4.350592	-0.178706	-1.237245
H	2.992525	-0.508823	2.356239
H	2.949362	0.933379	-1.325688
H	2.949362	0.933379	1.325688
H	2.992525	-0.508823	-2.356239

$[(PMe_3)_4W{\equiv}Sn(Mes)]^+$ (VII)
BP86

C	0.000643	3.353141	0.000000

C	0.005492	4.052722	1.226512
C	0.014742	5.451355	1.199235
C	0.017228	6.171236	0.000000
C	0.014742	5.451355	-1.199235
C	0.005492	4.052722	-1.226512
C	0.003489	3.366161	2.571884
C	-0.002217	7.678724	0.000000
C	0.003489	3.366161	-2.571884
Sn	-0.002025	1.200537	0.000000
W	-0.001269	-1.264756	0.000000
P	-0.001028	-1.936865	2.421802
C	1.379512	-3.032139	3.024359
P	-0.001028	-1.936865	-2.421802
C	1.379512	-3.032139	-3.024359
P	-2.496666	-1.194882	0.000000
C	-3.477141	-2.782220	0.000000
P	2.494225	-1.192774	0.000000
C	3.475451	-2.779682	0.000000
C	-1.379671	-3.034926	-3.023220
C	-0.002870	-0.641871	-3.741423
C	-3.367064	-0.305722	1.385481
C	-3.367064	-0.305722	-1.385481
C	3.364129	-0.303025	1.385420
C	3.364129	-0.303025	-1.385420
C	-1.379671	-3.034926	3.023220
C	-0.002870	-0.641871	3.741423
H	0.023693	5.995554	2.146762
H	0.023693	5.995554	-2.146762
H	1.213666	-3.297109	4.078001
H	1.399618	-3.959034	2.434234
H	2.354732	-2.541219	2.933763
H	-1.213415	-3.300478	4.076646
H	-1.398405	-3.961384	2.432340
H	-0.893953	-0.011297	3.634620
H	-2.355636	-2.545390	2.933022
H	0.887159	-0.009677	3.635482
H	-0.002912	-1.112517	4.735139
H	1.213666	-3.297109	-4.078001
H	1.399618	-3.959034	-2.434234
H	2.354732	-2.541219	-2.933763
H	-1.213415	-3.300478	-4.076646
H	-1.398405	-3.961384	-2.432340
H	-0.893953	-0.011297	-3.634620
H	-2.355636	-2.545390	-2.933022
H	0.887159	-0.009677	-3.635482
H	-0.002912	-1.112517	-4.735139
H	-4.554701	-2.566601	0.000000
H	-3.238960	-3.379498	0.888906
H	-3.238960	-3.379498	-0.888906
H	4.552916	-2.563573	0.000000
H	3.237562	-3.377095	0.888903
H	3.237562	-3.377095	-0.888903

H	-4.457137	-0.397202	1.277481
H	-3.074968	-0.698995	2.366201
H	-3.094457	0.757760	-1.350239
H	-3.094457	0.757760	1.350239
H	-3.074968	-0.698995	-2.366201
H	-4.457137	-0.397202	-1.277481
H	4.454244	-0.394252	1.277553
H	4.454244	-0.394252	-1.277553
H	3.072051	-0.696082	2.366217
H	3.091326	0.760397	-1.349847
H	3.091326	0.760397	1.349847
H	3.072051	-0.696082	-2.366217
H	0.009872	2.270608	-2.478003
H	-0.885453	3.642162	-3.155814
H	0.883764	3.652220	-3.163812
H	-1.037493	8.052055	0.000000
H	0.491947	8.087126	-0.889815
H	0.491947	8.087126	0.889815
H	0.009872	2.270608	2.478003
H	0.883764	3.652220	3.163812
H	-0.885453	3.642162	3.155814

PBE

C	3.330760	-0.424203	0.000000
C	4.024646	-0.501612	-1.226779
C	5.414386	-0.655232	-1.199455
C	6.129061	-0.735177	0.000000
C	5.414386	-0.655232	1.199455
C	4.024646	-0.501612	1.226779
C	3.341144	-0.423102	-2.570478
C	3.341144	-0.423102	2.570478
C	7.623055	-0.925879	0.000000
Sn	1.199236	-0.161285	0.000000
H	5.956978	-0.709922	-2.147319
H	5.956978	-0.709922	2.147319
H	2.251358	-0.303314	2.477704
H	3.523651	-1.332260	3.160852
H	3.717674	0.426859	3.157210
H	2.251358	-0.303314	-2.477704
H	3.717674	0.426859	-3.157210
H	3.523651	-1.332260	-3.160852
H	7.876672	-1.997270	0.000000
H	8.086061	-0.482119	-0.890248
H	8.086061	-0.482119	0.890248
W	-1.243729	0.154913	0.000000
P	-1.892995	0.239941	-2.419714
C	-2.796148	1.748282	-3.030090
P	-1.892995	0.239941	2.419714
C	-2.796148	1.748282	3.030090
P	-1.467826	-2.327704	0.000000
C	-3.156246	-3.118509	0.000000
P	-0.825255	2.612011	0.000000

C	-2.255521	3.807971	0.000000
C	-3.150954	-0.988520	3.029857
C	-0.595014	0.070803	3.723710
C	-0.683849	-3.292736	-1.385005
C	-0.683849	-3.292736	1.385005
C	0.179344	3.344458	-1.384998
C	0.179344	3.344458	1.384998
C	-3.150954	-0.988520	-3.029857
C	-0.595014	0.070803	-3.723710
H	-3.074124	1.615190	-4.085558
H	-3.716029	1.888314	-2.444177
H	-2.183160	2.652151	-2.936600
H	-3.385310	-0.789992	-4.085640
H	-4.076376	-0.888858	-2.444426
H	-0.084852	-0.894067	-3.607355
H	-2.788695	-2.018707	-2.935212
H	0.144538	0.873694	-3.608863
H	-1.051330	0.129087	-4.723040
H	-3.074124	1.615190	4.085558
H	-3.716029	1.888314	2.444177
H	-2.183160	2.652151	2.936600
H	-3.385310	-0.789992	4.085640
H	-4.076376	-0.888858	2.444426
H	-0.084852	-0.894067	3.607355
H	-2.788695	-2.018707	2.935212
H	0.144538	0.873694	3.608863
H	-1.051330	0.129087	4.723040
H	-3.066693	-4.214303	0.000000
H	-3.721276	-2.811071	-0.889526
H	-3.721276	-2.811071	0.889526
H	-1.889016	4.844533	0.000000
H	-2.880341	3.655072	-0.889527
H	-2.880341	3.655072	0.889527
H	-0.901964	-4.365372	-1.278414
H	-1.038185	-2.954104	-2.366146
H	0.404690	-3.144649	1.345823
H	0.404690	-3.144649	-1.345823
H	-1.038185	-2.954104	2.366146
H	-0.901964	-4.365372	1.278414
H	0.242479	4.437252	-1.278672
H	0.242479	4.437252	1.278672
H	-0.249727	3.107297	-2.366076
H	1.193949	2.923261	1.345649
H	1.193949	2.923261	-1.345649
H	-0.249727	3.107297	2.366076

PW91

C	0.001258	3.336633	0.000000
C	0.016696	4.032654	1.225489
C	0.049013	5.428918	1.198163
C	0.064074	6.146729	0.000000
C	0.049013	5.428918	-1.198163

C	0.016696	4.032654	-1.225489
C	0.002342	3.344431	2.566904
C	0.070305	7.650730	0.000000
C	0.002342	3.344431	-2.566904
Sn	-0.016920	1.190741	0.000000
W	-0.005034	-1.270533	0.000000
P	0.000042	-1.927257	2.418240
C	1.389838	-3.000926	3.028734
P	0.000042	-1.927257	-2.418240
C	1.389838	-3.000926	-3.028734
P	-2.493736	-1.204529	0.000000
C	-3.469679	-2.791298	0.000000
P	2.482413	-1.159604	0.000000
C	3.488478	-2.727475	0.000000
C	-1.365525	-3.032998	-3.024091
C	-0.016948	-0.620357	-3.720671
C	-3.360995	-0.315376	1.382961
C	-3.360995	-0.315376	-1.382961
C	3.333308	-0.253854	1.382576
C	3.333308	-0.253854	-1.382576
C	-1.365525	-3.032998	3.024091
C	-0.016948	-0.620357	3.720671
H	0.066811	5.973042	2.144192
H	0.066811	5.973042	-2.144192
H	1.224674	-3.261034	4.082545
H	1.420809	-3.929021	2.443968
H	2.357945	-2.499633	2.936356
H	-1.196482	-3.290628	4.077896
H	-1.373958	-3.960895	2.438207
H	-0.912829	-0.001019	3.603503
H	-2.344770	-2.554039	2.930434
H	0.866109	0.017782	3.607174
H	-0.013976	-1.079429	4.718254
H	1.224674	-3.261034	-4.082545
H	1.420809	-3.929021	-2.443968
H	2.357945	-2.499633	-2.936356
H	-1.196482	-3.290628	-4.077896
H	-1.373958	-3.960895	-2.438207
H	-0.912829	-0.001019	-3.603503
H	-2.344770	-2.554039	-2.930434
H	0.866109	0.017782	-3.607174
H	-0.013976	-1.079429	-4.718254
H	-4.546383	-2.578556	0.000000
H	-3.228602	-3.385947	0.887840
H	-3.228602	-3.385947	-0.887840
H	4.560931	-2.494261	0.000000
H	3.258795	-3.326589	0.887883
H	3.258795	-3.326589	-0.887883
H	-4.449952	-0.404040	1.273534
H	-3.070353	-0.709038	2.362730
H	-3.084632	0.745896	-1.346828
H	-3.084632	0.745896	1.346828

H	-3.070353	-0.709038	-2.362730
H	-4.449952	-0.404040	-1.273534
H	4.423742	-0.323501	1.274019
H	4.423742	-0.323501	-1.274019
H	3.048893	-0.650978	2.362756
H	3.038766	0.802501	-1.344824
H	3.038766	0.802501	1.344824
H	3.048893	-0.650978	-2.362756
H	-0.007013	2.250071	-2.472311
H	-0.882706	3.631803	-3.148884
H	0.884240	3.616576	-3.160641
H	-0.957102	8.040818	0.000000
H	0.570593	8.050419	-0.889101
H	0.570593	8.050419	0.889101
H	-0.007013	2.250071	2.472311
H	0.884240	3.616576	3.160641
H	-0.882706	3.631803	3.148884

$[(PMe_3)_4W{\equiv}Pb(Mes)]^+$ (VIII)
BP86/TZ2P

C	0.000049	3.453973	0.000000
C	0.006729	4.146214	1.227048
C	0.018852	5.546343	1.199076
C	0.023117	6.266081	0.000000
C	0.018852	5.546343	-1.199076
C	0.006729	4.146214	-1.227048
C	0.003535	3.462386	2.574909
C	0.007215	7.774074	0.000000
C	0.003535	3.462386	-2.574909
Pb	-0.004127	1.221372	0.000000
W	-0.001258	-1.299771	0.000000
P	0.000543	-1.954171	2.423972
C	1.379350	-3.049144	3.032871
P	0.000543	-1.954171	-2.423972
C	1.379350	-3.049144	-3.032871
P	-2.497100	-1.242798	0.000000
C	-3.462415	-2.839480	0.000000
P	2.494433	-1.237126	0.000000
C	3.463119	-2.831771	0.000000
C	-1.376921	-3.049076	-3.035571
C	0.002483	-0.652407	-3.738778
C	-3.377413	-0.359091	1.383565
C	-3.377413	-0.359091	-1.383565
C	3.372505	-0.351396	1.383625
C	3.372505	-0.351396	-1.383625
C	-1.376921	-3.049076	3.035571
C	0.002483	-0.652407	3.738778
H	0.028674	6.090162	2.146979
H	0.028674	6.090162	-2.146979
H	1.215655	-3.304541	4.089170
H	1.393289	-3.981099	2.450579

H	2.356711	-2.564244	2.935273
H	-1.210884	-3.304859	4.091411
H	-1.392410	-3.980821	2.452987
H	-0.887856	-0.021229	3.629276
H	-2.354397	-2.563922	2.940354
H	0.892691	-0.021546	3.626502
H	0.004088	-1.115166	4.736207
H	1.215655	-3.304541	-4.089170
H	1.393289	-3.981099	-2.450579
H	2.356711	-2.564244	-2.935273
H	-1.210884	-3.304859	-4.091411
H	-1.392410	-3.980821	-2.452987
H	-0.887856	-0.021229	-3.629276
H	-2.354397	-2.563922	-2.940354
H	0.892691	-0.021546	-3.626502
H	0.004088	-1.115166	-4.736207
H	-4.542175	-2.635142	0.000000
H	-3.217778	-3.434284	0.888801
H	-3.217778	-3.434284	-0.888801
H	4.542430	-2.625130	0.000000
H	3.219758	-3.427080	0.888823
H	3.219758	-3.427080	-0.888823
H	-4.466364	-0.465631	1.278534
H	-3.078012	-0.741991	2.365955
H	-3.120428	0.708110	-1.341943
H	-3.120428	0.708110	1.341943
H	-3.078012	-0.741991	-2.365955
H	-4.466364	-0.465631	-1.278534
H	4.461702	-0.455154	1.278451
H	4.461702	-0.455154	-1.278451
H	3.074190	-0.735135	2.366014
H	3.112813	0.715145	-1.342080
H	3.112813	0.715145	1.342080
H	3.074190	-0.735135	-2.366014
H	0.005787	2.366982	-2.487806
H	-0.883916	3.744166	-3.158314
H	0.885335	3.747790	-3.164894
H	-1.026749	8.150737	0.000000
H	0.502962	8.181138	-0.889564
H	0.502962	8.181138	0.889564
H	0.005787	2.366982	2.487806
H	0.885335	3.747790	3.164894
H	-0.883916	3.744166	3.158314

PBE

C	3.427963	-0.435946	0.000000
C	4.115148	-0.511516	-1.227196
C	5.506594	-0.662105	-1.199044
C	6.222033	-0.740651	0.000000
C	5.506594	-0.662105	1.199044
C	4.115148	-0.511516	1.227196

C	3.435312	-0.435617	-2.574277
C	3.435312	-0.435617	2.574277
C	7.716437	-0.930030	0.000000
Pb	1.219792	-0.163810	0.000000
H	6.048491	-0.716201	-2.147617
H	6.048491	-0.716201	2.147617
H	2.344180	-0.328083	2.490919
H	3.631463	-1.340825	3.166301
H	3.806351	0.420049	3.156310
H	2.344180	-0.328083	-2.490919
H	3.806351	0.420049	-3.156310
H	3.631463	-1.340825	-3.166301
H	7.970505	-2.001090	0.000000
H	8.177763	-0.484625	-0.890210
H	8.177763	-0.484625	0.890210
W	-1.275787	0.160193	0.000000
P	-1.912255	0.243596	-2.421911
C	-2.814553	1.749863	-3.040083
P	-1.912255	0.243596	2.421911
C	-2.814553	1.749863	3.040083
P	-1.516057	-2.321315	0.000000
C	-3.213770	-3.091051	0.000000
P	-0.873029	2.620371	0.000000
C	-2.317673	3.798277	0.000000
C	-3.170500	-0.982069	3.038523
C	-0.608463	0.072208	3.721151
C	-0.741506	-3.297793	-1.382941
C	-0.741506	-3.297793	1.382941
C	0.125605	3.365847	-1.383012
C	0.125605	3.365847	1.383012
C	-3.170500	-0.982069	-3.038523
C	-0.608463	0.072208	-3.721151
H	-3.083791	1.616500	-4.097795
H	-3.740093	1.885079	-2.461848
H	-2.207899	2.657232	-2.941458
H	-3.396344	-0.786051	-4.096649
H	-4.099929	-0.874757	-2.460680
H	-0.098945	-0.892423	-3.599736
H	-2.816509	-2.014383	-2.938059
H	0.131268	0.874416	-3.602225
H	-1.056243	0.129020	-4.724427
H	-3.083791	1.616500	4.097795
H	-3.740093	1.885079	2.461848
H	-2.207899	2.657232	2.941458
H	-3.396344	-0.786051	4.096649
H	-4.099929	-0.874757	2.460680
H	-0.098945	-0.892423	3.599736
H	-2.816509	-2.014383	2.938059
H	0.131268	0.874416	3.602225
H	-1.056243	0.129020	4.724427
H	-3.138855	-4.188024	0.000000
H	-3.775095	-2.776517	-0.889333

H	-3.775095	-2.776517	0.889333
H	-1.965110	4.839744	0.000000
H	-2.940680	3.637479	-0.889347
H	-2.940680	3.637479	0.889347
H	-0.973428	-4.367521	-1.276673
H	-1.087102	-2.955769	-2.365841
H	0.348977	-3.165295	1.340578
H	0.348977	-3.165295	-1.340578
H	-1.087102	-2.955769	2.365841
H	-0.973428	-4.367521	1.276673
H	0.174638	4.459390	-1.277403
H	0.174638	4.459390	1.277403
H	-0.295604	3.122743	-2.365853
H	1.146031	2.959182	1.340029
H	1.146031	2.959182	-1.340029
H	-0.295604	3.122743	2.365853

PW91

C	0.005804	3.435230	0.000000
C	0.016085	4.124773	1.225902
C	0.035298	5.522317	1.197716
C	0.042973	6.240170	0.000000
C	0.035298	5.522317	-1.197716
C	0.016085	4.124773	-1.225902
C	0.010034	3.440283	2.570666
C	0.035503	7.744841	0.000000
C	0.010034	3.440283	-2.570666
Pb	-0.009111	1.210879	0.000000
W	-0.002347	-1.305295	0.000000
P	-0.000189	-1.940480	2.420811
C	1.382447	-3.017774	3.041886
P	-0.000189	-1.940480	-2.420811
C	1.382447	-3.017774	-3.041886
P	-2.491315	-1.240468	0.000000
C	-3.460079	-2.831684	0.000000
P	2.485925	-1.213678	0.000000
C	3.472975	-2.793712	0.000000
C	-1.370615	-3.035329	-3.038917
C	-0.010352	-0.622326	-3.714182
C	-3.364500	-0.352059	1.380914
C	-3.364500	-0.352059	-1.380914
C	3.349540	-0.315192	1.380539
C	3.349540	-0.315192	-1.380539
C	-1.370615	-3.035329	3.038917
C	-0.010352	-0.622326	3.714182
H	0.048718	6.066243	2.144072
H	0.048718	6.066243	-2.144072
H	1.217319	-3.264965	4.098827
H	1.403700	-3.952724	2.467483
H	2.355341	-2.527385	2.942305
H	-1.204954	-3.280204	4.096319

H	-1.378462	-3.970599	2.464680
H	-0.903368	0.000127	3.590812
H	-2.349483	-2.557477	2.936811
H	0.875060	0.011348	3.593240
H	-0.008855	-1.069419	4.717328
H	1.217319	-3.264965	-4.098827
H	1.403700	-3.952724	-2.467483
H	2.355341	-2.527385	-2.942305
H	-1.204954	-3.280204	-4.096319
H	-1.378462	-3.970599	-2.464680
H	-0.903368	0.000127	-3.590812
H	-2.349483	-2.557477	-2.936811
H	0.875060	0.011348	-3.593240
H	-0.008855	-1.069419	-4.717328
H	-4.537998	-2.624889	0.000000
H	-3.215593	-3.425107	0.887812
H	-3.215593	-3.425107	-0.887812
H	4.548441	-2.574507	0.000000
H	3.235409	-3.389944	0.887815
H	3.235409	-3.389944	-0.887815
H	-4.452841	-0.451990	1.275099
H	-3.067718	-0.734761	2.363006
H	-3.100565	0.712163	-1.336964
H	-3.100565	0.712163	1.336964
H	-3.067718	-0.734761	-2.363006
H	-4.452841	-0.451990	-1.275099
H	4.438915	-0.403592	1.275021
H	4.438915	-0.403592	-1.275021
H	3.056626	-0.700288	2.362838
H	3.074564	0.746231	-1.335877
H	3.074564	0.746231	1.335877
H	3.056626	-0.700288	-2.362838
H	0.012044	2.345800	-2.485148
H	-0.877238	3.722079	-3.152122
H	0.889681	3.725049	-3.161960
H	-0.995022	8.126616	0.000000
H	0.532833	8.148971	-0.888857
H	0.532833	8.148971	0.888857
H	0.012044	2.345800	2.485148
H	0.889681	3.725049	3.161960
H	-0.877238	3.722079	3.152122

$[(PMe_3)_5W{\equiv}Si(Mes)]^+$ (IX)
BP86/TZ2P

C	-3.162738	0.608294	0.000000
C	-3.876108	0.774077	-1.219534
C	-5.236950	1.083339	-1.195536
C	-5.945129	1.240673	0.000000
C	-5.236950	1.083339	1.195536
C	-3.876108	0.774077	1.219534

C	-3.206171	0.615345	-2.558528
C	-7.408721	1.596959	0.000000
C	-3.206171	0.615345	2.558528
Si	-1.326445	0.120871	0.000000
H	-5.763227	1.202435	-2.144996
H	-5.763227	1.202435	2.144996
H	-2.299415	1.231360	2.624587
H	-3.874216	0.913624	3.374592
H	-2.908439	-0.426545	2.736174
H	-7.540290	2.689809	0.000000
H	-7.917625	1.207598	0.890205
H	-7.917625	1.207598	-0.890205
H	-2.299415	1.231360	-2.624587
H	-2.908439	-0.426545	-2.736174
H	-3.874216	0.913624	-3.374592
W	0.941195	-0.181622	0.000000
P	1.239179	-0.349437	-2.519220
C	2.378773	-1.695285	-3.136626
P	1.239179	-0.349437	2.519220
C	2.378773	-1.695285	3.136626
P	0.903483	2.351447	0.000000
C	2.419875	3.446953	0.000000
P	0.514209	-2.686949	0.000000
C	1.866074	-3.977623	0.000000
C	1.908930	1.061244	3.556211
C	-0.177445	-0.714855	3.664722
C	0.002802	3.216946	-1.382476
C	0.002802	3.216946	1.382476
C	-0.504792	-3.424851	-1.376554
C	-0.504792	-3.424851	1.376554
C	1.908930	1.061244	-3.556211
C	-0.177445	-0.714855	-3.664722
H	2.433060	-1.667249	-4.233561
H	3.393370	-1.587133	-2.736840
H	1.997415	-2.677475	-2.831396
H	2.278096	0.678375	-4.517918
H	2.714898	1.606457	-3.055792
H	-0.836913	0.157520	-3.708227
H	1.094613	1.765063	-3.766523
H	-0.759338	-1.578790	-3.329959
H	0.211057	-0.908662	-4.674256
H	2.433060	-1.667249	4.233561
H	3.393370	-1.587133	2.736840
H	1.997415	-2.677475	2.831396
H	2.278096	0.678375	4.517918
H	2.714898	1.606457	3.055792
H	-0.836913	0.157520	3.708227
H	1.094613	1.765063	3.766523
H	-0.759338	-1.578790	3.329959
H	0.211057	-0.908662	4.674256
H	2.119941	4.503739	0.000000
H	3.032048	3.265124	-0.892448

H	3.032048	3.265124	0.892448
H	1.422620	-4.982769	0.000000
H	2.500730	-3.876622	-0.889126
H	2.500730	-3.876622	0.889126
H	-0.002223	4.301917	-1.207656
H	0.480278	3.019771	-2.347769
H	-1.036291	2.862526	1.421843
H	-1.036291	2.862526	-1.421843
H	0.480278	3.019771	2.347769
H	-0.002223	4.301917	1.207656
H	-0.685595	-4.489200	-1.173034
H	-0.685595	-4.489200	1.173034
H	0.001709	-3.341291	-2.344975
H	-1.470491	-2.905423	1.436631
H	-1.470491	-2.905423	-1.436631
H	0.001709	-3.341291	2.344975
P	3.647337	-0.152724	0.000000
C	4.590573	0.666555	1.379832
H	4.367243	1.739227	1.407188
H	4.356354	0.232575	2.356864
H	5.665004	0.539618	1.189368
H	4.287129	-2.367797	0.887360
C	4.547557	-1.780173	0.000000
H	4.287129	-2.367797	-0.887360
H	5.630727	-1.595854	0.000000
H	5.665004	0.539618	-1.189368
C	4.590573	0.666555	-1.379832
H	4.367243	1.739227	-1.407188
H	4.356354	0.232575	-2.356864

$[(PMe_3)_5W{\equiv}Ge(Mes)]^+$ (X)
BP86/TZ2P

C	-3.247620	0.626021	0.000000
C	-3.954678	0.778278	-1.219704
C	-5.325045	1.051424	-1.195439
C	-6.037765	1.186149	0.000000
C	-5.325045	1.051424	1.195439
C	-3.954678	0.778278	1.219704
C	-3.277389	0.649351	-2.559169
C	-7.511160	1.502947	0.000000
C	-3.277389	0.649351	2.559169
Ge	-1.325828	0.136117	0.000000
H	-5.852657	1.165058	-2.145154
H	-5.852657	1.165058	2.145154
H	-2.337267	1.215773	2.585227
H	-3.918342	1.026383	3.364487
H	-3.037241	-0.397542	2.790028
H	-7.674500	2.591470	0.000000
H	-8.009276	1.098876	0.889794
H	-8.009276	1.098876	-0.889794
H	-2.337267	1.215773	-2.585227

H	-3.037241	-0.397542	-2.790028
H	-3.918342	1.026383	-3.364487
W	0.980721	-0.176041	0.000000
P	1.245466	-0.343597	-2.519537
C	2.353867	-1.705069	-3.155335
P	1.245466	-0.343597	2.519537
C	2.353867	-1.705069	3.155335
P	0.950886	2.362878	0.000000
C	2.467322	3.454179	0.000000
P	0.517449	-2.681419	0.000000
C	1.850382	-3.989823	0.000000
C	1.918964	1.055177	3.568930
C	-0.203751	-0.680150	3.632222
C	0.048396	3.227957	-1.382167
C	0.048396	3.227957	1.382167
C	-0.517232	-3.404088	-1.373750
C	-0.517232	-3.404088	1.373750
C	1.918964	1.055177	-3.568930
C	-0.203751	-0.680150	-3.632222
H	2.380581	-1.685695	-4.253497
H	3.379085	-1.600553	-2.781782
H	1.973608	-2.681863	-2.832324
H	2.254529	0.665635	-4.540218
H	2.749797	1.581074	-3.088823
H	-0.846803	0.205417	-3.654313
H	1.114980	1.776725	-3.757631
H	-0.794902	-1.532422	-3.284537
H	0.153308	-0.878067	-4.652671
H	2.380581	-1.685695	4.253497
H	3.379085	-1.600553	2.781782
H	1.973608	-2.681863	2.832324
H	2.254529	0.665635	4.540218
H	2.749797	1.581074	3.088823
H	-0.846803	0.205417	3.654313
H	1.114980	1.776725	3.757631
H	-0.794902	-1.532422	3.284537
H	0.153308	-0.878067	4.652671
H	2.169235	4.511599	0.000000
H	3.078930	3.270472	-0.892491
H	3.078930	3.270472	0.892491
H	1.391998	-4.988270	0.000000
H	2.486011	-3.896885	-0.889232
H	2.486011	-3.896885	0.889232
H	0.031908	4.311458	-1.199771
H	0.533237	3.042823	-2.346091
H	-0.986971	2.864109	1.430996
H	-0.986971	2.864109	-1.430996
H	0.533237	3.042823	2.346091
H	0.031908	4.311458	1.199771
H	-0.704401	-4.467733	-1.172572
H	-0.704401	-4.467733	1.172572
H	-0.020245	-3.320275	-2.346849

H	-1.480157	-2.878357	1.421944
H	-1.480157	-2.878357	-1.421944
H	-0.020245	-3.320275	2.346849
P	3.657908	-0.178735	0.000000
C	4.601919	0.635080	1.382029
H	4.378128	1.707650	1.414004
H	4.366160	0.196462	2.356841
H	5.676615	0.508558	1.192466
H	4.280432	-2.397423	0.887835
C	4.545716	-1.812206	0.000000
H	4.280432	-2.397423	-0.887835
H	5.630258	-1.635741	0.000000
H	5.676615	0.508558	-1.192466
C	4.601919	0.635080	-1.382029
H	4.378128	1.707650	-1.414004
H	4.366160	0.196462	-2.356841

$[(PMe_3)_5W{\equiv}Sn(Mes)]^+$ (XI)
BP86/TZ2P

C	-3.546582	0.636228	0.000000
C	-4.244678	0.773042	-1.221033
C	-5.617784	1.036713	-1.198010
C	-6.328030	1.171584	0.000000
C	-5.617784	1.036713	1.198010
C	-4.244678	0.773042	1.221033
C	-3.552385	0.640797	-2.555688
C	-7.803625	1.479419	0.000000
C	-3.552385	0.640797	2.555688
Sn	-1.424587	0.152696	0.000000
H	-6.150343	1.136529	-2.146616
H	-6.150343	1.136529	2.146616
H	-2.737205	1.372145	2.658030
H	-4.249076	0.809432	3.384903
H	-3.118090	-0.359935	2.688921
H	-7.973440	2.566904	0.000000
H	-8.299149	1.072095	0.889745
H	-8.299149	1.072095	-0.889745
H	-2.737205	1.372145	-2.658030
H	-3.118090	-0.359935	-2.688921
H	-4.249076	0.809432	-3.384903
W	1.083312	-0.175361	0.000000
P	1.297171	-0.324968	-2.516337
C	2.339614	-1.714315	-3.202231
P	1.297171	-0.324968	2.516337
C	2.339614	-1.714315	3.202231
P	1.097218	2.364822	0.000000
C	2.638590	3.421192	0.000000
P	0.592649	-2.678987	0.000000
C	1.910924	-4.002634	0.000000
C	1.997664	1.053740	3.574648
C	-0.212769	-0.583136	3.568763

C	0.221830	3.257769	-1.383459
C	0.221830	3.257769	1.383459
C	-0.448721	-3.399327	-1.371903
C	-0.448721	-3.399327	1.371903
C	1.997664	1.053740	-3.574648
C	-0.212769	-0.583136	-3.568763
H	2.301724	-1.709013	-4.300255
H	3.386781	-1.611058	-2.892240
H	1.975298	-2.683941	-2.842534
H	2.311748	0.651035	-4.547654
H	2.850383	1.553462	-3.104438
H	-0.849890	0.305154	-3.484551
H	1.215011	1.799290	-3.758682
H	-0.784843	-1.455389	-3.237259
H	0.073096	-0.715868	-4.622173
H	2.301724	-1.709013	4.300255
H	3.386781	-1.611058	2.892240
H	1.975298	-2.683941	2.842534
H	2.311748	0.651035	4.547654
H	2.850383	1.553462	3.104438
H	-0.849890	0.305154	3.484551
H	1.215011	1.799290	3.758682
H	-0.784843	-1.455389	3.237259
H	0.073096	-0.715868	4.622173
H	2.364280	4.484737	0.000000
H	3.245623	3.223473	-0.892287
H	3.245623	3.223473	0.892287
H	1.440746	-4.995243	0.000000
H	2.547270	-3.917004	-0.889222
H	2.547270	-3.917004	0.889222
H	0.222678	4.339770	-1.191544
H	0.714898	3.072977	-2.343144
H	-0.818856	2.912100	1.450626
H	-0.818856	2.912100	-1.450626
H	0.714898	3.072977	2.343144
H	0.222678	4.339770	1.191544
H	-0.615717	-4.468834	-1.184168
H	-0.615717	-4.468834	1.184168
H	0.029854	-3.292057	-2.351673
H	-1.421684	-2.890305	1.398701
H	-1.421684	-2.890305	-1.398701
H	0.029854	-3.292057	2.351673
P	3.719809	-0.233418	0.000000
C	4.682341	0.554791	1.384678
H	4.483294	1.631829	1.426199
H	4.437938	0.113162	2.356470
H	5.753863	0.405559	1.193243
H	4.305582	-2.461553	0.889055
C	4.579240	-1.881800	0.000000
H	4.305582	-2.461553	-0.889055
H	5.666428	-1.722171	0.000000
H	5.753863	0.405559	-1.193243

C	4.682341	0.554791	-1.384678
H	4.483294	1.631829	-1.426199
H	4.437938	0.113162	-2.356470

$[(PMe_3)_5W{\equiv}Pb(Mes)]^+$ (XII)
BP86/TZ2P

C	-3.654005	0.627506	0.000000
C	-4.346628	0.748585	-1.221576
C	-5.726360	0.983717	-1.198544
C	-6.438429	1.104174	0.000000
C	-5.726360	0.983717	1.198544
C	-4.346628	0.748585	1.221576
C	-3.647211	0.630764	-2.554773
C	-7.920701	1.381113	0.000000
C	-3.647211	0.630764	2.554773
Pb	-1.442161	0.173933	0.000000
H	-6.261356	1.071877	-2.147107
H	-6.261356	1.071877	2.147107
H	-2.860361	1.391979	2.663400
H	-4.348435	0.765918	3.386352
H	-3.176342	-0.354659	2.679557
H	-8.114051	2.464596	0.000000
H	-8.407663	0.963026	0.889506
H	-8.407663	0.963026	-0.889506
H	-2.860361	1.391979	-2.663400
H	-3.176342	-0.354659	-2.679557
H	-4.348435	0.765918	-3.386352
W	1.124399	-0.169439	0.000000
P	1.311635	-0.316021	-2.516206
C	2.320475	-1.723319	-3.217003
P	1.311635	-0.316021	2.516206
C	2.320475	-1.723319	3.217003
P	1.171991	2.370267	0.000000
C	2.728507	3.404246	0.000000
P	0.602536	-2.673248	0.000000
C	1.899791	-4.018142	0.000000
C	2.028760	1.048892	3.581958
C	-0.217200	-0.540467	3.552290
C	0.311304	3.279130	-1.383028
C	0.311304	3.279130	1.383028
C	-0.451519	-3.381135	-1.370423
C	-0.451519	-3.381135	1.370423
C	2.028760	1.048892	-3.581958
C	-0.217200	-0.540467	-3.552290
H	2.256046	-1.727705	-4.313815
H	3.375766	-1.625261	-2.933484
H	1.958183	-2.686464	-2.838916
H	2.329181	0.639303	-4.556352
H	2.893814	1.533046	-3.118019
H	-0.842499	0.354528	-3.446334

H	1.258709	1.808198	-3.762308
H	-0.794952	-1.410486	-3.224014
H	0.048962	-0.662845	-4.612155
H	2.256046	-1.727705	4.313815
H	3.375766	-1.625261	2.933484
H	1.958183	-2.686464	2.838916
H	2.329181	0.639303	4.556352
H	2.893814	1.533046	3.118019
H	-0.842499	0.354528	3.446334
H	1.258709	1.808198	3.762308
H	-0.794952	-1.410486	3.224014
H	0.048962	-0.662845	4.612155
H	2.468882	4.471552	0.000000
H	3.332856	3.198225	-0.892124
H	3.332856	3.198225	0.892124
H	1.412776	-5.002779	0.000000
H	2.537492	-3.942961	-0.889064
H	2.537492	-3.942961	0.889064
H	0.325067	4.360144	-1.186656
H	0.805932	3.092351	-2.341395
H	-0.733779	2.948412	1.456864
H	-0.733779	2.948412	-1.456864
H	0.805932	3.092351	2.341395
H	0.325067	4.360144	1.186656
H	-0.625095	-4.450273	-1.186572
H	-0.625095	-4.450273	1.186572
H	0.021016	-3.272203	-2.352784
H	-1.422385	-2.867433	1.389998
H	-1.422385	-2.867433	-1.389998
H	0.021016	-3.272203	2.352784
P	3.733181	-0.269947	0.000000
C	4.706769	0.506136	1.385699
H	4.518963	1.585003	1.430288
H	4.457470	0.064710	2.356455
H	5.776764	0.346350	1.194389
H	4.296715	-2.504109	0.889449
C	4.576455	-1.927797	0.000000
H	4.296715	-2.504109	-0.889449
H	5.665267	-1.779920	0.000000
H	5.776764	0.346350	-1.194389
C	4.706769	0.506136	-1.385699
H	4.518963	1.585003	-1.430288
H	4.457470	0.064710	-2.356455

[$(PMe_3)_4Mo$]

Energy = -266.87791945 eV

Mo	-0.001532	-1.427178	0.000000
P	-0.001498	-1.849279	2.396455
C	1.390317	-2.916912	3.064213
P	-0.001498	-1.849279	-2.396455
C	1.390317	-2.916912	-3.064213

P	-2.398898	-1.009626	0.000000
C	-3.763776	-2.297891	0.000000
P	2.395034	-1.004472	0.000000
C	3.762428	-2.290073	0.000000
C	-1.388114	-2.925883	-3.059954
C	-0.006910	-0.564009	-3.763712
C	-3.066723	0.062431	1.388292
C	-3.066723	0.062431	-1.388292
C	3.060174	0.069128	1.388366
C	3.060174	0.069128	-1.388366
C	-1.388114	-2.925883	3.059954
C	-0.006910	-0.564009	3.763712
H	1.239046	-3.163748	4.126147
H	1.434178	-3.850808	2.485759
H	2.355166	-2.406275	2.952759
H	-1.236425	-3.175236	4.121237
H	-1.427065	-3.858217	2.478598
H	-0.897346	0.071950	3.666455
H	-2.355323	-2.419537	2.949339
H	0.880792	0.076228	3.669167
H	-0.007230	-1.034552	4.759061
H	1.239046	-3.163748	-4.126147
H	1.434178	-3.850808	-2.485759
H	2.355166	-2.406275	-2.952759
H	-1.236425	-3.175236	-4.121237
H	-1.427065	-3.858217	-2.478598
H	-0.897346	0.071950	-3.666455
H	-2.355323	-2.419537	-2.949339
H	0.880792	0.076228	-3.669167
H	-0.007230	-1.034552	-4.759061
H	-4.759962	-1.829183	0.000000
H	-3.666576	-2.935783	0.889061
H	-3.666576	-2.935783	-0.889061
H	4.757712	-1.819460	0.000000
H	3.666381	-2.928166	0.889056
H	3.666381	-2.928166	-0.889056
H	-4.130338	0.303537	1.239502
H	-2.949292	-0.441783	2.355728
H	-2.492441	0.999303	-1.424108
H	-2.492441	0.999303	1.424108
H	-2.949292	-0.441783	-2.355728
H	-4.130338	0.303537	-1.239502
H	4.123572	0.311713	1.240377
H	4.123572	0.311713	-1.240377
H	2.942531	-0.434667	2.355986
H	2.484583	1.005233	-1.423097
H	2.484583	1.005233	1.423097
H	2.942531	-0.434667	-2.355986

[$(PMe_3)_4W$]
Energy = -267.55377629 eV

W	-0.001680	-1.108683	0.000000
P	0.000409	-2.603793	1.771850
C	1.407576	-3.812840	2.045363
P	0.000409	-2.603793	-1.771850
C	1.407576	-3.812840	-2.045363
P	-2.309033	-0.441177	0.000000
C	-3.894943	-1.441316	0.000000
P	2.305080	-0.439732	0.000000
C	3.891783	-1.438840	0.000000
C	-1.402687	-3.817697	-2.044759
C	-0.001577	-1.843813	-3.497008
C	-2.756894	0.704822	1.421177
C	-2.756894	0.704822	-1.421177
C	2.752359	0.706462	1.421215
C	2.752359	0.706462	-1.421215
C	-1.402687	-3.817697	2.044759
C	-0.001577	-1.843813	3.497008
H	1.246646	-4.423270	2.947345
H	1.497653	-4.477383	1.175661
H	2.349513	-3.257741	2.150254
H	-1.239680	-4.428098	2.946402
H	-1.490620	-4.482067	1.174699
H	-0.893616	-1.215039	3.626999
H	-2.346437	-3.265758	2.150036
H	0.888233	-1.212095	3.627950
H	-0.000766	-2.620958	4.275857
H	1.246646	-4.423270	-2.947345
H	1.497653	-4.477383	-1.175661
H	2.349513	-3.257741	-2.150254
H	-1.239680	-4.428098	-2.946402
H	-1.490620	-4.482067	-1.174699
H	-0.893616	-1.215039	-3.626999
H	-2.346437	-3.265758	-2.150036
H	0.888233	-1.212095	-3.627950
H	-0.000766	-2.620958	-4.275857
H	-4.776358	-0.781462	0.000000
H	-3.927094	-2.084701	0.888879
H	-3.927094	-2.084701	-0.888879
H	4.772710	-0.778337	0.000000
H	3.924471	-2.082209	0.888866
H	3.924471	-2.082209	-0.888866
H	-3.742249	1.168560	1.263326
H	-2.778527	0.139269	2.362561
H	-2.004061	1.500906	-1.513540
H	-2.004061	1.500906	1.513540
H	-2.778527	0.139269	-2.362561
H	-3.742249	1.168560	-1.263326
H	3.737508	1.170626	1.263353
H	3.737508	1.170626	-1.263353
H	2.774315	0.140850	2.362549
H	1.999190	1.502217	-1.513707
H	1.999190	1.502217	1.513707

H	2.774315	0.140850	-2.362549

[$(PMe_3)_5Mo$]

Mo	1.437790	-0.362634	0.000000
P	1.579737	-0.313714	-2.457159
C	2.750830	-1.528074	-3.286209
P	1.579737	-0.313714	2.457159
C	2.750830	-1.528074	3.286209
P	0.179881	1.610846	0.000000
C	1.073392	3.259677	0.000000
P	-0.385563	-1.964187	0.000000
C	0.322246	-3.705508	0.000000
C	2.161772	1.265313	3.284266
C	0.185109	-0.621194	3.682718
C	-1.042094	1.979647	-1.376207
C	-1.042094	1.979647	1.376207
C	-1.638147	-2.223373	-1.373128
C	-1.638147	-2.223373	1.373128
C	2.161772	1.265313	-3.284266
C	0.185109	-0.621194	-3.682718
H	2.735114	-1.406510	-4.379521
H	3.781358	-1.398913	-2.933860
H	2.433089	-2.552236	-3.042743
H	2.484067	1.070850	-4.318509
H	2.978554	1.731789	-2.726762
H	-0.732443	-0.100134	-3.386924
H	1.323744	1.974366	-3.311990
H	-0.027938	-1.694781	-3.750274
H	0.492632	-0.272611	-4.679410
H	2.735114	-1.406510	4.379521
H	3.781358	-1.398913	2.933860
H	2.433089	-2.552236	3.042743
H	2.484067	1.070850	4.318509
H	2.978554	1.731789	2.726762
H	-0.732443	-0.100134	3.386924
H	1.323744	1.974366	3.311990
H	-0.027938	-1.694781	3.750274
H	0.492632	-0.272611	4.679410
H	0.381329	4.116724	0.000000
H	1.716824	3.314167	-0.889321
H	1.716824	3.314167	0.889321
H	-0.477046	-4.462316	0.000000
H	0.948146	-3.854128	-0.891376
H	0.948146	-3.854128	0.891376
H	-1.552188	2.939692	-1.206465
H	-0.539408	2.017809	-2.350437
H	-1.794118	1.178770	1.408369
H	-1.794118	1.178770	-1.408369
H	-0.539408	2.017809	2.350437
H	-1.552188	2.939692	1.206465
H	-2.311656	-3.055337	-1.121664

H	-2.311656	-3.055337	1.121664
H	-1.136784	-2.450994	-2.318929
H	-2.237379	-1.313187	1.512650
H	-2.237379	-1.313187	-1.512650
H	-1.136784	-2.450994	2.318929
P	3.867239	0.126169	0.000000
C	4.950714	0.848679	1.359020
H	4.825096	1.940221	1.384588
H	4.697262	0.448634	2.346837
H	6.006867	0.625742	1.148728
H	4.279968	-2.160024	0.889888
C	4.603803	-1.604923	0.000000
H	4.279968	-2.160024	-0.889888
H	5.702470	-1.552311	0.000000
H	6.006867	0.625742	-1.148728
C	4.950714	0.848679	-1.359020
H	4.825096	1.940221	-1.384588
H	4.697262	0.448634	-2.346837

[$(PMe_3)_5W$]

W	1.437269	-0.356065	0.000000
P	1.572316	-0.311122	-2.459459
C	2.731553	-1.531138	-3.305099
P	1.572316	-0.311122	2.459459
C	2.731553	-1.531138	3.305099
P	0.184348	1.627886	0.000000
C	1.081437	3.280109	0.000000
P	-0.367920	-1.986136	0.000000
C	0.332965	-3.734538	0.000000
C	2.154303	1.260551	3.311974
C	0.164530	-0.614121	3.677971
C	-1.034695	2.022037	-1.376553
C	-1.034695	2.022037	1.376553
C	-1.624211	-2.259520	-1.372860
C	-1.624211	-2.259520	1.372860
C	2.154303	1.260551	-3.311974
C	0.164530	-0.614121	-3.677971
H	2.709797	-1.405539	-4.397860
H	3.765205	-1.408557	-2.958832
H	2.410620	-2.554663	-3.063615
H	2.459852	1.053086	-4.348728
H	2.982884	1.727790	-2.772447
H	-0.748207	-0.090359	-3.372398
H	1.321265	1.975569	-3.335334
H	-0.052883	-1.686301	-3.747444
H	0.463644	-0.263073	-4.676320
H	2.709797	-1.405539	4.397860
H	3.765205	-1.408557	2.958832
H	2.410620	-2.554663	3.063615
H	2.459852	1.053086	4.348728
H	2.982884	1.727790	2.772447

H	-0.748207	-0.090359	3.372398
H	1.321265	1.975569	3.335334
H	-0.052883	-1.686301	3.747444
H	0.463644	-0.263073	4.676320
H	0.391387	4.138975	0.000000
H	1.724768	3.333358	-0.889336
H	1.724768	3.333358	0.889336
H	-0.471745	-4.485344	0.000000
H	0.957631	-3.888515	-0.891254
H	0.957631	-3.888515	0.891254
H	-1.528498	2.989710	-1.201911
H	-0.529698	2.059427	-2.349667
H	-1.800507	1.234742	1.415164
H	-1.800507	1.234742	-1.415164
H	-0.529698	2.059427	2.349667
H	-1.528498	2.989710	1.201911
H	-2.294870	-3.091487	-1.113859
H	-2.294870	-3.091487	1.113859
H	-1.122474	-2.496498	-2.316373
H	-2.225547	-1.352259	1.520807
H	-2.225547	-1.352259	-1.520807
H	-1.122474	-2.496498	2.316373
P	3.866316	0.108712	0.000000
C	4.945538	0.845495	1.359144
H	4.806464	1.935219	1.384910
H	4.697016	0.441085	2.346449
H	6.004091	0.635199	1.147957
H	4.326768	-2.172119	0.890292
C	4.638478	-1.610486	0.000000
H	4.326768	-2.172119	-0.890292
H	5.735586	-1.533199	0.000000
H	6.004091	0.635199	-1.147957
C	4.945538	0.845495	-1.359144
H	4.806464	1.935219	-1.384910
H	4.697016	0.441085	-2.346449

Si(Mes)]$^{+}$

Energy = -116.16140127 eV

C	-0.000161	3.069182	0.000000
C	0.005724	3.772704	1.242381
C	0.013798	5.156314	1.220339
C	0.013534	5.866893	0.000000
C	0.013798	5.156314	-1.220339
C	0.005724	3.772704	-1.242381
C	0.006405	2.987756	2.530481
C	-0.014936	7.364093	0.000000
C	0.006405	2.987756	-2.530481
Si	-0.008535	1.267398	0.000000
H	0.023307	5.717295	2.156897
H	0.023307	5.717295	-2.156897

H	0.004864	1.889387	-2.351916
H	-0.881738	3.199474	-3.140414
H	0.895850	3.197663	-3.139115
H	-1.061602	7.711824	0.000000
H	0.461939	7.780647	-0.894513
H	0.461939	7.780647	0.894513
H	0.004864	1.889387	2.351916
H	0.895850	3.197663	3.139115
H	-0.881738	3.199474	3.140414

Ge(Mes)]$^{+}$

Energy = -115.72751137 eV

C	0.000649	3.059959	0.000000
C	0.006054	3.761949	1.240208
C	0.018017	5.147372	1.218303
C	0.020788	5.860220	0.000000
C	0.018017	5.147372	-1.218303
C	0.006054	3.761949	-1.240208
C	0.001646	2.989931	2.536349
C	0.000434	7.358423	0.000000
C	0.001646	2.989931	-2.536349
Ge	-0.004672	1.158419	0.000000
H	0.028545	5.706777	2.156127
H	0.028545	5.706777	-2.156127
H	-0.000327	1.890411	-2.372432
H	-0.887736	3.211298	-3.141363
H	0.888633	3.207922	-3.145985
H	-1.043380	7.714375	0.000000
H	0.480564	7.772654	-0.894067
H	0.480564	7.772654	0.894067
H	-0.000327	1.890411	2.372432
H	0.888633	3.207922	3.145985
H	-0.887736	3.211298	3.141363

Sn(Mes)]$^{+}$

Energy = -115.29087081 eV

C	-0.000413	3.420497	0.000000
C	0.005013	4.121422	1.234811
C	0.015074	5.509954	1.215249
C	0.015260	6.223873	0.000000
C	0.015074	5.509954	-1.215249
C	0.005013	4.121422	-1.234811
C	0.002155	3.366946	2.542828
C	-0.008735	7.723503	0.000000
C	0.002155	3.366946	-2.542828
Sn	-0.002827	1.309967	0.000000
H	0.025837	6.067676	2.154244
H	0.025837	6.067676	-2.154244
H	0.000879	2.263734	-2.399893
H	-0.886930	3.593072	-3.146381
H	0.889149	3.591338	-3.149979

H	-1.051942	8.079644	0.000000
H	0.473152	8.137379	-0.893286
H	0.473152	8.137379	0.893286
H	0.000879	2.263734	2.399893
H	0.889149	3.591338	3.149979
H	-0.886930	3.593072	3.146381

[Pb(Mes)]$^{+}$

Energy = -115.15204883 eV

C	-0.003009	3.565673	0.000000
C	0.004335	4.265338	1.232030
C	0.014586	5.655778	1.212749
C	0.015387	6.370793	0.000000
C	0.014586	5.655778	-1.212749
C	0.004335	4.265338	-1.232030
C	0.003077	3.524003	2.548026
C	-0.008376	7.871580	0.000000
C	0.003077	3.524003	-2.548026
Pb	-0.000028	1.360152	0.000000
H	0.025017	6.212364	2.152514
H	0.025017	6.212364	-2.152514
H	0.009227	2.420283	-2.420533
H	-0.888483	3.753000	-3.146817
H	0.886252	3.762614	-3.155285
H	-1.050476	8.229977	0.000000
H	0.475258	8.284742	-0.892728
H	0.475258	8.284742	0.892728
H	0.009227	2.420283	2.420533
H	0.886252	3.762614	3.155285
H	-0.888483	3.753000	3.146817