Assessment of density functionals and paucity of noncovalent interactions in aminoylyne complexes of molybdenum and tungsten [(η^5-C_5H_5)$(CO)_2$M≡EN($SiMe_3$)(R)] (E = Si, Ge, Sn, Pb): A dispersion-corrected DFT study

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Supporting Information

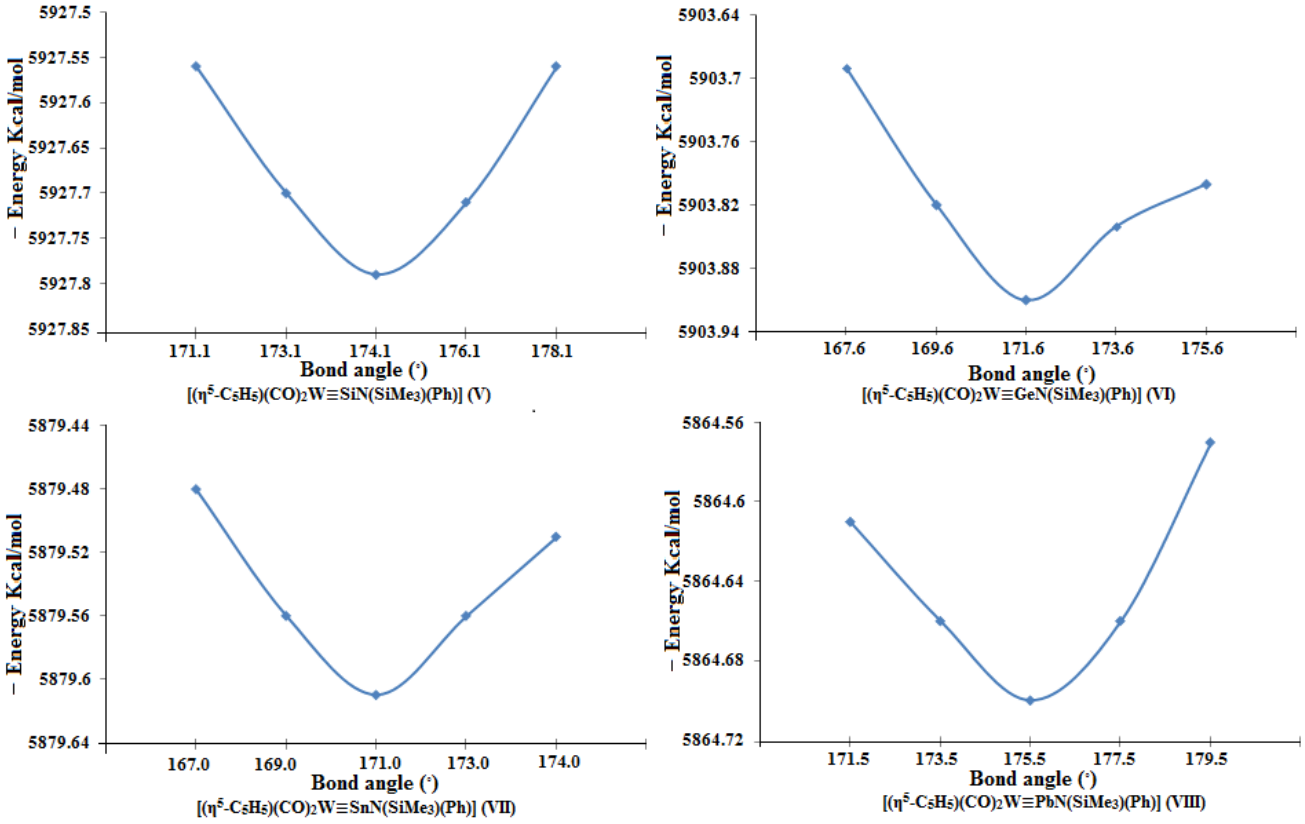

Fig. S1 The potential energy surface (PES) associated with M-E-N bond angles of the complexes [(η^5-C_5H_5)$(CO)_2$W≡EN($SiMe_3$)(Ph)] (E = Si – Pb) (**V-VII**).

Table S1 HOMO, LUMO energies and W-Sn-N bond angle in the complexe[(η^5-C_5H_5)$(CO)_2$W≡SnN($SiMe_3$)(Ph)] (**VII**).

Functional	HOMO[a]	LUMO[a]	ΔE[b]	W-Sn-N[C]
BP86	-4.747	-2.538	-2.209	173.4
PW91	-4.702	-2.507	-2.195	171.1
PBE	-4.644	-2.450	-2.194	171.0
RPBE	-4.556	-2.350	-2.206	171.9
M06-L	-4.571	-2.499	-2.072	155.1

[a]Energy in eV. [b]ΔE = HOMO-LUMO.[C]bond angle in degree.

Table S2 Results of natural hybrid orbital (NHO) analysis of M≡E bonds of the complexes [(η^5-C_5H_5)$(CO)_2$M≡EN($SiMe_3$)(Ph)] (M = Mo, W; E = Si – Pb) (**I** – **VIII**) and [(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)] (**IX**).

		M					E			
Complexes	Occupation	%	%s	%p	%d	%f	%	%s	%p	%d
M-E σ-bond										
[(η^5-C_5H_5)$(CO)_2$Mo≡SiN($SiMe_3$)(Ph)] (**I**)	1.891	38.8	20.3	49.6	30.1	0.0	61.2	81.9	18.1	0.0
[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ph)] (**II**)	1.903	37.5	20.3	51.0	28.6	0.1	62.5	86.5	13.5	0.0
[(η^5-C_5H_5)$(CO)_2$Mo≡SnN($SiMe_3$)(Ph)] (**III**)	1.931	37.0	17.7	47.8	34.5	0.0	63.0	89.8	10.2	0.0
[(η^5-C_5H_5)$(CO)_2$Mo≡PbN($SiMe_3$)(Ph)] (**IV**)	1.944	28.2	19.7	51.8	28.5	0.0	71.8	94.3	5.7	0.0
[(η^5-C_5H_5)$(CO)_2$W≡SiN($SiMe_3$)(Ph)] (**V**)	1.887	47.1	23.2	34.3	42.5	0.0	52.9	61.5	38.5	0.0
[(η^5-C_5H_5)$(CO)_2$W≡GeN($SiMe_3$)(Ph)] (**VI**)	1.852	47.9	22.9	36.3	40.7	0.0	52.1	60.1	39.9	0.0
[(η^5-C_5H_5)$(CO)_2$W≡SnN($SiMe_3$)(Ph)] (**VII**)	1.901	38.5	20.4	55.3	24.3	0.0	61.5	89.1	10.9	0.0
[(η^5-C_5H_5)$(CO)_2$W≡PbN($SiMe_3$)(Ph)] (**VIII**)	1.925	30.8	18.6	55.7	25.7	0.0	69.2	93.4	6.5	0.1
[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)](**IX**)	1.820	43.7	19.2	42.3	38.5	0.0	56.3	60.4	39.6	0.0
M-E π-bond (1)										
[(η^5-C_5H_5)$(CO)_2$Mo≡SiN($SiMe_3$)(Ph)] (**I**)	1.356	71.5	0.0	45.5	54.4	0.1	28.5	0.0	99.1	0.9
[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ph)] (**II**)	1.369	72.2	0.0	45.0	54.9	0.1	27.8	0.0	99.7	0.3
[(η^5-C_5H_5)$(CO)_2$Mo≡SnN($SiMe_3$)(Ph)] (**III**)	1.601	80.2	1.1	16.3	82.6	0.0	19.8	0.0	99.9	0.1
[(η^5-C_5H_5)$(CO)_2$Mo≡PbN($SiMe_3$)(Ph)] (**IV**)	1.640	81.4	0.4	15.1	84.5	0.0	18.6	0.0	100.0	0.0
[(η^5-C_5H_5)$(CO)_2$W≡SiN($SiMe_3$)(Ph)] (**V**)	1.701	77.7	0.0	11.7	88.3	0.0	22.3	0.0	99.2	0.8
[(η^5-C_5H_5)$(CO)_2$W≡GeN($SiMe_3$)(Ph)] (**VI**)	1.698	78.0	0.0	12.0	88.0	0.0	22.0	0.0	99.7	0.3
[(η^5-C_5H_5)$(CO)_2$W≡SnN($SiMe_3$)(Ph)] (**VII**)	1.377	71.1	0.0	46.2	53.7	0.1	28.9	0.0	99.9	0.1
[(η^5-C_5H_5)$(CO)_2$W≡PbN($SiMe_3$)(Ph)] (**VIII**)	1.648	79.8	0.1	14.1	85.8	0.0	20.2	0.0	100.0	0.0
[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)](**IX**)	1.693	80.7	0.1	10.7	89.2	0.0	19.3	0.0	99.7	0.3
M-E π-bond (2)										
[(η^5-C_5H_5)$(CO)_2$Mo≡SiN($SiMe_3$)(Ph)] (**I**)	1.565	78.4	0.6	23.6	75.8	0.0	21.6	6.0	93.3	0.7
[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ph)] (**II**)	1.563	79.3	0.5	23.5	76.0	0.0	20.7	5.4	94.3	0.3
[(η^5-C_5H_5)$(CO)_2$Mo≡SnN($SiMe_3$)(Ph)] (**III**)	1.603	83.7	1.2	14.8	84.0	0.0	16.3	6.0	93.9	0.1
[(η^5-C_5H_5)$(CO)_2$Mo≡PbN($SiMe_3$)(Ph)] (**IV**)	1.429	85.3	7.4	11.6	81.0	0.0	14.7	3.7	96.2	0.1
[(η^5-C_5H_5)$(CO)_2$W≡SiN($SiMe_3$)(Ph)] (**V**)	1.671	77.9	1.4	11.0	87.6	0.0	22.1	4.4	94.9	0.7
[(η^5-C_5H_5)$(CO)_2$W≡GeN($SiMe_3$)(Ph)] (**VI**)	1.671	79.0	1.2	10.5	88.3	0.0	21.0	4.0	95.7	0.3
[(η^5-C_5H_5)$(CO)_2$W≡SnN($SiMe_3$)(Ph)] (**VII**)	1.523	80.8	0.4	25.2	74.4	0.1	19.2	5.9	94.0	0.1
[(η^5-C_5H_5)$(CO)_2$W≡PbN($SiMe_3$)(Ph)] (**VIII**)	1.470	84.0	3.6	10.3	86.2	0.0	16.0	4.2	95.7	0.1
[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)](**IX**)	1.662	81.2	3.3	9.6	87.1	0.0	18.8	3.8	95.8	0.4

Table S3 Topological properties, electron densities, ρ(r) and Laplician, $\nabla^2\rho(r)$ (in a.u.) at bond critical points (BCPs) and ring critical points (RCPs) in the complex $[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$ at DFT-D3(BJ)/BP86 Level.

Bonds	distance (in Å)	ρ(r)	$\nabla^2\rho(r)$
Bond Critical Points (BCPs)			
Mo-Ge	2.303	0.0840	0.1764
E-C	1.842	0.1393	0.3086
O14---H7	2.721	0.0067	0.0219
O15---H10	2.721	0.0067	0.0219
C5---H44	2.598	0.0098	0.0345
C9---H49	2.598	0.0098	0.0345
Ring Critical Points (RCPs)			
Mo-Ge-N-Si-H7-O14-C		0.0053	0.0173
Mo-Ge-N-Si-H10-O15-C		0.0053	0.0173
Si-C5-H44-C-C-C-N		0.0056	0.0226
Si-C9-H49-C-C-C-N		0.0056	0.0226

Table S4 Results of energy decomposition analysis (EDA)[a] of M-E bonds for the studied aminoylyne complexes $[(\eta^5\text{-}C_5H_5)(CO)_2M{\equiv}EN(SiMe_3)(Ph)]$ (M = Mo, W; E = Si – Pb) (**I** – **VIII**) and $[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$ (**IX**) considering their neutral fragments.[b]

Complexes	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat} [c]	ΔE_{orb}	$\Delta E_{a'}$	$\Delta E_{a''}$[d]	ΔE_{prep}
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SiN(SiMe_3)(Ph)]$ (**I**)	-93.9	188.5	-106.3 (37.6%)	-176.1	-32.8	-143.3	12.3
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ph)]$ (**II**)	-85.1	161.7	-87.8 (35.6%)	-158.8	-17.5	-141.3	11.6
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SnN(SiMe_3)(Ph)]$ (**III**)	-75.9	125.5	-68.2 (33.9%)	-133.2	2.6	-135.8	11.2
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}PbN(SiMe_3)(Ph)]$ (**IV**)	-70.3	111.9	-57.7 (31.7%)	-124.5	10.7	-135.2	12.1
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiN(SiMe_3)(Ph)]$ (**V**)	-103.1	190.5	-112.7 (38.4%)	-180.9	-35.3	-145.6	15.3
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}GeN(SiMe_3)(Ph)]$ (**VI**)	-93.7	164.6	-93.7 (35.8%)	-169.0	-24.6	-144.4	14.4
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SnN(SiMe_3)(Ph)]$ (**VII**)	-83.0	136.8	-77.0 (35.0%)	-142.8	-5.9	-136.9	13.6
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}PbN(SiMe_3)(Ph)]$ (**VIII**)	-76.4	119.5	-63.8 (32.6%)	-132.1	4.5	-136.6	14.6
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)	-85.8	160.2	-88.1 (35.8%)	-157.9	-17.4	-140.5	10.6

[a] Energy contributions in kcal mol^{-1}. [b] neutral fragments $[(\eta^5\text{-}C_5H_5)(CO)_2M]$ and $[EN(SiMe_3)(Ph)]$ have been considered. [c]The values in parentheses are the percentage contribution to the total attractive interactions reflecting total ionic character of the bond.

Table S5 Comparison of the M≡E bond distances[a] and various bonding energy[b] parameters of M-E bonds for the metal-ylyne complexes $[(Cp)(CO)_2M{\equiv}EMe]$ and aminoylyne complexes $[(\eta^5\text{-}C_5H_5)(CO)_2M{\equiv}EN(SiMe_3)(Ph)]$ (M = Mo, W; E = Si – Pb) (**I** – **VIII**) considering their ionic fragments.[c]

Complexes	Bond Distance	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{orb}	$\Delta E_{a"}$	$\Delta E_{(-De)}$	Ref.
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SiMe]$	2.229	-220.9	117.0	-168.1	-169.7	-71.7	-211.0	28
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SiN(SiMe_3)(Ph)]$ (**I**)	2.247	-178.8	113.8	-145.6	-146.9	-55.4	-169.2	this work
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeMe]$	2.286	-210.5	107.7	-160.8	-157.4	-66.7	-204.7	28
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ph)]$ (**II**)	2.305	-173.4	96.6	-132.9	-137.1	-52.5	-163.7	this work
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SnMe]$	2.482	-193.6	90.7	-153.5	-130.8	-55.2	-185.7	28
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SnN(SiMe_3)(Ph)]$ (**III**)	2.503	-162.1	75.0	-122.5	-114.7	-46.0	-154.5	this work
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}PbMe]$	2.522	-180.3	92.7	-153.0	-120.0	-50.9	-172.9	28
$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}PbN(SiMe_3)(Ph)]$ (**IV**)	2.561	-152.4	69.5	-117.0	-104.8	-43.3	-145.9	this work
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiMe]$	2.239	-231.0	129.8	-180.7	-180.1	-74.9	-220.1	28
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiN(SiMe_3)(Ph)]$ (**V**)	2.252	-188.1	121.7	-153.3	-156.5	-58.5	-177.6	this work
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}GeMe]$	2.293	-220.2	115.9	-168.9	-167.5	-70.5	-213.2	28
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}GeN(SiMe_3)(Ph)]$ (**VI**)	2.303	-182.7	107.5	-143.2	-147.0	-56.6	-171.7	this work
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SnMe]$	2.483	-202.0	100.8	-162.8	-140.0	-58.3	-193.3	28
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SnN(SiMe_3)(Ph)]$ (**VII**)	2.503	-169.4	85.7	-131.5	-123.6	-48.3	-161.6	this work
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}PbMe]$	2.521	-187.9	104.9	-163.8	-129.1	-53.8	-179.9	28
$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}PbN(SiMe_3)(Ph)]$ (**VIII**)	2.562	-158.6	78.5	-124.2	-112.9	-45.6	-151.7	this work

[a] Bond distances are in (Å). [b] Energy contributions in kcal mol^{-1}. [c]Charged fragments $[(\eta^5\text{-}C_5H_5)(CO)_2M]^-$ and $[EMe]^+$ or $[EN(SiMe_3)(Ph)]^+$ have been considered.

Cartesian coordinate of the optimized geometries of the transition metal-aminoylyne complexes of molybdenum and tungsten [(η^5-C_5H_5)$(CO)_2$M≡EN($SiMe_3$)(Ph)] (M = Mo: **I**, E = Si; **II**, E = Ge; **III**, E = Sn; **IV**, E = Pb; M = W: **V**, E = Si; **VI**, E = Ge; **VII**, E = Sn; **VIII**, E = Pb), [(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)] (**IX**) and [(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ar*)] (**X**).

BP86/DFT

[(η^5-C_5H_5)$(CO)_2$Mo≡SiN($SiMe_3$)(Ph)] (**I**)

H	-3.736315	-3.623032	1.561713
H	-1.075389	-4.321890	0.000000
H	-3.736315	-3.623032	-1.561713
H	-2.812205	-2.398143	2.460429
C	-3.404959	-2.572734	1.550410
C	-0.808387	-3.252991	0.000000
H	-0.189146	-3.070849	0.889807
H	-4.303751	-1.940606	1.597426
C	-3.404959	-2.572734	-1.550410
H	-0.189146	-3.070849	-0.889807
H	-2.812205	-2.398143	-2.460429
Si	-2.387185	-2.236892	0.000000
H	-4.303751	-1.940606	-1.597426
O	2.083920	-1.824762	2.247092
O	2.083920	-1.824762	-2.247092
C	1.992660	-1.031502	1.387551
C	1.992660	-1.031502	-1.387551
N	-1.881316	-0.508212	0.000000
Mo	1.969650	0.351720	0.000000
H	5.019559	0.214325	0.000000
C	-2.898492	0.523962	0.000000
C	4.233482	0.961022	0.000000
C	-3.393774	1.030217	1.209519
C	-3.393774	1.030217	-1.209519
H	3.884835	1.337735	2.187595
Si	-0.260153	0.072561	0.000000
H	3.884835	1.337735	-2.187595
C	3.641366	1.568009	1.156177
C	3.641366	1.568009	-1.156177
C	-4.376854	2.021342	1.207205
C	-4.376854	2.021342	-1.207205
H	-4.753501	2.407484	2.153761
H	-4.753501	2.407484	-2.153761
C	-4.872984	2.518262	0.000000
C	2.694281	2.528661	0.716594
C	2.694281	2.528661	-0.716594
H	2.080052	3.157506	1.352689
H	2.080052	3.157506	-1.352689
H	-5.639547	3.292362	0.000000
H	-2.999658	0.639661	2.147039
H	-2.999658	0.639661	-2.147039

[(η^5-C_5H_5)(CO)$_2$Mo≡GeN(SiMe$_3$)(Ph)] (**II**)

H	-3.817954	-3.627095	1.534290
H	-1.155275	-4.288644	0.000000
H	-3.817954	-3.627095	-1.534290
H	-2.922533	-2.401388	2.461727
C	-3.498511	-2.572887	1.540506
C	-0.888603	-3.219687	0.000000
H	-0.269646	-3.038624	0.890406
H	-4.406175	-1.952847	1.582078
C	-3.498511	-2.572887	-1.540506
H	-0.269646	-3.038624	-0.890406
H	-2.922533	-2.401388	-2.461727
Si	-2.471245	-2.205482	0.000000
H	-4.406175	-1.952847	-1.582078
O	2.172486	-1.813332	2.252532
O	2.172486	-1.813332	-2.252532
C	2.070060	-1.024355	1.392134
C	2.070060	-1.024355	-1.392134
N	-1.984444	-0.483068	0.000000
Mo	2.052455	0.358187	0.000000
H	5.093254	0.162455	0.000000
C	-3.010885	0.528943	0.000000
C	4.319387	0.921900	0.000000
C	-3.529790	1.019316	1.208652
C	-3.529790	1.019316	-1.208652
H	3.975458	1.304059	2.187749
Ge	-0.240181	0.117624	0.000000
H	3.975458	1.304059	-2.187749
C	3.737736	1.539468	1.156180
C	3.737736	1.539468	-1.156180
C	-4.552562	1.969777	1.206716
C	-4.552562	1.969777	-1.206716
H	-4.947735	2.336731	2.153629
H	-4.947735	2.336731	-2.153629
C	-5.069701	2.446429	0.000000
C	2.807071	2.516751	0.716775
C	2.807071	2.516751	-0.716775
H	2.202495	3.154950	1.353030
H	2.202495	3.154950	-1.353030
H	-5.870479	3.185252	0.000000
H	-3.126811	0.639948	2.147528
H	-3.126811	0.639948	-2.147528

[(η^5-C_5H_5)(CO)$_2$Mo≡SnN(SiMe$_3$)(Ph)] (**III**)

H	-4.011243	-3.694696	1.533884
H	-1.313374	-4.274848	0.000000
H	-4.011243	-3.694696	-1.533884
H	-3.134537	-2.454400	2.461034
C	-3.711641	-2.634836	1.542050
C	-1.084048	-3.197491	0.000000
H	-0.467518	-3.004288	0.891117

H	-4.630475	-2.031702	1.591900
C	-3.711641	-2.634836	-1.542050
H	-0.467518	-3.004288	-0.891117
H	-3.134537	-2.454400	-2.461034
Si	-2.701319	-2.225584	0.000000
H	-4.630475	-2.031702	-1.591900
O	2.486434	-1.812508	2.232294
O	2.486434	-1.812508	-2.232294
C	2.309851	-1.024354	1.382794
C	2.309851	-1.024354	-1.382794
N	-2.239578	-0.515131	0.000000
Mo	2.214630	0.363931	0.000000
H	5.250687	0.282044	0.000000
C	-3.235429	0.515850	0.000000
C	4.446365	1.009064	0.000000
C	-3.740871	1.028143	1.207917
C	-3.740871	1.028143	-1.207917
H	4.091727	1.383151	2.188131
Sn	-0.273222	0.083965	0.000000
H	4.091727	1.383151	-2.188131
C	3.843537	1.606534	1.156315
C	3.843537	1.606534	-1.156315
C	-4.727962	2.015513	1.206159
C	-4.727962	2.015513	-1.206159
H	-5.108493	2.397240	2.153343
H	-5.108493	2.397240	-2.153343
C	-5.227696	2.512021	0.000000
C	2.881316	2.552923	0.716814
C	2.881316	2.552923	-0.716814
H	2.261824	3.176474	1.353395
H	2.261824	3.176474	-1.353395
H	-5.999339	3.281224	0.000000
H	-3.352418	0.636251	2.147957
H	-3.352418	0.636251	-2.147957

[(η^5-C_5H_5)$(CO)_2$Mo≡PbN($SiMe_3$)(Ph)] (**IV**)

H	-4.183917	-3.728339	1.528212
H	-1.497771	-4.358749	0.000000
H	-4.183917	-3.728339	-1.528212
H	-3.278066	-2.512307	2.460378
C	-3.860392	-2.675639	1.541295
C	-1.247337	-3.286191	0.000000
H	-0.627481	-3.107611	0.892376
H	-4.764931	-2.051587	1.596961
C	-3.860392	-2.675639	-1.541295
H	-0.627481	-3.107611	-0.892376
H	-3.278066	-2.512307	-2.460378
Si	-2.842542	-2.274313	0.000000
H	-4.764931	-2.051587	-1.596961
N	-2.349535	-0.583348	0.000000
C	-3.277919	0.497891	0.000000

C	-3.745182	1.049663	1.208020
C	-3.745182	1.049663	-1.208020
Pb	-0.279039	0.030649	0.000000
C	-4.651881	2.110644	1.206429
C	-4.651881	2.110644	-1.206429
H	-5.000544	2.521826	2.153634
H	-5.000544	2.521826	-2.153634
C	-5.109692	2.646318	0.000000
H	-5.815559	3.476140	0.000000
H	-3.386720	0.628480	2.147468
H	-3.386720	0.628480	-2.147468
Mo	2.255204	0.400611	0.000000
O	2.643726	-1.751985	2.239953
O	2.643726	-1.751985	-2.239953
C	2.414966	-0.980561	1.387526
C	2.414966	-0.980561	-1.387526
C	4.457997	1.107073	0.000000
C	3.838377	1.688019	1.156492
C	3.838377	1.688019	-1.156492
C	2.848229	2.605443	0.717063
C	2.848229	2.605443	-0.717063
H	2.212709	3.211765	1.354033
H	2.212709	3.211765	-1.354033
H	5.283309	0.403326	0.000000
H	4.092623	1.470775	2.188154
H	4.092623	1.470775	-2.188154

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiN(SiMe_3)(Ph)]$ (**V**)

H	-3.873358	-3.563828	1.573108
H	-1.236371	-4.359896	0.000000
H	-3.873358	-3.563828	-1.573108
H	-2.900375	-2.367986	2.459651
C	-3.504001	-2.526570	1.553794
C	-0.934465	-3.300276	0.000000
H	-0.307879	-3.138554	0.889401
H	-4.378155	-1.860848	1.601651
C	-3.504001	-2.526570	-1.553794
H	-0.307879	-3.138554	-0.889401
H	-2.900375	-2.367986	-2.459651
Si	-2.479886	-2.231342	0.000000
H	-4.378155	-1.860848	-1.601651
O	2.366207	-1.838210	2.265852
O	2.366207	-1.838210	-2.265852
C	2.176208	-1.070884	1.398290
C	2.176208	-1.070884	-1.398290
N	-1.902638	-0.528187	0.000000
W	1.979920	0.295803	0.000000
H	5.014718	0.632942	0.000000
C	-2.856693	0.560314	0.000000
C	4.120175	1.244031	0.000000
C	-3.323896	1.092931	1.209375

C	-3.323896	1.092931	-1.209375
H	3.715558	1.564692	2.189482
Si	-0.237021	-0.100008	0.000000
H	3.715558	1.564692	-2.189482
C	3.438026	1.749940	1.157969
C	3.438026	1.749940	-1.157969
C	-4.254335	2.133687	1.206982
C	-4.254335	2.133687	-1.206982
H	-4.611334	2.537962	2.153592
H	-4.611334	2.537962	-2.153592
C	-4.724940	2.655174	0.000000
C	2.352623	2.554259	0.717147
C	2.352623	2.554259	-0.717147
H	1.649023	3.080201	1.352901
H	1.649023	3.080201	-1.352901
H	-5.452059	3.466436	0.000000
H	-2.950484	0.683158	2.147118
H	-2.950484	0.683158	-2.147118

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}GeN(SiMe_3)(Ph)]$ (**VI**)

H	-3.997182	-3.547998	1.544843
H	-1.358262	-4.348046	0.000000
H	-3.997182	-3.547998	-1.544843
H	-3.032762	-2.366560	2.460718
C	-3.621601	-2.512595	1.543202
C	-1.046641	-3.291381	0.000000
H	-0.418989	-3.136960	0.890091
H	-4.493993	-1.843793	1.585426
C	-3.621601	-2.512595	-1.543202
H	-0.418989	-3.136960	-0.890091
H	-3.032762	-2.366560	-2.460718
Si	-2.580987	-2.203081	0.000000
H	-4.493993	-1.843793	-1.585426
O	2.455824	-1.801530	2.273280
O	2.455824	-1.801530	-2.273280
C	2.253704	-1.041988	1.403008
C	2.253704	-1.041988	-1.403008
N	-2.000243	-0.513040	0.000000
W	2.054254	0.321209	0.000000
H	5.084396	0.623656	0.000000
C	-2.947332	0.572168	0.000000
C	4.195021	1.242138	0.000000
C	-3.428340	1.099568	1.208616
C	-3.428340	1.099568	-1.208616
H	3.791037	1.565113	2.189542
Ge	-0.215160	-0.069338	0.000000
H	3.791037	1.565113	-2.189542
C	3.516995	1.754468	1.157718
C	3.516995	1.754468	-1.157718
C	-4.378676	2.122481	1.206685
C	-4.378676	2.122481	-1.206685

H	-4.746197	2.517337	2.153501
H	-4.746197	2.517337	-2.153501
C	-4.859592	2.635740	0.000000
C	2.438168	2.569183	0.717251
C	2.438168	2.569183	-0.717251
H	1.738347	3.100035	1.353374
H	1.738347	3.100035	-1.353374
H	-5.604230	3.431152	0.000000
H	-3.052516	0.693547	2.147510
H	-3.052516	0.693547	-2.147510

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SnN(SiMe_3)(Ph)]$ (**VII**)

H	-4.120081	-3.680705	1.539891
H	-1.451658	-4.358213	0.000000
H	-4.120081	-3.680705	-1.539891
H	-3.193597	-2.471762	2.459913
C	-3.782557	-2.632418	1.544708
C	-1.181832	-3.290050	0.000000
H	-0.558740	-3.119934	0.891281
H	-4.678197	-1.995822	1.599538
C	-3.782557	-2.632418	-1.544708
H	-0.558740	-3.119934	-0.891281
H	-3.193597	-2.471762	-2.459913
Si	-2.762443	-2.260122	0.000000
H	-4.678197	-1.995822	-1.599538
O	2.591335	-1.775503	2.243751
O	2.591335	-1.775503	-2.243751
C	2.371614	-1.001308	1.389216
C	2.371614	-1.001308	-1.389216
N	-2.244437	-0.566900	0.000000
W	2.199501	0.376752	0.000000
H	5.228969	0.455607	0.000000
C	-3.180329	0.518326	0.000000
C	4.387266	1.137852	0.000000
C	-3.647205	1.064835	1.208273
C	-3.647205	1.064835	-1.208273
H	4.008871	1.489440	2.189243
Sn	-0.272799	-0.016229	0.000000
H	4.008871	1.489440	-2.189243
C	3.749008	1.700085	1.157770
C	3.749008	1.700085	-1.157770
C	-4.556777	2.123821	1.206503
C	-4.556777	2.123821	-1.206503
H	-4.906097	2.534391	2.153607
H	-4.906097	2.534391	-2.153607
C	-5.015678	2.657728	0.000000
C	2.733957	2.593625	0.717383
C	2.733957	2.593625	-0.717383
H	2.076979	3.174931	1.355029
H	2.076979	3.174931	-1.355029
H	-5.723507	3.485979	0.000000

H	-3.286080	0.645664	2.147538
H	-3.286080	0.645664	-2.147538

[(η^5-C_5H_5)$(CO)_2$W≡PbN($SiMe_3$)(Ph)] (**VIII**)

H	-4.339103	-3.638477	1.529679
H	-1.689417	-4.403103	0.000000
H	-4.339103	-3.638477	-1.529679
H	-3.372031	-2.469266	2.460263
C	-3.963062	-2.603443	1.541987
C	-1.385350	-3.344503	0.000000
H	-0.757549	-3.195965	0.892279
H	-4.834900	-1.934560	1.598729
C	-3.963062	-2.603443	-1.541987
H	-0.757549	-3.195965	-0.892279
H	-3.372031	-2.469266	-2.460263
Si	-2.927251	-2.254594	0.000000
H	-4.834900	-1.934560	-1.598729
O	2.770582	-1.696699	2.254976
O	2.770582	-1.696699	-2.254976
C	2.500299	-0.945823	1.394144
C	2.500299	-0.945823	-1.394144
N	-2.354102	-0.589123	0.000000
W	2.251266	0.415820	0.000000
H	5.262304	0.664134	0.000000
C	-3.224710	0.539084	0.000000
C	4.381851	1.295554	0.000000
C	-3.662318	1.114479	1.208135
C	-3.662318	1.114479	-1.208135
H	3.984087	1.627062	2.189448
Pb	-0.264327	-0.071780	0.000000
H	3.984087	1.627062	-2.189448
C	3.712758	1.822029	1.157872
C	3.712758	1.822029	-1.157872
C	-4.511877	2.221643	1.206580
C	-4.511877	2.221643	-1.206580
H	-4.838740	2.650559	2.153683
H	-4.838740	2.650559	-2.153683
C	-4.940716	2.780584	0.000000
C	2.648342	2.656516	0.717599
C	2.648342	2.656516	-0.717599
H	1.963679	3.204653	1.355250
H	1.963679	3.204653	-1.355250
H	-5.602091	3.646313	0.000000
H	-3.325872	0.675417	2.147566
H	-3.325872	0.675417	-2.147566

[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)](**IX**)

H	-3.115551	-4.155086	1.415182
H	-0.367408	-4.446229	0.000000
H	-3.115551	-4.155086	-1.415182
H	-2.328406	-2.948454	2.452901

C	-2.889277	-3.081616	1.517179
C	-0.217122	-3.354626	0.000000
H	0.379664	-3.109672	0.890211
H	-3.849606	-2.552238	1.604624
C	-2.889277	-3.081616	-1.517179
H	0.379664	-3.109672	-0.890211
H	-2.328406	-2.948454	-2.452901
Si	-1.907033	-2.527299	0.000000
H	-3.849606	-2.552238	-1.604624
O	2.692503	-1.723519	2.247884
O	2.692503	-1.723519	-2.247884
C	2.508516	-0.947030	1.389465
C	2.508516	-0.947030	-1.389465
N	-1.608642	-0.761322	0.000000
Mo	2.352483	0.428205	0.000000
H	5.399220	0.530366	0.000000
C	-2.699603	0.193540	0.000000
C	4.555480	1.211362	0.000000
C	-3.231962	0.663323	1.223413
C	-3.231962	0.663323	-1.223413
H	4.176296	1.557871	2.187439
Ge	0.090816	-0.033872	0.000000
H	4.176296	1.557871	-2.187439
C	3.916117	1.768654	1.155948
C	3.916117	1.768654	-1.155948
C	-4.344307	1.512784	1.195343
C	-4.344307	1.512784	-1.195343
H	-4.761226	1.855122	2.145362
H	-4.761226	1.855122	-2.145362
C	-4.931286	1.936140	0.000000
C	2.894642	2.650943	0.716654
C	2.894642	2.650943	-0.716654
H	2.231894	3.228343	1.352878
H	2.231894	3.228343	-1.352878
C	-6.126212	2.859785	0.000000
H	-6.751623	2.705895	-0.888589
H	-6.751623	2.705895	0.888589
H	-5.812080	3.914811	0.000000
C	-2.619304	0.292592	2.551207
H	-2.754049	-0.770607	2.785468
H	-1.536045	0.481639	2.564210
H	-3.075596	0.877970	3.358430
C	-2.619304	0.292592	-2.551207
H	-1.536045	0.481639	-2.564210
H	-2.754049	-0.770607	-2.785468
H	-3.075596	0.877970	-3.358430

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ar^*)]$ (**X**)

C	3.086485	-1.187860	-4.984261
C	1.777822	-1.295873	-4.506013
C	4.132379	-1.001114	-4.079542

C	-3.003923	-3.680069	-3.199784
C	-3.476122	-2.341035	-3.154827
C	1.520756	-1.206994	-3.137977
C	3.872030	-0.918584	-2.708618
C	-3.756423	-4.448913	-2.251725
C	-4.529134	-2.269011	-2.187154
C	2.562379	-1.011243	-2.219756
C	-4.698616	-3.564260	-1.632066
C	-3.546947	2.334588	-1.452840
C	2.879104	4.100597	-1.285931
C	-0.801415	-3.831495	-1.035199
C	-4.739026	2.075027	-0.777194
C	2.448047	1.627929	-0.948528
C	-2.342983	2.435599	-0.747074
C	2.229761	-0.873394	-0.727343
C	2.090650	2.951518	-0.704771
C	1.751618	0.542475	-0.398299
C	3.563076	-2.757883	0.286271
C	3.371959	-1.372299	0.161882
C	0.970676	3.181210	0.100688
C	-4.721398	1.915221	0.611775
C	0.631413	0.793887	0.431748
C	-2.314517	2.285968	0.645794
C	4.611665	-3.271651	1.048359
C	-2.844021	-3.551102	0.783147
C	0.230455	2.138105	0.658327
C	4.259411	-0.516705	0.824964
C	-3.521609	2.022056	1.312976
C	5.495026	-2.407495	1.702264
C	-1.031384	2.445071	1.467381
C	5.314179	-1.029432	1.587884
C	-1.474336	4.972418	1.600096
C	-0.969597	3.799521	2.177989
C	-1.364436	6.200449	2.257630
C	0.549239	-2.682403	2.719977
C	-0.754115	6.276290	3.510750
C	-0.368190	3.888801	3.441512
C	-0.259187	5.112380	4.103688
C	-1.462097	-0.632900	3.725437
C	1.534849	0.159022	3.500100
H	3.289247	-1.258181	-6.052940
H	0.953813	-1.454879	-5.201665
H	5.158877	-0.925746	-4.438109
H	-2.219489	-4.060576	-3.844731
H	-3.104892	-1.513795	-3.751101
H	0.495887	-1.298646	-2.772451
H	-3.663091	-5.514154	-2.072682
H	-3.547147	2.459995	-2.535476
H	4.700271	-0.791511	-2.010280
H	-5.090281	-1.379765	-1.920585
H	3.590742	3.753159	-2.044246
H	2.218773	4.844148	-1.752770

H	3.294534	1.421401	-1.604872
H	-5.677453	1.998173	-1.326335
H	-5.423513	-3.841880	-0.874631
H	-1.415785	2.636145	-1.285478
H	3.449276	4.624580	-0.504419
H	2.881180	-3.438023	-0.226423
H	1.386439	-1.551080	-0.539847
H	0.660550	4.208252	0.298609
H	4.738551	-4.350587	1.133248
H	-5.645465	1.707825	1.150667
H	-1.965063	4.924138	0.627176
H	4.125113	0.562622	0.751719
H	-1.762170	7.100048	1.788246
H	6.314864	-2.807229	2.298927
H	-0.241729	-3.278118	2.241032
H	5.992975	-0.344292	2.095699
H	-3.518246	1.906289	2.397896
H	1.495704	-2.879639	2.196113
H	-1.090774	1.688240	2.257917
H	-2.314229	-1.119050	3.226366
H	2.499721	-0.074531	3.026927
H	-0.671079	7.233380	4.025444
H	0.022033	2.986506	3.914295
H	0.651777	-3.047234	3.754472
H	1.375293	1.243768	3.421945
H	-1.728671	0.418208	3.908171
H	0.211125	5.155897	5.085816
H	-1.342828	-1.116929	4.707899
H	1.611783	-0.097038	4.569011
N	-0.109874	-0.286896	1.037480
Si	0.137966	-0.845713	2.733570
Ge	-1.349644	-1.157148	-0.029631
Mo	-2.513358	-2.888223	-1.034530
O	0.186045	-4.460973	-1.103332
O	-3.123565	-4.004989	1.826306

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$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)

H	-3.047227	-4.010724	1.406054
H	-0.284128	-4.290484	0.000000
H	-3.047227	-4.010724	-1.406054
H	-2.235775	-2.818784	2.445831
C	-2.804687	-2.941832	1.513767
C	-0.129959	-3.199417	0.000000
H	0.464011	-2.952438	0.890832
H	-3.753685	-2.391901	1.600341
C	-2.804687	-2.941832	-1.513767
H	0.464011	-2.952438	-0.890832
H	-2.235775	-2.818784	-2.445831
Si	-1.824618	-2.391564	0.000000
H	-3.753685	-2.391901	-1.600341

O	2.511043	-1.776836	2.244474
O	2.511043	-1.776836	-2.244474
C	2.418963	-0.981355	1.388014
C	2.418963	-0.981355	-1.388014
N	-1.577175	-0.615577	0.000000
Mo	2.398522	0.401173	0.000000
H	5.443060	0.251325	0.000000
C	-2.740062	0.247581	0.000000
C	4.657242	0.998251	0.000000
C	-3.316559	0.659518	1.222978
C	-3.316559	0.659518	-1.222978
H	4.306717	1.374878	2.187959
Ge	0.112984	0.117444	0.000000
H	4.306717	1.374878	-2.187959
C	4.065934	1.606654	1.156162
C	4.065934	1.606654	-1.156162
C	-4.525008	1.364816	1.195863
C	-4.525008	1.364816	-1.195863
H	-4.979570	1.659313	2.144519
H	-4.979570	1.659313	-2.144519
C	-5.163022	1.704468	0.000000
C	3.120117	2.569339	0.716894
C	3.120117	2.569339	-0.716894
H	2.506881	3.199776	1.352878
H	2.506881	3.199776	-1.352878
C	-6.468611	2.463908	0.000000
H	-7.069035	2.229612	-0.888480
H	-7.069035	2.229612	0.888480
H	-6.293377	3.550530	0.000000
C	-2.642061	0.385128	2.543749
H	-2.620188	-0.683643	2.784121
H	-1.595962	0.724273	2.534855
H	-3.160570	0.906854	3.356934
C	-2.642061	0.385128	-2.543749
H	-1.595962	0.724273	-2.534855
H	-2.620188	-0.683643	-2.784121
H	-3.160570	0.906854	-3.356934

BP86/DFT-D3(BJ)

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)

H	-3.066243	-4.032967	1.413855
H	-0.264907	-4.297287	0.000000
H	-3.066243	-4.032967	-1.413855
H	-2.254455	-2.836723	2.446242
C	-2.824082	-2.963463	1.515345
C	-0.143541	-3.202666	0.000000
H	0.444634	-2.938212	0.889531
H	-3.774009	-2.416143	1.604237
C	-2.824082	-2.963463	-1.515345
H	0.444634	-2.938212	-0.889531
H	-2.254455	-2.836723	-2.446242

Si	-1.846600	-2.416312	0.000000
H	-3.774009	-2.416143	-1.604237
O	2.573177	-1.761613	2.247747
O	2.573177	-1.761613	-2.247747
C	2.446798	-0.974638	1.388580
C	2.446798	-0.974638	-1.388580
N	-1.584741	-0.647887	0.000000
Mo	2.382686	0.403830	0.000000
H	5.420370	0.310478	0.000000
C	-2.730140	0.232745	0.000000
C	4.621862	1.042985	0.000000
C	-3.292191	0.656515	1.222334
C	-3.292191	0.656515	-1.222334
H	4.259751	1.408341	2.187127
Ge	0.104163	0.083716	0.000000
H	4.259751	1.408341	-2.187127
C	4.016769	1.637506	1.155959
C	4.016769	1.637506	-1.155959
C	-4.477573	1.398646	1.196814
C	-4.477573	1.398646	-1.196814
H	-4.922907	1.704970	2.145775
H	-4.922907	1.704970	-2.145775
C	-5.102174	1.759528	0.000000
C	3.049899	2.578816	0.716729
C	3.049899	2.578816	-0.716729
H	2.418274	3.189828	1.352518
H	2.418274	3.189828	-1.352518
C	-6.381580	2.559697	0.000000
H	-6.987898	2.343615	-0.888625
H	-6.987898	2.343615	0.888625
H	-6.173385	3.640354	0.000000
C	-2.621769	0.353454	2.536332
H	-2.615675	-0.719505	2.758567
H	-1.570400	0.676483	2.529364
H	-3.133030	0.871410	3.355983
C	-2.621769	0.353454	-2.536332
H	-1.570400	0.676483	-2.529364
H	-2.615675	-0.719505	-2.758567
H	-3.133030	0.871410	-3.355983

PBE/DFT

[(η^5-C_5H_5)$(CO)_2$Mo≡SiN($SiMe_3$)(Ph)] (**I**)

H	-3.688501	-3.632808	1.571765
H	-1.013045	-4.295456	0.000000
H	-3.688501	-3.632808	-1.571765
H	-2.774685	-2.388638	2.458741
C	-3.370901	-2.577945	1.553070
C	-0.763333	-3.221878	0.000000
H	-0.147245	-3.028347	0.890992
H	-4.276526	-1.954387	1.597814
C	-3.370901	-2.577945	-1.553070

H	-0.147245	-3.028347	-0.890992
H	-2.774685	-2.388638	-2.458741
Si	-2.361513	-2.235177	0.000000
H	-4.276526	-1.954387	-1.597814
O	2.032542	-1.835002	2.229559
O	2.032542	-1.835002	-2.229559
C	1.962717	-1.030333	1.377670
C	1.962717	-1.030333	-1.377670
N	-1.881992	-0.500809	0.000000
Mo	1.966521	0.356786	0.000000
H	5.012011	0.184418	0.000000
C	-2.901764	0.524360	0.000000
C	4.234123	0.940833	0.000000
C	-3.398061	1.028692	1.209692
C	-3.398061	1.028692	-1.209692
H	3.887929	1.319148	2.188355
Si	-0.261935	0.080759	0.000000
H	3.887929	1.319148	-2.188355
C	3.648047	1.553378	1.156075
C	3.648047	1.553378	-1.156075
C	-4.381662	2.018729	1.207211
C	-4.381662	2.018729	-1.207211
H	-4.758522	2.405134	2.154467
H	-4.758522	2.405134	-2.154467
C	-4.877370	2.515681	0.000000
C	2.710899	2.523885	0.716367
C	2.710899	2.523885	-0.716367
H	2.100642	3.157709	1.352791
H	2.100642	3.157709	-1.352791
H	-5.643844	3.290963	0.000000
H	-3.002131	0.638220	2.147586
H	-3.002131	0.638220	-2.147586

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ph)]$ (**II**)

H	-3.749021	-3.626878	1.544118
H	-1.061245	-4.237529	0.000000
H	-3.749021	-3.626878	-1.544118
H	-2.870878	-2.377491	2.460576
C	-3.447057	-2.567162	1.542265
C	-0.819398	-3.162252	0.000000
H	-0.205138	-2.965235	0.891535
H	-4.363930	-1.959300	1.578563
C	-3.447057	-2.567162	-1.542265
H	-0.205138	-2.965235	-0.891535
H	-2.870878	-2.377491	-2.460576
Si	-2.427850	-2.189048	0.000000
H	-4.363930	-1.959300	-1.578563
O	2.098551	-1.827665	2.238641
O	2.098551	-1.827665	-2.238641
C	2.029907	-1.027473	1.383928
C	2.029907	-1.027473	-1.383928

N	-1.979511	-0.454436	0.000000
Mo	2.057184	0.356765	0.000000
H	5.088818	0.098990	0.000000
C	-3.024437	0.536032	0.000000
C	4.329285	0.873648	0.000000
C	-3.556196	1.013354	1.208328
C	-3.556196	1.013354	-1.208328
H	3.990503	1.261690	2.188907
Ge	-0.238630	0.148434	0.000000
H	3.990503	1.261690	-2.188907
C	3.758901	1.501660	1.156203
C	3.758901	1.501660	-1.156203
C	-4.600483	1.940018	1.206304
C	-4.600483	1.940018	-1.206304
H	-5.004748	2.297856	2.153761
H	-5.004748	2.297856	-2.153761
C	-5.127954	2.405451	0.000000
C	2.847448	2.496901	0.716558
C	2.847448	2.496901	-0.716558
H	2.253250	3.146042	1.352990
H	2.253250	3.146042	-1.352990
H	-5.945042	3.127462	0.000000
H	-3.146001	0.641661	2.148143
H	-3.146001	0.641661	-2.148143

[(η^5-C_5H_5)$(CO)_2$Mo≡SnN($SiMe_3$)(Ph)] (**III**)

H	-3.798738	-3.769741	1.543086
H	-1.076859	-4.196081	0.000000
H	-3.798738	-3.769741	-1.543086
H	-2.983531	-2.477353	2.458938
C	-3.558452	-2.694586	1.545825
C	-0.904843	-3.107445	0.000000
H	-0.299770	-2.881285	0.892094
H	-4.507560	-2.139624	1.598191
C	-3.558452	-2.694586	-1.545825
H	-0.299770	-2.881285	-0.892094
H	-2.983531	-2.477353	-2.458938
Si	-2.577618	-2.234308	0.000000
H	-4.507560	-2.139624	-1.598191
O	2.270280	-1.822238	2.218865
O	2.270280	-1.822238	-2.218865
C	2.167721	-1.013155	1.374904
C	2.167721	-1.013155	-1.374904
N	-2.222629	-0.496982	0.000000
Mo	2.204155	0.378055	0.000000
H	5.206835	-0.031631	0.000000
C	-3.266970	0.481569	0.000000
C	4.484578	0.777899	0.000000
C	-3.794233	0.971195	1.207840
C	-3.794233	0.971195	-1.207840
H	4.169497	1.185386	2.188748

Sn	-0.296114	0.204967	0.000000
H	4.169497	1.185386	-2.188748
C	3.947778	1.435475	1.156286
C	3.947778	1.435475	-1.156286
C	-4.819868	1.918009	1.206039
C	-4.819868	1.918009	-1.206039
H	-5.215245	2.285054	2.153753
H	-5.215245	2.285054	-2.153753
C	-5.337781	2.395284	0.000000
C	3.089874	2.477391	0.716714
C	3.089874	2.477391	-0.716714
H	2.535135	3.159630	1.354136
H	2.535135	3.159630	-1.354136
H	-6.138561	3.135158	0.000000
H	-3.388963	0.594386	2.148020
H	-3.388963	0.594386	-2.148020

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}PbN(SiMe_3)(Ph)]$ (**IV**)

H	-4.065729	-3.753443	1.531749
H	-1.346340	-4.289732	0.000000
H	-4.065729	-3.753443	-1.531749
H	-3.191841	-2.507608	2.459134
C	-3.773109	-2.691328	1.542471
C	-1.136030	-3.208178	0.000000
H	-0.522966	-3.005966	0.893176
H	-4.694652	-2.091429	1.597131
C	-3.773109	-2.691328	-1.542471
H	-0.522966	-3.005966	-0.893176
H	-3.191841	-2.507608	-2.459134
Si	-2.771083	-2.260388	0.000000
H	-4.694652	-2.091429	-1.597131
O	2.545188	-1.794286	2.229884
O	2.545188	-1.794286	-2.229884
C	2.357758	-1.007207	1.380592
C	2.357758	-1.007207	-1.380592
N	-2.339292	-0.551104	0.000000
Mo	2.266033	0.380445	0.000000
H	5.285535	0.243861	0.000000
C	-3.312669	0.487852	0.000000
C	4.491084	0.983064	0.000000
C	-3.808461	1.015167	1.207582
C	-3.808461	1.015167	-1.207582
H	4.139834	1.361774	2.189325
Pb	-0.281250	0.091693	0.000000
H	4.139834	1.361774	-2.189325
C	3.896970	1.590309	1.156525
C	3.896970	1.590309	-1.156525
C	-4.770785	2.025928	1.206056
C	-4.770785	2.025928	-1.206056
H	-5.141757	2.417906	2.153873
H	-5.141757	2.417906	-2.153873

C	-5.257527	2.535738	0.000000
C	2.948599	2.550817	0.716959
C	2.948599	2.550817	-0.716959
H	2.338677	3.184066	1.354378
H	2.338677	3.184066	-1.354378
H	-6.011323	3.323535	0.000000
H	-3.428137	0.613508	2.148055
H	-3.428137	0.613508	-2.148055

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiN(SiMe_3)(Ph)]$ (**V**)

H	-3.780294	-3.597737	1.585503
H	-1.128911	-4.325114	0.000000
H	-3.780294	-3.597737	-1.585503
H	-2.828470	-2.371649	2.456787
C	-3.437489	-2.551282	1.557655
C	-0.851465	-3.258120	0.000000
H	-0.228963	-3.081721	0.890595
H	-4.326564	-1.904925	1.607783
C	-3.437489	-2.551282	-1.557655
H	-0.228963	-3.081721	-0.890595
H	-2.828470	-2.371649	-2.456787
Si	-2.428187	-2.234472	0.000000
H	-4.326564	-1.904925	-1.607783
O	2.247012	-1.859359	2.246683
O	2.247012	-1.859359	-2.246683
C	2.105767	-1.070450	1.387950
C	2.105767	-1.070450	-1.387950
N	-1.901132	-0.514460	0.000000
W	1.975569	0.310736	0.000000
H	5.015259	0.525914	0.000000
C	-2.870942	0.555959	0.000000
C	4.145077	1.172640	0.000000
C	-3.342963	1.083534	1.209394
C	-3.342963	1.083534	-1.209394
H	3.750615	1.504327	2.190169
Si	-0.244357	-0.058531	0.000000
H	3.750615	1.504327	-2.190169
C	3.481368	1.702536	1.157969
C	3.481368	1.702536	-1.157969
C	-4.278533	2.119198	1.207083
C	-4.278533	2.119198	-1.207083
H	-4.636829	2.522778	2.154283
H	-4.636829	2.522778	-2.154283
C	-4.750469	2.639092	0.000000
C	2.426659	2.547228	0.716978
C	2.426659	2.547228	-0.716978
H	1.739765	3.095331	1.353548
H	1.739765	3.095331	-1.353548
H	-5.480351	3.448777	0.000000
H	-2.964808	0.675907	2.147225
H	-2.964808	0.675907	-2.147225

[(η^5-C_5H_5)$(CO)_2$W≡GeN($SiMe_3$)(Ph)] (**VI**)

H	-3.880525	-3.604515	1.541655
H	-1.201021	-4.309389	0.000000
H	-3.880525	-3.604515	-1.541655
H	-2.950984	-2.394436	2.460212
C	-3.536075	-2.557863	1.542581
C	-0.928746	-3.241434	0.000000
H	-0.307970	-3.061607	0.891252
H	-4.427546	-1.913608	1.582599
C	-3.536075	-2.557863	-1.542581
H	-0.307970	-3.061607	-0.891252
H	-2.950984	-2.394436	-2.460212
Si	-2.505331	-2.215745	0.000000
H	-4.427546	-1.913608	-1.582599
O	2.288276	-1.826229	2.245541
O	2.288276	-1.826229	-2.245541
C	2.146271	-1.036592	1.388742
C	2.146271	-1.036592	-1.388742
N	-1.995194	-0.500560	0.000000
W	2.048904	0.345777	0.000000
H	5.086097	0.372114	0.000000
C	-2.980495	0.547893	0.000000
C	4.256308	1.069856	0.000000
C	-3.475799	1.061294	1.208531
C	-3.475799	1.061294	-1.208531
H	3.878885	1.421843	2.190072
Ge	-0.234626	0.020841	0.000000
H	3.878885	1.421843	-2.190072
C	3.624410	1.638269	1.157669
C	3.624410	1.638269	-1.157669
C	-4.449084	2.062034	1.206556
C	-4.449084	2.062034	-1.206556
H	-4.825205	2.449156	2.154035
H	-4.825205	2.449156	-2.154035
C	-4.940455	2.565012	0.000000
C	2.620257	2.543984	0.717198
C	2.620257	2.543984	-0.717198
H	1.965502	3.129569	1.354508
H	1.965502	3.129569	-1.354508
H	-5.702041	3.345216	0.000000
H	-3.089636	0.663255	2.147734
H	-3.089636	0.663255	-2.147734

[(η^5-C_5H_5)$(CO)_2$W≡SnN($SiMe_3$)(Ph)] (**VII**)

H	-4.009538	-3.705684	1.546494
H	-1.309407	-4.293317	0.000000
H	-4.009538	-3.705684	-1.546494
H	-3.112906	-2.465438	2.458446
C	-3.703201	-2.647471	1.547317
C	-1.079664	-3.215396	0.000000

H	-0.462961	-3.021430	0.892087
H	-4.615967	-2.034726	1.602711
C	-3.703201	-2.647471	-1.547317
H	-0.462961	-3.021430	-0.892087
H	-3.112906	-2.465438	-2.458446
Si	-2.699756	-2.246733	0.000000
H	-4.615967	-2.034726	-1.602711
O	2.501063	-1.801913	2.235650
O	2.501063	-1.801913	-2.235650
C	2.317820	-1.013678	1.384439
C	2.317820	-1.013678	-1.384439
N	-2.241155	-0.534405	0.000000
W	2.204481	0.371480	0.000000
H	5.230339	0.328310	0.000000
C	-3.212159	0.516835	0.000000
C	4.414051	1.041934	0.000000
C	-3.698513	1.046003	1.208022
C	-3.698513	1.046003	-1.208022
H	4.047704	1.407071	2.190379
Sn	-0.279986	0.045201	0.000000
H	4.047704	1.407071	-2.190379
C	3.796649	1.627415	1.157895
C	3.796649	1.627415	-1.157895
C	-4.643915	2.072880	1.206240
C	-4.643915	2.072880	-1.206240
H	-5.007577	2.471372	2.154002
H	-5.007577	2.471372	-2.154002
C	-5.120521	2.591002	0.000000
C	2.816018	2.558982	0.717345
C	2.816018	2.558982	-0.717345
H	2.180657	3.165019	1.355305
H	2.180657	3.165019	-1.355305
H	-5.856814	3.395085	0.000000
H	-3.323011	0.638831	2.147982
H	-3.323011	0.638831	-2.147982

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}PbN(SiMe_3)(Ph)]$ (**VIII**)

H	-4.273124	-3.668187	1.537642
H	-1.599752	-4.384865	0.000000
H	-4.273124	-3.668187	-1.537642
H	-3.319305	-2.477338	2.457997
C	-3.914170	-2.626727	1.543964
C	-1.320861	-3.318971	0.000000
H	-0.697091	-3.154685	0.893197
H	-4.795545	-1.969588	1.599275
C	-3.914170	-2.626727	-1.543964
H	-0.697091	-3.154685	-0.893197
H	-3.319305	-2.477338	-2.457997
Si	-2.888453	-2.264294	0.000000
H	-4.795545	-1.969588	-1.599275
O	2.711490	-1.719364	2.246589

O	2.711490	-1.719364	-2.246589
C	2.463079	-0.956583	1.388627
C	2.463079	-0.956583	-1.388627
N	-2.346649	-0.586746	0.000000
W	2.250094	0.413696	0.000000
H	5.260855	0.574150	0.000000
C	-3.234546	0.526152	0.000000
C	4.398615	1.231351	0.000000
C	-3.680458	1.094987	1.207934
C	-3.680458	1.094987	-1.207934
H	4.006974	1.568575	2.189923
Pb	-0.269913	-0.041015	0.000000
H	4.006974	1.568575	-2.189923
C	3.742510	1.773717	1.157776
C	3.742510	1.773717	-1.157776
C	-4.541720	2.192881	1.206404
C	-4.541720	2.192881	-1.206404
H	-4.873576	2.618376	2.154032
H	-4.873576	2.618376	-2.154032
C	-4.976342	2.747179	0.000000
C	2.700108	2.636203	0.717617
C	2.700108	2.636203	-0.717617
H	2.027760	3.199811	1.356116
H	2.027760	3.199811	-1.356116
H	-5.646496	3.606995	0.000000
H	-3.338861	0.658464	2.147613
H	-3.338861	0.658464	-2.147613

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)

H	-3.046937	-4.150653	1.417078
H	-0.291057	-4.388988	0.000000
H	-3.046937	-4.150653	-1.417078
H	-2.273351	-2.930160	2.452148
C	-2.836842	-3.073431	1.518662
C	-0.158559	-3.294509	0.000000
H	0.433599	-3.038793	0.891405
H	-3.804286	-2.556115	1.607227
C	-2.836842	-3.073431	-1.518662
H	0.433599	-3.038793	-0.891405
H	-2.273351	-2.930160	-2.452148
Si	-1.866610	-2.504384	0.000000
H	-3.804286	-2.556115	-1.607227
O	2.626276	-1.750449	2.231305
O	2.626276	-1.750449	-2.231305
C	2.473252	-0.958175	1.379998
C	2.473252	-0.958175	-1.379998
N	-1.605965	-0.730733	0.000000
Mo	2.359237	0.424520	0.000000
H	5.402689	0.464652	0.000000
C	-2.711514	0.204754	0.000000
C	4.571468	1.161919	0.000000

C	-3.252264	0.665458	1.222935
C	-3.252264	0.665458	-1.222935
H	4.197506	1.514257	2.188256
Ge	0.090695	-0.002674	0.000000
H	4.197506	1.514257	-2.188256
C	3.942248	1.730484	1.155844
C	3.942248	1.730484	-1.155844
C	-4.379768	1.494463	1.194774
C	-4.379768	1.494463	-1.194774
H	-4.802579	1.830047	2.145572
H	-4.802579	1.830047	-2.145572
C	-4.974831	1.906851	0.000000
C	2.937792	2.632154	0.716495
C	2.937792	2.632154	-0.716495
H	2.284698	3.221487	1.353197
H	2.284698	3.221487	-1.353197
C	-6.185856	2.807255	0.000000
H	-6.808511	2.642006	-0.889077
H	-6.808511	2.642006	0.889077
H	-5.891404	3.868358	0.000000
C	-2.631625	0.309843	2.549870
H	-2.719804	-0.760447	2.774870
H	-1.557310	0.547048	2.570318
H	-3.117077	0.868786	3.359499
C	-2.631625	0.309843	-2.549870
H	-1.557310	0.547048	-2.570318
H	-2.719804	-0.760447	-2.774870
H	-3.117077	0.868786	-3.359499

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ar^*)]$ (**X**)

C	3.029724	-1.181077	-4.990088
C	1.722284	-1.283826	-4.507788
C	4.079955	-1.006945	-4.088021
C	-2.951951	-3.558959	-3.233615
C	-3.458085	-2.234581	-3.139162
C	1.470312	-1.202439	-3.138321
C	3.825140	-0.931398	-2.715910
C	-3.683977	-4.380962	-2.314869
C	-4.510933	-2.225013	-2.169329
C	2.516664	-1.018505	-2.223011
C	-4.646232	-3.543960	-1.661818
C	-3.532001	2.155026	-1.409584
C	2.891989	4.079773	-1.284711
C	-0.752256	-3.734259	-1.057591
C	-4.707288	1.850779	-0.723420
C	2.449108	1.611824	-0.939329
C	-2.332725	2.332579	-0.711376
C	2.191160	-0.889321	-0.729905
C	2.102699	2.938013	-0.693817
C	1.748627	0.532354	-0.382966
C	3.461231	-2.820876	0.271088

C	3.317009	-1.429316	0.151920
C	0.988295	3.177940	0.116812
C	-4.678024	1.726187	0.668707
C	0.645243	0.794496	0.464844
C	-2.292259	2.215458	0.684907
C	4.491788	-3.370375	1.032518
C	-2.779039	-3.546419	0.754987
C	0.249723	2.140370	0.685587
C	4.230889	-0.604595	0.817674
C	-3.483122	1.908841	1.362627
C	5.402430	-2.537591	1.689491
C	-1.012097	2.445491	1.492485
C	5.267487	-1.153961	1.579455
C	-1.521060	4.962045	1.529920
C	-0.981423	3.825996	2.147742
C	-1.436536	6.216640	2.138793
C	0.526550	-2.687627	2.752941
C	-0.816607	6.356255	3.381561
C	-0.368970	3.979070	3.399659
C	-0.284896	5.229458	4.012858
C	-1.471963	-0.626921	3.752982
C	1.534022	0.152657	3.550607
H	3.228269	-1.245907	-6.060717
H	0.894250	-1.433517	-5.202228
H	5.106366	-0.936655	-4.450242
H	-2.156809	-3.895244	-3.891424
H	-3.106454	-1.375477	-3.703056
H	0.445365	-1.291797	-2.768956
H	-3.561485	-5.449705	-2.173285
H	-3.541777	2.254782	-2.495631
H	4.657329	-0.815837	-2.018887
H	-5.091360	-1.358753	-1.866470
H	3.595180	3.725975	-2.048786
H	2.231218	4.826200	-1.747447
H	3.286153	1.398620	-1.607037
H	-5.642831	1.713197	-1.267400
H	-5.361233	-3.867523	-0.912024
H	-1.416916	2.564910	-1.258326
H	3.472062	4.603033	-0.509418
H	2.753216	-3.476387	-0.241312
H	1.330335	-1.548107	-0.550690
H	0.681305	4.208160	0.307945
H	4.583155	-4.453879	1.114892
H	-5.589622	1.484956	1.216273
H	-2.019062	4.863752	0.563598
H	4.130738	0.479676	0.746859
H	-1.862914	7.087569	1.639629
H	6.208836	-2.966189	2.285818
H	-0.280084	-3.269980	2.281558
H	5.968976	-0.492957	2.090100
H	-3.470837	1.815911	2.450570
H	1.465067	-2.897046	2.218680

H	-1.045456	1.719230	2.313616
H	-2.321715	-1.101475	3.236950
H	2.497019	-0.066843	3.065967
H	-0.754258	7.334840	3.859063
H	0.050894	3.104769	3.901628
H	0.632898	-3.054289	3.787043
H	1.363546	1.237791	3.491829
H	-1.731263	0.424974	3.945034
H	0.194318	5.323239	4.987966
H	-1.366517	-1.124962	4.730548
H	1.618668	-0.122141	4.614730
N	-0.096713	-0.277534	1.079227
Si	0.137036	-0.845799	2.774849
Ge	-1.344872	-1.119326	0.006096
Mo	-2.482772	-2.835815	-1.046461
O	0.255693	-4.333351	-1.123379
O	-3.026108	-4.027401	1.795334

PBE/DFT-D3

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)

H	-3.055463	-4.087457	1.416627
H	-0.289035	-4.348420	0.000000
H	-3.055463	-4.087457	-1.416627
H	-2.259860	-2.878442	2.449798
C	-2.827689	-3.014068	1.517927
C	-0.149258	-3.255007	0.000000
H	0.443245	-3.001897	0.891602
H	-3.785417	-2.478548	1.604694
C	-2.827689	-3.014068	-1.517927
H	0.443245	-3.001897	-0.891602
H	-2.259860	-2.878442	-2.449798
Si	-1.852136	-2.458106	0.000000
H	-3.785417	-2.478548	-1.604694
O	2.577001	-1.763893	2.232012
O	2.577001	-1.763893	-2.232012
C	2.450667	-0.967174	1.380188
C	2.450667	-0.967174	-1.380188
N	-1.593752	-0.683501	0.000000
Mo	2.378269	0.416648	0.000000
H	5.419814	0.369917	0.000000
C	-2.721606	0.224466	0.000000
C	4.609184	1.091004	0.000000
C	-3.278195	0.665532	1.222777
C	-3.278195	0.665532	-1.222777
H	4.243854	1.453302	2.188663
Ge	0.101446	0.044510	0.000000
H	4.243854	1.453302	-2.188663
C	3.996160	1.677181	1.155975
C	3.996160	1.677181	-1.155975
C	-4.444022	1.439651	1.195029
C	-4.444022	1.439651	-1.195029

H	-4.880979	1.758018	2.145287
H	-4.880979	1.758018	-2.145287
C	-5.060347	1.818644	0.000000
C	3.017275	2.606450	0.716595
C	3.017275	2.606450	-0.716595
H	2.380317	3.213516	1.353270
H	2.380317	3.213516	-1.353270
C	-6.318667	2.651852	0.000000
H	-6.931527	2.452608	-0.888971
H	-6.931527	2.452608	0.888971
H	-6.082134	3.727321	0.000000
C	-2.632109	0.348429	2.547197
H	-2.679582	-0.721047	2.786376
H	-1.566624	0.622996	2.551332
H	-3.127480	0.900203	3.355633
C	-2.632109	0.348429	-2.547197
H	-1.566624	0.622996	-2.551332
H	-2.679582	-0.721047	-2.786376
H	-3.127480	0.900203	-3.355633

PBE/DFT-D3(BJ)

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)

H	-3.044017	-4.082751	1.414091
H	-0.257623	-4.321730	0.000000
H	-3.044017	-4.082751	-1.414091
H	-2.248062	-2.874388	2.447781
C	-2.817386	-3.009365	1.516928
C	-0.135882	-3.226392	0.000000
H	0.452417	-2.962321	0.891037
H	-3.775293	-2.474892	1.606180
C	-2.817386	-3.009365	-1.516928
H	0.452417	-2.962321	-0.891037
H	-2.248062	-2.874388	-2.447781
Si	-1.846213	-2.449645	0.000000
H	-3.775293	-2.474892	-1.606180
O	2.580877	-1.763584	2.233581
O	2.580877	-1.763584	-2.233581
C	2.450662	-0.969478	1.380415
C	2.450662	-0.969478	-1.380415
N	-1.593953	-0.677419	0.000000
Mo	2.374592	0.412632	0.000000
H	5.411195	0.364754	0.000000
C	-2.723769	0.223836	0.000000
C	4.601083	1.085765	0.000000
C	-3.278304	0.662225	1.222339
C	-3.278304	0.662225	-1.222339
H	4.233588	1.445176	2.187945
Ge	0.099035	0.048950	0.000000
H	4.233588	1.445176	-2.187945
C	3.986937	1.670613	1.155810
C	3.986937	1.670613	-1.155810

C	-4.441426	1.439228	1.195651
C	-4.441426	1.439228	-1.195651
H	-4.878676	1.756724	2.145757
H	-4.878676	1.756724	-2.145757
C	-5.054874	1.820624	0.000000
C	3.006703	2.598213	0.716498
C	3.006703	2.598213	-0.716498
H	2.366488	3.201276	1.352895
H	2.366488	3.201276	-1.352895
C	-6.308776	2.658565	0.000000
H	-6.921670	2.461314	-0.889140
H	-6.921670	2.461314	0.889140
H	-6.067862	3.732851	0.000000
C	-2.629122	0.336815	2.541440
H	-2.657798	-0.736932	2.762320
H	-1.568298	0.629091	2.548120
H	-3.134145	0.868304	3.357162
C	-2.629122	0.336815	-2.541440
H	-1.568298	0.629091	-2.548120
H	-2.657798	-0.736932	-2.762320
H	-3.134145	0.868304	-3.357162

PW91/DFT

[(η^5-C_5H_5)$(CO)_2$Mo≡SiN($SiMe_3$)(Ph)] (**I**)

H	-3.689450	-3.629926	1.568851
H	-1.024912	-4.296794	0.000000
H	-3.689450	-3.629926	-1.568851
H	-2.781412	-2.385306	2.455243
C	-3.374289	-2.576268	1.549923
C	-0.772099	-3.225946	0.000000
H	-0.156715	-3.034453	0.889486
H	-4.279668	-1.955559	1.592101
C	-3.374289	-2.576268	-1.549923
H	-0.156715	-3.034453	-0.889486
H	-2.781412	-2.385306	-2.455243
Si	-2.364158	-2.235062	0.000000
H	-4.279668	-1.955559	-1.592101
O	2.044630	-1.832896	2.234373
O	2.044630	-1.832896	-2.234373
C	1.968406	-1.033233	1.380796
C	1.968406	-1.033233	-1.380796
N	-1.879742	-0.506223	0.000000
Mo	1.962533	0.351925	0.000000
H	5.008374	0.208133	0.000000
C	-2.895084	0.522253	0.000000
C	4.225307	0.956244	0.000000
C	-3.388157	1.029310	1.208069
C	-3.388157	1.029310	-1.208069
H	3.877013	1.332110	2.184756
Si	-0.262229	0.074284	0.000000

H	3.877013	1.332110	-2.184756
C	3.635518	1.563490	1.154464
C	3.635518	1.563490	-1.154464
C	-4.364263	2.024034	1.205478
C	-4.364263	2.024034	-1.205478
H	-4.738823	2.411807	2.150637
H	-4.738823	2.411807	-2.150637
C	-4.856031	2.523633	0.000000
C	2.692604	2.525506	0.715691
C	2.692604	2.525506	-0.715691
H	2.079384	3.154239	1.350876
H	2.079384	3.154239	-1.350876
H	-5.617921	3.300586	0.000000
H	-2.995108	0.637734	2.144465
H	-2.995108	0.637734	-2.144465

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ph)]$ (**II**)

H	-3.758859	-3.628796	1.539425
H	-1.072130	-4.242845	0.000000
H	-3.758859	-3.628796	-1.539425
H	-2.867989	-2.393068	2.456033
C	-3.449263	-2.573640	1.541114
C	-0.828980	-3.169766	0.000000
H	-0.215361	-2.974491	0.890005
H	-4.359349	-1.959563	1.584938
C	-3.449263	-2.573640	-1.541114
H	-0.215361	-2.974491	-0.890005
H	-2.867989	-2.393068	-2.456033
Si	-2.433799	-2.195639	0.000000
H	-4.359349	-1.959563	-1.584938
O	2.128257	-1.829746	2.235164
O	2.128257	-1.829746	-2.235164
C	2.043040	-1.030776	1.382988
C	2.043040	-1.030776	-1.382988
N	-1.983681	-0.466497	0.000000
Mo	2.048185	0.355248	0.000000
H	5.081675	0.133769	0.000000
C	-3.020810	0.530677	0.000000
C	4.315320	0.898808	0.000000
C	-3.542584	1.017630	1.206911
C	-3.542584	1.017630	-1.206911
H	3.974363	1.283125	2.185199
Ge	-0.244536	0.132274	0.000000
H	3.974363	1.283125	-2.185199
C	3.739422	1.519982	1.154700
C	3.739422	1.519982	-1.154700
C	-4.566218	1.964153	1.204865
C	-4.566218	1.964153	-1.204865
H	-4.960982	2.331124	2.150437
H	-4.960982	2.331124	-2.150437
C	-5.082819	2.440152	0.000000

C	2.819120	2.504193	0.715845
C	2.819120	2.504193	-0.715845
H	2.220847	3.147158	1.351316
H	2.220847	3.147158	-1.351316
H	-5.883139	3.177811	0.000000
H	-3.137834	0.640997	2.145228
H	-3.137834	0.640997	-2.145228

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SnN(SiMe_3)(Ph)]$ (**III**)

H	-3.868371	-3.737728	1.547053
H	-1.154289	-4.214051	0.000000
H	-3.868371	-3.737728	-1.547053
H	-3.030230	-2.458602	2.454734
C	-3.609725	-2.668898	1.545355
C	-0.968585	-3.129791	0.000000
H	-0.360993	-2.912639	0.890570
H	-4.547085	-2.098022	1.598051
C	-3.609725	-2.668898	-1.545355
H	-0.360993	-2.912639	-0.890570
H	-3.030230	-2.458602	-2.454734
Si	-2.624481	-2.228468	0.000000
H	-4.547085	-2.098022	-1.598051
O	2.370744	-1.831149	2.221328
O	2.370744	-1.831149	-2.221328
C	2.235195	-1.030118	1.377232
C	2.235195	-1.030118	-1.377232
N	-2.231699	-0.503684	0.000000
Mo	2.202365	0.363297	0.000000
H	5.227547	0.164788	0.000000
C	-3.246680	0.503154	0.000000
C	4.452030	0.920283	0.000000
C	-3.757138	1.008441	1.206200
C	-3.757138	1.008441	-1.206200
H	4.111073	1.305577	2.185261
Sn	-0.286396	0.136776	0.000000
H	4.111073	1.305577	-2.185261
C	3.872344	1.538466	1.154799
C	3.872344	1.538466	-1.154799
C	-4.749010	1.987585	1.204328
C	-4.749010	1.987585	-1.204328
H	-5.131366	2.367250	2.150256
H	-5.131366	2.367250	-2.150256
C	-5.249395	2.481581	0.000000
C	2.946847	2.518115	0.716065
C	2.946847	2.518115	-0.716065
H	2.350099	3.161881	1.351920
H	2.350099	3.161881	-1.351920
H	-6.023073	3.247295	0.000000
H	-3.364622	0.619696	2.144798
H	-3.364622	0.619696	-2.144798

[(η^5-C_5H_5)(CO)$_2$Mo≡PbN(SiMe$_3$)(Ph)] (**IV**)

H	-3.986303	-3.787081	1.535889
H	-1.274003	-4.270964	0.000000
H	-3.986303	-3.787081	-1.535889
H	-3.144255	-2.518259	2.454798
C	-3.721320	-2.720084	1.541869
C	-1.082085	-3.187909	0.000000
H	-0.473334	-2.976339	0.891496
H	-4.655745	-2.144196	1.595538
C	-3.721320	-2.720084	-1.541869
H	-0.473334	-2.976339	-0.891496
H	-3.144255	-2.518259	-2.454798
Si	-2.731522	-2.270599	0.000000
H	-4.655745	-2.144196	-1.595538
O	2.489087	-1.802505	2.227665
O	2.489087	-1.802505	-2.227665
C	2.317976	-1.011460	1.380479
C	2.317976	-1.011460	-1.380479
N	-2.334226	-0.556355	0.000000
Mo	2.257925	0.378097	0.000000
H	5.272126	0.160421	0.000000
C	-3.318174	0.470422	0.000000
C	4.500122	0.920408	0.000000
C	-3.816001	0.994255	1.206584
C	-3.816001	0.994255	-1.206584
H	4.161233	1.309646	2.185876
Pb	-0.289999	0.119376	0.000000
H	4.161233	1.309646	-2.185876
C	3.924816	1.544498	1.155155
C	3.924816	1.544498	-1.155155
C	-4.778376	2.002101	1.204660
C	-4.778376	2.002101	-1.204660
H	-5.149206	2.393078	2.150553
H	-5.149206	2.393078	-2.150553
C	-5.264274	2.511112	0.000000
C	3.005646	2.530077	0.716067
C	3.005646	2.530077	-0.716067
H	2.415676	3.179656	1.352347
H	2.415676	3.179656	-1.352347
H	-6.014284	3.299703	0.000000
H	-3.435520	0.593784	2.144931
H	-3.435520	0.593784	-2.144931

[(η^5-C_5H_5)(CO)$_2$W≡SiN(SiMe$_3$)(Ph)] (**V**)

H	-3.772844	-3.591941	1.575300
H	-1.126575	-4.315677	0.000000
H	-3.772844	-3.591941	-1.575300
H	-2.836327	-2.363652	2.454665
C	-3.437214	-2.544734	1.552461
C	-0.852610	-3.249928	0.000000
H	-0.231680	-3.071324	0.889119

H	-4.329563	-1.905728	1.597437
C	-3.437214	-2.544734	-1.552461
H	-0.231680	-3.071324	-0.889119
H	-2.836327	-2.363652	-2.454665
Si	-2.424899	-2.225392	0.000000
H	-4.329563	-1.905728	-1.597437
O	2.241798	-1.852557	2.248585
O	2.241798	-1.852557	-2.248585
C	2.100109	-1.066698	1.389094
C	2.100109	-1.066698	-1.389094
N	-1.897023	-0.509219	0.000000
W	1.974817	0.311769	0.000000
H	5.016851	0.498633	0.000000
C	-2.873368	0.555607	0.000000
C	4.154863	1.153146	0.000000
C	-3.349239	1.077918	1.207122
C	-3.349239	1.077918	-1.207122
H	3.765021	1.488714	2.186532
Si	-0.245451	-0.044299	0.000000
H	3.765021	1.488714	-2.186532
C	3.498555	1.689821	1.156502
C	3.498555	1.689821	-1.156502
C	-4.295706	2.101987	1.205276
C	-4.295706	2.101987	-1.205276
H	-4.658717	2.500000	2.150853
H	-4.658717	2.500000	-2.150853
C	-4.773211	2.616062	0.000000
C	2.453990	2.545700	0.716320
C	2.453990	2.545700	-0.716320
H	1.774884	3.100743	1.351784
H	1.774884	3.100743	-1.351784
H	-5.512008	3.414678	0.000000
H	-2.968434	0.674504	2.143600
H	-2.968434	0.674504	-2.143600

[(η^5-C_5H_5)$(CO)_2$W≡GeN($SiMe_3$)(Ph)] (**VI**)

H	-3.864800	-3.596545	1.548434
H	-1.203516	-4.296993	0.000000
H	-3.864800	-3.596545	-1.548434
H	-2.942445	-2.377098	2.455732
C	-3.528597	-2.549265	1.542585
C	-0.929293	-3.231365	0.000000
H	-0.309199	-3.053690	0.889822
H	-4.422737	-1.912025	1.582454
C	-3.528597	-2.549265	-1.542585
H	-0.309199	-3.053690	-0.889822
H	-2.942445	-2.377098	-2.455732
Si	-2.503268	-2.206648	0.000000
H	-4.422737	-1.912025	-1.582454
O	2.295419	-1.824827	2.248515
O	2.295419	-1.824827	-2.248515

C	2.151000	-1.039552	1.390356
C	2.151000	-1.039552	-1.390356
N	-1.994264	-0.495004	0.000000
W	2.047530	0.340029	0.000000
H	5.085562	0.395882	0.000000
C	-2.978134	0.552779	0.000000
C	4.251580	1.085419	0.000000
C	-3.473895	1.064846	1.207405
C	-3.473895	1.064846	-1.207405
H	3.873675	1.435700	2.186601
Ge	-0.233719	0.016495	0.000000
H	3.873675	1.435700	-2.186601
C	3.617137	1.648775	1.156084
C	3.617137	1.648775	-1.156084
C	-4.448276	2.061666	1.205131
C	-4.448276	2.061666	-1.205131
H	-4.824465	2.447769	2.150696
H	-4.824465	2.447769	-2.150696
C	-4.940302	2.562500	0.000000
C	2.608355	2.546741	0.716336
C	2.608355	2.546741	-0.716336
H	1.952423	3.128741	1.352218
H	1.952423	3.128741	-1.352218
H	-5.702569	3.339275	0.000000
H	-3.087401	0.668739	2.145030
H	-3.087401	0.668739	-2.145030

[(η^5-C_5H_5)$(CO)_2$W≡SnN($SiMe_3$)(Ph)] (**VII**)

H	-3.995732	-3.713482	1.546382
H	-1.301324	-4.294226	0.000000
H	-3.995732	-3.713482	-1.546382
H	-3.104292	-2.471052	2.454127
C	-3.694203	-2.655877	1.545879
C	-1.074811	-3.217614	0.000000
H	-0.459615	-3.022534	0.890534
H	-4.607571	-2.047686	1.602028
C	-3.694203	-2.655877	-1.545879
H	-0.459615	-3.022534	-0.890534
H	-3.104292	-2.471052	-2.454127
Si	-2.694320	-2.253226	0.000000
H	-4.607571	-2.047686	-1.602028
O	2.498342	-1.800469	2.232554
O	2.498342	-1.800469	-2.232554
C	2.313590	-1.012903	1.383146
C	2.313590	-1.012903	-1.383146
N	-2.238574	-0.544678	0.000000
W	2.196294	0.371949	0.000000
H	5.222401	0.346513	0.000000
C	-3.198541	0.514155	0.000000
C	4.404750	1.055277	0.000000
C	-3.677813	1.049192	1.207176

C	-3.677813	1.049192	-1.207176
H	4.038513	1.419374	2.186964
Sn	-0.283238	0.038058	0.000000
H	4.038513	1.419374	-2.186964
C	3.786506	1.637973	1.156575
C	3.786506	1.637973	-1.156575
C	-4.607473	2.087401	1.204641
C	-4.607473	2.087401	-1.204641
H	-4.965325	2.490614	2.150178
H	-4.965325	2.490614	-2.150178
C	-5.075595	2.611298	0.000000
C	2.803702	2.565156	0.716609
C	2.803702	2.565156	-0.716609
H	2.168469	3.168841	1.353235
H	2.168469	3.168841	-1.353235
H	-5.798702	3.424503	0.000000
H	-3.308514	0.637997	2.145275
H	-3.308514	0.637997	-2.145275

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}PbN(SiMe_3)(Ph)]$ (**VIII**)

H	-4.283506	-3.656874	1.534477
H	-1.623014	-4.382056	0.000000
H	-4.283506	-3.656874	-1.534477
H	-3.329434	-2.471096	2.454757
C	-3.923450	-2.618064	1.542047
C	-1.338525	-3.319636	0.000000
H	-0.714760	-3.159007	0.891524
H	-4.802237	-1.960762	1.598400
C	-3.923450	-2.618064	-1.542047
H	-0.714760	-3.159007	-0.891524
H	-3.329434	-2.471096	-2.454757
Si	-2.897916	-2.258259	0.000000
H	-4.802237	-1.960762	-1.598400
O	2.727454	-1.709955	2.250222
O	2.727454	-1.709955	-2.250222
C	2.473058	-0.953515	1.390788
C	2.473058	-0.953515	-1.390788
N	-2.348559	-0.586934	0.000000
W	2.248570	0.412301	0.000000
H	5.257963	0.612782	0.000000
C	-3.229426	0.530643	0.000000
C	4.389663	1.257944	0.000000
C	-3.671196	1.101218	1.206318
C	-3.671196	1.101218	-1.206318
H	3.996937	1.593221	2.186711
Pb	-0.268372	-0.051740	0.000000
H	3.996937	1.593221	-2.186711
C	3.729771	1.793642	1.156228
C	3.729771	1.793642	-1.156228
C	-4.525018	2.202112	1.204985
C	-4.525018	2.202112	-1.204985

H	-4.853911	2.628598	2.150850
H	-4.853911	2.628598	-2.150850
C	-4.955101	2.759084	0.000000
C	2.679879	2.644379	0.716604
C	2.679879	2.644379	-0.716604
H	2.004087	3.201583	1.353710
H	2.004087	3.201583	-1.353710
H	-5.619653	3.620686	0.000000
H	-3.332394	0.663944	2.144449
H	-3.332394	0.663944	-2.144449

[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)](**IX**)

H	-3.038277	-4.161923	1.422612
H	-0.289908	-4.398914	0.000000
H	-3.038277	-4.161923	-1.422612
H	-2.266878	-2.936531	2.448271
C	-2.831590	-3.085665	1.518730
C	-0.159740	-3.306117	0.000000
H	0.430899	-3.049859	0.889828
H	-3.798445	-2.571479	1.607699
C	-2.831590	-3.085665	-1.518730
H	0.430899	-3.049859	-0.889828
H	-2.266878	-2.936531	-2.448271
Si	-1.865930	-2.518384	0.000000
H	-3.798445	-2.571479	-1.607699
O	2.633644	-1.741953	2.233111
O	2.633644	-1.741953	-2.233111
C	2.472237	-0.954024	1.381728
C	2.472237	-0.954024	-1.381728
N	-1.606790	-0.749747	0.000000
Mo	2.345188	0.426752	0.000000
H	5.386994	0.493336	0.000000
C	-2.702654	0.193959	0.000000
C	4.551877	1.182802	0.000000
C	-3.235464	0.661278	1.221362
C	-3.235464	0.661278	-1.221362
H	4.176581	1.532334	2.184594
Ge	0.082814	-0.015585	0.000000
H	4.176581	1.532334	-2.184594
C	3.919616	1.746196	1.154257
C	3.919616	1.746196	-1.154257
C	-4.346628	1.508892	1.193549
C	-4.346628	1.508892	-1.193549
H	-4.762539	1.851632	2.142337
H	-4.762539	1.851632	-2.142337
C	-4.932057	1.932477	0.000000
C	2.910323	2.639335	0.715786
C	2.910323	2.639335	-0.715786
H	2.254843	3.223544	1.351549
H	2.254843	3.223544	-1.351549
C	-6.121606	2.857330	0.000000

H	-6.746793	2.705696	-0.887915
H	-6.746793	2.705696	0.887915
H	-5.804666	3.909880	0.000000
C	-2.622331	0.292253	2.546628
H	-2.754164	-0.770110	2.780708
H	-1.540583	0.483951	2.559315
H	-3.079390	0.876203	3.352685
C	-2.622331	0.292253	-2.546628
H	-1.540583	0.483951	-2.559315
H	-2.754164	-0.770110	-2.780708
H	-3.079390	0.876203	-3.352685

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ar^*)]$(**X**)

C	2.978193	-1.131778	-5.001360
C	1.675533	-1.227163	-4.510179
C	4.036358	-0.977490	-4.106721
C	-2.921502	-3.554029	-3.224895
C	-3.409182	-2.224487	-3.134226
C	1.435921	-1.158555	-3.140045
C	3.793535	-0.915477	-2.733726
C	-3.676640	-4.366122	-2.319132
C	-4.473159	-2.201646	-2.179304
C	2.489957	-0.995657	-2.232455
C	-4.633621	-3.517799	-1.677512
C	-3.484049	2.129188	-1.438528
C	2.925071	4.078975	-1.229733
C	-0.752158	-3.770778	-1.018907
C	-4.665940	1.823202	-0.768795
C	2.460631	1.614977	-0.913851
C	-2.297454	2.315049	-0.725578
C	2.177582	-0.883403	-0.737473
C	2.125395	2.939127	-0.655084
C	1.750692	0.536681	-0.371296
C	3.435308	-2.841243	0.219396
C	3.301662	-1.448133	0.127812
C	1.009304	3.180429	0.150086
C	-4.656050	1.704281	0.622492
C	0.649883	0.800143	0.475609
C	-2.276030	2.205278	0.670849
C	4.464344	-3.412213	0.963073
C	-2.802932	-3.531806	0.774743
C	0.260587	2.144808	0.702588
C	4.224613	-0.644708	0.802317
C	-3.473831	1.896199	1.332212
C	5.383816	-2.600816	1.629532
C	-1.009894	2.446760	1.493674
C	5.259900	-1.216185	1.546794
C	-1.535629	4.955879	1.511065
C	-0.996606	3.829022	2.141520
C	-1.471977	6.211721	2.114684
C	0.533876	-2.662651	2.772427

C	-0.874829	6.361843	3.365040
C	-0.405324	3.992534	3.400383
C	-0.343724	5.244555	4.008987
C	-1.464921	-0.603268	3.764358
C	1.534754	0.179156	3.550103
H	3.167161	-1.187421	-6.072174
H	0.842026	-1.360831	-5.198073
H	5.058594	-0.912886	-4.475465
H	-2.124458	-3.899458	-3.872005
H	-3.039774	-1.371044	-3.691609
H	0.415544	-1.243028	-2.764198
H	-3.571742	-5.435118	-2.178763
H	-3.479022	2.223961	-2.523279
H	4.630815	-0.815806	-2.043249
H	-5.044582	-1.329309	-1.883660
H	3.634663	3.726848	-1.986113
H	2.273609	4.829084	-1.695773
H	3.295599	1.402600	-1.581091
H	-5.590983	1.678975	-1.324283
H	-5.361888	-3.832137	-0.939747
H	-1.377157	2.549438	-1.259664
H	3.496791	4.595184	-0.446192
H	2.721694	-3.480686	-0.300222
H	1.312769	-1.535488	-0.562406
H	0.708730	4.209272	0.346242
H	4.546953	-4.495686	1.024330
H	-5.572232	1.460952	1.156358
H	-2.017366	4.849071	0.539558
H	4.133344	0.439245	0.752444
H	-1.897015	7.074827	1.605771
H	6.188259	-3.046460	2.211496
H	-0.264672	-3.248167	2.296266
H	5.968449	-0.572327	2.064038
H	-3.476961	1.808990	2.418383
H	1.475785	-2.870755	2.247551
H	-1.049131	1.725420	2.316763
H	-2.312083	-1.089626	3.259883
H	2.491681	-0.027399	3.052138
H	-0.829033	7.341339	3.838411
H	0.012819	3.125831	3.912304
H	0.631944	-3.025058	3.806432
H	1.354757	1.261318	3.503518
H	-1.730438	0.447762	3.942922
H	0.117850	5.346737	4.989459
H	-1.351636	-1.085899	4.746346
H	1.635745	-0.103897	4.608503
N	-0.094639	-0.268171	1.089136
Si	0.139417	-0.824485	2.784402
Ge	-1.326581	-1.126432	0.016178
Mo	-2.467614	-2.841615	-1.029353
O	0.244328	-4.386310	-1.075922
O	-3.075342	-3.995841	1.814559

RPBE/DFT

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SiN(SiMe_3)(Ph)]$ (**I**)

H	-3.709764	-3.672337	1.576309
H	-1.093536	-4.359937	0.000000
H	-3.709764	-3.672337	-1.576309
H	-2.819990	-2.414410	2.470320
C	-3.408801	-2.611241	1.560203
C	-0.806528	-3.294578	0.000000
H	-0.185953	-3.120334	0.892038
H	-4.325348	-2.002700	1.600977
C	-3.408801	-2.611241	-1.560203
H	-0.185953	-3.120334	-0.892038
H	-2.819990	-2.414410	-2.470320
Si	-2.388572	-2.261715	0.000000
H	-4.325348	-2.002700	-1.600977
O	2.059250	-1.832701	2.247972
O	2.059250	-1.832701	-2.247972
C	1.981212	-1.031401	1.387667
C	1.981212	-1.031401	-1.387667
N	-1.888618	-0.520086	0.000000
Mo	1.973494	0.357251	0.000000
H	5.037780	0.221652	0.000000
C	-2.904870	0.525394	0.000000
C	4.251212	0.970122	0.000000
C	-3.397827	1.040624	1.214083
C	-3.397827	1.040624	-1.214083
H	3.902006	1.349568	2.193211
Si	-0.263398	0.078311	0.000000
H	3.902006	1.349568	-2.193211
C	3.658751	1.580766	1.160275
C	3.658751	1.580766	-1.160275
C	-4.375009	2.045232	1.211382
C	-4.375009	2.045232	-1.211382
H	-4.747816	2.435549	2.159750
H	-4.747816	2.435549	-2.159750
C	-4.868737	2.549174	0.000000
C	2.709673	2.546063	0.719145
C	2.709673	2.546063	-0.719145
H	2.094395	3.175919	1.356007
H	2.094395	3.175919	-1.356007
H	-5.628972	3.331927	0.000000
H	-3.008601	0.649296	2.154928
H	-3.008601	0.649296	-2.154928

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ph)]$ (**II**)

H	-3.790974	-3.690957	1.552863
H	-1.149094	-4.330428	0.000000
H	-3.790974	-3.690957	-1.552863
H	-2.925736	-2.432699	2.471525
C	-3.499604	-2.626983	1.551389

C	-0.876149	-3.261480	0.000000
H	-0.257108	-3.081431	0.892386
H	-4.423369	-2.028612	1.587766
C	-3.499604	-2.626983	-1.551389
H	-0.257108	-3.081431	-0.892386
H	-2.925736	-2.432699	-2.471525
Si	-2.471996	-2.244601	0.000000
H	-4.423369	-2.028612	-1.587766
O	2.158399	-1.825695	2.246669
O	2.158399	-1.825695	-2.246669
C	2.062643	-1.025006	1.389332
C	2.062643	-1.025006	-1.389332
N	-1.999377	-0.505832	0.000000
Mo	2.051660	0.365634	0.000000
H	5.105115	0.179373	0.000000
C	-3.018441	0.525486	0.000000
C	4.328816	0.938561	0.000000
C	-3.527477	1.033407	1.213104
C	-3.527477	1.033407	-1.213104
H	3.983758	1.322694	2.193174
Ge	-0.249793	0.114550	0.000000
H	3.983758	1.322694	-2.193174
C	3.744929	1.557921	1.160180
C	3.744929	1.557921	-1.160180
C	-4.528047	2.015292	1.210867
C	-4.528047	2.015292	-1.210867
H	-4.912054	2.394477	2.159524
H	-4.912054	2.394477	-2.159524
C	-5.033875	2.508890	0.000000
C	2.809833	2.537450	0.719329
C	2.809833	2.537450	-0.719329
H	2.204016	3.176250	1.356546
H	2.204016	3.176250	-1.356546
H	-5.813853	3.272122	0.000000
H	-3.135147	0.647716	2.155546
H	-3.135147	0.647716	-2.155546

[(η^5-C_5H_5)$(CO)_2$Mo≡SnN($SiMe_3$)(Ph)] (**III**)

H	-3.927451	-3.773373	1.553826
H	-1.254489	-4.295920	0.000000
H	-3.927451	-3.773373	-1.553826
H	-3.102438	-2.486643	2.470770
C	-3.674525	-2.699747	1.553387
C	-1.030782	-3.215701	0.000000
H	-0.415912	-3.017788	0.892907
H	-4.618829	-2.134585	1.599805
C	-3.674525	-2.699747	-1.553387
H	-0.415912	-3.017788	-0.892907
H	-3.102438	-2.486643	-2.470770
Si	-2.672138	-2.261200	0.000000
H	-4.618829	-2.134585	-1.599805

O	2.408434	-1.822388	2.237553
O	2.408434	-1.822388	-2.237553
C	2.263035	-1.022946	1.385068
C	2.263035	-1.022946	-1.385068
N	-2.247932	-0.527543	0.000000
Mo	2.219120	0.371659	0.000000
H	5.261081	0.191268	0.000000
C	-3.257861	0.500865	0.000000
C	4.480362	0.945784	0.000000
C	-3.765327	1.018113	1.212287
C	-3.765327	1.018113	-1.212287
H	4.137443	1.334532	2.193842
Sn	-0.286259	0.129298	0.000000
H	4.137443	1.334532	-2.193842
C	3.897043	1.566591	1.160539
C	3.897043	1.566591	-1.160539
C	-4.753219	2.012396	1.210286
C	-4.753219	2.012396	-1.210286
H	-5.132358	2.396234	2.159212
H	-5.132358	2.396234	-2.159212
C	-5.253002	2.513570	0.000000
C	2.963973	2.548020	0.719502
C	2.963973	2.548020	-0.719502
H	2.363571	3.191713	1.357072
H	2.363571	3.191713	-1.357072
H	-6.022189	3.287672	0.000000
H	-3.379224	0.627725	2.155621
H	-3.379224	0.627725	-2.155621

[(η^5-C_5H_5)$(CO)_2$Mo≡PbN($SiMe_3$)(Ph)] (**IV**)

H	-4.060709	-3.827363	1.543597
H	-1.389868	-4.362929	0.000000
H	-4.060709	-3.827363	-1.543597
H	-3.222315	-2.556165	2.470603
C	-3.795929	-2.756594	1.551145
C	-1.156960	-3.284787	0.000000
H	-0.539983	-3.094747	0.893753
H	-4.734147	-2.181455	1.602497
C	-3.795929	-2.756594	-1.551145
H	-0.539983	-3.094747	-0.893753
H	-3.222315	-2.556165	-2.470603
Si	-2.789889	-2.310686	0.000000
H	-4.734147	-2.181455	-1.602497
O	2.543691	-1.796968	2.230205
O	2.543691	-1.796968	-2.230205
C	2.356718	-1.000797	1.382372
C	2.356718	-1.000797	-1.382372
N	-2.355687	-0.592131	0.000000
Mo	2.267625	0.395417	0.000000
H	5.302956	0.254433	0.000000
C	-3.315179	0.471493	0.000000

C	4.511750	0.998372	0.000000
C	-3.794539	1.019647	1.212287
C	-3.794539	1.019647	-1.212287
H	4.163407	1.382157	2.193853
Pb	-0.292629	0.092163	0.000000
H	4.163407	1.382157	-2.193853
C	3.920047	1.612045	1.160652
C	3.920047	1.612045	-1.160652
C	-4.720921	2.070928	1.210470
C	-4.720921	2.070928	-1.210470
H	-5.075810	2.477344	2.159486
H	-5.075810	2.477344	-2.159486
C	-5.189186	2.602122	0.000000
C	2.972478	2.579916	0.719772
C	2.972478	2.579916	-0.719772
H	2.366157	3.217134	1.357959
H	2.366157	3.217134	-1.357959
H	-5.908256	3.422911	0.000000
H	-3.431056	0.607065	2.155377
H	-3.431056	0.607065	-2.155377

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiN(SiMe_3)(Ph)]$ (**V**)

H	-3.816195	-3.631154	1.587689
H	-1.205258	-4.382103	0.000000
H	-3.816195	-3.631154	-1.587689
H	-2.888283	-2.392611	2.469635
C	-3.487351	-2.578635	1.563757
C	-0.901930	-3.321067	0.000000
H	-0.275874	-3.158241	0.891276
H	-4.387111	-1.945466	1.608274
C	-3.487351	-2.578635	-1.563757
H	-0.275874	-3.158241	-0.891276
H	-2.888283	-2.392611	-2.469635
Si	-2.465621	-2.257937	0.000000
H	-4.387111	-1.945466	-1.608274
O	2.315448	-1.848653	2.270911
O	2.315448	-1.848653	-2.270911
C	2.147545	-1.071384	1.400699
C	2.147545	-1.071384	-1.400699
N	-1.913016	-0.532834	0.000000
W	1.979818	0.303604	0.000000
H	5.029832	0.596152	0.000000
C	-2.873117	0.561913	0.000000
C	4.144151	1.222845	0.000000
C	-3.338288	1.101791	1.213852
C	-3.338288	1.101791	-1.213852
H	3.742258	1.551200	2.195282
Si	-0.245266	-0.079507	0.000000
H	3.742258	1.551200	-2.195282
C	3.467893	1.741852	1.162153
C	3.467893	1.741852	-1.162153

C	-4.261649	2.156025	1.211169
C	-4.261649	2.156025	-1.211169
H	-4.613673	2.565272	2.159518
H	-4.613673	2.565272	-2.159518
C	-4.728769	2.684979	0.000000
C	2.391627	2.566475	0.719731
C	2.391627	2.566475	-0.719731
H	1.694089	3.102355	1.356680
H	1.694089	3.102355	-1.356680
H	-5.447531	3.505986	0.000000
H	-2.968649	0.692045	2.154785
H	-2.968649	0.692045	-2.154785

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}GeN(SiMe_3)(Ph)]$ (**VI**)

H	-3.958468	-3.625145	1.565514
H	-1.336158	-4.388391	0.000000
H	-3.958468	-3.625145	-1.565514
H	-3.026014	-2.406038	2.470736
C	-3.614496	-2.577141	1.555019
C	-1.023414	-3.330303	0.000000
H	-0.395870	-3.174825	0.891791
H	-4.507019	-1.933018	1.594835
C	-3.614496	-2.577141	-1.555019
H	-0.395870	-3.174825	-0.891791
H	-3.026014	-2.406038	-2.470736
Si	-2.576695	-2.248352	0.000000
H	-4.507019	-1.933018	-1.594835
O	2.432906	-1.812887	2.270133
O	2.432906	-1.812887	-2.270133
C	2.237978	-1.041506	1.401501
C	2.237978	-1.041506	-1.401501
N	-2.017238	-0.537792	0.000000
W	2.049135	0.330685	0.000000
H	5.092246	0.607550	0.000000
C	-2.958186	0.563911	0.000000
C	4.208339	1.236647	0.000000
C	-3.425942	1.108597	1.212964
C	-3.425942	1.108597	-1.212964
H	3.805670	1.565401	2.195351
Ge	-0.228677	-0.066956	0.000000
H	3.805670	1.565401	-2.195351
C	3.533148	1.757926	1.162016
C	3.533148	1.757926	-1.162016
C	-4.345779	2.166156	1.210859
C	-4.345779	2.166156	-1.210859
H	-4.697989	2.575192	2.159499
H	-4.697989	2.575192	-2.159499
C	-4.811148	2.697915	0.000000
C	2.458943	2.586714	0.719913
C	2.458943	2.586714	-0.719913
H	1.763373	3.124814	1.357236

H	1.763373	3.124814	-1.357236
H	-5.527942	3.520782	0.000000
H	-3.062598	0.694991	2.155129
H	-3.062598	0.694991	-2.155129

[(η^5-C_5H_5)$(CO)_2$W≡SnN($SiMe_3$)(Ph)] (**VII**)

H	-4.055832	-3.750290	1.554677
H	-1.408297	-4.373158	0.000000
H	-4.055832	-3.750290	-1.554677
H	-3.174538	-2.500071	2.469728
C	-3.759579	-2.687857	1.554934
C	-1.141154	-3.302673	0.000000
H	-0.518932	-3.129337	0.892984
H	-4.679577	-2.084452	1.606993
C	-3.759579	-2.687857	-1.554934
H	-0.518932	-3.129337	-0.892984
H	-3.174538	-2.500071	-2.469728
Si	-2.744963	-2.286076	0.000000
H	-4.679577	-2.084452	-1.606993
O	2.549129	-1.797597	2.242430
O	2.549129	-1.797597	-2.242430
C	2.348711	-1.009133	1.388903
C	2.348711	-1.009133	-1.388903
N	-2.259623	-0.571512	0.000000
W	2.205598	0.378799	0.000000
H	5.245920	0.411554	0.000000
C	-3.205939	0.515162	0.000000
C	4.413516	1.107616	0.000000
C	-3.673380	1.067400	1.212692
C	-3.673380	1.067400	-1.212692
H	4.039158	1.468332	2.195257
Sn	-0.283530	0.012198	0.000000
H	4.039158	1.468332	-2.195257
C	3.782429	1.682834	1.162133
C	3.782429	1.682834	-1.162133
C	-4.580693	2.135508	1.210692
C	-4.580693	2.135508	-1.210692
H	-4.927142	2.548947	2.159622
H	-4.927142	2.548947	-2.159622
C	-5.038550	2.674796	0.000000
C	2.778157	2.595994	0.720095
C	2.778157	2.595994	-0.720095
H	2.130215	3.189399	1.358607
H	2.130215	3.189399	-1.358607
H	-5.741842	3.509137	0.000000
H	-3.315161	0.649805	2.155486
H	-3.315161	0.649805	-2.155486

[(η^5-C_5H_5)$(CO)_2$W≡PbN($SiMe_3$)(Ph)] (**VIII**)

H	-4.293078	-3.705061	1.545116
H	-1.667602	-4.426993	0.000000

H	-4.293078	-3.705061	-1.545116
H	-3.366172	-2.495059	2.469860
C	-3.953995	-2.655444	1.551483
C	-1.360826	-3.367453	0.000000
H	-0.732735	-3.219392	0.893899
H	-4.849516	-2.015966	1.603866
C	-3.953995	-2.655444	-1.551483
H	-0.732735	-3.219392	-0.893899
H	-3.366172	-2.495059	-2.469860
Si	-2.920487	-2.281693	0.000000
H	-4.849516	-2.015966	-1.603866
O	2.745883	-1.720107	2.255814
O	2.745883	-1.720107	-2.255814
C	2.488618	-0.956984	1.394402
C	2.488618	-0.956984	-1.394402
N	-2.370177	-0.597767	0.000000
W	2.261740	0.415204	0.000000
H	5.285187	0.628684	0.000000
C	-3.249572	0.533113	0.000000
C	4.411619	1.272217	0.000000
C	-3.688587	1.113661	1.212537
C	-3.688587	1.113661	-1.212537
H	4.016123	1.610393	2.195325
Pb	-0.273156	-0.051370	0.000000
H	4.016123	1.610393	-2.195325
C	3.747313	1.809771	1.162185
C	3.747313	1.809771	-1.162185
C	-4.538002	2.227916	1.210747
C	-4.538002	2.227916	-1.210747
H	-4.863438	2.658471	2.159633
H	-4.863438	2.658471	-2.159633
C	-4.966922	2.791081	0.000000
C	2.689616	2.661034	0.720451
C	2.689616	2.661034	-0.720451
H	2.010834	3.218370	1.359328
H	2.010834	3.218370	-1.359328
H	-5.625862	3.660886	0.000000
H	-3.354997	0.675981	2.155357
H	-3.354997	0.675981	-2.155357

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)

H	-3.049048	-4.256822	1.430401
H	-0.334773	-4.497836	0.000000
H	-3.049048	-4.256822	-1.430401
H	-2.313325	-3.010026	2.463505
C	-2.867490	-3.172802	1.526623
C	-0.183957	-3.404709	0.000000
H	0.411828	-3.158418	0.892268
H	-3.849396	-2.680863	1.607415
C	-2.867490	-3.172802	-1.526623
H	0.411828	-3.158418	-0.892268

H	-2.313325	-3.010026	-2.463505
Si	-1.893900	-2.589259	0.000000
H	-3.849396	-2.680863	-1.607415
O	2.685911	-1.728214	2.245913
O	2.685911	-1.728214	-2.245913
C	2.503329	-0.942653	1.388088
C	2.503329	-0.942653	-1.388088
N	-1.624677	-0.806666	0.000000
Mo	2.341227	0.438921	0.000000
H	5.397363	0.582539	0.000000
C	-2.704566	0.175311	0.000000
C	4.544175	1.254207	0.000000
C	-3.224360	0.668328	1.228588
C	-3.224360	0.668328	-1.228588
H	4.159947	1.598367	2.192805
Ge	0.076878	-0.053868	0.000000
H	4.159947	1.598367	-2.192805
C	3.896492	1.806255	1.159920
C	3.896492	1.806255	-1.159920
C	-4.304915	1.566814	1.198476
C	-4.304915	1.566814	-1.198476
H	-4.706513	1.928058	2.149586
H	-4.706513	1.928058	-2.149586
C	-4.875104	2.019012	0.000000
C	2.861062	2.679535	0.719193
C	2.861062	2.679535	-0.719193
H	2.190846	3.250177	1.356433
H	2.190846	3.250177	-1.356433
C	-6.029594	3.005365	0.000000
H	-6.662861	2.883152	-0.889620
H	-6.662861	2.883152	0.889620
H	-5.662122	4.044629	0.000000
C	-2.639493	0.277192	2.573780
H	-2.852231	-0.769069	2.828970
H	-1.545711	0.392378	2.595075
H	-3.060191	0.908386	3.367481
C	-2.639493	0.277192	-2.573780
H	-1.545711	0.392378	-2.595075
H	-2.852231	-0.769069	-2.828970
H	-3.060191	0.908386	-3.367481

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ar^*)]$(**X**)

C	2.978175	-1.271533	-5.014616
C	1.693014	-1.407778	-4.470079
C	4.060403	-1.024856	-4.160452
C	-2.988201	-3.630451	-3.211140
C	-3.340192	-2.249579	-3.181589
C	1.494916	-1.288161	-3.088855
C	3.859655	-0.910858	-2.776501
C	-3.857140	-4.331906	-2.303645
C	-4.434560	-2.083590	-2.264619

C	2.572931	-1.031227	-2.219344
C	-4.749635	-3.363772	-1.725438
C	-3.529088	2.480486	-1.616875
C	2.827866	4.128531	-1.328839
C	-0.910534	-3.979927	-0.922990
C	-4.749249	2.193101	-0.993414
C	2.456631	1.640145	-0.945701
C	-2.345162	2.544877	-0.864532
C	2.303042	-0.873595	-0.703850
C	2.061811	2.962823	-0.729385
C	1.788054	0.541461	-0.373814
C	3.729993	-2.725432	0.273655
C	3.501568	-1.339604	0.145734
C	0.922705	3.176316	0.060556
C	-4.777288	1.967746	0.391181
C	0.653335	0.778676	0.456490
C	-2.360152	2.328047	0.525862
C	4.822431	-3.214194	0.999345
C	-2.993929	-3.485680	0.811368
C	0.201179	2.122625	0.637860
C	4.401780	-0.459408	0.770679
C	-3.596208	2.035633	1.138946
C	5.716859	-2.324704	1.613976
C	-1.097430	2.432849	1.408000
C	5.500806	-0.946727	1.496545
C	-1.510880	4.977958	1.639276
C	-1.038423	3.766999	2.179996
C	-1.412534	6.177984	2.359007
C	0.586839	-2.734202	2.800727
C	-0.847098	6.190825	3.640721
C	-0.483031	3.794484	3.474262
C	-0.386121	4.989931	4.198332
C	-1.399849	-0.646487	3.815274
C	1.625451	0.106437	3.584342
H	3.134698	-1.365644	-6.091024
H	0.841556	-1.613407	-5.122117
H	5.068533	-0.927253	-4.567867
H	-2.207526	-4.079737	-3.818134
H	-2.865709	-1.456660	-3.753978
H	0.488311	-1.404673	-2.680514
H	-3.868767	-5.403067	-2.126287
H	-3.491713	2.656531	-2.693626
H	4.719085	-0.738927	-2.125973
H	-4.925613	-1.145522	-2.021129
H	3.552079	3.788257	-2.080636
H	2.150457	4.849492	-1.809758
H	3.310075	1.446252	-1.597458
H	-5.670153	2.145450	-1.578028
H	-5.535749	-3.576590	-1.006791
H	-1.402611	2.764708	-1.368640
H	3.382606	4.678418	-0.551979
H	3.045076	-3.428698	-0.205848

H	1.489101	-1.571691	-0.471587
H	0.580602	4.199191	0.227976
H	4.974944	-4.291498	1.084837
H	-5.720418	1.738902	0.890500
H	-1.969082	4.986414	0.648713
H	4.246343	0.617852	0.700030
H	-1.784888	7.103498	1.915743
H	6.569881	-2.703491	2.180101
H	-0.231022	-3.326505	2.361890
H	6.185451	-0.242139	1.972720
H	-3.634492	1.865336	2.217469
H	1.512433	-2.959957	2.251130
H	-1.206837	1.650869	2.165645
H	-2.259679	-1.131658	3.325169
H	2.591584	-0.156683	3.129244
H	-0.773543	7.123884	4.202548
H	-0.120189	2.869311	3.925935
H	0.718364	-3.079470	3.840552
H	1.494942	1.195119	3.499038
H	-1.659496	0.407419	3.998867
H	0.047246	4.981605	5.200180
H	-1.273068	-1.129364	4.799171
H	1.676996	-0.146903	4.657291
N	-0.056149	-0.320672	1.093684
Si	0.203405	-0.877060	2.807186
Ge	-1.288306	-1.220651	0.021517
Mo	-2.534274	-2.885867	-1.005973
O	0.022504	-4.698701	-0.942029
O	-3.344353	-3.888761	1.860059

TPSS/DFT

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SiN(SiMe_3)(Ph)]$ (**I**)

H	-3.939861	-3.580120	1.590446
H	-1.291434	-4.414894	0.000000
H	-3.939861	-3.580120	-1.590446
H	-2.945416	-2.394689	2.453703
C	-3.557072	-2.552281	1.556758
C	-0.999822	-3.356673	0.000000
H	-0.372771	-3.193193	0.885245
H	-4.416169	-1.873555	1.607999
C	-3.557072	-2.552281	-1.556758
H	-0.372771	-3.193193	-0.885245
H	-2.945416	-2.394689	-2.453703
Si	-2.539156	-2.273276	0.000000
H	-4.416169	-1.873555	-1.607999
O	2.565481	-1.821584	2.270503
O	2.565481	-1.821584	-2.270503
C	2.302010	-1.081097	1.405428
C	2.302010	-1.081097	-1.405428
N	-1.904507	-0.612121	0.000000
Mo	1.944641	0.265897	0.000000

H	4.899875	1.032218	0.000000
C	-2.759122	0.559198	0.000000
C	3.927717	1.502490	0.000000
C	-3.160179	1.139624	1.208943
C	-3.160179	1.139624	-1.208943
H	3.488124	1.768484	2.182521
Si	-0.221413	-0.273075	0.000000
H	3.488124	1.768484	-2.182521
C	3.184894	1.907828	1.155123
C	3.184894	1.907828	-1.155123
C	-3.957428	2.283336	1.205825
C	-3.957428	2.283336	-1.205825
H	-4.260809	2.727480	2.148596
H	-4.260809	2.727480	-2.148596
C	-4.358332	2.858789	0.000000
C	1.998726	2.547016	0.715941
C	1.998726	2.547016	-0.715941
H	1.235264	2.978298	1.346863
H	1.235264	2.978298	-1.346863
H	-4.976250	3.750965	0.000000
H	-2.835015	0.693356	2.142990
H	-2.835015	0.693356	-2.142990

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Ph)]$ (**II**)

H	-3.775019	-3.644887	1.551912
H	-1.100967	-4.259183	0.000000
H	-3.775019	-3.644887	-1.551912
H	-2.898144	-2.397984	2.455138
C	-3.478440	-2.588008	1.544059
C	-0.864959	-3.186946	0.000000
H	-0.249630	-2.991815	0.886191
H	-4.393136	-1.986047	1.591416
C	-3.478440	-2.588008	-1.544059
H	-0.249630	-2.991815	-0.886191
H	-2.898144	-2.397984	-2.455138
Si	-2.469097	-2.204706	0.000000
H	-4.393136	-1.986047	-1.591416
O	2.247294	-1.834728	2.253236
O	2.247294	-1.834728	-2.253236
C	2.112435	-1.049464	1.397043
C	2.112435	-1.049464	-1.397043
N	-1.997456	-0.493647	0.000000
Mo	2.031529	0.340398	0.000000
H	5.072895	0.294827	0.000000
C	-2.998719	0.544853	0.000000
C	4.260710	1.006452	0.000000
C	-3.494055	1.053494	1.208170
C	-3.494055	1.053494	-1.208170
H	3.901995	1.376201	2.182308
Ge	-0.246492	0.060652	0.000000
H	3.901995	1.376201	-2.182308

C	3.650656	1.594967	1.154974
C	3.650656	1.594967	-1.154974
C	-4.470001	2.049458	1.205494
C	-4.470001	2.049458	-1.205494
H	-4.844790	2.434556	2.148643
H	-4.844790	2.434556	-2.148643
C	-4.961527	2.550651	0.000000
C	2.673762	2.523822	0.716182
C	2.673762	2.523822	-0.716182
H	2.045699	3.133762	1.349389
H	2.045699	3.133762	-1.349389
H	-5.720686	3.326163	0.000000
H	-3.106357	0.661140	2.142866
H	-3.106357	0.661140	-2.142866

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SnN(SiMe_3)(Ph)]$ (**III**)

H	-3.884683	-3.743864	1.551729
H	-1.180957	-4.223069	0.000000
H	-3.884683	-3.743864	-1.551729
H	-3.054097	-2.464224	2.453986
C	-3.633141	-2.675455	1.546395
C	-0.999406	-3.140334	0.000000
H	-0.390074	-2.923512	0.887034
H	-4.571667	-2.112126	1.605889
C	-3.633141	-2.675455	-1.546395
H	-0.390074	-2.923512	-0.887034
H	-3.054097	-2.464224	-2.453986
Si	-2.652075	-2.228638	0.000000
H	-4.571667	-2.112126	-1.605889
O	2.455047	-1.819988	2.240458
O	2.455047	-1.819988	-2.240458
C	2.281273	-1.033336	1.391378
C	2.281273	-1.033336	-1.391378
N	-2.240888	-0.517451	0.000000
Mo	2.190430	0.361891	0.000000
H	5.217187	0.241423	0.000000
C	-3.237919	0.514297	0.000000
C	4.420371	0.970481	0.000000
C	-3.732726	1.032017	1.207103
C	-3.732726	1.032017	-1.207103
H	4.073320	1.354290	2.183138
Sn	-0.287216	0.098726	0.000000
H	4.073320	1.354290	-2.183138
C	3.826120	1.576691	1.155489
C	3.826120	1.576691	-1.155489
C	-4.697578	2.038532	1.204791
C	-4.697578	2.038532	-1.204791
H	-5.067318	2.427875	2.148446
H	-5.067318	2.427875	-2.148446
C	-5.183825	2.546678	0.000000
C	2.875685	2.532415	0.716146

C	2.875685	2.532415	-0.716146
H	2.268329	3.162926	1.349465
H	2.268329	3.162926	-1.349465
H	-5.932741	3.332164	0.000000
H	-3.350363	0.636106	2.142923
H	-3.350363	0.636106	-2.142923

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}PbN(SiMe_3)(Ph)]$ (**IV**)

H	-4.129036	-3.728206	1.543974
H	-1.455648	-4.318857	0.000000
H	-4.129036	-3.728206	-1.543974
H	-3.256356	-2.482149	2.454736
C	-3.836739	-2.669969	1.542570
C	-1.225431	-3.245484	0.000000
H	-0.607576	-3.057700	0.888441
H	-4.754090	-2.071673	1.598441
C	-3.836739	-2.669969	-1.542570
H	-0.607576	-3.057700	-0.888441
H	-3.256356	-2.482149	-2.454736
Si	-2.833090	-2.252557	0.000000
H	-4.754090	-2.071673	-1.598441
O	2.678149	-1.751181	2.251737
O	2.678149	-1.751181	-2.251737
C	2.435645	-0.989683	1.396670
C	2.435645	-0.989683	-1.396670
N	-2.349602	-0.570586	0.000000
Mo	2.239009	0.391700	0.000000
H	5.259783	0.498423	0.000000
C	-3.265699	0.523461	0.000000
C	4.408911	1.164183	0.000000
C	-3.721467	1.081387	1.206869
C	-3.721467	1.081387	-1.206869
H	4.032471	1.518872	2.183022
Pb	-0.274850	0.005164	0.000000
H	4.032471	1.518872	-2.183022
C	3.769575	1.722859	1.155241
C	3.769575	1.722859	-1.155241
C	-4.604672	2.159841	1.204917
C	-4.604672	2.159841	-1.204917
H	-4.943629	2.576527	2.148807
H	-4.943629	2.576527	-2.148807
C	-5.050109	2.705035	0.000000
C	2.747924	2.602727	0.716347
C	2.747924	2.602727	-0.716347
H	2.097527	3.188441	1.350162
H	2.097527	3.188441	-1.350162
H	-5.735118	3.547075	0.000000
H	-3.372298	0.655914	2.143063
H	-3.372298	0.655914	-2.143063

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiN(SiMe_3)(Ph)]$ (**V**)

H	-4.078729	-3.504577	1.582385
H	-1.480649	-4.471811	0.000000
H	-4.078729	-3.504577	-1.582385
H	-3.031949	-2.372146	2.454541
C	-3.645549	-2.496576	1.553772
C	-1.131485	-3.431013	0.000000
H	-0.496657	-3.300658	0.885063
H	-4.471173	-1.777297	1.602523
C	-3.645549	-2.496576	-1.553772
H	-0.496657	-3.300658	-0.885063
H	-3.031949	-2.372146	-2.454541
Si	-2.609808	-2.268417	0.000000
H	-4.471173	-1.777297	-1.602523
O	2.711428	-1.772023	2.281990
O	2.711428	-1.772023	-2.281990
C	2.391642	-1.060164	1.409647
C	2.391642	-1.060164	-1.409647
N	-1.895557	-0.636949	0.000000
W	1.957791	0.252187	0.000000
H	4.862555	1.143134	0.000000
C	-2.721939	0.555665	0.000000
C	3.870686	1.568648	0.000000
C	-3.117683	1.139667	1.208781
C	-3.117683	1.139667	-1.208781
H	3.414855	1.810918	2.184498
Si	-0.203260	-0.353786	0.000000
H	3.414855	1.810918	-2.184498
C	3.106304	1.937006	1.157305
C	3.106304	1.937006	-1.157305
C	-3.906722	2.289275	1.205680
C	-3.906722	2.289275	-1.205680
H	-4.207763	2.734766	2.148631
H	-4.207763	2.734766	-2.148631
C	-4.304556	2.866726	0.000000
C	1.890173	2.521701	0.716543
C	1.890173	2.521701	-0.716543
H	1.105382	2.910584	1.347769
H	1.105382	2.910584	-1.347769
H	-4.918108	3.761960	0.000000
H	-2.798306	0.689387	2.142919
H	-2.798306	0.689387	-2.142919

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}GeN(SiMe_3)(Ph)]$ (**VI**)

H	-3.910228	-3.579289	1.558658
H	-1.261547	-4.307811	0.000000
H	-3.910228	-3.579289	-1.558658
H	-2.978779	-2.367161	2.454914
C	-3.569512	-2.535846	1.546165
C	-0.983777	-3.245510	0.000000
H	-0.360322	-3.073972	0.885933
H	-4.457812	-1.895482	1.594261

C	-3.569512	-2.535846	-1.546165
H	-0.360322	-3.073972	-0.885933
H	-2.978779	-2.367161	-2.454914
Si	-2.547581	-2.199065	0.000000
H	-4.457812	-1.895482	-1.594261
O	2.453141	-1.811651	2.265563
O	2.453141	-1.811651	-2.265563
C	2.248661	-1.048526	1.401226
C	2.248661	-1.048526	-1.401226
N	-2.000452	-0.510411	0.000000
W	2.038821	0.319420	0.000000
H	5.060038	0.619936	0.000000
C	-2.947623	0.577801	0.000000
C	4.170064	1.229986	0.000000
C	-3.418228	1.109218	1.207787
C	-3.418228	1.109218	-1.207787
H	3.767502	1.555628	2.184377
Ge	-0.222152	-0.068404	0.000000
H	3.767502	1.555628	-2.184377
C	3.491878	1.741439	1.156896
C	3.491878	1.741439	-1.156896
C	-4.346985	2.149187	1.205357
C	-4.346985	2.149187	-1.205357
H	-4.703721	2.550969	2.148668
H	-4.703721	2.550969	-2.148668
C	-4.814887	2.672726	0.000000
C	2.412204	2.552528	0.716736
C	2.412204	2.552528	-0.716736
H	1.716458	3.083354	1.349516
H	1.716458	3.083354	-1.349516
H	-5.537370	3.482629	0.000000
H	-3.049548	0.699162	2.142679
H	-3.049548	0.699162	-2.142679

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SnN(SiMe_3)(Ph)]$ (**VII**)

H	-3.975749	-3.733573	1.553016
H	-1.289018	-4.284717	0.000000
H	-3.975749	-3.733573	-1.553016
H	-3.110199	-2.477225	2.454244
C	-3.696257	-2.672224	1.547696
C	-1.077901	-3.207418	0.000000
H	-0.462917	-3.006769	0.886774
H	-4.619323	-2.084489	1.609202
C	-3.696257	-2.672224	-1.547696
H	-0.462917	-3.006769	-0.886774
H	-3.110199	-2.477225	-2.454244
Si	-2.705492	-2.251518	0.000000
H	-4.619323	-2.084489	-1.609202
O	2.558401	-1.790331	2.242692
O	2.558401	-1.790331	-2.242692
C	2.348782	-1.013003	1.390136

C	2.348782	-1.013003	-1.390136
N	-2.245269	-0.552406	0.000000
W	2.185450	0.368672	0.000000
H	5.206319	0.415492	0.000000
C	-3.189874	0.527783	0.000000
C	4.369852	1.096814	0.000000
C	-3.652841	1.073545	1.207293
C	-3.652841	1.073545	-1.207293
H	3.996838	1.456952	2.184249
Sn	-0.281257	0.008303	0.000000
H	3.996838	1.456952	-2.184249
C	3.737768	1.665663	1.157019
C	3.737768	1.665663	-1.157019
C	-4.553873	2.137443	1.205209
C	-4.553873	2.137443	-1.205209
H	-4.897671	2.549394	2.148810
H	-4.897671	2.549394	-2.148810
C	-5.007655	2.674857	0.000000
C	2.731307	2.566525	0.716620
C	2.731307	2.566525	-0.716620
H	2.085889	3.156216	1.350391
H	2.085889	3.156216	-1.350391
H	-5.704315	3.506762	0.000000
H	-3.293848	0.655794	2.142783
H	-3.293848	0.655794	-2.142783

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}PbN(SiMe_3)(Ph)]$ **(VIII)**

H	-4.199755	-3.652335	1.549529
H	-1.537441	-4.308943	0.000000
H	-4.199755	-3.652335	-1.549529
H	-3.286081	-2.431535	2.453665
C	-3.877755	-2.602972	1.545531
C	-1.283946	-3.240896	0.000000
H	-0.661354	-3.067230	0.887895
H	-4.776768	-1.978416	1.607268
C	-3.877755	-2.602972	-1.545531
H	-0.661354	-3.067230	-0.887895
H	-3.286081	-2.431535	-2.453665
Si	-2.869353	-2.213206	0.000000
H	-4.776768	-1.978416	-1.607268
O	2.769547	-1.723014	2.259831
O	2.769547	-1.723014	-2.259831
C	2.503216	-0.974574	1.397785
C	2.503216	-0.974574	-1.397785
N	-2.347979	-0.541528	0.000000
W	2.244525	0.387840	0.000000
H	5.245491	0.702754	0.000000
C	-3.240676	0.572585	0.000000
C	4.349496	1.303663	0.000000
C	-3.687735	1.136661	1.206784
C	-3.687735	1.136661	-1.206784

H	3.947448	1.632125	2.184589
Pb	-0.258712	-0.056659	0.000000
H	3.947448	1.632125	-2.184589
C	3.669969	1.815040	1.157040
C	3.669969	1.815040	-1.157040
C	-4.557116	2.226166	1.204955
C	-4.557116	2.226166	-1.204955
H	-4.891147	2.646910	2.148586
H	-4.891147	2.646910	-2.148586
C	-4.995821	2.776538	0.000000
C	2.587784	2.623989	0.716940
C	2.587784	2.623989	-0.716940
H	1.897514	3.160909	1.350847
H	1.897514	3.160909	-1.350847
H	-5.671412	3.625992	0.000000
H	-3.343625	0.707469	2.142930
H	-3.343625	0.707469	-2.142930

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$(**IX**)

H	-3.041535	-4.211183	1.433008
H	-0.288310	-4.426440	0.000000
H	-3.041535	-4.211183	-1.433008
H	-2.285953	-2.973895	2.447246
C	-2.849492	-3.133524	1.521013
C	-0.179507	-3.333648	0.000000
H	0.409507	-3.069372	0.886176
H	-3.820395	-2.633652	1.615620
C	-2.849492	-3.133524	-1.521013
H	0.409507	-3.069372	-0.886176
H	-2.285953	-2.973895	-2.447246
Si	-1.894091	-2.556179	0.000000
H	-3.820395	-2.633652	-1.615620
O	2.747836	-1.722099	2.252462
O	2.747836	-1.722099	-2.252462
C	2.533724	-0.954881	1.395750
C	2.533724	-0.954881	-1.395750
N	-1.623361	-0.801429	0.000000
Mo	2.315234	0.419263	0.000000
H	5.348399	0.667761	0.000000
C	-2.685921	0.185942	0.000000
C	4.471788	1.298363	0.000000
C	-3.192665	0.677054	1.221441
C	-3.192665	0.677054	-1.221441
H	4.079827	1.631729	2.182026
Ge	0.076016	-0.095065	0.000000
H	4.079827	1.631729	-2.182026
C	3.808088	1.825380	1.154783
C	3.808088	1.825380	-1.154783
C	-4.256591	1.582456	1.194154
C	-4.256591	1.582456	-1.194154

H	-4.651727	1.945730	2.140582
H	-4.651727	1.945730	-2.140582
C	-4.816799	2.037263	0.000000
C	2.746526	2.656622	0.716044
C	2.746526	2.656622	-0.716044
H	2.063902	3.204665	1.349331
H	2.063902	3.204665	-1.349331
C	-5.954856	3.031456	0.000000
H	-6.584381	2.912338	-0.885972
H	-6.584381	2.912338	0.885972
H	-5.575814	4.060349	0.000000
C	-2.595777	0.274347	2.548940
H	-2.765092	-0.781709	2.770581
H	-1.512119	0.434057	2.563907
H	-3.037380	0.867181	3.353601
C	-2.595777	0.274347	-2.548940
H	-1.512119	0.434057	-2.563907
H	-2.765092	-0.781709	-2.770581
H	-3.037380	0.867181	-3.353601

[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ar*)] (**X**)

C	2.926122	-1.094473	-5.034771
C	1.634601	-1.240205	-4.526484
C	3.989326	-0.899907	-4.154846
C	-2.918864	-3.554847	-3.176367
C	-3.320519	-2.197667	-3.074104
C	1.410906	-1.179329	-3.152706
C	3.763741	-0.846092	-2.778460
C	-3.726534	-4.326024	-2.278819
C	-4.384566	-2.115452	-2.120957
C	2.470125	-0.972327	-2.260870
C	-4.632661	-3.423836	-1.634112
C	-3.449437	2.348361	-1.554322
C	2.929986	4.100847	-1.225731
C	-0.755097	-3.908796	-0.988749
C	-4.649459	2.009456	-0.932427
C	2.465785	1.632427	-0.915389
C	-2.276688	2.471824	-0.805306
C	2.174694	-0.869980	-0.757807
C	2.122885	2.955600	-0.658743
C	1.755509	0.552580	-0.377286
C	3.438529	-2.842668	0.158295
C	3.311208	-1.447828	0.087300
C	0.997493	3.194448	0.133345
C	-4.670397	1.792803	0.446263
C	0.652046	0.815333	0.464922
C	-2.288954	2.269266	0.579706
C	4.469146	-3.429458	0.886960
C	-2.829248	-3.593668	0.826528
C	0.248555	2.155647	0.681133

C	4.241870	-0.657002	0.766339
C	-3.502019	1.924694	1.192383
C	5.396962	-2.631096	1.558623
C	-1.039356	2.453056	1.451264
C	5.279242	-1.244611	1.495297
C	-1.470210	4.982817	1.517831
C	-1.025885	3.814546	2.148201
C	-1.419550	6.212097	2.175423
C	0.512777	-2.620115	2.808210
C	-0.935310	6.292943	3.480679
C	-0.548199	3.908411	3.460501
C	-0.502686	5.133371	4.124001
C	-1.486321	-0.543904	3.744331
C	1.523993	0.221842	3.563898
H	3.102548	-1.142677	-6.105143
H	0.800351	-1.406495	-5.201982
H	5.000642	-0.799327	-4.537327
H	-2.149637	-3.944227	-3.827256
H	-2.901870	-1.366733	-3.624052
H	0.403118	-1.300057	-2.762591
H	-3.698071	-5.398618	-2.157436
H	-3.420191	2.517369	-2.626618
H	4.603396	-0.722937	-2.100810
H	-4.899893	-1.213675	-1.824315
H	3.614969	3.752438	-2.002505
H	2.280214	4.866402	-1.660723
H	3.300020	1.423102	-1.578215
H	-5.561541	1.917172	-1.514805
H	-5.384758	-3.697858	-0.908817
H	-1.344984	2.723343	-1.302585
H	3.524741	4.585673	-0.443199
H	2.721848	-3.469770	-0.364402
H	1.312139	-1.517724	-0.578484
H	0.692580	4.218014	0.329091
H	4.546133	-4.511396	0.932228
H	-5.598176	1.523908	0.941776
H	-1.873346	4.928294	0.511162
H	4.151822	0.424229	0.737649
H	-1.769543	7.106445	1.668893
H	6.200341	-3.087538	2.128567
H	-0.274584	-3.201125	2.311811
H	5.991752	-0.613014	2.017309
H	-3.529678	1.763976	2.266401
H	1.463898	-2.842193	2.313343
H	-1.116371	1.705418	2.241978
H	-2.326699	-1.014887	3.218290
H	2.488009	-0.024347	3.106206
H	-0.903229	7.248619	3.994848
H	-0.210487	3.010380	3.970447
H	0.575337	-2.980298	3.843701
H	1.374071	1.302815	3.468757
H	-1.747222	0.505603	3.923615

H	-0.133382	5.180447	5.143829
H	-1.404441	-1.033065	4.724000
H	1.586114	-0.020029	4.633308
N	-0.084121	-0.256542	1.093142
Si	0.133076	-0.778258	2.790485
Ge	-1.272616	-1.192568	0.049114
Mo	-2.436299	-2.890506	-0.976141
O	0.206026	-4.573353	-1.067671
O	-3.143709	-4.048993	1.856439

TPSS/DFT-D3

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}GeN(SiMe_3)(Mes)]$ (**IX**)

H	-2.979957	-4.158211	1.429937
H	-0.219278	-4.357812	0.000000
H	-2.979957	-4.158211	-1.429937
H	-2.213968	-2.923256	2.441813
C	-2.782532	-3.081959	1.518674
C	-0.111924	-3.265012	0.000000
H	0.474137	-2.997739	0.886609
H	-3.748848	-2.572857	1.610819
C	-2.782532	-3.081959	-1.518674
H	0.474137	-2.997739	-0.886609
H	-2.213968	-2.923256	-2.441813
Si	-1.830986	-2.505314	0.000000
H	-3.748848	-2.572857	-1.610819
O	2.611252	-1.753204	2.245973
O	2.611252	-1.753204	-2.245973
C	2.456592	-0.967599	1.392697
C	2.456592	-0.967599	-1.392697
N	-1.600978	-0.745369	0.000000
Mo	2.328426	0.418983	0.000000
H	5.369568	0.486372	0.000000
C	-2.706278	0.192318	0.000000
C	4.531701	1.167732	0.000000
C	-3.232919	0.659244	1.221696
C	-3.232919	0.659244	-1.221696
H	4.158839	1.522216	2.182229
Ge	0.077658	-0.004890	0.000000
H	4.158839	1.522216	-2.182229
C	3.899553	1.732692	1.154932
C	3.899553	1.732692	-1.154932
C	-4.339854	1.511013	1.194775
C	-4.339854	1.511013	-1.194775
H	-4.750893	1.858626	2.140199
H	-4.750893	1.858626	-2.140199
C	-4.921009	1.936390	0.000000
C	2.887946	2.623955	0.716148
C	2.887946	2.623955	-0.716148
H	2.236988	3.209516	1.349567
H	2.236988	3.209516	-1.349567
C	-6.103368	2.877846	0.000000

H	-6.726904	2.730473	-0.886014
H	-6.726904	2.730473	0.886014
H	-5.769068	3.922069	0.000000
C	-2.604860	0.293045	2.545463
H	-2.722440	-0.767742	2.774441
H	-1.529383	0.501270	2.545106
H	-3.062317	0.870183	3.352479
C	-2.604860	0.293045	-2.545463
H	-1.529383	0.501270	-2.545106
H	-2.722440	-0.767742	-2.774441
H	-3.062317	0.870183	-3.352479

[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ar*)] (**X**)

C	2.687993	-1.050684	-5.033601
C	1.407560	-1.148714	-4.485835
C	3.789367	-0.932140	-4.186516
C	-2.852265	-3.397508	-3.216809
C	-3.353091	-2.080595	-3.044289
C	1.233089	-1.114113	-3.104870
C	3.612814	-0.905908	-2.802231
C	-3.590452	-4.270533	-2.353112
C	-4.410106	-2.126429	-2.080905
C	2.332194	-0.985449	-2.247783
C	-4.553794	-3.471942	-1.657251
C	-3.303483	1.934421	-1.488395
C	3.017704	4.065871	-1.113991
C	-0.644631	-3.682395	-1.058718
C	-4.488626	1.547017	-0.867499
C	2.475151	1.606345	-0.869038
C	-2.167460	2.214233	-0.724785
C	1.738951	0.539230	-0.340893
C	3.362492	-2.899827	0.066867
C	3.214619	-1.505820	0.085189
C	1.080460	3.191457	0.254475
C	-4.532718	1.436697	0.523466
C	0.668406	0.818787	0.527922
C	-2.204583	2.116267	0.672524
C	4.365927	-3.517138	0.806976
C	-2.687470	-3.596501	0.791728
C	0.309182	2.161464	0.781570
C	4.096473	-0.746051	0.856031
C	-3.401969	1.722038	1.284281
C	5.244501	-2.750516	1.576297
C	-0.984891	2.443818	1.538086
C	5.106691	-1.364889	1.597239
C	-1.564821	4.933816	1.412772
C	-1.032230	3.850571	2.119016
C	-1.534605	6.218416	1.955759
C	0.593619	-2.636595	2.743175
C	-0.976530	6.437218	3.214951
C	-0.479377	4.079886	3.383420

C	-0.451261	5.360880	3.930854
C	-1.492171	-0.649956	3.739574
C	1.491848	0.232273	3.578962
H	2.826168	-1.075785	-6.110378
H	0.544268	-1.256066	-5.136486
H	4.790309	-0.866744	-4.602242
H	-2.059637	-3.694318	-3.888322
H	-2.998584	-1.193588	-3.550566
H	0.235680	-1.199093	-2.680280
H	-3.478052	-5.342235	-2.283187
H	-3.255795	2.018538	-2.569745
H	4.475435	-0.836373	-2.145971
H	-4.983811	-1.281046	-1.731212
H	3.673074	3.720940	-1.917457
H	2.384470	4.866912	-1.507724
H	3.290277	1.385448	-1.551500
H	-5.372513	1.332831	-1.460822
H	-5.273110	-3.836443	-0.938503
H	-1.243326	2.503279	-1.215652
H	3.645553	4.503320	-0.329368
H	2.676068	-3.496400	-0.525195
H	1.206911	-1.506384	-0.542430
H	0.806480	4.219271	0.471863
H	4.459053	-4.598469	0.787721
H	-5.448345	1.125514	1.016110
H	-2.009652	4.768581	0.436467
H	3.986489	0.332980	0.890437
H	-1.952426	7.048743	1.394797
H	6.026296	-3.231619	2.156013
H	-0.176736	-3.219843	2.223533
H	5.780965	-0.758978	2.194774
H	-3.443341	1.637395	2.365921
H	1.546211	-2.790501	2.225241
H	-1.021319	1.755894	2.385052
H	-2.310082	-1.122092	3.179659
H	2.451375	0.052928	3.082488
H	-0.957312	7.436545	3.638693
H	-0.063799	3.244812	3.941039
H	0.683267	-3.043263	3.758856
H	1.271896	1.303596	3.508443
H	-1.771636	0.393118	3.929277
H	-0.021201	5.518343	4.915065
H	-1.424247	-1.158610	4.709589
H	1.600429	-0.028064	4.639510
N	-0.098505	-0.235040	1.136329
Si	0.141469	-0.816541	2.803482
Ge	-1.323214	-1.086313	0.072822
Mo	-2.396834	-2.805289	-0.993629
O	0.370897	-4.256573	-1.169746
O	-2.927165	-4.104935	1.817270

TPSS/DFT-D3(BJ)

[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Mes)] (**IX**)

H	-3.005881	-4.158024	1.432620
H	-0.208917	-4.349712	0.000000
H	-3.005881	-4.158024	-1.432620
H	-2.228523	-2.928505	2.441676
C	-2.799631	-3.083370	1.519570
C	-0.123635	-3.255274	0.000000
H	0.458114	-2.975820	0.885739
H	-3.762065	-2.567846	1.615259
C	-2.799631	-3.083370	-1.519570
H	0.458114	-2.975820	-0.885739
H	-2.228523	-2.928505	-2.441676
Si	-1.848107	-2.511780	0.000000
H	-3.762065	-2.567846	-1.615259
O	2.659177	-1.744094	2.246408
O	2.659177	-1.744094	-2.246408
C	2.480477	-0.965080	1.392344
C	2.480477	-0.965080	-1.392344
N	-1.607103	-0.756203	0.000000
Mo	2.321448	0.416619	0.000000
H	5.355386	0.525316	0.000000
C	-2.704136	0.187276	0.000000
C	4.509160	1.195467	0.000000
C	-3.221998	0.658691	1.220994
C	-3.221998	0.658691	-1.220994
H	4.128641	1.541337	2.181479
Ge	0.074324	-0.025339	0.000000
H	4.128641	1.541337	-2.181479
C	3.868070	1.749727	1.154645
C	3.868070	1.749727	-1.154645
C	-4.315993	1.526190	1.195514
C	-4.315993	1.526190	-1.195514
H	-4.722111	1.878349	2.141114
H	-4.722111	1.878349	-2.141114
C	-4.889756	1.959657	0.000000
C	2.842701	2.624862	0.715942
C	2.842701	2.624862	-0.715942
H	2.180099	3.196491	1.349024
H	2.180099	3.196491	-1.349024
C	-6.059066	2.915160	0.000000
H	-6.683519	2.774882	-0.886204
H	-6.683519	2.774882	0.886204
H	-5.712395	3.955159	0.000000
C	-2.591731	0.280150	2.538107
H	-2.704564	-0.783894	2.753844
H	-1.516857	0.492006	2.535691
H	-3.050044	0.847476	3.351280
C	-2.591731	0.280150	-2.538107
H	-1.516857	0.492006	-2.535691
H	-2.704564	-0.783894	-2.753844

H	-3.050044	0.847476	-3.351280

M06-L/DFT

[(η^5-C_5H_5)$(CO)_2$Mo≡SiN($SiMe_3$)(Ph)] (**I**)

H	-3.698591	-3.357878	1.554457
H	-1.040322	-4.133744	0.000000
H	-3.698591	-3.357878	-1.554457
H	-2.802966	-2.121809	2.431214
C	-3.339493	-2.329157	1.505315
C	-0.758121	-3.080107	0.000000
H	-0.140982	-2.912117	0.882150
H	-4.219256	-1.684369	1.479820
C	-3.339493	-2.329157	-1.505315
H	-0.140982	-2.912117	-0.882150
H	-2.802966	-2.121809	-2.431214
Si	-2.294732	-2.060867	0.000000
H	-4.219256	-1.684369	-1.479820
O	1.950331	-2.012749	2.171785
O	1.950331	-2.012749	-2.171785
C	1.993414	-1.177641	1.365367
C	1.993414	-1.177641	-1.365367
N	-1.792384	-0.352576	0.000000
Mo	2.048738	0.265799	0.000000
H	5.079691	0.535818	0.000000
C	-2.861648	0.607559	0.000000
C	4.210234	1.167625	0.000000
C	-3.408261	1.048865	1.196776
C	-3.408261	1.048865	-1.196776
H	3.822044	1.500014	2.167680
Si	-0.149647	0.069504	0.000000
H	3.822044	1.500014	-2.167680
C	3.559644	1.695969	1.143272
C	3.559644	1.695969	-1.143272
C	-4.505333	1.887993	1.194715
C	-4.505333	1.887993	-1.194715
H	-4.932598	2.216802	2.131534
H	-4.932598	2.216802	-2.131534
C	-5.060811	2.301936	0.000000
C	2.514347	2.520607	0.707818
C	2.514347	2.520607	-0.707818
H	1.827483	3.061696	1.335735
H	1.827483	3.061696	-1.335735
H	-5.924204	2.952231	0.000000
H	-2.979032	0.706380	2.127643
H	-2.979032	0.706380	-2.127643

[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ph)] (**II**)

H	-3.558846	-3.463259	1.568789
H	-0.943060	-4.059466	0.000000
H	-3.558846	-3.463259	-1.568789
H	-2.792094	-2.133869	2.428487

C	-3.310804	-2.402763	1.508030
C	-0.708836	-2.994198	0.000000
H	-0.101147	-2.799935	0.882417
H	-4.252272	-1.852928	1.484325
C	-3.310804	-2.402763	-1.508030
H	-0.101147	-2.799935	-0.882417
H	-2.792094	-2.133869	-2.428487
Si	-2.293338	-2.047177	0.000000
H	-4.252272	-1.852928	-1.484325
O	1.770622	-1.842547	2.216953
O	1.770622	-1.842547	-2.216953
C	1.850286	-1.038516	1.381662
C	1.850286	-1.038516	-1.381662
N	-1.912246	-0.316275	0.000000
Mo	2.093953	0.354041	0.000000
H	5.068388	-0.215408	0.000000
C	-3.064891	0.531364	0.000000
C	4.402825	0.628436	0.000000
C	-3.662503	0.912439	1.195251
C	-3.662503	0.912439	-1.195251
H	4.115497	1.053726	2.168066
Ge	-0.211539	0.350939	0.000000
H	4.115497	1.053726	-2.168066
C	3.920993	1.316381	1.143534
C	3.920993	1.316381	-1.143534
C	-4.847688	1.623341	1.193762
C	-4.847688	1.623341	-1.193762
H	-5.310136	1.896875	2.131926
H	-5.310136	1.896875	-2.131926
C	-5.448162	1.972534	0.000000
C	3.140316	2.396137	0.708212
C	3.140316	2.396137	-0.708212
H	2.625135	3.103630	1.335761
H	2.625135	3.103630	-1.335761
H	-6.383323	2.514436	0.000000
H	-3.201606	0.618263	2.127882
H	-3.201606	0.618263	-2.127882

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SnN(SiMe_3)(Ph)]$ (**III**)

H	-3.453989	-3.644033	1.600709
H	-0.783714	-3.985859	0.000000
H	-3.453989	-3.644033	-1.600709
H	-2.783062	-2.241861	2.425689
C	-3.296390	-2.568433	1.520227
C	-0.660224	-2.902355	0.000000
H	-0.072763	-2.653034	0.882862
H	-4.278748	-2.094641	1.510169
C	-3.296390	-2.568433	-1.520227
H	-0.072763	-2.653034	-0.882862
H	-2.783062	-2.241861	-2.425689
Si	-2.335102	-2.118902	0.000000

H	-4.278748	-2.094641	-1.510169
O	1.780180	-1.761640	2.243396
O	1.780180	-1.761640	-2.243396
C	1.869150	-0.970755	1.394297
C	1.869150	-0.970755	-1.394297
N	-2.135152	-0.377105	0.000000
Mo	2.233704	0.377445	0.000000
H	5.062387	-0.679731	0.000000
C	-3.330265	0.390713	0.000000
C	4.546482	0.262950	0.000000
C	-3.940574	0.757827	1.194427
C	-3.940574	0.757827	-1.194427
H	4.334886	0.733526	2.166872
Sn	-0.309678	0.507094	0.000000
H	4.334886	0.733526	-2.166872
C	4.185091	1.023430	1.142049
C	4.185091	1.023430	-1.142049
C	-5.135879	1.448358	1.192589
C	-5.135879	1.448358	-1.192589
H	-5.597332	1.722889	2.130677
H	-5.597332	1.722889	-2.130677
C	-5.739523	1.792357	0.000000
C	3.597265	2.219923	0.707923
C	3.597265	2.219923	-0.707923
H	3.215228	3.004896	1.338610
H	3.215228	3.004896	-1.338610
H	-6.674798	2.333448	0.000000
H	-3.467128	0.482124	2.126843
H	-3.467128	0.482124	-2.126843

[(η^5-C_5H_5)$(CO)_2$Mo≡PbN($SiMe_3$)(Ph)] (**IV**)

H	-3.495517	-3.708293	1.556948
H	-0.803018	-3.983567	0.000000
H	-3.495517	-3.708293	-1.556948
H	-2.850379	-2.323819	2.429969
C	-3.348501	-2.628611	1.508628
C	-0.693940	-2.898185	0.000000
H	-0.109034	-2.642588	0.884340
H	-4.337675	-2.168644	1.501056
C	-3.348501	-2.628611	-1.508628
H	-0.109034	-2.642588	-0.884340
H	-2.850379	-2.323819	-2.429969
Si	-2.385944	-2.134775	0.000000
H	-4.337675	-2.168644	-1.501056
O	1.814499	-1.870939	2.234889
O	1.814499	-1.870939	-2.234889
C	1.923364	-1.074399	1.392243
C	1.923364	-1.074399	-1.392243
N	-2.218058	-0.392868	0.000000
Mo	2.306501	0.281075	0.000000
H	5.143802	-0.737078	0.000000

C	-3.423619	0.345202	0.000000
C	4.607647	0.194346	0.000000
C	-4.061808	0.673411	1.194347
C	-4.061808	0.673411	-1.194347
H	4.385312	0.662309	2.168070
Pb	-0.275231	0.492589	0.000000
H	4.385312	0.662309	-2.168070
C	4.234730	0.949426	1.142588
C	4.234730	0.949426	-1.142588
C	-5.310112	1.253295	1.192665
C	-5.310112	1.253295	-1.192665
H	-5.799975	1.477444	2.131324
H	-5.799975	1.477444	-2.131324
C	-5.947530	1.536964	0.000000
C	3.624843	2.133755	0.707921
C	3.624843	2.133755	-0.707921
H	3.226039	2.911103	1.337317
H	3.226039	2.911103	-1.337317
H	-6.935159	1.976216	0.000000
H	-3.578494	0.422232	2.128037
H	-3.578494	0.422232	-2.128037

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}SiN(SiMe_3)(Ph)]$ (**V**)

H	-3.624570	-3.347652	1.533221
H	-1.034638	-4.072773	0.000000
H	-3.624570	-3.347652	-1.533221
H	-2.785494	-2.089476	2.432048
C	-3.307347	-2.304011	1.499644
C	-0.732205	-3.024074	0.000000
H	-0.115056	-2.865597	0.883070
H	-4.213285	-1.697108	1.475647
C	-3.307347	-2.304011	-1.499644
H	-0.115056	-2.865597	-0.883070
H	-2.785494	-2.089476	-2.432048
Si	-2.262984	-2.003311	0.000000
H	-4.213285	-1.697108	-1.475647
O	1.777494	-1.903465	2.192564
O	1.777494	-1.903465	-2.192564
C	1.874390	-1.087368	1.366756
C	1.874390	-1.087368	-1.366756
N	-1.799194	-0.269875	0.000000
W	2.052624	0.321954	0.000000
H	5.085781	0.208909	0.000000
C	-2.930179	0.618580	0.000000
C	4.299461	0.939984	0.000000
C	-3.521176	1.003376	1.195340
C	-3.521176	1.003376	-1.195340
H	3.944236	1.317582	2.169702
Si	-0.171513	0.207721	0.000000
H	3.944236	1.317582	-2.169702
C	3.710464	1.541645	1.144605

C	3.710464	1.541645	-1.144605
C	-4.707028	1.714446	1.193141
C	-4.707028	1.714446	-1.193141
H	-5.171480	1.985885	2.130870
H	-5.171480	1.985885	-2.130870
C	-5.310906	2.056663	0.000000
C	2.769446	2.488724	0.708254
C	2.769446	2.488724	-0.708254
H	2.144968	3.100014	1.336195
H	2.144968	3.100014	-1.336195
H	-6.253308	2.586734	0.000000
H	-3.063441	0.704725	2.127862
H	-3.063441	0.704725	-2.127862

$[(\eta^5\text{-}C_5H_5)(CO)_2W{\equiv}GeN(SiMe_3)(Ph)]$ (**VI**)

H	-3.592302	-3.439072	1.561594
H	-0.966255	-4.032463	0.000000
H	-3.592302	-3.439072	-1.561594
H	-2.831377	-2.111853	2.429177
C	-3.344399	-2.378120	1.504966
C	-0.736747	-2.966101	0.000000
H	-0.128953	-2.768914	0.882451
H	-4.286632	-1.829616	1.477381
C	-3.344399	-2.378120	-1.504966
H	-0.128953	-2.768914	-0.882451
H	-2.831377	-2.111853	-2.429177
Si	-2.323337	-2.023453	0.000000
H	-4.286632	-1.829616	-1.477381
O	1.824943	-1.851504	2.217016
O	1.824943	-1.851504	-2.217016
C	1.892208	-1.047103	1.377183
C	1.892208	-1.047103	-1.377183
N	-1.928739	-0.292970	0.000000
W	2.100204	0.341912	0.000000
H	5.097648	-0.097307	0.000000
C	-3.071901	0.565032	0.000000
C	4.391662	0.711448	0.000000
C	-3.672658	0.941237	1.195815
C	-3.672658	0.941237	-1.195815
H	4.077277	1.125733	2.170146
Ge	-0.207792	0.298129	0.000000
H	4.077277	1.125733	-2.170146
C	3.870600	1.373765	1.144718
C	3.870600	1.373765	-1.144718
C	-4.862273	1.642355	1.194116
C	-4.862273	1.642355	-1.194116
H	-5.332470	1.905481	2.131227
H	-5.332470	1.905481	-2.131227
C	-5.465070	1.985978	0.000000
C	3.033053	2.414577	0.708238
C	3.033053	2.414577	-0.708238

H	2.477041	3.088507	1.337106
H	2.477041	3.088507	-1.337106
H	-6.407529	2.514803	0.000000
H	-3.211884	0.645947	2.127931
H	-3.211884	0.645947	-2.127931

[(η^5-C_5H_5)(CO)$_2$W≡SnN(SiMe$_3$)(Ph)] (**VII**)

H	-3.493218	-3.602516	1.595641
H	-0.826460	-3.955132	0.000000
H	-3.493218	-3.602516	-1.595641
H	-2.801805	-2.213309	2.425022
C	-3.324533	-2.528119	1.520788
C	-0.693133	-2.872545	0.000000
H	-0.101276	-2.630505	0.882813
H	-4.301445	-2.043243	1.519791
C	-3.324533	-2.528119	-1.520788
H	-0.101276	-2.630505	-0.882813
H	-2.801805	-2.213309	-2.425022
Si	-2.365064	-2.082483	0.000000
H	-4.301445	-2.043243	-1.519791
O	1.847749	-1.818841	2.216372
O	1.847749	-1.818841	-2.216372
C	1.928707	-1.011481	1.376998
C	1.928707	-1.011481	-1.376998
N	-2.153085	-0.341506	0.000000
W	2.240261	0.354292	0.000000
H	5.131773	-0.495722	0.000000
C	-3.336116	0.442159	0.000000
C	4.542197	0.401355	0.000000
C	-3.945813	0.809426	1.197079
C	-3.945813	0.809426	-1.197079
H	4.297244	0.859159	2.170396
Sn	-0.292091	0.444400	0.000000
H	4.297244	0.859159	-2.170396
C	4.122887	1.133437	1.145384
C	4.122887	1.133437	-1.145384
C	-5.141317	1.498871	1.194881
C	-5.141317	1.498871	-1.194881
H	-5.605594	1.771973	2.132199
H	-5.605594	1.771973	-2.132199
C	-5.744482	1.841923	0.000000
C	3.442366	2.284309	0.708800
C	3.442366	2.284309	-0.708800
H	2.998463	3.035967	1.338663
H	2.998463	3.035967	-1.338663
H	-6.680982	2.380752	0.000000
H	-3.472510	0.531555	2.128861
H	-3.472510	0.531555	-2.128861

[(η^5-C_5H_5)(CO)$_2$W≡PbN(SiMe$_3$)(Ph)] (**VIII**)

H	-3.514640	-3.692152	1.575380

H	-0.849931	-3.979147	0.000000
H	-3.514640	-3.692152	-1.575380
H	-2.864927	-2.295587	2.426178
C	-3.372001	-2.612797	1.513970
C	-0.732706	-2.894669	0.000000
H	-0.143647	-2.645863	0.883337
H	-4.361453	-2.153782	1.511355
C	-3.372001	-2.612797	-1.513970
H	-0.143647	-2.645863	-0.883337
H	-2.864927	-2.295587	-2.426178
Si	-2.418580	-2.128051	0.000000
H	-4.361453	-2.153782	-1.511355
O	1.876268	-1.868498	2.218088
O	1.876268	-1.868498	-2.218088
C	1.974125	-1.063738	1.378945
C	1.974125	-1.063738	-1.378945
N	-2.244122	-0.388580	0.000000
W	2.305162	0.302903	0.000000
H	5.206626	-0.496736	0.000000
C	-3.430948	0.378910	0.000000
C	4.595662	0.385440	0.000000
C	-4.051995	0.736828	1.195671
C	-4.051995	0.736828	-1.195671
H	4.340930	0.839773	2.170235
Pb	-0.278941	0.431332	0.000000
H	4.340930	0.839773	-2.170235
C	4.162097	1.110281	1.145215
C	4.162097	1.110281	-1.145215
C	-5.265249	1.395624	1.194305
C	-5.265249	1.395624	-1.194305
H	-5.738404	1.652713	2.131980
H	-5.738404	1.652713	-2.131980
C	-5.878918	1.721158	0.000000
C	3.459454	2.247238	0.708937
C	3.459454	2.247238	-0.708937
H	3.003684	2.991503	1.338996
H	3.003684	2.991503	-1.338996
H	-6.832092	2.230433	0.000000
H	-3.576044	0.465938	2.127984
H	-3.576044	0.465938	-2.127984

$[(\eta^5\text{-}C_5H_5)(CO)_2Mo{\equiv}SiN(SiMe_3)(Mes)]$ (**IX**)

H	-2.912581	-3.859441	1.361963
H	-0.255091	-4.151674	0.000000
H	-2.912581	-3.859441	-1.361963
H	-2.125972	-2.702435	2.419904
C	-2.678005	-2.800631	1.485749
C	-0.067421	-3.076385	0.000000
H	0.528749	-2.856989	0.882820
H	-3.625931	-2.272005	1.589841
C	-2.678005	-2.800631	-1.485749

H	0.528749	-2.856989	-0.882820
H	-2.125972	-2.702435	-2.419904
Si	-1.714036	-2.244593	0.000000
H	-3.625931	-2.272005	-1.589841
O	2.092665	-1.656400	2.289873
O	2.092665	-1.656400	-2.289873
C	2.156689	-0.896768	1.411567
C	2.156689	-0.896768	-1.411567
N	-1.514986	-0.474005	0.000000
Mo	2.433433	0.445779	0.000000
H	5.339929	-0.397960	0.000000
C	-2.772133	0.237262	0.000000
C	4.758610	0.506277	0.000000
C	-3.401880	0.551228	1.209069
C	-3.401880	0.551228	-1.209069
H	4.515330	0.960240	2.166818
Ge	0.102744	0.395833	0.000000
H	4.515330	0.960240	-2.166818
C	4.347009	1.240388	1.142142
C	4.347009	1.240388	-1.142142
C	-4.681513	1.079191	1.179450
C	-4.681513	1.079191	-1.179450
H	-5.167086	1.305156	2.122215
H	-5.167086	1.305156	-2.122215
C	-5.353931	1.336077	0.000000
C	3.670662	2.389345	0.707956
C	3.670662	2.389345	-0.707956
H	3.232139	3.143875	1.338791
H	3.232139	3.143875	-1.338791
C	-6.715303	1.936356	0.000000
H	-7.287555	1.646793	-0.878810
H	-7.287555	1.646793	0.878810
H	-6.666714	3.026093	0.000000
C	-2.709326	0.392277	2.515064
H	-2.292799	-0.599608	2.656589
H	-1.874293	1.090386	2.596837
H	-3.384683	0.600438	3.341263
C	-2.709326	0.392277	-2.515064
H	-1.874293	1.090386	-2.596837
H	-2.292799	-0.599608	-2.656589
H	-3.384683	0.600438	-3.341263

[(η^5-C_5H_5)$(CO)_2$Mo≡GeN($SiMe_3$)(Ar*)] (**X**)

C	3.469873	-0.278758	-5.051780
C	2.111768	-0.328217	-4.794833
C	4.364420	-0.431263	-4.011445
C	-2.949604	-4.170108	-2.919918
C	-3.491331	-2.879160	-3.018515
C	1.659465	-0.511072	-3.505069
C	3.907935	-0.622153	-2.722992
C	-3.637130	-4.858272	-1.888811

C	-4.523034	-2.757367	-2.058624
C	2.550680	-0.649374	-2.452349
C	-4.611694	-3.973394	-1.366266
C	-3.298886	2.306691	-1.473689
C	3.196442	4.079830	-0.848637
C	-0.684578	-3.945202	-0.743001
C	-4.490355	1.990045	-0.853806
C	2.441552	1.704483	-0.950202
C	-2.144031	2.463340	-0.731365
C	2.015130	-0.724523	-1.047564
C	2.249284	2.988211	-0.502468
C	1.628105	0.647297	-0.573743
C	3.088781	-2.808352	-0.243661
C	2.953951	-1.434004	-0.111572
C	1.147363	3.223069	0.301611
C	-4.522674	1.833331	0.519311
C	0.553101	0.884834	0.291721
C	-2.166065	2.313276	0.646049
C	3.929632	-3.521544	0.579874
C	-2.690274	-3.538177	1.057884
C	0.301676	2.208194	0.693258
C	3.709924	-0.783793	0.850029
C	-3.369953	1.996986	1.258857
C	4.665226	-2.865312	1.547748
C	-0.935364	2.502856	1.493525
C	4.559083	-1.497421	1.674547
C	-1.305034	5.003321	1.610987
C	-0.892134	3.823591	2.206438
C	-1.125324	6.212311	2.252594
C	0.518886	-2.409172	2.584438
C	-0.546672	6.262208	3.504528
C	-0.338256	3.884317	3.475290
C	-0.160971	5.088726	4.121429
C	-1.566464	-0.451306	3.502605
C	1.354918	0.466534	3.259835
H	3.827512	-0.129492	-6.060097
H	1.403544	-0.218829	-5.603185
H	5.427145	-0.406021	-4.203250
H	-2.159253	-4.570020	-3.528955
H	-3.179391	-2.111013	-3.704953
H	0.595390	-0.531924	-3.301075
H	-3.486625	-5.881423	-1.597519
H	-3.263509	2.436732	-2.545584
H	4.614947	-0.745463	-1.913432
H	-5.124769	-1.881751	-1.889323
H	3.886970	3.778693	-1.631130
H	2.677726	4.974471	-1.185902
H	3.280569	1.499537	-1.604261
H	-5.392233	1.875669	-1.437049
H	-5.306521	-4.197361	-0.577143
H	-1.213168	2.705133	-1.227452
H	3.790802	4.372830	0.016064

H	2.509682	-3.320229	-0.998364
H	1.111806	-1.333205	-1.092997
H	0.950728	4.230437	0.643006
H	4.004371	-4.593065	0.470622
H	-5.449238	1.589359	1.016666
H	-1.747613	4.976160	0.624289
H	3.630441	0.288166	0.963515
H	-1.433009	7.126272	1.766019
H	5.322209	-3.421702	2.200089
H	-0.248572	-3.039829	2.134236
H	5.138679	-0.976293	2.422597
H	-3.397249	1.886177	2.335029
H	1.449607	-2.575660	2.043821
H	-0.999848	1.748658	2.271062
H	-2.378477	-0.979946	3.000130
H	2.313681	0.272844	2.781636
H	-0.401373	7.210710	4.000793
H	-0.027575	2.968971	3.959885
H	0.656753	-2.756509	3.608830
H	1.142371	1.526844	3.140930
H	-1.884509	0.579990	3.651578
H	0.284055	5.113105	5.105058
H	-1.460328	-0.898831	4.491442
H	1.468298	0.264603	4.325911
N	-0.229654	-0.178132	0.851147
Si	0.034408	-0.626565	2.561245
Ge	-1.436927	-1.184296	-0.125455
Mo	-2.468264	-3.115526	-0.872304
O	0.320082	-4.511498	-0.722805
O	-2.877104	-3.829781	2.158601