Supplementary Information

Structural and spin diversity of M(indenyl)$_2$ transition-metal complexes: A DFT Investigation

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Figure S1. The π MO diagram of the indenylide anion $C_9H_7^-$

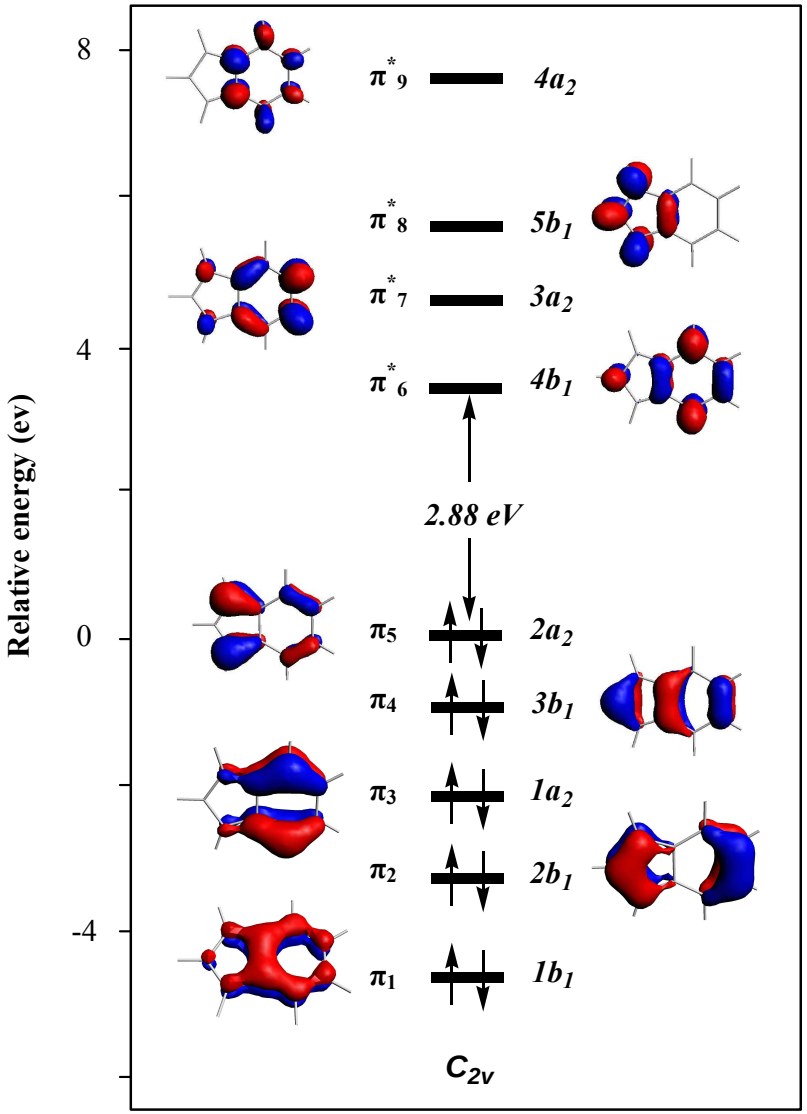

Table S1. Selected bond distances (in Å) for the $[Sc(Ind)_2]^+$ isomers of lowest energy.

TNE = 20		
Isomer	$[Sc(\eta^{5+2}\text{-Ind})_2]^+$	$[Sc(\eta^9\text{-Ind})(\eta^5\text{-Ind})]^+$
Spin state and symmetry	S = 0 *(C_1)*	S = 0 *(C_s)*
Sc-C(1)	2.501	2.438
Sc-C(2)	2.538	2.442
Sc-C(3)	2.544	2.438
Sc-C(4)	2.963	-
Sc-C(5)	-	-
Sc-C(6)	-	-
Sc-C(7)	2.921	-
Sc-C(8)	2.492	2.500
Sc-C(9)	2.512	2.500
Sc-C'(1)	2.529	2.611
Sc-C'(2)	2.544	2.759
Sc-C'(3)	2.562	2.611
Sc-C'(4)	2.961	2.733
Sc-C'(5)	-	2.980
Sc-C'(6)	-	2.980
Sc-C'(7)	2.943	2.733
Sc-C'(8)	2.478	2.322
Sc-C'(9)	2.482	2.322

Table S2. Selected bond distances (in Å) for the $Sc(Ind)_2$ isomers of lowest energy.

TNE = 21		
Isomer	$Sc(\eta^{5+2}\text{-Ind})_2$	$Sc(\eta^{9}\text{-Ind})(\eta^{5}\text{-Ind})$
Spin state and symmetry	S = 1/2 *(C_1)*	S = 1/2 *(C_s)*
Sc-C(1)	2.536	2.497
Sc-C(2)	2.556	2.474
Sc-C(3)	2.563	2.497
Sc-C(4)	3.003	-
Sc-C(5)	-	-
Sc-C(6)	-	-
Sc-C(7)	2.991	-
Sc-C(8)	2.632	2.581
Sc-C(9)	2.598	2.581
Sc-C'(1)	2.541	2.809
Sc-C'(2)	2.570	2.911
Sc-C'(3)	2.573	2.809
Sc-C'(4)	2.986	2.522
Sc-C'(5)	-	2.656
Sc-C'(6)	-	2.656
Sc-C'(7)	3.001	2.522
Sc-C'(8)	2.522	2.325
Sc-C'(9)	2.534	2.325

Table S3. Selected bond distances (in Å) for the $[Y(Ind)_2]^+$ isomers of lowest energy.

TNE = 20		
Isomer	$[Y(\eta^{5+2}\text{-Ind})_2]^+$	$[Y(\eta^9\text{-Ind})(\eta^5\text{-Ind})]^{++}$
Spin state and symmetry	S = 0 *(C_1)*	S = 0 *(C_s)*
Y-C(1)	2.690	2.622
Y-C(2)	2.810	2.646
Y-C(3)	2.720	2.622
Y-C(4)	3.014	-
Y-C(5)	-	-
Y-C(6)	-	-
Y-C(7)	2.931	-
Y-C(8)	2.475	2.645
Y-C(9)	2.502	2.645
Y-C'(1)	2.709	2.770
Y-C'(2)	2.794	2.913
Y-C'(3)	2.662	2.770
Y-C'(4)	2.961	2.890
Y-C'(5)	-	3.031
Y-C'(6)	-	3.031
Y-C'(7)	3.048	2.890
Y-C'(8)	2.506	2.493
Y-C'(9)	2.480	2.493

Table S4. Selected bond distances (in Å) for the Y(Ind)$_2$ isomers of lowest energy.

TNE = 21		
Isomer	Y(η^{5+2}-Ind)$_2$	Y(η^9-Ind)(η^5-Ind)
Spin state and symmetry	S = 1/2 *(C_1)*	S = 1/2 *(C_s)*
Y-C(1)	2.684	2.691
Y-C(2)	2.811	2.675
Y-C(3)	2.725	2.691
Y-C(4)	3.102	-
Y-C(5)	-	-
Y-C(6)	-	-
Y-C(7)	3.089	-
Y-C(8)	2.513	2.761
Y-C(9)	2.524	2.761
Y-C'(1)	2.712	2.878
Y-C'(2)	2.777	2.975
Y-C'(3)	2.684	2.875
Y-C'(4)	3.089	2.831
Y-C'(5)	-	2.840
Y-C'(6)	-	2.840
Y-C'(7)	3.111	2.831
Y-C'(8)	2.599	2.462
Y-C'(9)	2.589	2.462

Table S5. Selected bond distances (in Å) for the $Ti(Ind)_2$ isomers of lowest energy.

TNE = 22						
Isomer	Ti(η^9-Ind)(η^5-Ind)	Ti(η^9-Ind)(η^6-Ind)	Ti(η^5-Ind)$_2$	Ti(η^5-Ind)(η^6Ind)	Ti(η^5-Ind)(η^6-Ind)	Ti(η^5-Ind)$_2$
Spin state and Symmetry	S = 0 *(C_1)*	S = 0 *(C_s)*	S = 0 *(C_{2v})*	S = 1 *(C_1)*	S = 1*(C_s)*	S = 1 *(C_{2v})*
Ti-C(1)	2.601	2.597	2.298	2.376	-	2.376
Ti-C(2)	2.806	2.824	2.225	2.376	-	2.356
Ti-C(3)	2.558	2.597	2.298	2.383	-	2.376
Ti-C(4)	-	2.369	-	-	2.446	-
Ti-C(5)	-	2.458	-	-	2.436	-
Ti-C(6)	-	2.458	-	-	2.436	-
Ti-C(7)	-	2.369	-	-	2.446	-
Ti-C(8)	2.191	2.196	2.500	2.434	2.438	2.475
Ti-C(9)	2.172	2.196	2.500	2.442	2.438	2.475
Ti-C'(1)	2.329	-	2.298	-	-	2.376
Ti-C'(2)	2.333	-	2.225	-	-	2.356
Ti-C'(3)	2.383	-	2.298	-	-	2.376
Ti-C'(4)	2.301	2.386	-	2.423	2.447	-
Ti-C'(5)	2.439	2.368	-	2.424	2.433	-
Ti-C'(6)	2.446	2.368	-	2.441	2.433	-
Ti-C'(7)	2.326	2.386	-	2.445	2.447	-
Ti-C'(8)	2.471	2.508	2.500	2.429	2.442	2.475
Ti-C'(9)	2.505	2.508	2.500	2.425	2.442	2.475

Table S6. Selected bond distances (in Å) for the $Zr(Ind)_2$ isomers of lowest energy.

TNE = 22						
Isomer	$Zr(\eta^9\text{-Ind})(\eta^5\text{-Ind})$	$Zr(\eta^9\text{-Ind})(\eta^6\text{-Ind})$	$Zr(\eta^5\text{-Ind})_2$	$Zr(\eta^5\text{-Ind})(\eta^6\text{Ind})$	$Zr(\eta^5\text{-Ind})(\eta^6\text{-Ind})$	$Zr(\eta^5\text{-Ind})_2$
Spin state and symmetry	S = 0 *(C_1)*	S = 0 *(C_s)*	S = 0 *(C_{2v})*	S = 1 *(C_1)*	S = 1*(C_s)*	S = 1 *(C_{2v})*
Zr-C(1)	2.501	2.683	2.442	2.542	2.530	2.526
Zr-C(2)	2.524	2.879	2.384	2.556	2.511	2.543
Zr-C(3)	2.555	2.683	2.442	2.556	2.530	2.526
Zr-C(4)	-	2.344	-	-	3.136	-
Zr-C(5)	-	2.614	-	-	4.131	-
Zr-C(6)	-	2.614	-	-	4.131	-
Zr-C(7)	-	2.344	-	-	3.131	-
Zr-C(8)	2.652	2.519	2.601	2.553	2.567	2.541
Zr-C(9)	2.621	2.519	2.601	2.542	2.567	2.541
Zr-C'(1)	2.672	-	2.442	-	-	2.526
Zr-C'(2)	2.860	-	2.384	-	-	2.543
Zr-C'(3)	2.640	-	2.442	-	-	2.526
Zr-C'(4)	2.428	2.651	-	2.555	2.576	-
Zr-C'(5)	2.570	2.681	-	2.584	2.571	-
Zr-C'(6)	2.586	2.681	-	2.611	2.571	-
Zr-C'(7)	2.465	2.651	-	2.588	2.576	-
Zr-C'(8)	2.310	2.680	2.601	2.532	2.572	2.541
Zr-C'(9)	2.322	2.680	2.601	2.532	2.572	2.541

Table S7. Selected bond distances (in Å) for the $V(Ind)_2$ isomers of lowest energy.

TNE = 23						
Isomer	$V(\eta^5\text{-Ind})_2$		$V(\eta^5\text{-Ind})(\eta^6\text{-Ind})$		$V(\eta^6\text{-Ind})_2$	
Spin state and symmetry	S = 1/2 *(C_{2v})*	S = 3/2 *(C_{2v})*	S = 1/2 *(C_s)*	S = 3/2 *(C_1)*	S = 1/2 *(C_{2h})*	S = 3/2 *(C_{2v})*
V-C(1)/V-C(4)	2.307	2.221	2.264	2.307	2.272	2.385
V-C(2)/V-C(5)	2.302	2.172	2.226	2.299	2.299	2.281
V-C(3)/V-C(6)	2.307	2.221	2.264	2.315	2.299	2.281
V-C(7)	-	-	-	-	2.272	2.385
V-C(8)	2.368	2.387	2.419	2.376	2.307	2.500
V-C(9)	2.368	2.387	2.419	2.364	2.307	2.500
V-C'(1)/V-C'(4)	2.307	2.221	2.285	2.373	2.272	2.385
V-C'(2)/V-C'(5)	2.302	2.172	2.277	2.314	2.299	2.281
V-C'(3)/V-C'(6)	2.307	2.221	2.277	2.315	2.299	2.281
V-C'(7)	-	-	2.285	2.365	2.272	2.385
V-C'(8)	2.368	2.387	2.275	2.432	2.307	2.500
V-C'(9)	2.368	2.387	2.275	2.436	2.307	2.500

Table S8. Selected bond distances (in Å) for the $Nb(Ind)_2$ isomers of lowest energy.

TNE = 23						
Isomer	$Nb(\eta^5\text{-Ind})_2$		$Nb(\eta^5\text{-Ind})(\eta^6\text{-Ind})$		$Nb(\eta^6\text{-Ind})_2$	
Spin state and Symmetry	S = 1/2 *(C_{2v})*	S = 3/2 *(C_{2v})*	S = 1/2 *(C_s)*	S = 3/2 *(C_1)*	S = 1/2 *(C_{2h})*	S = 3/2 *(C_{2v})*
Nb-C(1)/Nb-C(4)	2.307	2.221	2.422	2.446	2.432	2.510
Nb-C(2)/Nb-C(5)	2.302	2.172	2.403	2.450	2.434	2.438
Nb-C(3)/Nb-C(6)	2.307	2.221	2.422	2.446	2.434	2.425
Nb-C(7)	-	-	-	-	2.432	2.474
Nb-C(8)	2.368	2.387	2.538	2.507	2.481	2.546
Nb-C(9)	2.368	2.387	2.538	2.510	2.481	2.569
Nb-C’(1)/Nb-C’(4)	2.307	2.221	2.365	2.552	2.432	2.474
Nb-C’(2)/Nb-C’(5)	2.302	2.172	2.405	2.461	2.434	2.425
Nb-C’(3)/Nb-C’(6)	2.307	2.221	2.405	2.460	2.434	2.438
Nb-C’(7)	-	-	2.365	2.494	2.432	2.510
Nb-C’(8)	2.368	2.387	2.406	2.544	2.481	2.569
Nb-C’(9)	2.368	2.387	2.406	2.562	2.481	2.546

Table S9. Selected bond distances (in Å) for the $Cr(Ind)_2$ isomers of lowest energy.

TNE = 24				
Isomer	$Cr(\eta^5\text{-Ind})_2$		$Cr(\eta^5\text{-Ind})(\eta^6\text{-Ind})$	$Cr(\eta^6\text{-Ind})_2$
Spin state and symmetry	S = 1 (C_{2v})	S = 2 (C_{2v})	S = 1 (C_s)	S = 1 (C_{2h})
Cr-C(1)/Cr-C(4)	2.178	2.314	2.194	2.234
Cr-C(2)/Cr-C(5)	2.132	2.264	2.157	2.214
Cr-C(3)/Cr-C(6)	2.178	2.314	2.194	2.214
Cr-C(7)	-	-	-	2.234
Cr-C(8)	2.317	2.554	2.326	2.332
Cr-C(9)	2.317	2.554	2.326	2.332
Cr-C'(1)/Cr-C'(4)	2.178	2.314	2.211	2.234
Cr-C'(2)/Cr-C'(5)	2.132	2.264	2.196	2.214
Cr-C'(3)/Cr-C'(6)	2.178	2.314	2.196	2.214
Cr-C'(7)	-	-	2.211	2.234
Cr-C'(8)	2.317	2.554	2.319	2.332
Cr-C'(9)	2.317	2.554	2.319	2.332

Table S10. Selected bond distances (in Å) for the $Mo(Ind)_2$ isomers of lowest energy.

TNE = 24					
Isomer	$Mo(\eta^5\text{-Ind})_2$		$Mo(\eta^5\text{-Ind})(\eta^6\text{-Ind})$		$Mo(\eta^6\text{-Ind})_2$
Spin state and symmetry	S = 0 *(C_{2v})*	S = 1 *(C_{2v})*	S = 0 *(C_s)*	S = 1 *(C_s)*	S = 0 *(C_2)*
Mo-C(1)/Mo-C(4)	2.301	2.321	2.335	2.342	2.295
Mo-C(2)/Mo-C(5)	2.291	2.282	2.329	2.311	2.383
Mo-C(3)/Mo-C(6)	2.301	2.321	2.335	2.342	2.425
Mo-C(7)	-	-	-	-	2.399
Mo-C(8)	2.403	2.472	2.448	2.472	2.336
Mo-C(9)	2.403	2.472	2.446	2.472	2.215
Mo-C’(1)/Mo-C’(4)	2.301	2.321	2.329	2.352	2.399
Mo-C’(2)/Mo-C’(5)	2.291	2.282	2.359	2.311	2.425
Mo-C’(3)/Mo-C’(6)	2.301	2.321	2.359	2.311	2.383
Mo-C’(7)	-	-	2.329	2.352	2.295
Mo-C’(8)	2.403	2.472	2.373	2.447	2.215
Mo-C’(9)	2.403	2.472	2.373	2.447	2.336

Table S11. Selected bond distances (in Å) for the $M(Ind)_2$ (M = Mn, Re) isomers of lowest energy.

TNE = 25							
Isomer	$Mn(\eta^5\text{-Ind})_2$			$Mn(\eta^5\text{-Ind})(\eta^6\text{-Ind})$	$Re(\eta^5\text{-Ind})_2$	$Re(\eta^5\text{-Ind})(\eta^6\text{-Ind})$	$Re(\eta^6\text{-Ind})_2$
Spin state and symmetry	S = 5/2 (C_2)	S = 3/2 (C_{2h})	S = 1/2 (C_{2v})	S = 5/2 (C_s)	S = 1/2 (C_{2v})	S = 1/2 (C_s)	S = 1/2 (C_{2h})
M-C(1)/M-C(4)	2.261	2.191	2.128	2.389	2.248	2.261	2.303
M-C(2)/M-C(5)	2.304	2.112	2.088	2.281	2.249	2.271	2.285
M-C(3)/M-C(6)	2.562	2.191	2.128	2.389	2.248	2.261	2.285
M-C(7)	-	-	-	-	-	-	2.303
M-C(8)	2.563	2.517	2.262	2.600	2.319	2.336	2.348
M-C(9)	2.601	2.517	2.262	2.600	2.319	2.336	2.348
M-C'(1)/M-C'(4)	2.562	2.191	2.128	2.567	2.248	2.290	2.303
M-C'(2)/M-C'(5)	2.304	2.112	2.088	2.319	2.249	2.263	2.285
M-C'(3)/M-C'(6)	2.261	2.191	2.128	2.319	2.248	2.263	2.285
M-C'(7)	-	-	-	2.567	-	2.290	2.303
M-C'(8)	2.601	2.517	2.262	2.760	2.319	2.314	2.348
M-C'(9)	2.563	2.517	2.262	2.760	2.319	2.314	2.348

Table S12. Selected bond distances (in Å) for the $M(Ind)_2$ (M = Fe, Ru) isomers of lowest energy.

	$Fe(Ind)_2$			$Ru(Ind)_2$	
Isomer	$Fe(\eta^5\text{-Ind})_2$		$Fe(\eta^5\text{-Ind})(\eta^6\text{-Ind})$	$Ru(\eta^5\text{-Ind})_2$	$Ru(\eta^5\text{-Ind}\eta)(\eta^6\text{-Ind})$
Spin state and symmetry	S = 0 *(C_{2v})*	S = 1 *(C_{2v})*	S = 0 *(C_s)*	S = 0 *(C_{2v})*	S = 0 *(C_s)*
M-C(1)/M-C(4)	2.079	2.147	2.063	2.241	2.242
M-C(2)/M-C(5)	2.063	2.125	2.049	2.228	2.222
M-C(3)/M-C(6)	2.079	2.147	2.063	2.241	2.242
M-C(7)	-	-	-	-	-
M-C(8)	2.153	2.362	2.148	2.309	2.340
M-C(9)	2.153	2.362	2.148	2.309	2.340
M-C'(1)/M-C'(4)	2.079	2.147	2.143	2.241	2.320
M-C'(2)/M-C'(5)	2.063	2.125	2.309	2.228	2.213
M-C'(3)/M-C'(6)	2.079	2.147	2.309	2.241	2.213
M-C'(7)	2.153	2.362	2.143	-	2.320
M-C'(8)	2.153	2.362	2.368	2.309	2.524
M-C'(9)	2.153	2.362	2.368	2.309	2.524

Table S13. Selected bond distances (in Å) for the $M(Ind)_2$ (M = Co, Re) isomers of lowest energy.

	$Co(Ind)_2$		$Rh(Ind)_2$ S = 1/2	
Isomer	$Co(\eta^5\text{-Ind})_2$	$Co(\eta^5\text{-Ind})(\eta^6\text{-Ind})$	$Rh(\eta^5\text{-Ind})_2$	$Re(\eta^5\text{-Ind})(\eta^4\text{-Ind})$
Spin state and symmetry	S = 1/2 *(C_{2v})*	S = 1/2 *(C_1)*	S = 1/2 *(C_{2v})*	S = 1/2 *(C_s)*
M-C(1)/M-C(4)	2.104	2.095	2.263	2.259
M-C(2)/MC(5)	2.101	2.077	2.239	2.219
M-C(3)/M-C(6)	2.104	2.091	2.263	2.259
M-C(7)	-	-	-	-
M-C(8)	2.271	2.332	2.461	2.518
M-C(9)	2.271	2.340	2.461	2.518
M-C'(1)/M-C'(4)	2.104	2.214	2.263	2.398
M-C'(2)/M-C'(5)	2.101	2.123	2.239	2.229
M-C'(3)/M-C'(6)	2.104	2.135	2.263	2.229
M-C'(7)	-	2.286	-	2.398
M-C'(8)	2.271	2.399	2.461	2.746
M-C'(9)	2.271	2.334	2.461	2.746

Table S14. Selected bond distances (in Å) for the $M(Ind)_2$ (M = Ni, Pd) isomers of lowest energy.

	$Ni(Ind)_2$			$Pd(Ind)_2$	
Isomer	$Ni(\eta^3\text{-}Ind)_2$	$Ni(\eta^3\text{-}Ind)(\eta^4\text{-}Ind)$	$Ni(\eta^5\text{-}Ind)_2$	$Pd(\eta^3\text{-}Ind)_2$	$Pd(\eta^3\text{-}Ind)(\eta^4\text{-}Ind)$
Spin state and symmetry	S = 0 *(C_{2h})*	S = 0 *(C_s)*	S = 1 *(C_{2h})*	S = 0 *(C_{2h})*	S = 0 *(C_s)*
M-C(1)/M-C(4)	2.125	2.226	2.222	2.355	2.370
M-C(2)/M-C(5)	2.034	2.175	2.127	2.227	2.220
M-C(3)/M-C(6)	2.125	2.226	2.222	2.355	2.370
M-C(7)	-	-	-	-	-
M-C(8)	2.525	2.573	2.407	2.798	2.820
M-C(9)	2.525	2.573	2.407	2.798	2.820
M-C'(1)/M-C'(4)	2.125	2.468	2.222	2.355	2.787
M-C'(2)/M-C'(5)	2.034	2.133	2.127	2.227	2.295
M-C'(3)/M-C'(6)	2.125	2.133	2.222	2.355	2.295
M-C'(7)	-	2.468	-	-	2.787
M-C'(8)	2.525	2.780	2.407	2.798	3.247
M-C'(9)	2.525	2.780	2.407	2.798	3.247

Table S15.

The total bonding energies in (eV) and cartesian coordinates in (Å) are given for the $M(Ind)_2$ compounds (M = Sc-Ni, Y-Mo, Re, Ru-Pd) obtained from BP86 optimizations and the corresponding B3LYP single-point calculations.

Compounds for TNE = 20

$[Sc(\eta^{5+2}\text{-Ind})_2]^+$ (C_1) S = 0, E_T (BP86) = -201.866, E_T (B3LYP/BP86) = -237.556.

Atom	X	Y	Z
1.Sc	-0.013592	0.007260	-0.248662
2.C	2.359616	0.016877	-0.821264
3.C	2.074027	-1.213688	-0.098266
4.C	1.701141	-0.851679	1.242009
5.C	1.818175	0.561112	1.355432
6.C	2.171582	1.109109	0.100210
7.C	2.054508	-2.450046	-0.796716
8.C	2.340721	-2.457004	-2.153821
9.C	2.639857	-1.257656	-2.855487
10.C	2.646206	-0.030237	-2.212546
11.H	1.470125	-1.540118	2.049635
12.H	1.645438	1.131972	2.263767
13.H	2.340818	2.161815	-0.114332
14.H	1.848785	-3.380278	-0.266472
15.H	2.353495	-3.403284	-2.694621
16.H	2.876709	-1.310548	-3.917799
17.H	2.887859	0.882969	-2.757149
18.C	-2.373086	-0.020191	-0.801021
19.C	-2.089528	1.209717	-0.074884
20.C	-1.721853	0.845587	1.265884
21.C	-1.836247	-0.567308	1.375449
22.C	-2.187991	-1.113266	0.119165
23.C	-2.035722	2.442770	-0.777889
24.C	-2.284923	2.448681	-2.142752
25.C	-2.582400	1.250644	-2.847348
26.C	-2.623437	0.026201	-2.199479
27.H	-1.489944	1.532724	2.074251
28.H	-1.663378	-1.140725	2.282125
29.H	-2.354110	-2.165801	-0.098082
30.H	-1.828479	3.371958	-0.246308
31.H	-2.268626	3.392591	-2.687407
32.H	-2.788783	1.300887	-3.916068
33.H	-2.862392	-0.885614	-2.747704

$[Sc(\eta^{9}\text{-Ind})(\eta^{5}\text{-Ind})]^+$ (C_S) S = 0, E_T (BP86) =-201.751, E_T (B3LYP/BP86) = -237.367.

Atom	X	Y	Z
1.Sc	0.261035	0.434700	0.000000
2.C	-2.115319	0.158141	0.726874
3.C	-2.115319	0.158141	-0.726874
4.C	-1.630936	1.444453	-1.158875
5.C	-1.394132	2.230222	0.000000
6.C	-1.630936	1.444453	1.158875

7.C	-2.589252	-0.983318	-1.433775
8.C	-3.062197	-2.060979	-0.712294
9.C	-3.062197	-2.060979	0.712294
10.C	-2.589252	-0.983318	1.433775
11.H	-1.558901	1.789555	-2.188062
12.H	-1.065087	3.267282	0.000000
13.H	-1.558901	1.789555	2.188062
14.H	-2.619948	-0.982493	-2.523996
15.H	-3.464196	-2.925945	-1.240168
16.H	-3.464196	-2.925945	1.240168
17.H	-2.619948	-0.982493	2.523996
18.C	2.300890	-0.397222	0.735134
19.C	2.556175	0.817347	1.434276
20.C	2.694501	1.999083	0.715400
21.C	2.694501	1.999083	-0.715400
22.C	2.556175	0.817347	-1.434276
23.C	2.300890	-0.397222	-0.735134
24.C	1.533951	-1.528251	1.159281
25.C	1.080541	-2.200113	0.000000
26.C	1.533951	-1.528251	-1.159281
27.H	2.547030	0.835541	2.525699
28.H	2.824047	2.942619	-1.245125
29.H	2.547030	0.835541	-2.525699
30.H	2.824047	2.942619	1.245125
31.H	1.342801	-1.822841	2.187969
32.H	0.460035	-3.092898	0.000000
33.H	1.342801	-1.822841	-2.187969

$[Y(\eta^{5+2}\text{-Ind})_2]^+$ (C_1) S = 0, E_T (BP86) = -202.123, E_T (B3LYP/BP86) = -237.012.

Atom	X	Y	Z
1.Y	-0.001988	0.004306	-0.359281
2.C	2.561266	0.018474	-0.700031
3.C	2.209169	-1.280404	-0.144236
4.C	1.780675	-1.069000	1.211537
5.C	1.917600	0.315798	1.493331
6.C	2.346947	1.000204	0.330425
7.C	2.159945	-2.417036	-0.994356
8.C	2.472288	-2.267433	-2.339445
9.C	2.835489	-1.003320	-2.877673
10.C	2.878381	0.131557	-2.080237
11.H	1.507669	-1.842144	1.924157
12.H	1.717292	0.781548	2.455129
13.H	2.568576	2.062453	0.258884
14.H	1.909690	-3.398341	-0.589144
15.H	2.459107	-3.138238	-2.994857
16.H	3.095634	-0.930450	-3.933646
17.H	3.173724	1.093464	-2.501978
18.C	-2.560298	-0.021226	-0.695767
19.C	-2.213828	1.278762	-0.137590
20.C	-1.786160	1.067270	1.218059
21.C	-1.917405	-0.318246	1.498138
22.C	-2.343773	-1.003155	0.334214

23.C	-2.161867	2.415721	-0.986974
24.C	-2.464771	2.266040	-2.334271
25.C	-2.821236	1.001117	-2.875193
26.C	-2.868371	-0.133964	-2.077967
27.H	-1.516508	1.840913	1.931461
28.H	-1.715615	-0.784188	2.459567
29.H	-2.560889	-2.066276	0.261923
30.H	-1.916057	3.397263	-0.579397
31.H	-2.448842	3.137152	-2.989249
32.H	-3.074175	0.927705	-3.932888
33.H	-3.159884	-1.095583	-2.503253

$[Y(\eta^9\text{-Ind})(\eta^5\text{-Ind})]^+$ (C_S) S = 0, E_T (BP86) =-201.894, E_T (B3LYP/BP86) = -236.990.

Atom	X	Y	Z
1.Y	0.247792	0.406166	0.000000
2.C	-2.309218	0.224468	0.727579
3.C	-2.309218	0.224468	-0.727579
4.C	-1.825427	1.511318	-1.160623
5.C	-1.589920	2.294772	0.000000
6.C	-1.825427	1.511318	1.160623
7.C	-2.774465	-0.921768	-1.432384
8.C	-3.235046	-2.008178	-0.711327
9.C	-3.235046	-2.008178	0.711327
10.C	-2.774465	-0.921768	1.432384
11.H	-1.781754	1.866391	-2.188137
12.H	-1.277723	3.337487	0.000000
13.H	-1.781754	1.866391	2.188137
14.H	-2.810133	-0.922430	-2.522815
15.H	-3.626411	-2.877105	-1.240506
16.H	-3.626411	-2.877105	1.240506
17.H	-2.810133	-0.922430	2.522815
18.C	2.488494	-0.405567	0.736244
19.C	2.676427	0.820157	1.433392
20.C	2.731416	2.012388	0.716411
21.C	2.731416	2.012388	-0.716411
22.C	2.676427	0.820157	-1.433392
23.C	2.488494	-0.405567	-0.736244
24.C	1.836754	-1.602965	1.160746
25.C	1.450585	-2.315257	0.000000
26.C	1.836754	-1.602965	-1.160746
27.H	2.684650	0.836102	2.525298
28.H	2.814703	2.961126	-1.246182
29.H	2.684650	0.836102	-2.525298
30.H	2.814703	2.961126	1.246182
31.H	1.694429	-1.927220	2.188951
32.H	0.933941	-3.272514	0.000000
33.H	1.694429	-1.927220	-2.188951

Compounds for TNE = 21

$[Sc(\eta^{5+2}\text{-Ind})_2]$ (C_1) S = 1/2, E_T (BP86) = -206.825, E_T (B3LYP/BP86) = -242.355.

Atom	X	Y	Z
1.Sc	-0.004342	0.008688	-0.194103
2.C	2.387979	0.015041	-0.726753
3.C	2.082766	-1.289346	-0.165212
4.C	1.746606	-1.093676	1.215217
5.C	1.893087	0.287757	1.501209
6.C	2.247919	0.984986	0.322648
7.C	2.007759	-2.421455	-1.016870
8.C	2.304710	-2.271791	-2.369988
9.C	2.596466	-1.000154	-2.918023
10.C	2.606983	0.144671	-2.126082
11.H	1.488621	-1.871910	1.927375
12.H	1.727763	0.746604	2.472872
13.H	2.432117	2.052189	0.240349
14.H	1.761829	-3.400621	-0.604857
15.H	2.286431	-3.142761	-3.025486
16.H	2.798243	-0.915714	-3.986320
17.H	2.817066	1.122185	-2.561338
18.C	-2.390646	-0.020471	-0.721323
19.C	-2.092461	1.283127	-0.154447
20.C	-1.761027	1.085347	1.226657
21.C	-1.902801	-0.297288	1.507461
22.C	-2.247675	-0.992926	0.325023
23.C	-1.996042	2.414710	-1.005481
24.C	-2.278855	2.267030	-2.362481
25.C	-2.570751	0.997336	-2.914300
26.C	-2.591541	-0.148782	-2.123299
27.H	-1.508875	1.862611	1.942000
28.H	-1.738531	-0.758888	2.478119
29.H	-2.425200	-2.060909	0.238675
30.H	-1.748826	3.392257	-0.590441
31.H	-2.247554	3.138088	-3.017390
32.H	-2.757786	0.913224	-3.985403
33.H	-2.794967	-1.125992	-2.562397

[Sc(η^9-Ind)(η^5-Ind)] (C_S) S = 1/2, E_T (BP86) =-207.076, E_T (B3LYP/BP86) = -242.339.

Atom	X	Y	Z
1.Sc	0.331307	0.387579	0.000000
2.C	-2.141374	0.247304	0.726718
3.C	-2.141374	0.247304	-0.726718
4.C	-1.579334	1.495122	-1.164255
5.C	-1.287800	2.258461	0.000000
6.C	-1.579334	1.495122	1.164255
7.C	-2.670052	-0.872089	-1.427642
8.C	-3.195556	-1.931555	-0.711900
9.C	-3.195556	-1.931555	0.711900
10.C	-2.670052	-0.872089	1.427642
11.H	-1.488126	1.834078	-2.192421
12.H	-0.883779	3.268394	0.000000
13.H	-1.488126	1.834078	2.192421
14.H	-2.685215	-0.877146	-2.519146
15.H	-3.625027	-2.781887	-1.243445
16.H	-3.625027	-2.781887	1.243445
17.H	-2.685215	-0.877146	2.519146

18.C	2.380739	-0.432024	0.730724
19.C	2.351983	0.811361	1.448695
20.C	2.312008	2.007553	0.711001
21.C	2.312008	2.007553	-0.711001
22.C	2.351983	0.811361	-1.448695
23.C	2.380739	-0.432024	-0.730724
24.C	1.838945	-1.681951	1.154883
25.C	1.527180	-2.433659	0.000000
26.C	1.838945	-1.681951	-1.154883
27.H	2.324484	0.823194	2.537752
28.H	2.232570	2.959712	-1.235768
29.H	2.324484	0.823194	-2.537752
30.H	2.232570	2.959712	1.235768
31.H	1.690996	-1.993354	2.185945
32.H	1.100414	-3.434792	0.000000
33.H	1.690996	-1.993354	-2.185945

$Y(\eta^{5+2}\text{-Ind})_2$ (C_1) S = 0, E_T (BP86) = -207.117, E_T (B3LYP/BP86) = -241.687.

Atom	X	Y	Z
1.Y	0.119618	0.530292	-0.095796
2.C	1.190203	0.316744	2.251694
3.C	0.362860	-0.868384	2.081004
4.C	-1.008253	-0.452993	2.165942
5.C	-1.019892	0.941036	2.403098
6.C	0.309326	1.436547	2.423488
7.C	0.968084	-2.100374	1.705097
8.C	2.355602	-2.160930	1.570130
9.C	3.158656	-1.009385	1.728010
10.C	2.589035	0.232950	2.019122
11.H	-1.879351	-1.100909	2.113266
12.H	-1.915138	1.543106	2.545154
13.H	0.607183	2.463651	2.618008
14.H	0.355785	-2.992040	1.560046
15.H	2.828586	-3.109064	1.310838
16.H	4.237350	-1.086184	1.586441
17.H	3.214449	1.121493	2.120695
18.C	1.119354	-0.281576	-2.970391
19.C	0.364898	0.872252	-2.610364
20.C	-1.056975	0.744267	-2.326165
21.C	-1.666852	-0.539966	-2.377744
22.C	-0.918059	-1.633490	-2.838988
23.C	0.455211	-1.504777	-3.127780
24.C	-1.481882	1.964166	-1.702660
25.C	-0.358483	2.828009	-1.642187
26.C	0.778338	2.172780	-2.167328
27.H	2.189697	-0.199579	-3.164291
28.H	-2.723035	-0.654613	-2.129185
29.H	-1.394729	-2.610335	-2.928385
30.H	1.020006	-2.384136	-3.440357
31.H	-2.495442	2.208305	-1.395301
32.H	-0.369607	3.843497	-1.25123
33.H	1.775937	2.594047	-2.258879

Y(η^9-Ind)(η^5-Ind) (C_S) S = 0, E_T (BP86) =-207.187, E_T (B3LYP/BP86) = -241.671.

Atom	X	Y	Z
1.Y	0.374459	0.405127	0.000000
2.C	-2.283963	0.243668	0.727359
3.C	-2.283963	0.243668	-0.727359
4.C	-1.781764	1.516429	-1.164035
5.C	-1.523343	2.290677	0.000000
6.C	-1.781764	1.516429	1.164035
7.C	-2.764730	-0.897514	-1.427918
8.C	-3.242956	-1.980147	-0.711773
9.C	-3.242956	-1.980147	0.711773
10.C	-2.764730	-0.897514	1.427918
11.H	-1.723943	1.865085	-2.191883
12.H	-1.182165	3.324663	0.000000
13.H	-1.723943	1.865085	2.191883
14.H	-2.781669	-0.903797	-2.519462
15.H	-3.634290	-2.848534	-1.243648
16.H	-3.634290	-2.848534	1.243648
17.H	-2.781669	-0.903797	2.519462
18.C	2.561613	-0.468000	0.728358
19.C	2.609965	0.775462	1.454150
20.C	2.627482	1.973241	0.709466
21.C	2.627482	1.973241	-0.709466
22.C	2.609965	0.775462	-1.454150
23.C	2.561613	-0.468000	-0.728358
24.C	1.924331	-1.674960	1.155177
25.C	1.547701	-2.398691	0.000000
26.C	1.924331	-1.674960	-1.155177
27.H	2.613116	0.788014	2.543101
28.H	2.617051	2.931263	-1.232480
29.H	2.613116	0.788014	-2.543101
30.H	2.617051	2.931263	1.232480
31.H	1.765336	-1.980603	2.186299
32.H	1.042157	-3.362997	0.00000
33.H	1.765336	-1.980603	-2.186299

Compounds for TNE = 22

[Ti(η^9-Ind)(η^5-Ind)] (C_1) S = 0, E_T (BP86) = -208.692, E_T (B3LYP/BP86) = -244.142.

Atom	X	Y	Z
1.Ti	-0.129608	0.365946	-0.348916
2.C	1.107173	0.285065	1.788483
3.C	0.642178	-1.066028	1.555547
4.C	-0.796322	-1.017563	1.472552
5.C	-1.219903	0.319514	1.713682
6.C	-0.051335	1.136417	1.847338
7.C	1.581164	-2.125402	1.457146
8.C	2.930763	-1.848744	1.606412
9.C	3.388550	-0.523113	1.819702
10.C	2.501261	0.539324	1.889834

11.H	-1.449321	-1.874233	1.332820
12.H	-2.248092	0.654092	1.806894
13.H	-0.043780	2.205691	2.044517
14.H	1.239209	-3.149796	1.297854
15.H	3.657181	-2.661256	1.556551
16.H	4.458365	-0.340158	1.930730
17.H	2.861891	1.554374	2.066339
18.C	0.919143	-0.509701	-2.231342
19.C	0.446265	0.852531	-2.405973
20.C	-0.948992	1.179251	-2.188551
21.C	-1.899175	0.148733	-1.803966
22.C	-1.412195	-1.182673	-1.729619
23.C	-0.049561	-1.498349	-1.929688
24.C	-0.986518	2.460049	-1.541239
25.C	0.341526	2.925117	-1.398777
26.C	1.225478	1.950673	-1.904148
27.H	1.971354	-0.757674	-2.352519
28.H	-2.946601	0.387432	-1.635059
29.H	-2.078010	-1.972009	-1.380117
30.H	0.284204	-2.514230	-1.716026
31.H	-1.887893	2.973872	-1.218064
32.H	0.634921	3.871732	-0.947827
33.H	2.311606	1.989749	-1.888822

[Ti(η^9-Ind)(η^5-Ind)] (C_1) S = 1, E_T (BP86) = -208.552, E_T (B3LYP/BP86) = -243.939

Atom	X	Y	Z
1.Ti	-0.101619	0.026447	-0.175477
2.C	1.112247	0.211898	1.926582
3.C	0.638454	-1.158696	1.827762
4.C	-0.798150	-1.116239	1.795947
5.C	-1.195879	0.244648	1.922171
6.C	-0.040995	1.073942	1.955742
7.C	1.575230	-2.221341	1.722618
8.C	2.930418	-1.933473	1.769431
9.C	3.393995	-0.595257	1.869146
10.C	2.509827	0.470966	1.922825
11.H	-1.463040	-1.975102	1.754085
12.H	-2.223496	0.596579	1.969077
13.H	-0.032366	2.155188	2.061675
14.H	1.226828	-3.252609	1.642252
15.H	3.657077	-2.745497	1.718907
16.H	4.467862	-0.405409	1.895403
17.H	2.877396	1.496424	1.992196
18.C	0.903093	-0.318375	-2.377788
19.C	0.483136	1.040559	-2.304302
20.C	-0.935147	1.348318	-2.030191
21.C	-1.853489	0.279087	-1.829801
22.C	-1.401680	-1.053683	-1.912876
23.C	-0.034694	-1.349114	-2.191364
24.C	-1.050901	2.763916	-1.966548

25.C	0.225239	3.310423	-2.188947
26.C	1.171618	2.278264	-2.372209
27.H	1.948902	-0.564885	-2.567910
28.H	-2.901862	0.483693	-1.608687
29.H	-2.101599	-1.871621	-1.745196
30.H	0.290660	-2.388100	-2.232001
31.H	-1.966816	3.319904	-1.780882
32.H	0.455229	4.374174	-2.195033
33.H	2.236662	2.404370	-2.552378

[Ti(η^9-Ind)(η^6-Ind)] (C_S) S = 0, E_T (BP86) = -207.762, E_T (B3LYP/BP86) = -243.579.

Atom	X	Y	Z
1.Ti	0.117847	0.364846	0.000000
2.C	2.133207	0.851085	0.725102
3.C	2.133207	0.851085	-0.725102
4.C	1.836079	-0.358866	-1.461044
5.C	1.537637	-1.511626	-0.710667
6.C	1.537637	-1.511626	0.710667
7.C	1.836079	-0.358866	1.461044
8.C	1.637717	2.129049	-1.150343
9.C	1.362876	2.899824	0.000000
10.C	1.637717	2.129049	1.150343
11.H	1.794738	-0.356855	-2.547921
12.H	1.178199	-2.404432	-1.220808
13.H	1.178199	-2.404432	1.220808
14.H	1.794738	-0.356855	2.547921
15.H	1.484458	2.430190	-2.183288
16.H	0.969468	3.914995	0.000000
17.H	1.484458	2.430190	2.183288
18.C	-1.936223	1.304212	0.710328
19.C	-1.759254	0.110067	1.451412
20.C	-1.754123	-1.130801	0.741275
21.C	-1.754123	-1.130801	-0.741275
22.C	-1.759254	0.110067	-1.451412
23.C	-1.936223	1.304212	-0.710328
24.C	-1.764022	-2.483319	-1.159029
25.C	-1.801019	-3.285927	0.000000
26.C	-1.764022	-2.483319	1.159029
27.H	-1.984981	2.256933	1.237886
28.H	-1.984981	2.256933	-1.237886
29.H	-1.767994	0.133206	-2.540251
30.H	-1.767994	0.133206	2.540251
31.H	-1.779381	-2.831968	-2.189113
32.H	-1.852568	-4.373984	0.000000
33.H	-1.779381	-2.831968	2.189113

[Ti(η^9-Ind)(η^6-Ind)] (C_S) S = 1, E_T (BP86) = -207.763, E_T (B3LYP/BP86) = -243.945.

Atom	X	Y	Z
1.Ti	-0.012373	-0.053862	0.000000

2.C	2.009307	1.085822	0.739852
3.C	2.009307	1.085822	-0.739852
4.C	1.964498	-0.154377	-1.436384
5.C	1.915550	-1.360234	-0.713761
6.C	1.915550	-1.360234	0.713761
7.C	1.964498	-0.154377	1.436384
8.C	2.014850	2.443017	-1.156639
9.C	2.038506	3.247855	0.000000
10.C	2.014850	2.443017	1.156639
11.H	1.955366	-0.173179	-2.527393
12.H	1.856244	-2.309087	-1.245572
13.H	1.856244	-2.309087	1.245572
14.H	1.955366	-0.173179	2.527393
15.H	2.016843	2.792468	-2.186362
16.H	2.054716	4.336383	0.000000
17.H	2.016843	2.792468	2.186362
18.C	-1.939242	1.249320	0.713870
19.C	-1.990985	0.043437	1.436387
20.C	-2.039749	-1.196698	0.740034
21.C	-2.039749	-1.196698	-0.740034
22.C	-1.990985	0.043437	-1.436387
23.C	-1.939242	1.249320	-0.713870
24.C	-2.056000	-2.553633	-1.156817
25.C	-2.085623	-3.357982	0.000000
26.C	-2.056000	-2.553633	1.156817
27.H	-1.877682	2.198344	1.245097
28.H	-1.877682	2.198344	-1.245097
29.H	-1.982038	0.062416	-2.527417
30.H	-1.982038	0.062416	2.527417
31.H	-2.059582	-2.903216	-2.186497
32.H	-2.109563	-4.446347	0.000000
33.H	-2.059582	-2.903216	2.186497

[Ti(η^5-Ind)$_2$] (C_{2v}) S = 0, E_T (BP86) = -207.951, E_T (B3LYP/BP86) = -244.166.

Atom	X	Y	Z
1.Ti	0.000000	0.000000	0.676990
2.C	-0.725653	2.337510	0.168812
3.C	0.725653	2.337510	0.168812
4.C	1.171828	1.822074	1.443419
5.C	0.000000	1.571185	2.253082
6.C	-1.171828	1.822074	1.443419
7.C	1.423800	2.726761	-1.003854
8.C	0.707826	3.131310	-2.123386
9.C	-0.707826	3.131310	-2.123386
10.C	-1.423800	2.726761	-1.003854
11.H	2.204086	1.771824	1.777569
12.H	0.000000	1.328949	3.309104
13.H	-2.204086	1.771824	1.777569
14.H	2.515386	2.730408	-1.016459
15.H	1.242750	3.445162	-3.021583

16.H	-1.242750	3.445162	-3.021583
17.H	-2.515386	2.730408	-1.016459
18.C	-0.725653	-2.337510	0.168812
19.C	-1.171828	-1.822074	1.443419
20.C	0.000000	-1.571185	2.253082
21.C	1.171828	-1.822074	1.443419
22.C	0.725653	-2.337510	0.168812
23.C	-1.423800	-2.726761	-1.003854
24.C	-0.707826	-3.131310	-2.123386
25.C	0.707826	-3.131310	-2.123386
26.C	1.423800	-2.726761	-1.003854
27.H	0.000000	-1.328949	3.309104
28.H	2.204086	-1.771824	1.777569
29.H	-2.204086	-1.771824	1.777569
30.H	-2.515386	-2.730408	-1.016459
31.H	-1.242750	-3.445162	-3.021583
32.H	1.242750	-3.445162	-3.021583
33.H	2.515386	-2.730408	-1.016459

[Ti(η^5-Ind)$_2$] (C_{2v}) S = 1, E_T (BP86) = -208.399, E_T (B3LYP/BP86) = -244.805.

Atom	X	Y	Z
1.Ti	0.000000	0.000000	0.728952
2.C	-0.725744	2.266372	0.166948
3.C	0.725744	2.266372	0.166948
4.C	1.162223	1.918949	1.493346
5.C	0.000000	1.760511	2.299456
6.C	-1.162223	1.918949	1.493346
7.C	1.427381	2.497478	-1.044711
8.C	0.708221	2.774518	-2.200503
9.C	-0.708221	2.774518	-2.200503
10.C	-1.427381	2.497478	-1.044711
11.H	2.191003	1.877194	1.837789
12.H	0.000000	1.538916	3.362782
13.H	-2.191003	1.877194	1.837789
14.H	2.518607	2.488605	-1.057109
15.H	1.242139	2.980843	-3.129680
16.H	-1.242139	2.980843	-3.129680
17.H	-2.518607	2.488605	-1.057109
18.C	-0.725744	-2.266372	0.166948
19.C	-1.162223	-1.918949	1.493346
20.C	0.000000	-1.760511	2.299456
21.C	1.162223	-1.918949	1.493346
22.C	0.725744	-2.266372	0.166948
23.C	-1.427381	-2.497478	-1.044711
24.C	-0.708221	-2.774518	-2.200503
25.C	0.708221	-2.774518	-2.200503
26.C	1.427381	-2.497478	-1.044711
27.H	0.000000	-1.538916	3.362782
28.H	2.191003	-1.877194	1.837789

29.H	-2.191003	-1.877194	1.837789
30.H	-2.518607	-2.488605	-1.057109
31.H	-1.242139	-2.980843	-3.129680
32.H	1.242139	-2.980843	-3.129680
33.H	2.518607	-2.488605	-1.057109

[Zr(η^9-Ind)(η^5-Ind)] (C_1) S = 0, E_T (BP86) = -208.552, E_T (B3LYP/BP86) = -243.357.

Atom	X	Y	Z
1.Zr	-0.115404	0.388390	-0.342475
2.C	1.152377	0.253051	1.947488
3.C	0.656907	-1.090636	1.718991
4.C	-0.783272	-1.019801	1.682056
5.C	-1.173012	0.321094	1.947895
6.C	0.007851	1.123364	2.044473
7.C	1.576858	-2.162983	1.576525
8.C	2.935388	-1.910372	1.686658
9.C	3.421579	-0.595248	1.893307
10.C	2.553888	0.482140	1.997507
11.H	-1.456796	-1.866375	1.577272
12.H	-2.192537	0.669805	2.079239
13.H	0.034762	2.186479	2.271916
14.H	1.212452	-3.179107	1.415545
15.H	3.645371	-2.734502	1.604198
16.H	4.497267	-0.429241	1.963405
17.H	2.939129	1.489549	2.163816
18.C	0.915639	-0.462238	-2.414098
19.C	0.403704	0.898684	-2.547872
20.C	-0.995695	1.193189	-2.320323
21.C	-1.931234	0.136616	-1.934173
22.C	-1.406628	-1.192553	-1.904135
23.C	-0.041675	-1.477679	-2.130740
24.C	-1.056522	2.472505	-1.661866
25.C	0.264018	2.965325	-1.523939
26.C	1.166237	2.010940	-2.043166
27.H	1.959806	-0.693876	-2.609109
28.H	-2.992831	0.338942	-1.819723
29.H	-2.056076	-2.008364	-1.582939
30.H	0.308428	-2.497705	-1.967611
31.H	-1.968047	2.972955	-1.347389
32.H	0.540272	3.918629	-1.075499
33.H	2.250235	2.081630	-2.048880

[Zr(η^5-Ind)(η^6-Ind)] (C_1) S = 1, E_T (BP86) = -208.018, E_T (B3LYP/BP86) = -243.154.

Atom	X	Y	Z
1.Zr	-0.065161	0.005628	-0.213621
2.C	1.110282	0.305941	2.019664
3.C	0.626819	-1.064754	1.998169
4.C	-0.809084	-1.017290	2.002195
5.C	-1.195082	0.350143	2.072298
6.C	-0.037901	1.173196	2.044562
7.C	1.552042	-2.131860	1.843288
8.C	2.913459	-1.849242	1.798887

9.C	3.384132	-0.515160	1.823925
10.C	2.503926	0.559687	1.894273
11.H	-1.477826	-1.873555	2.031359
12.H	-2.218584	0.711703	2.137901
13.H	-0.022824	2.257756	2.104124
14.H	1.195602	-3.162554	1.803023
15.H	3.629906	-2.667200	1.714417
16.H	4.456496	-0.326830	1.760773
17.H	2.876552	1.585055	1.889079
18.C	0.845915	-0.266853	-2.620872
19.C	0.453813	1.094773	-2.439138
20.C	-0.951988	1.411086	-2.123963
21.C	-1.890533	0.347763	-1.968908
22.C	-1.464458	-0.986510	-2.146799
23.C	-0.111217	-1.288079	-2.481006
24.C	-1.029847	2.818961	-1.930600
25.C	0.256290	3.355019	-2.119084
26.C	1.175202	2.314901	-2.392582
27.H	1.880567	-0.518239	-2.856497
28.H	-2.931395	0.559642	-1.721966
29.H	-2.177816	-1.801805	-2.029179
30.H	0.186495	-2.328598	-2.606460
31.H	-1.931665	3.376131	-1.688320
32.H	0.515602	4.408036	-2.027616
33.H	2.242770	2.426699	-2.566628

[Zr(η^9-Ind)(η^6-Ind)] (C_S) S = 0, E_T (BP86) = -208.275, E_T (B3LYP/BP86) = -243.450.

Atom	X	Y	Z
1.Zr	0.370267	0.434107	0.000000
2.C	-2.161973	0.231578	0.726280
3.C	-2.161973	0.231578	-0.726280
4.C	-1.631874	1.489840	-1.169762
5.C	-1.358195	2.260518	0.000000
6.C	-1.631874	1.489840	1.169762
7.C	-2.661768	-0.901449	-1.427960
8.C	-3.164493	-1.970022	-0.712639
9.C	-3.164493	-1.970022	0.712639
10.C	-2.661768	-0.901449	1.427960
11.H	-1.573253	1.834592	-2.196689
12.H	-0.998312	3.286095	0.000000
13.H	-1.573253	1.834592	2.196689
14.H	-2.674476	-0.905737	-2.518451
15.H	-3.575449	-2.829389	-1.243384
16.H	-3.575449	-2.829389	1.243384
17.H	-2.674476	-0.905737	2.518451
18.C	2.440960	-0.331840	0.723801
19.C	2.247610	0.907215	1.473347
20.C	2.176587	2.107980	0.705864
21.C	2.176587	2.107980	-0.705864
22.C	2.247610	0.907215	-1.473347
23.C	2.440960	-0.331840	-0.723801
24.C	1.800845	-1.546147	1.149735
25.C	1.437311	-2.283106	0.000000
26.C	1.800845	-1.546147	-1.149735

27.H	2.294534	0.922659	2.558787
28.H	1.993988	3.051831	-1.221341
29.H	2.294534	0.922659	-2.558787
30.H	1.993988	3.051831	1.221341
31.H	1.632954	-1.837107	2.183171
32.H	0.942988	-3.253303	0.000000
33.H	1.632954	-1.837107	-2.183171

[Zr(η^5-Ind)(η^6-Ind)] (C_S) S = 1, E_T (BP86) = -207.863, E_T (B3LYP/BP86) = -243.201.

Atom	X	Y	Z
1.Zr	-0.207647	0.529704	0.000000
2.C	2.254738	0.531745	0.725952
3.C	2.254738	0.531745	-0.725952
4.C	2.699225	-0.619776	-1.427223
5.C	3.196102	-1.702422	-0.706060
6.C	3.196102	-1.702422	0.706060
7.C	2.699225	-0.619776	1.427223
8.C	1.665058	1.772427	-1.160819
9.C	1.355508	2.533399	0.000000
10.C	1.665058	1.772427	1.160819
11.H	2.688233	-0.635729	-2.518280
12.H	3.571654	-2.576695	-1.238981
13.H	3.571654	-2.576695	1.238981
14.H	2.688233	-0.635729	2.518280
15.H	1.564827	2.106994	-2.189713
16.H	0.947167	3.541273	0.000000
17.H	1.564827	2.106994	2.189713
18.C	-2.499205	1.452425	0.713673
19.C	-2.325691	0.257962	1.441075
20.C	-2.161636	-0.971769	0.738345
21.C	-2.161636	-0.971769	-0.738345
22.C	-2.325691	0.257962	-1.441075
23.C	-2.499205	1.452425	-0.713673
24.C	-1.907058	-2.303336	-1.155070
25.C	-1.779382	-3.102536	0.000000
26.C	-1.907058	-2.303336	1.155070
27.H	-2.626622	2.395366	1.244382
28.H	-2.626622	2.395366	-1.244382
29.H	-2.332009	0.276900	-2.531421
30.H	-2.332009	0.276900	2.531421
31.H	-1.837320	-2.644318	-2.185171
32.H	-1.579299	-4.171869	0.000000
33.H	-1.837320	-2.644318	2.185171

[Zr(η^5-Ind)2] (C_{2v}) S = 0, E_T (BP86) = -208.023, E_T (B3LYP/BP86) = -243.075.

Atom	X	Y	Z
1.Zr	0.000000	0.000000	0.659953
2.C	-0.726126	2.451761	0.181191
3.C	0.726126	2.451761	0.181191
4.C	1.173016	1.981421	1.472515
5.C	0.000000	1.744068	2.284688

6.C	-1.173016	1.981421	1.472515
7.C	1.421840	2.772496	-1.013536
8.C	0.706633	3.123442	-2.154722
9.C	-0.706633	3.123442	-2.154722
10.C	-1.421840	2.772496	-1.013536
11.H	2.202331	1.974284	1.820146
12.H	0.000000	1.554006	3.353520
13.H	-2.202331	1.974284	1.820146
14.H	2.513610	2.771767	-1.027251
15.H	1.242739	3.389568	-3.066543
16.H	-1.242739	3.389568	-3.066543
17.H	-2.513610	2.771767	-1.027251
18.C	-0.726126	-2.451761	0.181191
19.C	-1.173016	-1.981421	1.472515
20.C	0.000000	-1.744068	2.284688
21.C	1.173016	-1.981421	1.472515
22.C	0.726126	-2.451761	0.181191
23.C	-1.421840	-2.772496	-1.013536
24.C	-0.706633	-3.123442	-2.154722
25.C	0.706633	-3.123442	-2.154722
26.C	1.421840	-2.772496	-1.013536
27.H	0.000000	-1.554006	3.353520
28.H	2.202331	-1.974284	1.820146
29.H	-2.202331	-1.974284	1.820146
30.H	-2.513610	-2.771767	-1.027251
31.H	-1.242739	-3.389568	-3.066543
32.H	1.242739	-3.389568	-3.066543
33.H	2.513610	-2.771767	-1.027251

[Zr(η^5-Ind)2] (C_{2v}) S = 1, E_T (BP86) = -208.335, E_T (B3LYP/BP86) = -243.500.

Atom	X	Y	Z
1.Zr	0.000000	0.000000	0.723608
2.C	-0.725133	2.407631	0.159359
3.C	0.725133	2.407631	0.159359
4.C	1.164147	2.099355	1.496151
5.C	0.000000	1.962570	2.307844
6.C	-1.164147	2.099355	1.496151
7.C	1.425654	2.583449	-1.062680
8.C	0.706397	2.828460	-2.229192
9.C	-0.706397	2.828460	-2.229192
10.C	-1.425654	2.583449	-1.062680
11.H	2.192667	2.090165	1.845523
12.H	0.000000	1.793079	3.381794
13.H	-2.192667	2.090165	1.845523
14.H	2.516822	2.570354	-1.076163
15.H	1.240910	3.000356	-3.164237
16.H	-1.240910	3.000356	-3.164237
17.H	-2.516822	2.570354	-1.076163
18.C	-0.725133	-2.407631	0.159359
19.C	-1.164147	-2.099355	1.496151
20.C	0.000000	-1.962570	2.307844

21.C	1.164147	-2.099355	1.496151
22.C	0.725133	-2.407631	0.159359
23.C	-1.425654	-2.583449	-1.062680
24.C	-0.706397	-2.828460	-2.229192
25.C	0.706397	-2.828460	-2.229192
26.C	1.425654	-2.583449	-1.062680
27.H	0.000000	-1.793079	3.381794
28.H	2.192667	-2.090165	1.845523
29.H	-2.192667	-2.090165	1.845523
30.H	-2.516822	-2.570354	-1.076163
31.H	-1.240910	-3.000356	-3.164237
32.H	1.240910	-3.000356	-3.164237
33.H	2.516822	-2.570354	-1.076163

Compounds for TNE = 23

[V(η^5-Ind)2] (C_{2v}) S = 1/2, E_T (BP86) = -209.610, E_T (B3LYP/BP86) = -246.208.

Atom	X	Y	Z
1.V	0.000000	0.000000	0.560554
2.C	-0.722606	2.181910	-0.090469
3.C	0.722606	2.181910	-0.090469
4.C	1.168242	1.761465	1.220550
5.C	0.000000	1.579387	2.041622
6.C	-1.168242	1.761465	1.220550
7.C	1.422055	2.464585	-1.290327
8.C	0.705983	2.787788	-2.437657
9.C	-0.705983	2.787788	-2.437657
10.C	-1.422055	2.464585	-1.290327
11.H	2.200607	1.725828	1.557815
12.H	0.000000	1.390358	3.110371
13.H	-2.200607	1.725828	1.557815
14.H	2.513505	2.458041	-1.303079
15.H	1.241247	3.030449	-3.356726
16.H	-1.241247	3.030449	-3.356726
17.H	-2.513505	2.458041	-1.303079
18.C	-0.722606	-2.181910	-0.090469
19.C	-1.168242	-1.761465	1.220550
20.C	0.000000	-1.579387	2.041622
21.C	1.168242	-1.761465	1.220550
22.C	0.722606	-2.181910	-0.090469
23.C	-1.422055	-2.464585	-1.290327
24.C	-0.705983	-2.787788	-2.437657
25.C	0.705983	-2.787788	-2.437657
26.C	1.422055	-2.464585	-1.290327
27.H	0.000000	-1.390358	3.110371
28.H	2.200607	-1.725828	1.557815
29.H	-2.200607	-1.725828	1.557815
30.H	-2.513505	-2.458041	-1.303079
31.H	-1.241247	-3.030449	-3.356726
32.H	1.241247	-3.030449	-3.356726
33.H	2.513505	-2.458041	-1.303079

[V(η^5-Ind)2] (C_{2v}) S = 3/2, E_T (BP86) = -209.730, E_T (B3LYP/BP86) = -247.061.

Atom	X	Y	Z
1.V	0.000000	0.000000	0.799282
2.C	-0.728202	2.041935	-0.140436
3.C	0.728202	2.041935	-0.140436
4.C	1.162617	1.949666	1.227962
5.C	0.000000	1.939255	2.052636
6.C	-1.162617	1.949666	1.227962
7.C	1.430029	2.116778	-1.378294
8.C	0.712937	2.204659	-2.553621
9.C	-0.712937	2.204659	-2.553621
10.C	-1.430029	2.116778	-1.378294
11.H	2.192218	1.956261	1.575447
12.H	0.000000	1.907683	3.139493
13.H	-2.192218	1.956261	1.575447
14.H	2.521366	2.127763	-1.388608
15.H	1.242456	2.276336	-3.504433
16.H	-1.242456	2.276336	-3.504433
17.H	-2.521366	2.127763	-1.388608
18.C	-0.728202	-2.041935	-0.140436
19.C	-1.162617	-1.949666	1.227962
20.C	0.000000	-1.939255	2.052636
21.C	1.162617	-1.949666	1.227962
22.C	0.728202	-2.041935	-0.140436
23.C	-1.430029	-2.116778	-1.378294
24.C	-0.712937	-2.204659	-2.553621
25.C	0.712937	-2.204659	-2.553621
26.C	1.430029	-2.116778	-1.378294
27.H	0.000000	-1.907683	3.139493
28.H	2.192218	-1.956261	1.575447
29.H	-2.192218	-1.956261	1.575447
30.H	-2.521366	-2.127763	-1.388608
31.H	-1.242456	-2.276336	-3.504433
32.H	1.242456	-2.276336	-3.504433
33.H	2.521366	-2.127763	-1.388608

[V(η^6-Ind)2] (C_{2v}) S = 3/2, E_T (BP86) = -208.520, E_T (B3LYP/BP86) = -245.817.

Atom	X	Y	Z
1.V	0.000000	0.000000	0.787031
2.C	0.746130	-2.028635	-0.469030
3.C	-0.746130	-2.028635	-0.469030
4.C	-1.433907	-1.905029	0.761104
5.C	-0.716577	-1.810679	1.975688
6.C	0.716577	-1.810679	1.975688
7.C	1.433907	-1.905029	0.761104
8.C	-1.161490	-2.152454	-1.812506
9.C	0.000000	-2.239553	-2.606859
10.C	1.161490	-2.152454	-1.812506
11.H	-2.524189	-1.876371	0.778907
12.H	-1.254337	-1.723995	2.918675
13.H	1.254337	-1.723995	2.918675
14.H	2.524189	-1.876371	0.778907
15.H	-2.188339	-2.179874	-2.165286
16.H	0.000000	-2.354046	-3.689344

17.H	2.188339	-2.179874	-2.165286
18.C	0.746130	2.028635	-0.469030
19.C	1.433907	1.905029	0.761104
20.C	0.716577	1.810679	1.975688
21.C	-0.716577	1.810679	1.975688
22.C	-1.433907	1.905029	0.761104
23.C	-0.746130	2.028635	-0.469030
24.C	1.161490	2.152454	-1.812506
25.C	0.000000	2.239553	-2.606859
26.C	-1.161490	2.152454	-1.812506
27.H	1.254337	1.723995	2.918675
28.H	-1.254337	1.723995	2.918675
29.H	-2.524189	1.876371	0.778907
30.H	2.524189	1.876371	0.778907
31.H	2.188339	2.179874	-2.165286
32.H	0.000000	2.354046	-3.689344
33.H	-2.188339	2.179874	-2.165286

[V(η^6-Ind)2] (C_{2h}) S = 1/2, E_T (BP86) = -208.779, E_T (B3LYP/BP86) = -245.553.

Atom	X	Y	Z
1.V	0.000000	0.000000	0.000000
2.C	1.953115	0.985917	-0.733391
3.C	1.953115	0.985917	0.733391
4.C	0.838867	1.543035	1.442059
5.C	-0.195422	2.177023	0.711265
6.C	-0.195422	2.177023	-0.711265
7.C	0.838867	1.543035	-1.442059
8.C	3.141148	0.320221	1.153093
9.C	3.859954	-0.047353	0.000000
10.C	3.141148	0.320221	-1.153093
11.H	0.801513	1.512618	2.530791
12.H	-1.054605	2.590210	1.238585
13.H	-1.054605	2.590210	-1.238585
14.H	0.801513	1.512618	-2.530791
15.H	3.437142	0.142150	2.184413
16.H	4.817750	-0.564275	0.000000
17.H	3.437142	0.142150	-2.184413
18.C	0.195422	-2.177023	-0.711265
19.C	-0.838867	-1.543035	-1.442059
20.C	-1.953115	-0.985917	-0.733391
21.C	-1.953115	-0.985917	0.733391
22.C	-0.838867	-1.543035	1.442059
23.C	0.195422	-2.177023	0.711265
24.C	-3.141148	-0.320221	1.153093
25.C	-3.859954	0.047353	0.000000
26.C	-3.141148	-0.320221	-1.153093
27.H	1.054605	-2.590210	-1.238585
28.H	1.054605	-2.590210	1.238585
29.H	-0.801513	-1.512618	2.530791
30.H	-0.801513	-1.512618	-2.530791
31.H	-3.437142	-0.142150	2.184413
32.H	-4.817750	0.564275	0.000000
33.H	-3.437142	-0.142150	-2.184413

[V(η^5-Ind)(η^6-Ind)] (C_S) S = 1/2, E_T (BP86) = -209.120, E_T (B3LYP/BP86) = -245.922.

Atom	X	Y	Z
1.V	0.277254	0.712160	0.000000
2.C	-1.986175	0.260950	0.724319
3.C	-1.986175	0.260950	-0.724319
4.C	-1.478183	1.539588	-1.165141
5.C	-1.244346	2.336843	0.000000
6.C	-1.478183	1.539588	1.165141
7.C	-2.416466	-0.894323	-1.426351
8.C	-2.857914	-1.993548	-0.709066
9.C	-2.857914	-1.993548	0.709066
10.C	-2.416466	-0.894323	1.426351
11.H	-1.414902	1.878079	-2.195664
12.H	-0.935142	3.378718	0.000000
13.H	-1.414902	1.878079	2.195664
14.H	-2.421815	-0.903754	-2.517723
15.H	-3.209931	-2.878858	-1.240633
16.H	-3.209931	-2.878858	1.240633
17.H	-2.421815	-0.903754	2.517723
18.C	1.999194	-0.583844	0.729458
19.C	1.966262	0.665685	1.447105
20.C	2.103266	1.872896	0.709911
21.C	2.103266	1.872896	-0.709911
22.C	1.966262	0.665685	-1.447105
23.C	1.999194	-0.583844	-0.729458
24.C	1.848203	-1.938748	1.148197
25.C	1.795548	-2.751448	0.000000
26.C	1.848203	-1.938748	-1.148197
27.H	1.921274	0.685894	2.535298
28.H	2.094103	2.827491	-1.236353
29.H	1.921274	0.685894	-2.535298
30.H	2.094103	2.827491	1.236353
31.H	1.790602	-2.277979	2.180352
32.H	1.680090	-3.833442	0.000000
33.H	1.790602	-2.277979	-2.180352

[V(η^5-Ind)(η^6-Ind)] (C_1) S = 3/2, E_T (BP86) = -209.295, E_T (B3LYP/BP86) = -246.504.

Atom	X	Y	Z
1.V	-0.058094	-0.057796	-0.074262
2.C	1.138252	0.022742	1.969717
3.C	0.270992	-1.145452	1.998419
4.C	-1.087018	-0.679500	1.881164
5.C	-1.054173	0.746160	1.835778
6.C	0.299653	1.183894	1.836281
7.C	0.844579	-2.443550	2.119242
8.C	2.216347	-2.564480	2.230526
9.C	3.066448	-1.420646	2.196653
10.C	2.550012	-0.147073	2.055511
11.H	-1.979829	-1.299144	1.901147
12.H	-1.922951	1.395731	1.766860

13.H	0.637663	2.215241	1.783462
14.H	0.202259	-3.325313	2.152956
15.H	2.662558	-3.553066	2.347989
16.H	4.144713	-1.558640	2.287884
17.H	3.206765	0.724225	2.040359
18.C	1.361208	0.018107	-1.974446
19.C	0.657069	1.250240	-2.000408
20.C	-0.831189	1.234215	-1.984605
21.C	-1.508831	-0.014612	-1.941830
22.C	-0.776359	-1.222952	-1.941504
23.C	0.654500	-1.205410	-1.952835
24.C	-1.262377	2.583155	-1.996987
25.C	-0.109943	3.395205	-2.034059
26.C	1.059046	2.609132	-2.022028
27.H	2.452118	0.008311	-1.952864
28.H	-2.598988	-0.046735	-1.903197
29.H	-1.301101	-2.176697	-1.907679
30.H	1.202359	-2.146159	-1.919083
31.H	-2.294595	2.924311	-1.999189
32.H	-0.121732	4.483639	-2.069244
33.H	2.083902	2.971429	-2.045083

[Nb(η^5-Ind)$_2$] (C_{2v}) S = 1/2, E_T (BP86) = -209.525, E_T (B3LYP/BP86) = -245.962.

Atom	X	Y	Z
1.Nb	0.046937	0.003657	0.543613
2.C	-0.740025	2.355919	0.013643
3.C	0.707148	2.397576	0.036576
4.C	1.146267	1.941693	1.338174
5.C	-0.027366	1.690334	2.132063
6.C	-1.189388	1.868267	1.300077
7.C	1.415037	2.725279	-1.143671
8.C	0.702336	3.079533	-2.289992
9.C	-0.705370	3.040585	-2.311370
10.C	-1.430000	2.643069	-1.187338
11.H	2.169759	1.954342	1.701751
12.H	-0.036375	1.491874	3.200245
13.H	-2.223162	1.817360	1.630470
14.H	2.506272	2.739790	-1.142121
15.H	1.244366	3.369477	-3.190177
16.H	-1.235890	3.298591	-3.228483
17.H	-2.519687	2.594111	-1.219498
18.C	-0.715658	-2.365259	0.043366
19.C	-1.161774	-1.868349	1.327777
20.C	0.004003	-1.664498	2.148910
21.C	1.175512	-1.910156	1.349262
22.C	0.732423	-2.385429	0.055230
23.C	-1.408965	-2.678268	-1.149469
24.C	-0.685946	-3.072153	-2.275880
25.C	0.722322	-3.086001	-2.265738
26.C	1.437264	-2.709026	-1.128969
27.H	-0.002112	-1.456737	3.214989
28.H	2.201573	-1.908901	1.705695
29.H	-2.192992	-1.827002	1.666632

30.H	-2.499507	-2.649207	-1.174554
31.H	-1.218135	-3.348531	-3.185849
32.H	1.262443	-3.373409	-3.168269
33.H	2.528605	-2.704179	-1.136082

[Nb(η^5-Ind)$_2$] (C_{2v}) S = 3/2, E_T (BP86) = -209.807, E_T (B3LYP/BP86) = -246.786.

Atom	X	Y	Z
1.Nb	0.010890	0.003957	0.787006
2.C	-0.748289	2.274763	-0.005128
3.C	0.707202	2.305361	0.031155
4.C	1.112106	2.108278	1.397372
5.C	-0.069235	2.007604	2.188622
6.C	-1.212186	2.060804	1.339101
7.C	1.435738	2.516707	-1.173931
8.C	0.743128	2.722818	-2.351708
9.C	-0.681671	2.693556	-2.386949
10.C	-1.423593	2.457869	-1.245587
11.H	2.131520	2.125165	1.773150
12.H	-0.094064	1.899761	3.270212
13.H	-2.249106	2.031872	1.662769
14.H	2.526518	2.544067	-1.155407
15.H	1.292595	2.907158	-3.275454
16.H	-1.192244	2.856783	-3.336670
17.H	-2.513988	2.440273	-1.282306
18.C	-0.711317	-2.293317	0.052119
19.C	-1.134049	-2.072226	1.409074
20.C	0.036287	-1.981246	2.217950
21.C	1.191345	-2.065995	1.387762
22.C	0.744845	-2.289161	0.039214
23.C	-1.423889	-2.502282	-1.162966
24.C	-0.715886	-2.729683	-2.327411
25.C	0.709480	-2.726364	-2.339713
26.C	1.436816	-2.495489	-1.187987
27.H	0.046300	-1.857516	3.298122
28.H	2.223396	-2.051619	1.727646
29.H	-2.159425	-2.063583	1.768412
30.H	-2.515084	-2.509873	-1.162402
31.H	-1.254151	-2.910565	-3.258558
32.H	1.232132	-2.905492	-3.279929
33.H	2.527791	-2.498033	-1.206566

[Nb(η^5-Ind)(η^6-Ind)] (C_s) S = 1/2, E_T (BP86) = -209.460, E_T (B3LYP/BP86) = -246.293.

Atom	X	Y	Z
1.Nb	0.257380	0.676469	0.000000
2.C	-2.143800	0.290116	0.724712
3.C	-2.143800	0.290116	-0.724712
4.C	-1.664079	1.579283	-1.165894
5.C	-1.441429	2.375336	0.000000
6.C	-1.664079	1.579283	1.165894
7.C	-2.538203	-0.878533	-1.426529
8.C	-2.963071	-1.987944	-0.707920
9.C	-2.963071	-1.987944	0.707920

10.C	-2.538203	-0.878533	1.426529
11.H	-1.621929	1.925113	-2.194334
12.H	-1.152564	3.423052	0.000000
13.H	-1.621929	1.925113	2.194334
14.H	-2.536158	-0.891268	-2.517506
15.H	-3.293781	-2.880744	-1.240500
16.H	-3.293781	-2.880744	1.240500
17.H	-2.536158	-0.891268	2.517506
18.C	2.154164	-0.611276	0.728412
19.C	2.122301	0.635250	1.454349
20.C	2.250272	1.841358	0.710799
21.C	2.250272	1.841358	-0.710799
22.C	2.122301	0.635250	-1.454349
23.C	2.154164	-0.611276	-0.728412
24.C	1.996874	-1.966081	1.147712
25.C	1.944337	-2.781392	0.000000
26.C	1.996874	-1.966081	-1.147712
27.H	2.123702	0.654318	2.542693
28.H	2.260392	2.796321	-1.236186
29.H	2.123702	0.654318	-2.542693
30.H	2.260392	2.796321	1.236186
31.H	1.941802	-2.304459	2.179968
32.H	1.826372	-3.862723	0.000000
33.H	1.941802	-2.304459	-2.179968

[Nb(η^6-Ind)$_2$] (C_{2v}) S = 1/2, E_T (BP86) = -209.169, E_T (B3LYP/BP86) = -245.919

Atom	X	Y	Z
1.Nb	0.000000	0.000000	0.670526
2.C	0.733629	-2.105818	-0.416527
3.C	-0.733629	-2.105818	-0.416527
4.C	-1.447183	-1.948565	0.816573
5.C	-0.713544	-1.891123	2.026099
6.C	0.713544	-1.891123	2.026099
7.C	1.447183	-1.948565	0.816573
8.C	-1.151937	-2.200987	-1.771458
9.C	0.000000	-2.282132	-2.578023
10.C	1.151937	-2.200987	-1.771458
11.H	-2.536516	-1.941328	0.836211
12.H	-1.240795	-1.794990	2.975131
13.H	1.240795	-1.794990	2.975131
14.H	2.536516	-1.941328	0.836211
15.H	-2.182639	-2.203614	-2.117454
16.H	0.000000	-2.357643	-3.663295
17.H	2.182639	-2.203614	-2.117454
18.C	0.733629	2.105818	-0.416527
19.C	1.447183	1.948565	0.816573
20.C	0.713544	1.891123	2.026099
21.C	-0.713544	1.891123	2.026099
22.C	-1.447183	1.948565	0.816573
23.C	-0.733629	2.105818	-0.416527
24.C	1.151937	2.200987	-1.771458
25.C	0.000000	2.282132	-2.578023
26.C	-1.151937	2.200987	-1.771458
27.H	1.240795	1.794990	2.975131

28.H	-1.240795	1.794990	2.975131
29.H	-2.536516	1.941328	0.836211
30.H	2.536516	1.941328	0.836211
31.H	2.182639	2.203614	-2.117454
32.H	0.000000	2.357643	-3.663295
33.H	-2.182639	2.203614	-2.117454

[Nb(η^5-Ind)(η^6-Ind)] (C_1) S = 3/2, E_T (BP86) = -209.334, E_T (B3LYP/BP86) = -245.313

Atom	X	Y	Z
1.Nb	0.067062	-0.013032	-0.083165
2.C	1.211279	-0.079011	2.146737
3.C	0.217662	-1.140308	2.153983
4.C	-1.075929	-0.524080	2.018280
5.C	-0.883622	0.887318	1.987419
6.C	0.510982	1.172534	2.010107
7.C	0.635651	-2.495705	2.273382
8.C	1.982195	-2.775177	2.416015
9.C	2.956396	-1.737227	2.404391
10.C	2.591435	-0.411518	2.252709
11.H	-2.033611	-1.037363	2.034060
12.H	-1.674998	1.629450	1.924872
13.H	0.958368	2.162064	2.004532
14.H	-0.105720	-3.296314	2.285118
15.H	2.308506	-3.808830	2.537438
16.H	4.009996	-1.997279	2.512809
17.H	3.344476	0.377876	2.248404
18.C	1.367294	0.219882	-2.231061
19.C	0.529483	1.366656	-2.191427
20.C	-0.942497	1.186522	-2.086757
21.C	-1.479710	-0.130941	-2.035720
22.C	-0.619543	-1.249773	-2.096080
23.C	0.798680	-1.074135	-2.179380
24.C	-1.522414	2.481423	-2.073791
25.C	-0.472599	3.416875	-2.184003
26.C	0.773950	2.764907	-2.239930
27.H	2.450751	0.330013	-2.293792
28.H	-2.557759	-0.282302	-1.959439
29.H	-1.034825	-2.255801	-2.064672
30.H	1.444714	-1.950121	-2.205593
31.H	-2.584626	2.704370	-2.015573
32.H	-0.608519	4.496992	-2.218033
33.H	1.748387	3.239177	-2.321932

[Nb(η^6-Ind)$_2$] (C_2) S = 3/2, E_T (BP86) = -209.087, E_T (B3LYP/BP86) = -245.795

Atom	X	Y	Z
1.V	0.000000	0.000000	0.130808
2.C	1.991366	0.062996	-1.322304
3.C	1.942617	-1.261605	-0.649044
4.C	1.839610	-1.314578	0.767034
5.C	1.809445	-0.120192	1.522158
6.C	1.845159	1.155239	0.871160
7.C	1.919025	1.241556	-0.537058
8.C	2.005403	-2.246151	-1.664663

9.C	2.106884	-1.573731	-2.901094
10.C	2.084427	-0.178910	-2.714606
11.H	1.782203	-2.275988	1.279924
12.H	1.733690	-0.166860	2.607777
13.H	1.790053	2.064630	1.468302
14.H	1.905360	2.220692	-1.018121
15.H	2.001296	-3.322831	-1.513045
16.H	2.185512	-2.067165	-3.868772
17.H	2.126362	0.578785	-3.492374
18.C	-1.991366	-0.062996	-1.322304
19.C	-1.942617	1.261605	-0.649044
20.C	-1.839610	1.314578	0.767034
21.C	-1.809445	0.120192	1.522158
22.C	-1.845159	-1.155239	0.871160
23.C	-1.919025	-1.241556	-0.537058
24.C	-2.005403	2.246151	-1.664663
25.C	-2.106884	1.573731	-2.901094
26.C	-2.084427	0.178910	-2.714606
27.H	-1.782203	2.275988	1.279924
28.H	-1.733690	0.166860	2.607777
29.H	-1.790053	-2.064630	1.468302
30.H	-1.905360	-2.220692	-1.018121
31.H	-2.001296	3.322831	-1.513045
32.H	-2.185512	2.067165	-3.868772
33.H	-2.126362	-0.578785	-3.492374

Compounds for TNE = 24

$Cr(\eta^5\text{-Ind})_2$ (C_{2v}) S = 1, E_T (BP86) = -210.142, E_T (B3LYP/BP86) = -248.077.

Atom	X	Y	Z
1.Cr	0.000000	0.000000	0.868948
2.C	-0.726078	2.055681	0.066605
3.C	0.726078	2.055681	0.066605
4.C	1.165666	1.761172	1.406699
5.C	0.000000	1.631574	2.242497
6.C	-1.165666	1.761172	1.406699
7.C	1.427404	2.289560	-1.147980
8.C	0.710950	2.543203	-2.303373
9.C	-0.710950	2.543203	-2.303373
10.C	-1.427404	2.289560	-1.147980
11.H	2.198589	1.724232	1.742962
12.H	0.000000	1.516359	3.322229
13.H	-2.198589	1.724232	1.742962
14.H	2.519212	2.296368	-1.155966
15.H	1.241917	2.744072	-3.235264
16.H	-1.241917	2.744072	-3.235264
17.H	-2.519212	2.296368	-1.155966
18.C	-0.726078	-2.055681	0.066605
19.C	-1.165666	-1.761172	1.406699
20.C	0.000000	-1.631574	2.242497

21.C	1.165666	-1.761172	1.406699
22.C	0.726078	-2.055681	0.066605
23.C	-1.427404	-2.289560	-1.147980
24.C	-0.710950	-2.543203	-2.303373
25.C	0.710950	-2.543203	-2.303373
26.C	1.427404	-2.289560	-1.147980
27.H	0.000000	-1.516359	3.322229
28.H	2.198589	-1.724232	1.742962
29.H	-2.198589	-1.724232	1.742962
30.H	-2.519212	-2.296368	-1.155966
31.H	-1.241917	-2.744072	-3.235264
32.H	1.241917	-2.744072	-3.235264
33.H	2.519212	-2.296368	-1.155966

$Cr(\eta^5\text{-Ind})_2$ (C_{2v}) S = 2, E_T (BP86) = -209.955, E_T (B3LYP/BP86) = -248.516.

Atom	X	Y	Z
1.Cr	0.000000	0.000000	1.203111
2.C	-0.723580	2.097540	-0.011180
3.C	0.723580	2.097540	-0.011180
4.C	1.157306	2.001272	1.369287
5.C	0.000000	2.053807	2.196382
6.C	-1.157306	2.001272	1.369287
7.C	1.427136	2.178581	-1.232742
8.C	0.706691	2.280007	-2.418992
9.C	-0.706691	2.280007	-2.418992
10.C	-1.427136	2.178581	-1.232742
11.H	2.187524	2.037283	1.714734
12.H	0.000000	2.073142	3.284041
13.H	-2.187524	2.037283	1.714734
14.H	2.518559	2.179284	-1.242804
15.H	1.239996	2.362859	-3.366935
16.H	-1.239996	2.362859	-3.366935
17.H	-2.518559	2.179284	-1.242804
18.C	-0.723580	-2.097540	-0.011180
19.C	-1.157306	-2.001272	1.369287
20.C	0.000000	-2.053807	2.196382
21.C	1.157306	-2.001272	1.369287
22.C	0.723580	-2.097540	-0.011180
23.C	-1.427136	-2.178581	-1.232742
24.C	-0.706691	-2.280007	-2.418992
25.C	0.706691	-2.280007	-2.418992
26.C	1.427136	-2.178581	-1.232742
27.H	0.000000	-2.073142	3.284041
28.H	2.187524	-2.037283	1.714734
29.H	-2.187524	-2.037283	1.714734
30.H	-2.518559	-2.179284	-1.242804
31.H	-1.239996	-2.362859	-3.366935
32.H	1.239996	-2.362859	-3.366935
33.H	2.518559	-2.179284	-1.242804

Cr(η^5-Ind)(η^6-Ind) (C_S) S = 1, E_T (BP86) = -209.692, E_T (B3LYP/BP86) = -247.456

Atom	X	Y	Z
1.Cr	0.229747	0.820486	0.000000
2.C	-1.902468	0.238521	0.726018
3.C	-1.902468	0.238521	-0.726018
4.C	-1.480829	1.545961	-1.165801
5.C	-1.281354	2.359195	0.000000
6.C	-1.480829	1.545961	1.165801
7.C	-2.252312	-0.947756	-1.429948
8.C	-2.606590	-2.072388	-0.712343
9.C	-2.606590	-2.072388	0.712343
10.C	-2.252312	-0.947756	1.429948
11.H	-1.406671	1.878313	-2.197722
12.H	-1.022105	3.414252	0.000000
13.H	-1.406671	1.878313	2.197722
14.H	-2.257820	-0.956130	-2.521334
15.H	-2.889225	-2.983362	-1.241639
16.H	-2.889225	-2.983362	1.241639
17.H	-2.257820	-0.956130	2.521334
18.C	1.852525	-0.672829	0.738512
19.C	1.887996	0.574371	1.441263
20.C	2.069829	1.783244	0.713611
21.C	2.069829	1.783244	-0.713611
22.C	1.887996	0.574371	-1.441263
23.C	1.852525	-0.672829	-0.738512
24.C	1.745234	-2.024125	1.157397
25.C	1.708795	-2.827325	0.000000
26.C	1.745234	-2.024125	-1.157397
27.H	1.819742	0.602921	2.528982
28.H	2.106731	2.735071	-1.243147
29.H	1.819742	0.602921	-2.528982
30.H	2.106731	2.735071	1.243147
31.H	1.714638	-2.371042	2.187907
32.H	1.645258	-3.914501	0.000000
33.H	1.714638	-2.371042	-2.187907

Cr(η^6-Ind)$_2$ (C_{2h}) S = 1, E_T (BP86) = -209.450, E_T (B3LYP/BP86) = -247.718

Atom	X	Y	Z
1.Cr	0.000000	0.000000	0.000000
2.C	1.973561	0.998855	-0.739488
3.C	1.973561	0.998855	0.739488
4.C	0.829800	1.493657	1.439526
5.C	-0.237786	2.082642	0.713269
6.C	-0.237786	2.082642	-0.713269
7.C	0.829800	1.493657	-1.439526
8.C	3.186602	0.394888	1.158814
9.C	3.915171	0.059316	0.000000
10.C	3.186602	0.394888	-1.158814
11.H	0.779754	1.445054	2.527320
12.H	-1.121909	2.436819	1.241847
13.H	-1.121909	2.436819	-1.241847
14.H	0.779754	1.445054	-2.527320

15.H	3.498895	0.243027	2.189184
16.H	4.899546	-0.406023	0.000000
17.H	3.498895	0.243027	-2.189184
18.C	0.237786	-2.082642	-0.713269
19.C	-0.829800	-1.493657	-1.439526
20.C	-1.973561	-0.998855	-0.739488
21.C	-1.973561	-0.998855	0.739488
22.C	-0.829800	-1.493657	1.439526
23.C	0.237786	-2.082642	0.713269
24.C	-3.186602	-0.394888	1.158814
25.C	-3.915171	-0.059316	0.000000
26.C	-3.186602	-0.394888	-1.158814
27.H	1.121909	-2.436819	-1.241847
28.H	1.121909	-2.436819	1.241847
29.H	-0.779754	-1.445054	2.527320
30.H	-0.779754	-1.445054	-2.527320
31.H	-3.498895	-0.243027	2.189184
32.H	-4.899546	0.406023	0.000000
33.H	-3.498895	-0.243027	-2.189184

$Mo(\eta^5\text{-Ind})_2$ (C_{2v}) S = 1, E_T (BP86) = -209.917, E_T (B3LYP/BP86) = -246.331.

1.Mo	0.000000	0.000000	0.858892
2.C	-0.726425	2.228290	0.069088
3.C	0.726425	2.228290	0.069088
4.C	1.166511	1.932818	1.410648
5.C	0.000000	1.811056	2.246792
6.C	-1.166511	1.932818	1.410648
7.C	1.427937	2.471654	-1.144259
8.C	0.711106	2.738500	-2.297099
9.C	-0.711106	2.738500	-2.297099
10.C	-1.427937	2.471654	-1.144259
11.H	2.198040	1.918627	1.751533
12.H	0.000000	1.712453	3.328244
13.H	-2.198040	1.918627	1.751533
14.H	2.519229	2.475852	-1.153543
15.H	1.242617	2.947566	-3.226210
16.H	-1.242617	2.947566	-3.226210
17.H	-2.519229	2.475852	-1.153543
18.C	-0.726425	-2.228290	0.069088
19.C	-1.166511	-1.932818	1.410648
20.C	0.000000	-1.811056	2.246792
21.C	1.166511	-1.932818	1.410648
22.C	0.726425	-2.228290	0.069088
23.C	-1.427937	-2.471654	-1.144259
24.C	-0.711106	-2.738500	-2.297099
25.C	0.711106	-2.738500	-2.297099
26.C	1.427937	-2.471654	-1.144259
27.H	0.000000	-1.712453	3.328244
28.H	2.198040	-1.918627	1.751533
29.H	-2.198040	-1.918627	1.751533
30.H	-2.519229	-2.475852	-1.153543
31.H	-1.242617	-2.947566	-3.226210
32.H	1.242617	-2.947566	-3.226210
33.H	2.519229	-2.475852	-1.153543

Mo(η^5-Ind)$_2$ (C_{2v}) S = 1, E_T (BP86) = -209.695, E_T (B3LYP/BP86) = -246.131.

Atom	X	Y	Z
1.Mo	0.000000	0.000000	0.757947
2.C	-0.723314	2.212296	0.152135
3.C	0.723314	2.212296	0.152135
4.C	1.168775	1.845627	1.482119
5.C	0.000000	1.695117	2.298448
6.C	-1.168775	1.845627	1.482119
7.C	1.422239	2.310129	-1.070480
8.C	0.700018	2.529549	-2.255400
9.C	-0.700018	2.529549	-2.255400
10.C	-1.422239	2.310129	-1.070480
11.H	2.198312	1.837400	1.827885
12.H	0.000000	1.509647	3.369082
13.H	-2.198312	1.837400	1.827885
14.H	2.511875	2.256766	-1.085177
15.H	1.238020	2.655155	-3.195693
16.H	-1.238020	2.655155	-3.195693
17.H	-2.511875	2.256766	-1.085177
18.C	-0.723314	-2.212296	0.152135
19.C	-1.168775	-1.845627	1.482119
20.C	0.000000	-1.695117	2.298448
21.C	1.168775	-1.845627	1.482119
22.C	0.723314	-2.212296	0.152135
23.C	-1.422239	-2.310129	-1.070480
24.C	-0.700018	-2.529549	-2.255400
25.C	0.700018	-2.529549	-2.255400
26.C	1.422239	-2.310129	-1.070480
27.H	0.000000	-1.509647	3.369082
28.H	2.198312	-1.837400	1.827885
29.H	-2.198312	-1.837400	1.827885
30.H	-2.511875	-2.256766	-1.085177
31.H	-1.238020	-2.655155	-3.195693
32.H	1.238020	-2.655155	-3.195693
33.H	2.511875	-2.256766	-1.085177

Mo(η^5-Ind)(η^6-Ind) (C_s) S = 0, E_T (BP86) = -209.309, E_T (B3LYP/BP86) = -245.755.

Atom	X	Y	Z
1.Mo	0.221487	0.760042	0.000000
2.C	-2.076537	0.325430	0.722751
3.C	-2.076537	0.325430	-0.722751
4.C	-1.611496	1.622194	-1.161564
5.C	-1.404481	2.427450	0.000000
6.C	-1.611496	1.622194	1.161564
7.C	-2.416930	-0.853835	-1.424488
8.C	-2.820589	-1.978155	-0.703736
9.C	-2.820589	-1.978155	0.703736
10.C	-2.416930	-0.853835	1.424488
11.H	-1.570216	1.966765	-2.190796
12.H	-1.149189	3.483416	0.000000
13.H	-1.570216	1.966765	2.190796
14.H	-2.396069	-0.870801	-2.514483

15.H	-3.115895	-2.880599	-1.239296
16.H	-3.115895	-2.880599	1.239296
17.H	-2.396069	-0.870801	2.514483
18.C	2.038661	-0.580811	0.729234
19.C	2.041232	0.662467	1.449771
20.C	2.180808	1.865660	0.711004
21.C	2.180808	1.865660	-0.711004
22.C	2.041232	0.662467	-1.449771
23.C	2.038661	-0.580811	-0.729234
24.C	1.939529	-1.941080	1.146408
25.C	1.914404	-2.755936	0.000000
26.C	1.939529	-1.941080	-1.146408
27.H	2.034647	0.683551	2.538884
28.H	2.213318	2.820370	-1.237352
29.H	2.034647	0.683551	-2.538884
30.H	2.213318	2.820370	1.237352
31.H	1.881289	-2.281297	2.177398
32.H	1.822032	-3.839043	0.000000
33.H	1.881289	-2.281297	-2.177398

Mo(η^5-Ind)(η^6-Ind) (C_S) S = 1, E_T (BP86) = -209.397, E_T (B3LYP/BP86) = -245.906.

Atom	X	Y	Z
1.Mo	0.221650	0.805881	0.000000
2.C	-2.090175	0.316950	0.725735
3.C	-2.090175	0.316950	-0.725735
4.C	-1.641402	1.614986	-1.166243
5.C	-1.430709	2.422194	0.000000
6.C	-1.641402	1.614986	1.166243
7.C	-2.477577	-0.857015	-1.428455
8.C	-2.877915	-1.967209	-0.711771
9.C	-2.877915	-1.967209	0.711771
10.C	-2.477577	-0.857015	1.428455
11.H	-1.588166	1.954022	-2.196304
12.H	-1.174094	3.477476	0.000000
13.H	-1.588166	1.954022	2.196304
14.H	-2.482850	-0.867238	-2.518577
15.H	-3.197380	-2.863242	-1.244185
16.H	-3.197380	-2.863242	1.244185
17.H	-2.482850	-0.867238	2.518577
18.C	2.068851	-0.620348	0.736401
19.C	2.065911	0.620119	1.447285
20.C	2.160981	1.838501	0.717058
21.C	2.160981	1.838501	-0.717058
22.C	2.065911	0.620119	-1.447285
23.C	2.068851	-0.620348	-0.736401
24.C	2.025611	-1.981864	1.155466
25.C	2.022423	-2.786525	0.000000
26.C	2.025611	-1.981864	-1.155466
27.H	2.037451	0.639295	2.535902
28.H	2.181002	2.788956	-1.248839
29.H	2.037451	0.639295	-2.535902
30.H	2.181002	2.788956	1.248839
31.H	2.006334	-2.327933	2.185067
32.H	2.000482	-3.874406	0.000000

33.H	2.006334	-2.327933	-2.185067

Mo(η^6-Ind)$_2$ (C_2) S = 0, E_T (BP86) = -209.236, E_T (B3LYP/BP86) = -245.236.

Atom	X	Y	Z
1.Mo	0.000000	0.000000	-0.080495
2.C	2.005437	-0.262343	-1.403087
3.C	2.013567	-1.258274	-0.330490
4.C	1.876308	-0.838934	1.030160
5.C	1.821880	0.548022	1.315975
6.C	1.819633	1.516357	0.270207
7.C	1.856970	1.125875	-1.084139
8.C	2.157119	-2.540601	-0.949979
9.C	2.251467	-2.343218	-2.335971
10.C	2.126723	-0.968858	-2.632373
11.H	1.881099	-1.566305	1.842924
12.H	1.743643	0.883824	2.350903
13.H	1.727160	2.573026	0.524204
14.H	1.827530	1.878646	-1.872422
15.H	2.196056	-3.495119	-0.430181
16.H	2.361543	-3.134131	-3.075511
17.H	2.118473	-0.522493	-3.623860
18.C	-2.005437	0.262343	-1.403087
19.C	-2.013567	1.258274	-0.330490
20.C	-1.876308	0.838934	1.030160
21.C	-1.821880	-0.548022	1.315975
22.C	-1.819633	-1.516357	0.270207
23.C	-1.856970	-1.125875	-1.084139
24.C	-2.157119	2.540601	-0.949979
25.C	-2.251467	2.343218	-2.335971
26.C	-2.126723	0.968858	-2.632373
27.H	-1.881099	1.566305	1.842924
28.H	-1.743643	-0.883824	2.350903
29.H	-1.727160	-2.573026	0.524204
30.H	-1.827530	-1.878646	-1.872422
31.H	-2.196056	3.495119	-0.430181
32.H	-2.361543	3.134131	-3.075511
33.H	-2.118473	0.522493	-3.623860

Compounds for TNE = 25

Mn(η^5-Ind)$_2$ (C_2) S = 5/2, E_T (BP86) = -209.635, E_T (B3LYP/BP86) = -248.832.

Atom	X	Y	Z
1.Mn	0.000000	0.000000	-0.037947
2.C	2.296003	-0.269925	-1.144610
3.C	2.389243	-1.308083	-0.130439
4.C	2.163162	-0.692065	1.147685
5.C	1.968245	0.697235	0.936293
6.C	1.992974	0.974947	-0.473382
7.C	2.654288	-2.644282	-0.519513
8.C	2.848559	-2.933244	-1.862317
9.C	2.771306	-1.916644	-2.850093
10.C	2.490008	-0.601298	-2.507895
11.H	2.175542	-1.192408	2.112922

12.H	1.846039	1.444133	1.718444
13.H	1.985669	1.962828	-0.927756
14.H	2.723765	-3.433659	0.232015
15.H	3.070262	-3.957176	-2.168457
16.H	2.939997	-2.176701	-3.896202
17.H	2.434054	0.172285	-3.276844
18.C	-2.296003	0.269925	-1.144610
19.C	-2.389243	1.308083	-0.130439
20.C	-2.163162	0.692065	1.147685
21.C	-1.968245	-0.697235	0.936293
22.C	-1.992974	-0.974947	-0.473382
23.C	-2.654288	2.644282	-0.519513
24.C	-2.848559	2.933244	-1.862317
25.C	-2.771306	1.916644	-2.850093
26.C	-2.490008	0.601298	-2.507895
27.H	-2.175542	1.192408	2.112922
28.H	-1.846039	-1.444133	1.718444
29.H	-1.985669	-1.962828	-0.927756
30.H	-2.723765	3.433659	0.232015
31.H	-3.070262	3.957176	-2.168457
32.H	-2.939997	2.176701	-3.896202
33.H	-2.434054	-0.172285	-3.276844

$Mn(\eta^5\text{-Ind})_2$ (C_{2h}) S = 3/2, E_T (BP86) = -209.913, E_T (B3LYP/BP86) = -248.496.

Atom	X	Y	Z
1.Mn	0.000000	0.000000	0.000000
2.C	0.997442	-1.861645	0.000000
3.C	0.154420	-1.851359	-1.162279
4.C	-1.216311	-2.081898	-0.721397
5.C	-1.216311	-2.081898	0.721397
6.C	0.154420	-1.851359	1.162279
7.C	-3.605649	-2.432540	-0.705035
8.C	-2.424548	-2.248021	-1.424086
9.C	-3.605649	-2.432540	0.705035
10.C	-2.424548	-2.248021	1.424086
11.H	2.084648	-1.849323	0.000000
12.H	0.497119	-1.884330	-2.193296
13.H	0.497119	-1.884330	2.193296
14.H	-4.544079	-2.584348	-1.240360
15.H	-2.434464	-2.246284	-2.515703
16.H	-4.544079	-2.584348	1.240360
17.H	-2.434464	-2.246284	2.515703
18.C	1.216311	2.081898	0.721397
19.C	-0.154420	1.851359	1.162279
20.C	-0.997442	1.861645	0.000000
21.C	-0.154420	1.851359	-1.162279
22.C	1.216311	2.081898	-0.721397
23.C	3.605649	2.432540	-0.705035
24.C	2.424548	2.248021	-1.424086
25.C	3.605649	2.432540	0.705035
26.C	2.424548	2.248021	1.424086
27.H	-2.084648	1.849323	0.000000
28.H	-0.497119	1.884330	2.193296
29.H	-0.497119	1.884330	-2.193296

30.H	4.544079	2.584348	-1.240360
31.H	2.434464	2.246284	-2.515703
32.H	4.544079	2.584348	1.240360
33.H	2.434464	2.246284	2.515703

Mn(η^5-Ind)$_2$ (C_{2v}) S = 1/2, E_T (BP86) = -209.973, E_T (B3LYP/BP86) = -248.234.

Atom	X	Y	Z
1.Mn	0.000000	0.000000	0.900353
2.C	-0.725478	1.972728	0.064079
3.C	0.725478	1.972728	0.064079
4.C	1.167508	1.705208	1.408828
5.C	0.000000	1.602532	2.239481
6.C	-1.167508	1.705208	1.408828
7.C	1.429110	2.150389	-1.159729
8.C	0.711453	2.362458	-2.322767
9.C	-0.711453	2.362458	-2.322767
10.C	-1.429110	2.150389	-1.159729
11.H	2.199550	1.681058	1.748818
12.H	0.000000	1.476422	3.319150
13.H	-2.199550	1.681058	1.748818
14.H	2.520499	2.144260	-1.169272
15.H	1.241579	2.521273	-3.262977
16.H	-1.241579	2.521273	-3.262977
17.H	-2.520499	2.144260	-1.169272
18.C	-0.725478	-1.972728	0.064079
19.C	-1.167508	-1.705208	1.408828
20.C	0.000000	-1.602532	2.239481
21.C	1.167508	-1.705208	1.408828
22.C	0.725478	-1.972728	0.064079
23.C	-1.429110	-2.150389	-1.159729
24.C	-0.711453	-2.362458	-2.322767
25.C	0.711453	-2.362458	-2.322767
26.C	1.429110	-2.150389	-1.159729
27.H	0.000000	-1.476422	3.319150
28.H	2.199550	-1.681058	1.748818
29.H	-2.199550	-1.681058	1.748818
30.H	-2.520499	-2.144260	-1.169272
31.H	-1.241579	-2.521273	-3.262977
32.H	1.241579	-2.521273	-3.262977
33.H	2.520499	-2.144260	-1.169272

Re(η^5-Ind)$_2$ (C_{2v}) S = 1/2, E_T (BP86) = -212.019, E_T (B3LYP/BP86) = -247.871.

Atom	X	Y	Z
1.Re	0.000000	0.000000	0.949639
2.C	-0.726161	2.008275	0.045142
3.C	0.726161	2.008275	0.045142
4.C	1.169332	1.863390	1.413213
5.C	0.000000	1.839141	2.244755
6.C	-1.169332	1.863390	1.413213
7.C	1.428598	2.012598	-1.188292
8.C	0.709494	2.064135	-2.371210
9.C	-0.709494	2.064135	-2.371210
10.C	-1.428598	2.012598	-1.188292

11.H	2.191842	1.926453	1.762827
12.H	0.000000	1.840658	3.328666
13.H	-2.191842	1.926453	1.762827
14.H	2.517485	1.977981	-1.198760
15.H	1.240979	2.082722	-3.323420
16.H	-1.240979	2.082722	-3.323420
17.H	-2.517485	1.977981	-1.198760
18.C	-0.726161	-2.008275	0.045142
19.C	-1.169332	-1.863390	1.413213
20.C	0.000000	-1.839141	2.244755
21.C	1.169332	-1.863390	1.413213
22.C	0.726161	-2.008275	0.045142
23.C	-1.428598	-2.012598	-1.188292
24.C	-0.709494	-2.064135	-2.371210
25.C	0.709494	-2.064135	-2.371210
26.C	1.428598	-2.012598	-1.188292
27.H	0.000000	-1.840658	3.328666
28.H	2.191842	-1.926453	1.762827
29.H	-2.191842	-1.926453	1.762827
30.H	-2.517485	-1.977981	-1.198760
31.H	-1.240979	-2.082722	-3.323420
32.H	1.240979	-2.082722	-3.323420
33.H	2.517485	-1.977981	-1.198760

Re(η^5-Ind)(η^6-Ind) (C_S) S = 1/2, E_T (BP86) = -211.858, E_T (B3LYP/BP86) = -247.625.

Atom	X	Y	Z
1.Re	0.241567	0.861689	0.000000
2.C	-1.879854	0.208535	0.727371
3.C	-1.879854	0.208535	-0.727371
4.C	-1.569422	1.551761	-1.165261
5.C	-1.449343	2.377398	0.000000
6.C	-1.569422	1.551761	1.165261
7.C	-2.147094	-0.998591	-1.432290
8.C	-2.407830	-2.144817	-0.712880
9.C	-2.407830	-2.144817	0.712880
10.C	-2.147094	-0.998591	1.432290
11.H	-1.580604	1.903445	-2.189654
12.H	-1.321343	3.453681	0.000000
13.H	-1.580604	1.903445	2.189654
14.H	-2.143061	-1.010749	-2.521685
15.H	-2.620285	-3.076109	-1.240218
16.H	-2.620285	-3.076109	1.240218
17.H	-2.143061	-1.010749	2.521685
18.C	1.800116	-0.686062	0.729317
19.C	1.987973	0.527656	1.442733
20.C	2.206550	1.727466	0.713045
21.C	2.206550	1.727466	-0.713045
22.C	1.987973	0.527656	-1.442733
23.C	1.800116	-0.686062	-0.729317
24.C	1.566802	-2.042261	1.150339
25.C	1.445607	-2.836866	0.000000
26.C	1.566802	-2.042261	-1.150339
27.H	2.002598	0.541998	2.530182
28.H	2.370123	2.661482	-1.245587

29.H	2.002598	0.541998	-2.530182
30.H	2.370123	2.661482	1.245587
31.H	1.467772	-2.377198	2.179136
32.H	1.255516	-3.908796	0.000000
33.H	1.467772	-2.377198	-2.179136

Re(η^6-Ind) (C_{2h}) S = 1/2, E_T (BP86) = -211.499, E_T (B3LYP/BP86) = -247.062.

Atom	X	Y	Z
1.Re	0.000000	0.000000	0.000000
2.C	2.006135	0.973522	-0.735500
3.C	2.006135	0.973522	0.735500
4.C	0.909616	1.550632	1.438680
5.C	-0.141832	2.165737	0.714634
6.C	-0.141832	2.165737	-0.714634
7.C	0.909616	1.550632	-1.438680
8.C	3.223040	0.360977	1.154983
9.C	3.945298	0.018674	0.000000
10.C	3.223040	0.360977	-1.154983
11.H	0.892428	1.556655	2.526795
12.H	-0.981075	2.607463	1.247165
13.H	-0.981075	2.607463	-1.247165
14.H	0.892428	1.556655	-2.526795
15.H	3.526642	0.187496	2.183156
16.H	4.924390	-0.457961	0.000000
17.H	3.526642	0.187496	-2.183156
18.C	0.141832	-2.165737	-0.714634
19.C	-0.909616	-1.550632	-1.438680
20.C	-2.006135	-0.973522	-0.735500
21.C	-2.006135	-0.973522	0.735500
22.C	-0.909616	-1.550632	1.438680
23.C	0.141832	-2.165737	0.714634
24.C	-3.223040	-0.360977	1.154983
25.C	-3.945298	-0.018674	0.000000
26.C	-3.223040	-0.360977	-1.154983
27.H	0.981075	-2.607463	-1.247165
28.H	0.981075	-2.607463	1.247165
29.H	-0.892428	-1.556655	2.526795
30.H	-0.892428	-1.556655	-2.526795
31.H	-3.526642	-0.187496	2.183156
32.H	-4.924390	0.457961	0.000000
33.H	-3.526642	-0.187496	-2.183156

Compounds for TNE = 26

Fe(η^5-Ind)$_2$ (C_{2v}) S = 0, E_T (BP86) = -209.776, E_T (B3LYP/BP86) = -247.836.

Atom	X	Y	Z
1.Fe	0.000000	0.000000	0.997801
2.C	-0.730645	1.785963	0.040862
3.C	0.730645	1.785963	0.040862
4.C	1.167719	1.670395	1.408502
5.C	0.000000	1.643862	2.243907
6.C	-1.167719	1.670395	1.408502
7.C	1.433515	1.877478	-1.199175

8.C	0.716291	1.983930	-2.369003
9.C	-0.716291	1.983930	-2.369003
10.C	-1.433515	1.877478	-1.199175
11.H	2.198544	1.652459	1.752751
12.H	0.000000	1.592920	3.329627
13.H	-2.198544	1.652459	1.752751
14.H	2.524925	1.895937	-1.208308
15.H	1.243402	2.079587	-3.319529
16.H	-1.243402	2.079587	-3.319529
17.H	-2.524925	1.895937	-1.208308
18.C	-0.730645	-1.785963	0.040862
19.C	-1.167719	-1.670395	1.408502
20.C	0.000000	-1.643862	2.243907
21.C	1.167719	-1.670395	1.408502
22.C	0.730645	-1.785963	0.040862
23.C	-1.433515	-1.877478	-1.199175
24.C	-0.716291	-1.983930	-2.369003
25.C	0.716291	-1.983930	-2.369003
26.C	1.433515	-1.877478	-1.199175
27.H	0.000000	-1.592920	3.329627
28.H	2.198544	-1.652459	1.752751
29.H	-2.198544	-1.652459	1.752751
30.H	-2.524925	-1.895937	-1.208308
31.H	-1.243402	-2.079587	-3.319529
32.H	1.243402	-2.079587	-3.319529
33.H	2.524925	-1.895937	-1.208308

Fe(η^5-Ind)(η^6-Ind) (C_s) S = 0, E_T (BP86) = -209.260, E_T (B3LYP/BP86) = -247.100

Atom	X	Y	Z
1.Fe	0.617969	0.930405	0.000000
2.C	-1.426511	1.046387	0.729198
3.C	-1.426511	1.046387	-0.729198
4.C	-0.610807	2.151073	-1.164859
5.C	-0.150792	2.849972	0.000000
6.C	-0.610807	2.151073	1.164859
7.C	-2.145357	0.037244	-1.434324
8.C	-2.830016	-0.916352	-0.715184
9.C	-2.830016	-0.916352	0.715184
10.C	-2.145357	0.037244	1.434324
11.H	-0.411497	2.431055	-2.196308
12.H	0.455432	3.752672	0.000000
13.H	-0.411497	2.431055	2.196308
14.H	-2.159671	0.034424	-2.525550
15.H	-3.388169	-1.691503	-1.241985
16.H	-3.388169	-1.691503	1.241985
17.H	-2.159671	0.034424	2.525550
18.C	1.441733	-1.160359	0.744792
19.C	1.926717	-0.018334	1.432525
20.C	2.551383	1.043232	0.716456
21.C	2.551383	1.043232	-0.716456
22.C	1.926717	-0.018334	-1.432525
23.C	1.441733	-1.160359	-0.744792

24.C	0.834561	-2.364483	1.163844
25.C	0.493338	-3.085781	0.000000
26.C	0.834561	-2.364483	-1.163844
27.H	1.856778	0.042690	2.519899
28.H	2.958033	1.899807	-1.255184
29.H	1.856778	0.042690	-2.519899
30.H	2.958033	1.899807	1.255184
31.H	0.681122	-2.682360	2.192081
32.H	0.037350	-4.075646	0.000000
33.H	0.681122	-2.682360	-2.192081

Fe(η^5-Ind)$_2$ (C_{2v}) S = 1, E_T (BP86) = -209.396, E_T (B3LYP/BP86) = -248.022.

Atom	X	Y	Z
1.Fe	0.000000	0.000000	1.047153
2.C	-0.721975	2.000582	0.017458
3.C	0.721975	2.000582	0.017458
4.C	1.157567	1.776609	1.386882
5.C	0.000000	1.768325	2.225179
6.C	-1.157567	1.776609	1.386882
7.C	1.426175	2.144484	-1.196511
8.C	0.705827	2.319155	-2.376067
9.C	-0.705827	2.319155	-2.376067
10.C	-1.426175	2.144484	-1.196511
11.H	2.190124	1.779090	1.726579
12.H	0.000000	1.728114	3.311169
13.H	-2.190124	1.779090	1.726579
14.H	2.517602	2.134753	-1.207521
15.H	1.239533	2.453447	-3.318153
16.H	-1.239533	2.453447	-3.318153
17.H	-2.517602	2.134753	-1.207521
18.C	-0.721975	-2.000582	0.017458
19.C	-1.157567	-1.776609	1.386882
20.C	0.000000	-1.768325	2.225179
21.C	1.157567	-1.776609	1.386882
22.C	0.721975	-2.000582	0.017458
23.C	-1.426175	-2.144484	-1.196511
24.C	-0.705827	-2.319155	-2.376067
25.C	0.705827	-2.319155	-2.376067
26.C	1.426175	-2.144484	-1.196511
27.H	0.000000	-1.728114	3.311169
28.H	2.190124	-1.779090	1.726579
29.H	-2.190124	-1.779090	1.726579
30.H	-2.517602	-2.134753	-1.207521
31.H	-1.239533	-2.453447	-3.318153
32.H	1.239533	-2.453447	-3.318153
33.H	2.517602	-2.134753	-1.207521

Fe(η^5-Ind)(η^6-Ind) (C_s) S = 1, E_T (BP86) = -208.854, E_T (B3LYP/BP86) = -247.207.

Atom	X	Y	Z
1.Fe	0.693264	0.855689	0.000000
2.C	-1.640142	1.018738	0.719479
3.C	-1.640142	1.018738	-0.719479
4.C	-0.681202	2.028966	-1.152613

5.C	-0.232282	2.744247	0.000000
6.C	-0.681202	2.028966	1.152613
7.C	-2.461733	0.123451	-1.425350
8.C	-3.297266	-0.731670	-0.703821
9.C	-3.297266	-0.731670	0.703821
10.C	-2.461733	0.123451	1.425350
11.H	-0.505798	2.319994	-2.186023
12.H	0.383623	3.640180	0.000000
13.H	-0.505798	2.319994	2.186023
14.H	-2.463357	0.114447	-2.516897
15.H	-3.960401	-1.414942	-1.236217
16.H	-3.960401	-1.414942	1.236217
17.H	-2.463357	0.114447	2.516897
18.C	1.635820	-1.129573	0.736674
19.C	2.145721	0.006471	1.423785
20.C	2.797607	1.047941	0.707378
21.C	2.797607	1.047941	-0.707378
22.C	2.145721	0.006471	-1.423785
23.C	1.635820	-1.129573	-0.736674
24.C	1.029804	-2.344681	1.156111
25.C	0.689090	-3.073993	0.000000
26.C	1.029804	-2.344681	-1.156111
27.H	2.093620	0.058308	2.512656
28.H	3.223416	1.892198	-1.249585
29.H	2.093620	0.058308	-2.512656
30.H	3.223416	1.892198	1.249585
31.H	0.864162	-2.654170	2.185680
32.H	0.214203	-4.053512	0.000000
33.H	0.864162	-2.654170	-2.185680

Ru(η^5-Ind)$_2$(C_{2v}) S = 0, E_T (BP86) = -209.046, E_T (B3LYP/BP86) = -248.022.

1.Ru	0.000000	0.000000	0.986361
2.C	-0.729894	1.973663	0.028791
3.C	0.729894	1.973663	0.028791
4.C	1.167587	1.867344	1.396868
5.C	0.000000	1.843871	2.232395
6.C	-1.167587	1.867344	1.396868
7.C	1.434866	2.091973	-1.209681
8.C	0.716609	2.215404	-2.376965
9.C	-0.716609	2.215404	-2.376965
10.C	-1.434866	2.091973	-1.209681
11.H	2.197419	1.887250	1.743630
12.H	0.000000	1.835632	3.319187
13.H	-2.197419	1.887250	1.743630
14.H	2.525633	2.102407	-1.218508
15.H	1.243496	2.321403	-3.326142
16.H	-1.243496	2.321403	-3.326142
17.H	-2.525633	2.102407	-1.218508
18.C	-0.729894	-1.973663	0.028791
19.C	-1.167587	-1.867344	1.396868
20.C	0.000000	-1.843871	2.232395
21.C	1.167587	-1.867344	1.396868
22.C	0.729894	-1.973663	0.028791

23.C	-1.434866	-2.091973	-1.209681
24.C	-0.716609	-2.215404	-2.376965
25.C	0.716609	-2.215404	-2.376965
26.C	1.434866	-2.091973	-1.209681
27.H	0.000000	-1.835632	3.319187
28.H	2.197419	-1.887250	1.743630
29.H	-2.197419	-1.887250	1.743630
30.H	-2.525633	-2.102407	-1.218508
31.H	-1.243496	-2.321403	-3.326142
32.H	1.243496	-2.321403	-3.326142
33.H	2.525633	-2.102407	-1.218508

Ru(η^5-Ind)(η^6-Ind) (C_S) S = 0, E_T (BP86) = -208.505, E_T (B3LYP/BP86) = -244.593.

1.Ru	0.176323	0.901845	-0.001383
2.C	-1.956382	0.272969	0.728751
3.C	-1.955642	0.270804	-0.728062
4.C	-1.606935	1.598978	-1.167135
5.C	-1.443429	2.422763	-0.003463
6.C	-1.606647	1.602678	1.162937
7.C	-2.277255	-0.927507	-1.432399
8.C	-2.591754	-2.057894	-0.711518
9.C	-2.593118	-2.055324	0.719143
10.C	-2.279460	-0.922626	1.437066
11.H	-1.571307	1.942163	-2.198152
12.H	-1.263617	3.494929	-0.005264
13.H	-1.568666	1.949199	2.192775
14.H	-2.283223	-0.937809	-2.523117
15.H	-2.846835	-2.979259	-1.236374
16.H	-2.849767	-2.974570	1.246966
17.H	-2.287000	-0.929034	2.527787
18.C	1.928457	-0.754097	0.746098
19.C	1.947546	0.484990	1.437121
20.C	2.106767	1.707308	0.721603
21.C	2.109741	1.708981	-0.714961
22.C	1.954405	0.488919	-1.434323
23.C	1.931185	-0.751459	-0.746185
24.C	1.857689	-2.100701	1.161909
25.C	1.837976	-2.894758	-0.004756
26.C	1.860869	-2.096140	-1.167757
27.H	1.903121	0.508033	2.527727
28.H	2.208388	2.651985	-1.253599
29.H	1.915126	0.514454	-2.524963
30.H	2.203597	2.648981	1.262767
31.H	1.839708	-2.455671	2.188889
32.H	1.816820	-3.984247	-0.006870
33.H	1.847682	-2.446893	-2.196183

Compounds for TNE = 27

Co(η^5-Ind)$_2$ (C_{2v}) S = 1/2, E_T (BP86) = -208.865, E_T (B3LYP/BP86) = -246.829.

Atom	X	Y	Z

1.Co	0.000000	0.000000	1.060339
2.C	-0.724397	1.880342	0.013196
3.C	0.724397	1.880342	0.013196
4.C	1.157529	1.724934	1.391585
5.C	0.000000	1.744218	2.230748
6.C	-1.157529	1.724934	1.391585
7.C	1.428911	1.987983	-1.208087
8.C	0.708641	2.110133	-2.389511
9.C	-0.708641	2.110133	-2.389511
10.C	-1.428911	1.987983	-1.208087
11.H	2.189115	1.717194	1.733388
12.H	0.000000	1.719448	3.316742
13.H	-2.189115	1.717194	1.733388
14.H	2.520458	1.987658	-1.217902
15.H	1.240406	2.208090	-3.336879
16.H	-1.240406	2.208090	-3.336879
17.H	-2.520458	1.987658	-1.217902
18.C	-0.724397	-1.880342	0.013196
19.C	-1.157529	-1.724934	1.391585
20.C	0.000000	-1.744218	2.230748
21.C	1.157529	-1.724934	1.391585
22.C	0.724397	-1.880342	0.013196
23.C	-1.428911	-1.987983	-1.208087
24.C	-0.708641	-2.110133	-2.389511
25.C	0.708641	-2.110133	-2.389511
26.C	1.428911	-1.987983	-1.208087
27.H	0.000000	-1.719448	3.316742
28.H	2.189115	-1.717194	1.733388
29.H	-2.189115	-1.717194	1.733388
30.H	-2.520458	-1.987658	-1.217902
31.H	-1.240406	-2.208090	-3.336879
32.H	1.240406	-2.208090	-3.336879
33.H	2.520458	-1.987658	-1.217902

Co(η^5-Ind)(η^6-Ind) (*C1*) S = 1/2, E_T (BP86) = -208.258, E_T (B3LYP/BP86) = -246.015.

Atom	X	Y	Z
1.Co	-0.272076	-0.174944	-0.108627
2.C	0.991331	0.116192	1.829893
3.C	0.456357	-1.223336	1.852649
4.C	-0.981381	-1.116317	1.623196
5.C	-1.334509	0.270413	1.619933
6.C	-0.125196	1.025096	1.597165
7.C	1.316286	-2.323116	2.035762
8.C	2.680251	-2.085168	2.203504
9.C	3.203999	-0.774814	2.172682
10.C	2.374893	0.329304	1.978576
11.H	-1.681571	-1.948240	1.619891
12.H	-2.341081	0.676414	1.561974
13.H	-0.053359	2.107373	1.518948
14.H	0.920212	-3.339864	2.060627
15.H	3.355942	-2.925552	2.368001
16.H	4.275633	-0.625011	2.310586
17.H	2.784704	1.339939	1.951464
18.C	1.131519	-0.351749	-1.812283

19.C	0.765902	1.022047	-1.822950
20.C	-0.677878	1.403032	-1.868990
21.C	-1.656553	0.377459	-1.841332
22.C	-1.260469	-0.978479	-1.822358
23.C	0.131582	-1.348657	-1.830555
24.C	-0.737003	2.812370	-1.876838
25.C	0.594020	3.287901	-1.853404
26.C	1.514300	2.223357	-1.803919
27.H	2.181769	-0.641578	-1.756085
28.H	-2.718651	0.626095	-1.812351
29.H	-2.016878	-1.762337	-1.789498
30.H	0.408926	-2.401734	-1.806756
31.H	-1.639638	3.417243	-1.906853
32.H	0.871697	4.341630	-1.870554
33.H	2.598229	2.301581	-1.786725

$Rh(\eta^5\text{-Ind})_2$ (C_{2v}) S = 1/2, E_T (BP86) = -207.550, E_T (B3LYP/BP86) = -243.602.

Atom	X	Y	Z
1.Rh	0.000000	0.000000	1.059542
2.C	-0.723969	2.106056	0.009849
3.C	0.723969	2.106056	0.009849
4.C	1.157366	1.918071	1.381728
5.C	0.000000	1.915637	2.219295
6.C	-1.157366	1.918071	1.381728
7.C	1.429588	2.278289	-1.202351
8.C	0.707922	2.465422	-2.375929
9.C	-0.707922	2.465422	-2.375929
10.C	-1.429588	2.278289	-1.202351
11.H	2.188855	1.935190	1.727180
12.H	0.000000	1.904917	3.305908
13.H	-2.188855	1.935190	1.727180
14.H	2.521016	2.281774	-1.211495
15.H	1.239666	2.621060	-3.315940
16.H	-1.239666	2.621060	-3.315940
17.H	-2.521016	2.281774	-1.211495
18.C	-0.723969	-2.106056	0.009849
19.C	-1.157366	-1.918071	1.381728
20.C	0.000000	-1.915637	2.219295
21.C	1.157366	-1.918071	1.381728
22.C	0.723969	-2.106056	0.009849
23.C	-1.429588	-2.278289	-1.202351
24.C	-0.707922	-2.465422	-2.375929
25.C	0.707922	-2.465422	-2.375929
26.C	1.429588	-2.278289	-1.202351
27.H	0.000000	-1.904917	3.305908
28.H	2.188855	-1.935190	1.727180
29.H	-2.188855	-1.935190	1.727180
30.H	-2.521016	-2.281774	-1.211495
31.H	-1.239666	-2.621060	-3.315940
32.H	1.239666	-2.621060	-3.315940
33.H	2.521016	-2.281774	-1.211495

Rh(η^5-Ind)(η^6-Ind) (C_S) S = 1/2, E_T (BP86) = -206.401, E_T (B3LYP/BP86) = -242.845.

Atom	X	Y	Z
1.Rh	0.185694	0.993905	0.000000
2.C	-2.111946	0.258648	0.722443
3.C	-2.111946	0.258648	-0.722443
4.C	-1.667081	1.574066	-1.155470
5.C	-1.527967	2.403622	0.000000
6.C	-1.667081	1.574066	1.155470
7.C	-2.506698	-0.894228	-1.428871
8.C	-2.917222	-2.012670	-0.705951
9.C	-2.917222	-2.012670	0.705951
10.C	-2.506698	-0.894228	1.428871
11.H	-1.629509	1.916475	-2.187581
12.H	-1.345223	3.474630	0.000000
13.H	-1.629509	1.916475	2.187581
14.H	-2.510062	-0.903108	-2.519843
15.H	-3.249535	-2.905416	-1.237314
16.H	-3.249535	-2.905416	1.237314
17.H	-2.510062	-0.903108	2.519843
18.C	2.122510	-0.806415	0.740016
19.C	2.037545	0.435301	1.416961
20.C	2.186872	1.667243	0.714148
21.C	2.186872	1.667243	-0.714148
22.C	2.037545	0.435301	-1.416961
23.C	2.122510	-0.806415	-0.740016
24.C	2.155685	-2.148680	1.162546
25.C	2.197203	-2.953198	0.000000
26.C	2.155685	-2.148680	-1.162546
27.H	1.970901	0.460216	2.507513
28.H	2.286532	2.603599	-1.262464
29.H	1.970901	0.460216	-2.507513
30.H	2.286532	2.603599	1.262464
31.H	2.163648	-2.501621	2.190711
32.H	2.260116	-4.040319	0.000000
33.H	2.163648	-2.501621	-2.190711

Compounds for TNE = 28

Ni(η^3-Ind)(η^3-Ind) (C_{2h}) S = 0, E_T (BP86) = -205.950, E_T (B3LYP/BP86) = -241.886.

Atom	X	Y	Z
1.Ni	0.000000	0.000000	0.000000
2.C	0.983168	-1.769972	0.000000
3.C	0.134528	-1.755842	-1.151686
4.C	-1.231727	-2.051069	-0.718303
5.C	-1.231727	-2.051069	0.718303
6.C	0.134528	-1.755842	1.151686
7.C	-3.593137	-2.544142	-0.702316
8.C	-2.418408	-2.288681	-1.422836
9.C	-3.593137	-2.544142	0.702316
10.C	-2.418408	-2.288681	1.422836
11.H	2.069144	-1.716123	0.000000
12.H	0.474900	-1.760751	-2.184879

13.H	0.474900	-1.760751	2.184879
14.H	-4.519481	-2.756290	-1.238223
15.H	-2.426662	-2.289972	-2.514790
16.H	-4.519481	-2.756290	1.238223
17.H	-2.426662	-2.289972	2.514790
18.C	1.231727	2.051069	0.718303
19.C	-0.134528	1.755842	1.151686
20.C	-0.983168	1.769972	0.000000
21.C	-0.134528	1.755842	-1.151686
22.C	1.231727	2.051069	-0.718303
23.C	3.593137	2.544142	-0.702316
24.C	2.418408	2.288681	-1.422836
25.C	3.593137	2.544142	0.702316
26.C	2.418408	2.288681	1.422836
27.H	-2.069144	1.716123	0.000000
28.H	-0.474900	1.760751	2.184879
29.H	-0.474900	1.760751	-2.184879
30.H	4.519481	2.756290	-1.238223
31.H	2.426662	2.289972	-2.514790
32.H	4.519481	2.756290	1.238223
33.H	2.426662	2.289972	2.514790

Ni(η^4-Ind)(η^3-Ind) (C_S) S = 0, E_T (BP86) = -205.542, E_T (B3LYP/BP86) = -240.894.

Atom	X	Y	Z
1.Ni	0.233036	1.258917	0.000000
2.C	-1.979936	0.157879	0.718252
3.C	-1.979936	0.157879	-0.718252
4.C	-1.557434	1.492566	-1.150277
5.C	-1.479002	2.337705	0.000000
6.C	-1.557434	1.492566	1.150277
7.C	-2.300880	-1.004189	-1.422893
8.C	-2.641132	-2.160309	-0.699782
9.C	-2.641132	-2.160309	0.699782
10.C	-2.300880	-1.004189	1.422893
11.H	-1.527116	1.834162	-2.182752
12.H	-1.363936	3.418917	0.000000
13.H	-1.527116	1.834162	2.182752
14.H	-2.291721	-1.017155	-2.514412
15.H	-2.904140	-3.072043	-1.237387
16.H	-2.904140	-3.072043	1.237387
17.H	-2.291721	-1.017155	2.514412
18.C	1.919022	-0.825775	0.731618
19.C	1.941229	0.406685	1.411212
20.C	2.164880	1.631818	0.712176
21.C	2.164880	1.631818	-0.712176
22.C	1.941229	0.406685	-1.411212
23.C	1.919022	-0.825775	-0.731618
24.C	1.819655	-2.176196	1.154939
25.C	1.782126	-2.985249	0.000000
26.C	1.819655	-2.176196	-1.154939
27.H	1.864386	0.434960	2.500611
28.H	2.337330	2.554279	-1.265193
29.H	1.864386	0.434960	-2.500611

30.H	2.337330	2.554279	1.265193
31.H	1.787711	-2.524991	2.184781
32.H	1.724928	-4.071952	0.000000
33.H	1.787711	-2.524991	-2.184781

Ni(η^3-Ind)(η^3-Ind) (C_{2h}) S = 1, E_T (BP86) = -205.698, E_T (B3LYP/BP86) = -241.886.

Atom	X	Y	Z
1.Ni	0.000000	0.000000	0.000000
2.C	1.106745	-1.816596	0.000000
3.C	0.280093	-1.871123	-1.165951
4.C	-1.081463	-2.023066	-0.729791
5.C	-1.081463	-2.023066	0.729791
6.C	0.280093	-1.871123	1.165951
7.C	-3.479239	-2.327443	-0.712149
8.C	-2.306586	-2.168429	-1.430623
9.C	-3.479239	-2.327443	0.712149
10.C	-2.306586	-2.168429	1.430623
11.H	2.192291	-1.757354	0.000000
12.H	0.628208	-1.867350	-2.195046
13.H	0.628208	-1.867350	2.195046
14.H	-4.423510	-2.463319	-1.241687
15.H	-2.317531	-2.178649	-2.522247
16.H	-4.423510	-2.463319	1.241687
17.H	-2.317531	-2.178649	2.522247
18.C	1.081463	2.023066	0.729791
19.C	-0.280093	1.871123	1.165951
20.C	-1.106745	1.816596	0.000000
21.C	-0.280093	1.871123	-1.165951
22.C	1.081463	2.023066	-0.729791
23.C	3.479239	2.327443	-0.712149
24.C	2.306586	2.168429	-1.430623
25.C	3.479239	2.327443	0.712149
26.C	2.306586	2.168429	1.430623
27.H	-2.192291	1.757354	0.000000
28.H	-0.628208	1.867350	2.195046
29.H	-0.628208	1.867350	-2.195046
30.H	4.423510	2.463319	-1.241687
31.H	2.317531	2.178649	-2.522247
32.H	4.423510	2.463319	1.241687
33.H	2.317531	2.178649	2.522247

Pd(η^3-Ind)(η^3-Ind) (C_{2h}) S = 0, E_T (BP86) = -203.381, E_T (B3LYP/BP86) = -237.628.

Atom	X	Y	Z
1.Pd	-0.003381	0.004770	0.001541
2.C	0.852400	-2.040358	-0.002050
3.C	0.012673	-2.022702	-1.153020
4.C	-1.357434	-2.306624	-0.717327
5.C	-1.356305	-2.310390	0.714891
6.C	0.013892	-2.025769	1.149801

7.C	-3.714704	-2.811425	-0.701432
8.C	-2.538942	-2.546434	-1.422298
9.C	-3.713042	-2.817328	0.700368
10.C	-2.535724	-2.558769	1.420497
11.H	1.938677	-2.025786	-0.002672
12.H	0.361816	-2.052286	-2.181987
13.H	0.363771	-2.059619	2.178429
14.H	-4.639478	-3.025177	-1.238867
15.H	-2.547332	-2.544214	-2.513997
16.H	-4.636254	-3.036603	1.238424
17.H	-2.542145	-2.564741	2.512223
18.C	1.358105	2.313636	0.714707
19.C	-0.013333	2.033534	1.149574
20.C	-0.851661	2.051821	-0.002344
21.C	-0.011748	2.030341	-1.153132
22.C	1.359467	2.310440	-0.717006
23.C	3.720039	2.796788	-0.701806
24.C	2.541071	2.546144	-1.423003
25.C	3.718106	2.803584	0.700065
26.C	2.537668	2.558433	1.420511
27.H	-1.937906	2.041489	-0.003231
28.H	-0.363453	2.068611	2.178111
29.H	-0.360453	2.060347	-2.182248
30.H	4.646675	3.002518	-1.239099
31.H	2.549336	2.542899	-2.514601
32.H	4.643108	3.015132	1.238171
33.H	2.543472	2.565708	2.512300

Pd(η^4-Ind)(η^3-Ind) (C_S) S = 0, E_T (BP86) = -202.775, E_T (B3LYP/BP86) = -236.892.

Atom	X	Y	Z
1.Pd	0.205781	1.394851	0.000000
2.C	-2.208846	0.126645	0.717053
3.C	-2.208846	0.126645	-0.717053
4.C	-1.864683	1.480835	-1.150859
5.C	-1.821473	2.319363	0.000000
6.C	-1.864683	1.480835	1.150859
7.C	-2.490920	-1.043463	-1.421345
8.C	-2.789518	-2.212735	-0.699675
9.C	-2.789518	-2.212735	0.699675
10.C	-2.490920	-1.043463	1.421345
11.H	-1.873503	1.828750	-2.180903
12.H	-1.767800	3.404723	0.000000
13.H	-1.873503	1.828750	2.180903
14.H	-2.485210	-1.054935	-2.512735
15.H	-3.023514	-3.131620	-1.238328
16.H	-3.023514	-3.131620	1.238328
17.H	-2.485210	-1.054935	2.512735
18.C	2.222340	-1.043617	0.728062
19.C	2.266588	0.169723	1.421243
20.C	2.387269	1.397641	0.714221
21.C	2.387269	1.397641	-0.714221
22.C	2.266588	0.169723	-1.421243
23.C	2.222340	-1.043617	-0.728062
24.C	2.109020	-2.399455	1.150671

25.C	2.052474	-3.210815	0.000000
26.C	2.109020	-2.399455	-1.150671
27.H	2.242900	0.188214	2.513272
28.H	2.600139	2.317265	-1.257601
29.H	2.242900	0.188214	-2.513272
30.H	2.600139	2.317265	1.257601
31.H	2.072226	-2.745007	2.181739
32.H	1.969735	-4.295544	0.000000
33.H	2.072226	-2.745007	-2.181739