

Endo- and exohedral chloro-fulleride as η^5 ligands: A DFT study on the first-row transition metal complexes

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1. Crystal structural of the reference complex, Mn(CO)₃Cp

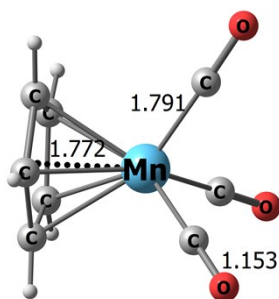


Fig. S1 Crystal structural of Mn(CO)₃Cp^{1,2}

2. Quantum Theory of Atoms In Molecules (QTAIM) analysis

The distance of interaction is labelled as d_1 for the metal Mn from the C atoms of the five membered ring, d_2 for Mn-CO distance, d_3 for C-O distance, d_4 for C-Cl distance and d_5 for C-C distance in C₆₀. QTAIM data analysis shows that the C-Cl interaction in the endohedral complex, Mn(CO)₃(η^5 -Cl@C₆₀) is purely non-covalent in nature, with avg. G/V value greater than one.³ In the case of the exohedral complex the ρ value for C-Cl bond critical point clearly indicates the covalent bonding. This is again supported by the parameters like the negative values of $\nabla^2\rho$ (-0.1068 a.u.) and H (-0.1384a.u.).

Table S1. QTAIM data of Mn(CO)₃ complexes. All values are given in a.u.

Complex	Parameter	avg. ρ	avg. $\nabla^2\rho$	V	G	avg. value of $ G/V $	avg. value of H
Mn(CO) ₃ (η^5 -C ₆₀)	d_1	0.0578	0.1844	-0.0705	0.0583	0.8270	-0.0122
	d_2	0.0193	0.0615	-0.0235	0.0194	0.2757	-0.0041
	d_3	0.4471	1.1129	-1.7511	1.0147	0.5794	-0.7364
	d_4	-	-	-	-	-	-
	d_5	0.2920	-0.7484	-0.3685	0.0907	0.2459	-0.2778
Mn(CO) ₃ (η^5 -Cl@C ₆₀)	d_1	0.0581	0.1922	-0.0714	0.0597	0.8367	-0.0117
	d_2	0.1478	0.6173	-0.2520	0.2031	0.8062	-0.0488
	d_3	0.4422	1.0622	-1.7182	0.9919	0.5773	-0.7263
	d_4	0.2930	-0.7555	-0.3704	0.0908	0.2582	-0.2797
	d_5	0.0069	0.0226	-0.0040	0.0048	1.2139	0.0008
Mn(CO) ₃ (η^5 -Cl-C ₆₀)	d_1	0.0608	0.2063	-0.0764	0.0640	0.8394	-0.0124
	d_2	0.1463	0.6167	-0.2495	0.2018	0.8091	-0.0476

d_3	0.4423	1.0609	-1.7184	0.9918	0.5772	-0.7266
d_4	0.2908	-0.7419	-0.3663	0.0904	0.2464	-0.2759
d_5	0.1513	-0.1068	-0.1384	0.0559	0.4036	-0.0826

3. Different exohedral complexes of $\text{Mn}(\text{CO})_3(\eta^5\text{-Cl-C}_{60})$

Variations in exohedral complex, $\text{Mn}(\text{CO})_3(\eta^5\text{-Cl-C}_{60})$ by changing the position of exohedral bonding of Cl^- with respect to the five membered ring attached to the metal fragment $[\text{Mn}(\text{CO})_3]^+$. When Cl^- is connected at $\alpha, \beta, \gamma, \delta, \epsilon, \zeta,$ and η positions the complexes are represented as A, B, C, D, E, F, and G respectively. Relative energies (kcal/mol) of each complex with respect to complex A with Cl^- at the α -position is given in Table S3, which shows that A is the most stable form among the various possible exohedral complexes of $\text{Mn}(\text{CO})_3(\eta^5\text{-Cl-C}_{60})$.

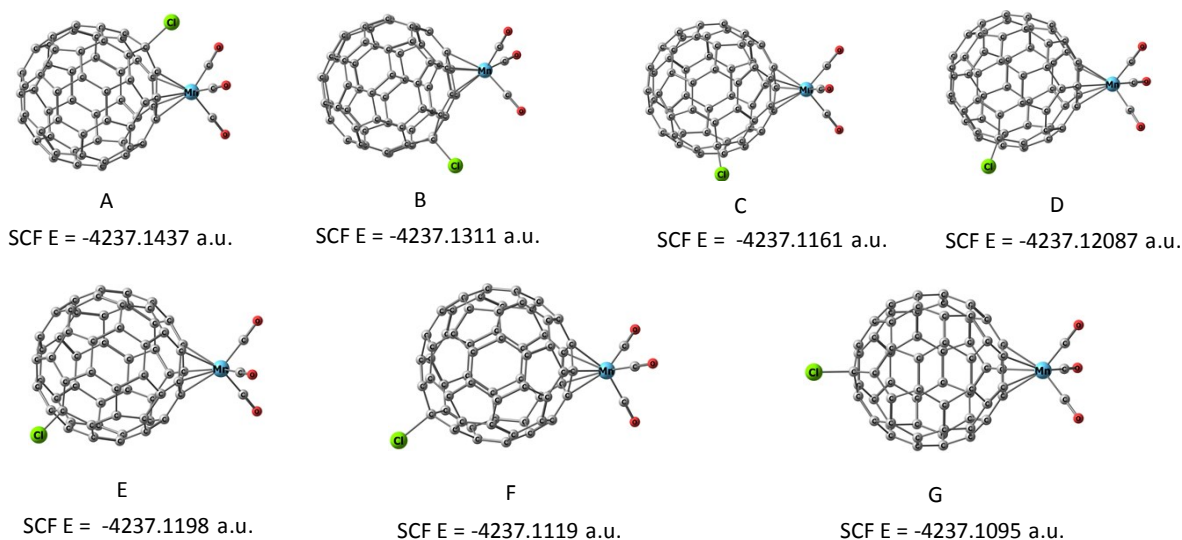


Fig. S2 The variations in exohedral bonding of Cl^- to C_{60} unit in $\text{Mn}(\text{CO})_3(\eta^5\text{-Cl-C}_{60})$ with their respective SCF energies in a.u.

Table S2. Relative energies in kcal/mol of the different exohedral complexes with respect to the most stable form A.

Complex	Relative energy (kcal/mol)
A	0
B	7.931977
C	17.35593
D	14.33415
E	15.01056
F	19.95949
G	21.46282

4. Cp⁻ complexes of the transition metals known in literature used in this study.

ful₂ScCO₄ (CAS Registry Number 209116-85-8)⁴
 CpTiCl₃ (CAS Registry Number 1270-98-0)^{5,6}
 CpTiCO₂Cl (CAS Registry Number 110141-99-6)⁷
 CpVCO₂ (CAS Registry Number 120610-59-5)⁸
 CpVCO₃ (CAS Registry Number 120610-58-4)⁹
 CpVCO₄ (CAS Registry Number 12108-04-2)^{10,11}
 CpCrCO₂Cl¹², CpCrCO₂H (CAS Registry Number 1384841-85-3)¹³ CpCrCO₂Cl
 CpMnNMe₃CO₂¹⁴, CpMnPMe₃CO₂¹⁵
 CpFeCO₂Cl, CpFeCO₂Br¹⁶
 CpCoCOPEt₃^{17,18}
 CpCoCONMe₃¹⁹
 CpNiPMe₃Cl (CAS Registry Number 85191-97-5)²⁰
 CpNiNEt₃Cl (CAS Registry Number 125026-88-2)²⁰
 CpCuPEt₃ (CAS Registry Number 12261-30-2)^{21,22}
 CpCuNMe₃ (CAS Registry Number 89989-39-9)²³
 CpCuCO (CAS Registry Number 31922-31-3)²⁴

5. Exceptional case of exohedral complexes of transition metals: Sc, Cu and Ti

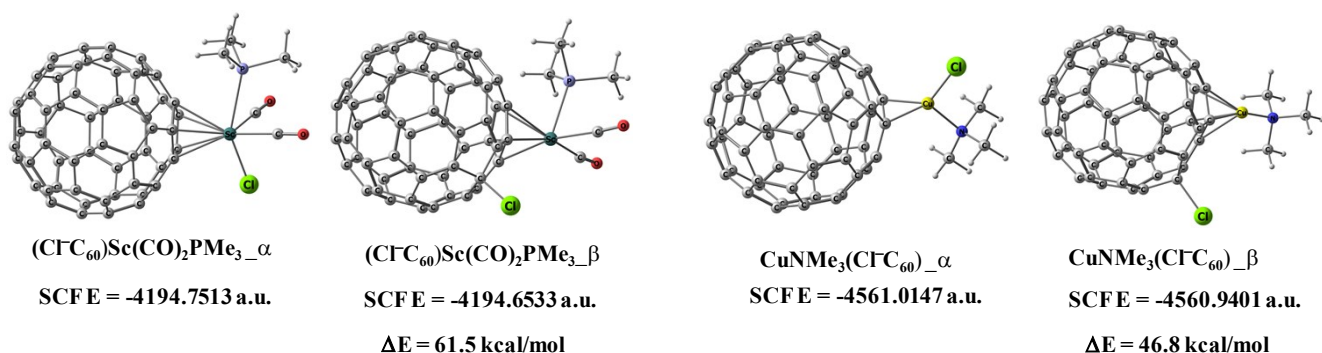


Fig. S3 Optimised geometries and SCF energy (a.u.) of [(Cl⁻C₆₀)Sc(CO)₂PMe₃] and [(Cl⁻C₆₀)CuNMe₃] with Cl⁻ at α and β positions. The difference in their SCF energies are given in kcal/mol.

In both the cases the α form is found to be more stabilized than corresponding β form with an energy difference of 61.5 kcal/mol for [(Cl⁻C₆₀)Sc(CO)₂PMe₃] and 46.8 kcal/mol for [(Cl⁻C₆₀)CuNMe₃]. In the case of Sc, α form has the metal coordinated to Cl⁻ also as another ligand. Here fullerene is not in the anionic form, but the negative charge resides in Cl⁻ itself. Whereas in the β form the exohedral anionic nature of the fullerene unit is reserved in the complexation and Cl⁻C₆₀ acts as the large anionic ligand. Similar is the observation with the Cu complex as well. In the case of TiCl₃, the non-bonded C₆₀...TiCl₄ is formed when the optimization is attempted for (Cl⁻C₆₀)(TiCl₃)⁺ with Cl⁻ at the α-position. Also, the optimization of the complex with Cl⁻ at the β-position yields the structure given in Fig. 5 wherein the fullerene part shows η¹ coordination with Ti. When the Cl⁻ is connected diametrically opposite to the metal coordination, η⁵ complex of [(Cl⁻C₆₀)(TiCl₃)⁺] is obtained.

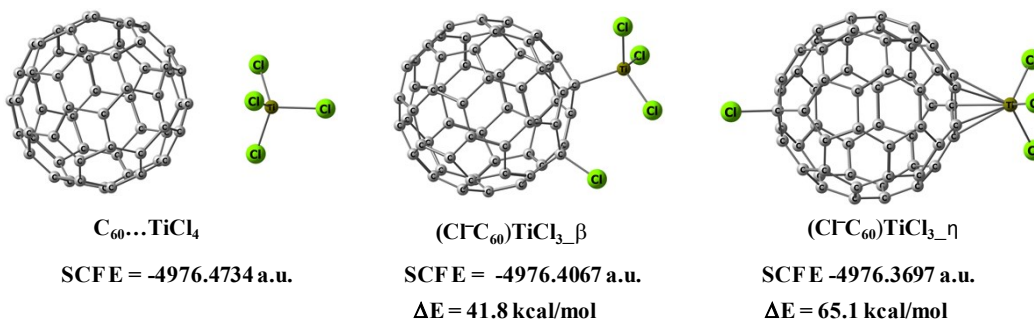


Fig. S4 Optimised geometries and SCF energy (a.u.) of $[(Cl^-C_{60})TiCl_3]$ with Cl^- at α , β and diametrically opposite to metal coordination (η) position. The difference in their SCF energies are given in kcal/mol.

6. Comparison of binding affinity of chloro-fulleride ligands in gas phase and solvent phase.

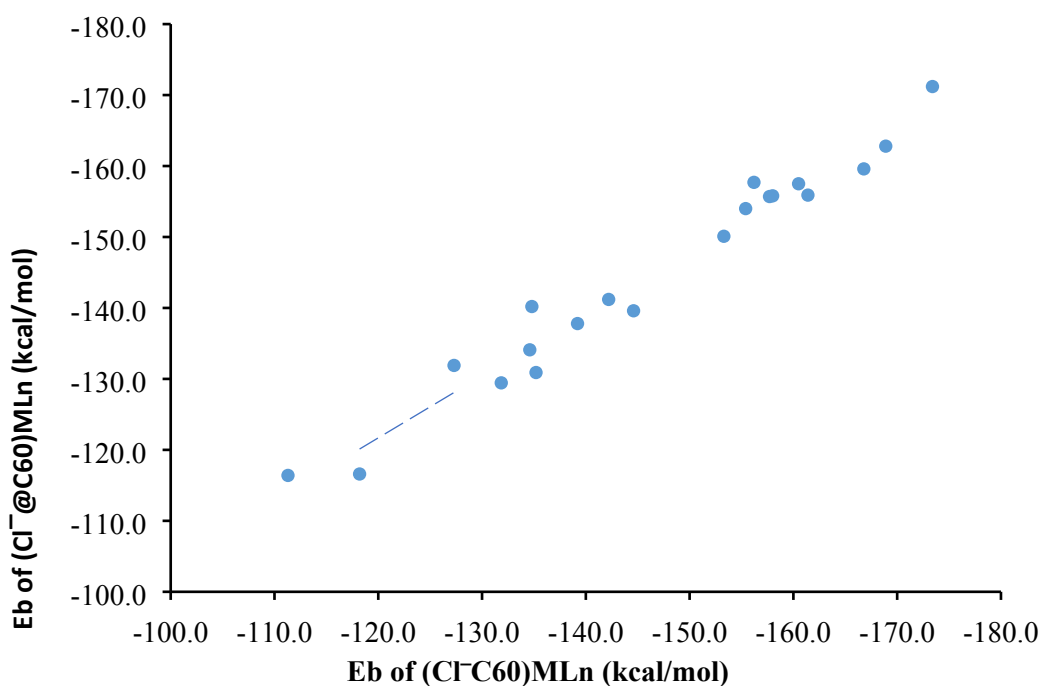


Fig. S5 Correlation between the E_b (kcal/mol) of $(Cl^-C_{60})ML_n$ against $(Cl^-@C_{60})ML_n$.

The E_b values of $(Cl^-C_{60})(ML_n)^+$ is having a good linear correlation (Fig.S5) with $(Cl^-@C_{60})(ML_n)^+$ with the correlation coefficient (R) of 0.9826. The correlation for the same complexes in gaseous state was having $R = 0.9834$. This similar values of R show that the trend in the complexation of the $(Cl^-@C_{60})(ML_n)^+$ and $(Cl^-C_{60})(ML_n)^+$ in gaseous state is conserved even under the influence of the solvent as well. This may be because in the ligands $Cl^-@C_{60}$ and Cl^-C_{60} , the negative charge is no longer on Cl atom alone but $Cl^-@C_{60}$ and Cl^-C_{60} are acting as the large anions with the extra electron delocalized over the whole fullerene unit.

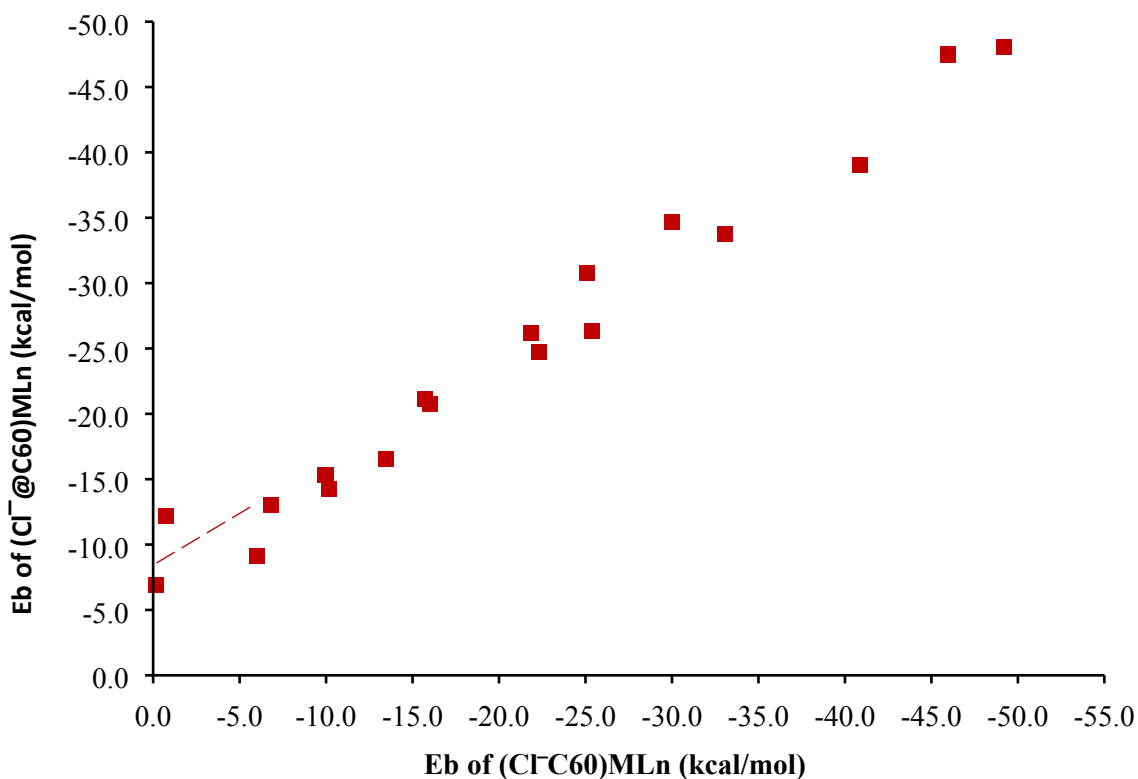


Fig. S6 Correlation between the E_{bs} (kcal/mol) of $(Cl^-@C_{60})ML_n$ against $(Cl^-@C_{60})ML_n$.

7. Comparison of binding affinity of chloro-fulleride ligands in η^6 and η^5 modes of coordination for Cr, Fe and Co complexes.

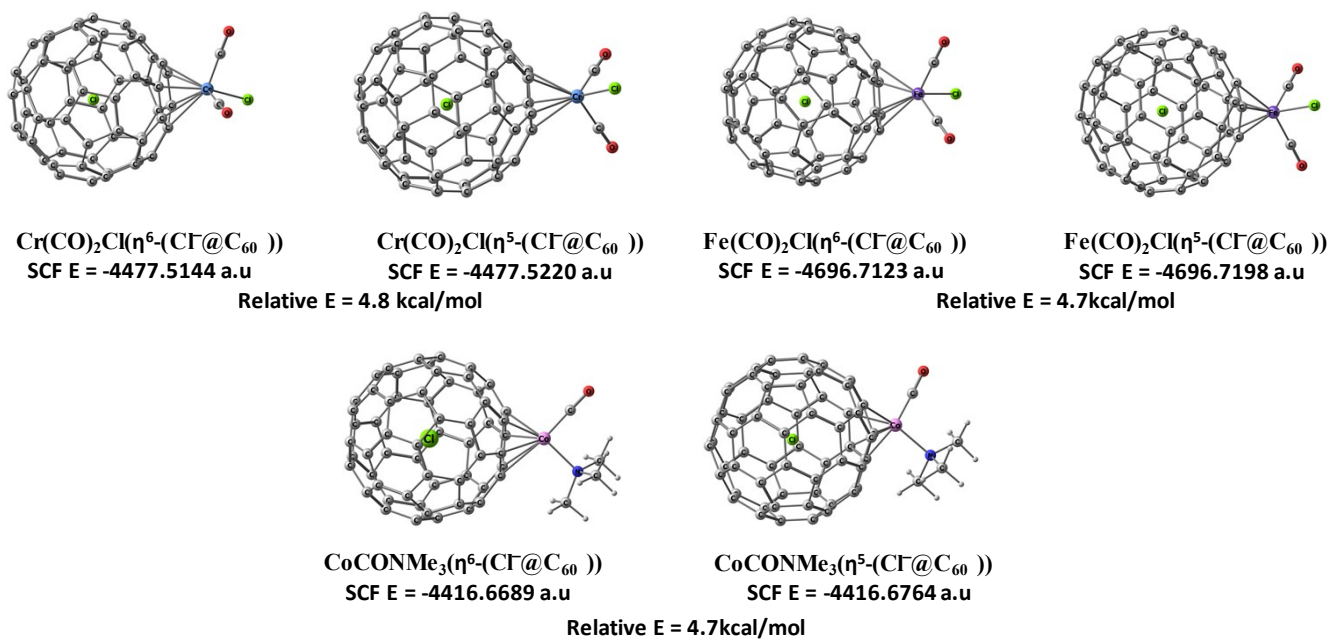


Fig. S7 Optimised geometries and SCF energy (a.u.) of $(Cl^-@C_{60})$ complexes of Cr, Fe, and Co in η^6 and η^5 modes of coordination.

8. Cartesian coordinates of optimized geometry of ligands Cp⁻, C₆₀, Cl⁻@C₆₀, Cl⁻C₆₀ at Mo6L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

Cp ⁻				C ₆₀			
6	0.686595000	-0.983427000	-0.000170000	6	-1.694235000	2.876716000	1.169945000
6	1.147387000	0.349077000	0.000089000	6	-1.015488000	3.388762000	0.000000000
6	0.022582000	1.199169000	0.000045000	6	-0.960156000	2.512413000	2.298722000
6	-1.133417000	0.392025000	0.000026000	6	0.373217000	3.517998000	0.000000000
6	-0.723145000	-0.956858000	-0.000073000	6	1.134317000	3.139925000	-1.170085000
1	-1.380692000	-1.826278000	0.000509000	6	-1.694235000	2.876716000	-1.169945000
1	-2.163722000	0.748146000	-0.000148000	6	-0.960156000	2.512413000	-2.298722000
1	0.043099000	2.289025000	-0.000137000	6	0.479726000	2.646349000	-2.298675000
1	2.190361000	0.666175000	-0.000045000	6	-2.355773000	0.506869000	2.590892000
1	1.310945000	-1.876986000	0.000324000	6	-3.116859000	0.884873000	1.420643000
				6	-1.296790000	1.305962000	3.021957000
				6	-2.791989000	2.048222000	0.723095000
				6	-2.791989000	2.048222000	-0.723095000
				6	-3.453682000	-0.321387000	0.697505000
				6	-3.453682000	-0.321387000	-0.697505000
				6	-3.116859000	0.884873000	-1.420643000
				6	0.064754000	-0.694450000	3.468855000
				6	-1.033200000	-1.522858000	3.021722000
				6	-0.064754000	0.694450000	3.468855000
				6	-2.221456000	-0.932987000	2.590584000
				6	-2.900087000	-1.444751000	1.420397000
				6	-0.479726000	-2.646349000	2.298675000
				6	-1.134317000	-3.139925000	1.170085000
				6	-2.366154000	-2.528337000	0.723070000
				6	2.221456000	0.932987000	2.590584000
				6	2.355773000	-0.506869000	2.590892000
				6	1.033200000	1.522858000	3.021722000
				6	1.296790000	-1.305962000	3.021957000
				6	0.960156000	-2.512413000	2.298722000
				6	3.116859000	-0.884873000	1.420643000
				6	2.791989000	-2.048222000	0.723095000
				6	1.694235000	-2.876716000	1.169945000
				6	1.134317000	3.139925000	1.170085000
				6	2.366154000	2.528337000	0.723070000
				6	0.479726000	2.646349000	2.298675000
				6	2.900087000	1.444751000	1.420397000
				6	3.453682000	0.321387000	0.697505000
				6	2.366154000	2.528337000	-0.723070000
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				6	3.453682000	0.321387000	-0.697505000
				6	1.694235000	-2.876716000	-1.169945000
				6	2.791989000	-2.048222000	-0.723095000
				6	3.116859000	-0.884873000	-1.420643000
				6	0.960156000	-2.512413000	-2.298722000
				6	-1.134317000	-3.139925000	-1.170085000
				6	-0.373217000	-3.517998000	0.000000000
				6	1.015488000	-3.388762000	0.000000000
				6	-0.479726000	-2.646349000	-2.298675000
				6	-2.221456000	-0.932987000	-2.590584000
				6	-2.900087000	-1.444751000	-1.420397000
				6	-2.366154000	-2.528337000	-0.723070000
				6	-1.033200000	-1.522858000	-3.021722000
				6	-0.064754000	0.694450000	-3.468855000
				6	-1.296790000	1.305962000	-3.021957000
				6	-2.355773000	0.506869000	-2.590892000
				6	0.064754000	-0.694450000	-3.468855000
				6	2.355773000	-0.506869000	-2.590892000
				6	2.221456000	0.932987000	-2.590584000
				6	1.033200000	1.522858000	-3.021722000

	6	1.296790000	-1.305962000	-3.021957000			
Cl ⁻ @C ₆₀	Cl ⁻ C ₆₀						
6	-0.194924000	3.374580000	1.039093000	6	-1.563033000	-2.644659000	1.462766000
6	-1.590454000	3.006658000	0.967021000	6	-2.334694000	-2.376697000	0.268142000
6	0.557331000	3.489766000	-0.129761000	6	-1.542514000	-1.715026000	2.504507000
6	-2.185378000	2.766747000	-0.271386000	6	-3.049518000	-1.186131000	0.155015000
6	-3.094585000	1.655183000	-0.433006000	6	-3.052970000	-0.458249000	-1.094452000
6	-1.883236000	2.143522000	2.088222000	6	-1.587311000	-2.880643000	-0.864703000
6	-2.761055000	1.070891000	1.932407000	6	-1.590638000	-2.177504000	-2.071107000
6	-3.377485000	0.822236000	0.649409000	6	-2.341422000	-0.945431000	-2.188584000
6	2.456156000	2.359492000	0.950655000	6	0.876917000	-2.072377000	2.808223000
6	1.676787000	2.240061000	2.161448000	6	0.855602000	-3.034240000	1.731284000
6	1.906228000	2.973009000	-0.174755000	6	-0.302465000	-1.422092000	3.183732000
6	0.374875000	2.738476000	2.204788000	6	-0.343779000	-3.311369000	1.068725000
6	-0.668557000	1.977778000	2.853029000	6	-0.358981000	-3.457159000	-0.370867000
6	1.982218000	0.963174000	2.764853000	6	2.079831000	-2.886675000	0.974668000
6	0.974917000	0.228999000	3.390551000	6	2.065166000	-3.027253000	-0.414376000
6	-0.373821000	0.745260000	3.435364000	6	0.826105000	-3.321135000	-1.100511000
6	2.883198000	1.244055000	-1.625530000	6	0.914024000	0.708987000	3.409930000
6	3.453022000	0.608542000	-0.459846000	6	2.132279000	0.036587000	3.014740000
6	2.123503000	2.405402000	-1.485608000	6	-0.283201000	-0.007934000	3.489901000
6	3.243317000	1.156388000	0.805656000	6	2.113741000	-1.327900000	2.719177000
6	2.950555000	0.293389000	1.927111000	6	2.858175000	-1.832074000	1.586022000
6	3.377552000	-0.822089000	-0.649341000	6	2.895275000	0.944939000	2.187394000
6	3.094603000	-1.654921000	0.433121000	6	3.614934000	0.458002000	1.094202000
6	2.877320000	-1.087418000	1.743938000	6	3.596359000	-0.955145000	0.788334000
6	0.496292000	1.569277000	-3.128891000	6	-1.502587000	1.849845000	2.436425000
6	1.283033000	0.366092000	-3.273710000	6	-0.264578000	2.588128000	2.346291000
6	0.908996000	2.571040000	-2.250640000	6	-1.511782000	0.571844000	2.999095000
6	2.455522000	0.206216000	-2.535470000	6	0.923591000	2.030699000	2.827684000
6	2.761142000	-1.070787000	-1.932348000	6	2.147584000	2.177667000	2.071212000
6	0.373880000	-0.745137000	-3.435320000	6	-0.268120000	3.316715000	1.096099000
6	0.668601000	-1.977693000	-2.853017000	6	0.916838000	3.463514000	0.368843000
6	1.883265000	-2.143395000	-2.088164000	6	2.144193000	2.880611000	0.864792000
6	-1.406128000	2.886090000	-1.482290000	6	-3.027413000	-0.222613000	1.233054000
6	-1.833641000	1.848137000	-2.392123000	6	-3.017490000	1.100326000	0.650006000
6	-0.059044000	3.241136000	-1.412786000	6	-2.292636000	-0.482342000	2.387974000
6	-0.899239000	1.201481000	-3.200718000	6	-2.273676000	2.119348000	1.241552000
6	-0.974860000	-0.228882000	-3.390400000	6	-1.508226000	3.027923000	0.414616000
6	-2.877260000	1.087548000	-1.743783000	6	-3.033167000	0.954877000	-0.788328000
6	-2.950438000	-0.293263000	-1.926951000	6	-2.303704000	1.833168000	-1.586870000
6	-1.982152000	-0.963067000	-2.764710000	6	-1.522692000	2.886520000	-0.974511000
6	0.194855000	-3.374378000	-1.039010000	6	2.120135000	2.645262000	-1.462953000
6	-0.374862000	-2.738448000	-2.204806000	6	0.901742000	3.317912000	-1.068019000
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6	-0.557410000	-3.489684000	0.129840000	6	2.099292000	1.714799000	-2.503783000
6	1.406146000	-2.885922000	1.482371000	6	3.590884000	0.222525000	-1.233398000
6	2.185296000	-2.766386000	0.271464000	6	3.611577000	1.185816000	-0.155079000
6	1.590366000	-3.006373000	-0.966916000	6	2.888620000	2.375417000	-0.267917000
6	0.059054000	-3.240962000	1.412830000	6	2.847197000	0.482132000	-2.386490000
6	-0.496249000	-1.569176000	3.129004000	6	2.059577000	-1.849424000	-2.436017000
6	0.899282000	-1.201387000	3.200882000	6	2.828574000	-2.118017000	-1.240737000
6	1.833695000	-1.848043000	2.392282000	6	3.581409000	-1.100785000	-0.650298000
6	-0.908967000	-2.570940000	2.250743000	6	2.068890000	-0.571784000	-2.999089000
6	-2.883112000	-1.243923000	1.625588000	6	-0.356047000	-0.705165000	-3.404531000
6	-2.455436000	-0.206089000	2.535533000	6	-0.365691000	-2.029317000	-2.821160000
6	-1.282967000	-0.365969000	3.273791000	6	0.822604000	-2.594154000	-2.347979000
6	-2.123489000	-2.405332000	1.485706000	6	0.841254000	0.010698000	-3.495592000
6	-2.456173000	-2.359512000	-0.950579000	6	-0.319059000	2.066641000	-2.805121000
6	-3.243199000	-1.156302000	-0.805549000	6	-1.556939000	1.328321000	-2.719646000
6	-3.452926000	-0.608422000	0.459913000	6	-1.575217000	-0.036521000	-3.014178000

6	-1.906335000	-2.973094000	0.174869000	6	0.860346000	1.421938000	-3.190213000
17	-0.000295000	-0.001266000	-0.000938000	17	-5.906679000	-0.000675000	-0.000649000

9. Cartesian coordinates of optimized geometry of CpML_n complexes at Mo6L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

CpScNMe₃(CO)₂				CpScPMe₃(CO)₂			
21	0.165302000	0.064846000	-0.000099000	21	-0.628725000	0.076819000	-0.496311000
7	-2.166173000	-0.142477000	-0.000161000	15	2.098354000	0.054761000	-0.372093000
8	1.066799000	2.339563000	-2.276747000	8	-0.406710000	2.362829000	1.923175000
8	1.066029000	2.338609000	2.277801000	8	-3.318623000	1.825169000	-1.459561000
6	0.716428000	1.547544000	-1.487867000	6	-0.466401000	1.596456000	1.038166000
6	0.715922000	1.546930000	1.488461000	6	-2.343558000	1.234729000	-1.202722000
6	-2.809041000	1.177606000	-0.000028000	6	2.910742000	1.701067000	-0.461055000
1	-2.503088000	1.736823000	0.888468000	1	2.831800000	2.118835000	-1.467845000
1	-2.503167000	1.736968000	-0.888460000	1	2.417180000	2.387376000	0.231736000
6	-2.534140000	-0.893714000	-1.207304000	6	2.559706000	-0.463292000	1.325591000
1	-2.026888000	-1.862849000	-1.197315000	1	2.212887000	-1.480206000	1.523372000
1	-3.620398000	-1.059886000	-1.266763000	1	3.644933000	-0.426523000	1.467999000
6	-2.534030000	-0.893894000	1.206907000	6	3.266752000	-0.959184000	-1.376409000
1	-3.620290000	-1.060022000	1.266466000	1	4.300877000	-0.846581000	-1.034291000
1	-2.208729000	-0.341408000	2.093411000	1	3.215389000	-0.667017000	-2.428213000
1	-2.026826000	-1.863050000	1.196700000	1	2.992009000	-2.015249000	-1.309202000
1	-3.906534000	1.091204000	0.000013000	1	3.970951000	1.636315000	-0.196364000
1	-2.208987000	-0.341072000	-2.093764000	1	2.076624000	0.203349000	2.043839000
6	2.393895000	-0.815938000	-0.705194000	6	-2.142213000	-0.820163000	1.159875000
6	1.372462000	-1.688282000	-1.152261000	6	-0.827426000	-1.274740000	1.475611000
6	0.734410000	-2.234279000	-0.000260000	6	-0.417432000	-2.158514000	0.438725000
6	1.372308000	-1.688454000	1.151910000	6	-1.464228000	-2.241095000	-0.508899000
6	2.393841000	-0.816084000	0.705091000	6	-2.527826000	-1.423893000	-0.066149000
1	1.140933000	-1.918312000	2.184559000	1	-0.269262000	-1.031991000	2.370463000
1	-0.048477000	-2.986319000	-0.000369000	1	0.523695000	-2.695548000	0.388730000
1	1.141211000	-1.917975000	-2.184975000	1	-1.452147000	-2.827566000	-1.420653000
1	3.044119000	-0.226111000	-1.338789000	1	-3.473120000	-1.282638000	-0.573536000
1	3.044029000	-0.226396000	1.338852000	1	-2.749921000	-0.159389000	1.762581000
CpSc(CO)₄				CpTi(CO)₂Cl			
6	0.644808000	-1.035293000	1.857954000	6	-1.651562000	-0.827841000	-1.153736000
6	1.178077000	0.274805000	1.836362000	6	-1.959107000	0.482117000	-0.705333000
6	-0.766208000	-0.938539000	1.831303000	6	-1.650981000	-0.826247000	1.154225000
6	-1.112606000	0.437721000	1.792370000	6	-1.469405000	-1.646650000	0.000732000
6	0.094639000	1.190767000	1.796089000	6	-1.958698000	0.483190000	0.704014000
21	0.008488000	-0.010961000	-0.309600000	22	0.236189000	-0.236352000	-0.000327000
6	-1.127878000	1.844770000	-0.890236000	17	2.161800000	-1.385094000	-0.001730000
8	-1.725566000	2.818472000	-1.068939000	8	0.755593000	1.939441000	2.300755000
6	1.137789000	-1.863685000	-0.928891000	8	0.754646000	1.944057000	-2.297402000
8	1.727009000	-2.831439000	-1.158104000	6	0.566234000	1.165016000	1.458864000
6	-1.864262000	-1.113649000	-0.907191000	6	0.565422000	1.167885000	-1.457093000
8	-2.851102000	-1.681220000	-1.109368000	1	-2.140920000	1.343433000	1.334514000
6	1.844813000	1.152172000	-0.907177000	1	-1.586617000	-1.143622000	2.186103000
8	2.800013000	1.770948000	-1.110924000	1	-1.223777000	-2.701140000	0.001365000
1	2.229172000	0.532691000	1.862496000	1	-1.587225000	-1.146557000	-2.185213000
1	1.217664000	-1.953149000	1.899723000	1	-2.141565000	1.341424000	-1.337040000
1	-1.459495000	-1.769655000	1.853213000				
1	-2.116711000	0.841575000	1.787471000				
1	0.173268000	2.270217000	1.793880000				
CpTiCl₃				CpV(CO)₂			
22	-0.212729000	0.002797000	-0.002505000				

17	-1.153564000	-1.389897000	-1.466865000	6	0.713189000	-1.417705000	1.020735000
17	-1.198598000	-0.525752000	1.925491000	6	-0.723935000	-1.412272000	1.020370000
17	-1.063343000	1.999444000	-0.512767000	6	1.151297000	-1.594702000	-0.324733000
6	1.758116000	-1.227420000	0.229862000	6	-0.005797000	-1.687619000	-1.133376000
6	1.785783000	-0.216331000	1.219973000	6	-1.162592000	-1.585824000	-0.325386000
6	1.813256000	1.033820000	0.564747000	23	0.001347000	0.303111000	-0.047513000
6	1.810402000	-0.599194000	-1.039914000	6	-1.594087000	1.376951000	-0.042386000
6	1.834565000	0.795720000	-0.834527000	8	-2.633477000	1.913336000	-0.011074000
1	1.717858000	-0.373366000	2.287046000	6	1.603965000	1.366433000	-0.042421000
1	1.770808000	2.005500000	1.038735000	8	2.646561000	1.896534000	-0.011089000
1	1.808993000	1.555615000	-1.603683000	1	-0.005745000	-1.753804000	-2.216379000
1	1.763906000	-1.102015000	-1.995639000	1	2.176784000	-1.654239000	-0.661652000
1	1.669326000	-2.291348000	0.408201000	1	1.357717000	-1.343324000	1.887471000
				1	-1.368328000	-1.333118000	1.886776000
				1	-2.188308000	-1.637599000	-0.662914000
CpV(CO)₃				CpV(CO)₄			
6	-1.924754000	1.150085000	-0.007506000	6	-2.001224000	-0.521707000	1.013121000
6	-2.252332000	0.000528000	-0.763132000	6	-1.984940000	0.870213000	0.761926000
6	-1.386619000	0.710617000	1.233418000	6	-1.919295000	-1.196145000	-0.229854000
6	-1.385847000	-0.716726000	1.230640000	6	-1.852056000	-0.215929000	-1.257356000
6	-1.923670000	-1.151790000	-0.012113000	6	-1.892810000	1.064863000	-0.639715000
23	-0.006370000	0.000107000	-0.326690000	23	-0.025267000	0.000245000	0.001276000
6	0.962759000	-1.620023000	-0.748812000	6	0.964633000	0.902611000	-1.400045000
8	1.522343000	-2.621635000	-0.952912000	8	1.530159000	1.448996000	-2.256124000
6	0.960218000	1.622081000	-0.748165000	6	0.857898000	-0.910269000	1.473272000
8	1.517656000	2.624871000	-0.952250000	8	1.362407000	-1.464408000	2.361345000
6	1.400379000	0.000582000	0.971493000	6	0.943958000	-1.434411000	-0.872382000
8	2.252310000	0.000837000	1.768526000	8	1.497248000	-2.304783000	-1.408469000
1	-1.059083000	-1.354703000	2.040070000	6	0.877642000	1.442201000	0.938594000
1	-1.059891000	1.345742000	2.045110000	8	1.393479000	2.318246000	1.501533000
1	-2.066231000	2.177158000	-0.315052000	1	-2.022798000	1.650222000	1.510669000
1	-2.643156000	0.002413000	-1.774491000	1	-2.051664000	-0.989529000	1.987367000
1	-2.064402000	-2.177772000	-0.323613000	1	-1.911035000	-2.268491000	-0.370897000
				1	-1.796930000	-0.409787000	-2.319811000
				1	-1.865618000	2.018985000	-1.148323000
CpCr(CO)₂Cl				CpCr(CO)₂H			
6	1.431650000	-0.992694000	-1.145328000	6	-1.468779000	1.233627000	0.409958000
6	1.052826000	-1.742266000	0.003893000	6	-0.927038000	0.304906000	1.353577000
6	2.104200000	0.186868000	0.700031000	6	-1.949434000	-0.885743000	-0.338826000
6	2.103959000	0.182946000	-0.703139000	6	-2.098235000	0.489810000	-0.617599000
6	1.432164000	-0.986396000	1.148962000	6	-1.220063000	-1.007453000	0.882353000
24	-0.018008000	0.109995000	-0.000434000	24	0.058809000	-0.015164000	-0.484412000
17	-0.315573000	2.301320000	-0.001935000	1	0.292754000	-1.286827000	-1.436611000
8	-2.180651000	-0.815209000	1.850866000	8	2.202659000	-1.949275000	0.210918000
8	-2.180632000	-0.819865000	-1.849585000	8	2.221185000	1.988076000	0.109384000
6	-1.341236000	-0.439086000	1.137478000	6	1.385644000	-1.160818000	-0.071053000
6	-1.341205000	-0.442097000	-1.137089000	6	1.374440000	1.226917000	-0.147403000
1	1.276133000	-1.285340000	-2.174894000	1	-1.424381000	2.312043000	0.478244000
1	2.465883000	0.982148000	-1.336714000	1	-2.564770000	0.904954000	-1.503317000
1	2.466437000	0.989571000	1.328963000	1	-2.315280000	-1.702018000	-0.945752000
1	1.277184000	-1.273709000	2.180109000	1	-0.957730000	-1.934354000	1.373767000
1	0.547410000	-2.698053000	0.006763000	1	-0.411972000	0.552265000	2.271103000
CpMn(CO)₂NMe₃				CpMn(CO)₂PMe₃			
25	0.387396000	0.163663000	0.000037000	25	-0.604715000	0.179437000	0.000266000
7	-1.669694000	-0.513282000	-0.000199000	15	1.539694000	-0.348823000	-0.001371000
8	-0.062088000	2.077353000	-2.178543000	8	-0.168304000	2.109987000	2.169451000
8	-0.062859000	2.076597000	2.179112000	8	-0.175121000	2.116017000	-2.164882000
6	0.074985000	1.322592000	-1.289489000	6	-0.322669000	1.353064000	1.286948000

6	0.074522000	1.322172000	1.289807000	6	-0.326100000	1.356322000	-1.284224000
6	-2.596376000	0.636546000	-0.000213000	6	2.701974000	1.060974000	-0.010031000
1	-2.423406000	1.247943000	0.886499000	1	2.522432000	1.673764000	-0.896977000
1	-2.423218000	1.248071000	-0.886801000	1	2.524216000	1.683085000	0.870788000
6	-1.953315000	-1.316019000	-1.202085000	6	2.154922000	-1.316783000	1.429877000
1	-1.309657000	-2.196919000	-1.225175000	1	1.616652000	-2.264757000	1.512215000
1	-3.003546000	-1.645261000	-1.216850000	1	3.225693000	-1.528755000	1.348082000
6	-1.953535000	-1.316191000	1.201512000	6	2.151116000	-1.331355000	-1.424338000
1	-3.003753000	-1.645483000	1.216014000	1	3.222378000	-1.541217000	-1.343586000
1	-1.754555000	-0.715101000	2.091201000	1	1.969170000	-0.773885000	-2.347031000
1	-1.309845000	-2.197070000	1.224615000	1	1.613797000	-2.280825000	-1.494751000
1	-3.640126000	0.287680000	-0.000345000	1	3.745401000	0.731428000	-0.009242000
1	-1.754112000	-0.714816000	-2.091644000	1	1.976387000	-0.749116000	2.347025000
6	2.330695000	-0.093584000	-0.708506000	6	-2.536877000	-0.261886000	0.704790000
6	1.542204000	-1.203880000	-1.155972000	6	-1.630059000	-1.271158000	1.155278000
6	1.072717000	-1.871404000	-0.000086000	6	-1.077040000	-1.889314000	0.004004000
6	1.542191000	-1.204168000	1.155926000	6	-1.624571000	-1.276213000	-1.152937000
6	2.330661000	-0.093727000	0.708807000	6	-2.533555000	-0.265239000	-0.710946000
1	2.840876000	0.617613000	1.344282000	1	-3.110595000	0.389654000	-1.349515000
1	2.841425000	0.617553000	-1.343794000	1	-1.399932000	-1.531245000	-2.179776000
1	1.362494000	-1.492016000	-2.182964000	1	-3.116701000	0.395996000	1.337707000
1	0.429815000	-2.744514000	-0.000206000	1	-1.409334000	-1.520766000	2.184303000
1	1.361651000	-1.491907000	2.182885000	1	-0.352520000	-2.695451000	0.007611000
CpMn(CO)₃				CpFe(CO)₂Br			
25	-0.054779000	0.001355000	-0.004389000	6	1.661947000	1.150479000	0.434752000
6	-1.061636000	-0.126922000	1.463385000	6	1.746032000	0.710630000	-0.927773000
8	-1.671488000	-0.214871000	2.449566000	6	1.661089000	-1.154645000	0.427085000
6	-1.017739000	1.363444000	-0.640856000	6	1.627141000	-0.004845000	1.250841000
8	-1.596700000	2.279904000	-1.062197000	6	1.745423000	-0.705829000	-0.932530000
6	-1.025786000	-1.224509000	-0.865461000	26	0.016838000	0.000333000	-0.094384000
8	-1.610083000	-2.052000000	-1.436749000	17	-1.354553000	-0.004581000	1.770324000
6	1.673478000	-0.073785000	1.224505000	8	-1.555556000	-2.170413000	-1.252700000
6	1.674233000	-1.178683000	0.332788000	8	-1.552983000	2.178767000	-1.241530000
6	1.702060000	-0.656225000	-0.995515000	6	-0.956843000	-1.297219000	-0.790986000
6	1.706582000	0.755251000	-0.916462000	6	-0.955376000	1.302512000	-0.784184000
6	1.683063000	1.123383000	0.463793000	1	1.786168000	-1.337754000	-1.809778000
1	1.635450000	-0.134784000	2.304131000	1	1.621983000	-2.181196000	0.762882000
1	1.666690000	-2.223771000	0.608183000	1	1.787421000	1.348382000	-1.800774000
1	1.698322000	-1.240782000	-1.905603000	1	1.623970000	2.174788000	0.777432000
1	1.708786000	1.438726000	-1.754594000	1	1.461909000	-0.008316000	2.319322000
1	1.680865000	2.130752000	0.855586000				
CpFe(CO)₂Cl				CpCoCONMe₃			
6	-1.504735000	-1.144099000	-1.152408000	27	-0.358100000	0.208449000	-0.000192000
6	-2.310972000	-0.044480000	-0.708540000	7	1.606186000	-0.391932000	0.000004000
6	-1.505395000	-1.143544000	1.152553000	8	0.223600000	3.031349000	-0.000034000
6	-1.033517000	-1.816591000	0.000388000	6	0.001077000	1.878063000	-0.000117000
6	-2.311347000	-0.044090000	0.707705000	6	2.576959000	0.720980000	-0.003878000
26	-0.402337000	0.185635000	0.000025000	1	2.423446000	1.337646000	-0.890468000
35	1.866499000	-0.654132000	-0.000139000	1	2.425176000	1.342409000	0.879672000
8	0.314035000	1.992504000	2.176817000	6	1.867307000	-1.202470000	1.204507000
8	0.313733000	1.993162000	-2.176290000	1	1.205039000	-2.068657000	1.220711000
6	0.053296000	1.286748000	1.299264000	1	2.912907000	-1.548318000	1.223065000
6	0.053129000	1.287131000	-1.298917000	6	1.866174000	-1.209520000	-1.199994000
1	-2.817452000	0.671874000	1.341588000	1	2.911858000	-1.555141000	-1.217626000
1	-1.284668000	-1.404503000	2.177979000	1	1.667893000	-0.609976000	-2.089985000
1	-2.816682000	0.671198000	-1.343065000	1	1.204257000	-2.076047000	-1.210378000
1	-1.283425000	-1.405570000	-2.177577000	1	3.605301000	0.329847000	-0.003788000
1	-0.329366000	-2.636678000	0.000796000	1	1.670132000	-0.597600000	2.091129000
				6	-2.220892000	0.196889000	0.718700000
				6	-1.579665000	-0.982793000	1.175903000

	6	-1.146645000	-1.672769000	0.003132000
	6	-1.576852000	-0.987881000	-1.173932000
	6	-2.219380000	0.193603000	-0.723774000
	1	-2.639549000	0.971489000	-1.347502000
	1	-1.460620000	-1.324650000	-2.195011000
	1	-0.588398000	-2.603798000	0.005894000
	1	-1.466699000	-1.314984000	2.198835000
	1	-2.642654000	0.977773000	1.337599000
CpCoCOPEt ₃				
27		-0.930658000	0.331911000	-0.081593000
8		-0.215979000	3.116647000	-0.129043000
6		-0.511587000	1.981122000	-0.133035000
6		-2.834440000	0.361775000	0.599357000
6		-2.160236000	-0.746794000	1.166838000
6		-1.686932000	-1.538916000	0.075080000
6		-2.120312000	-0.960768000	-1.162044000
6		-2.811623000	0.228581000	-0.833374000
15		1.119573000	-0.246105000	0.039795000
6		1.846381000	-1.270491000	-1.316824000
1		1.763175000	-0.678133000	-2.234485000
1		2.920418000	-1.383908000	-1.110241000
6		1.192955000	-2.626672000	-1.512937000
1		0.143189000	-2.521260000	-1.800362000
1		1.230316000	-3.236503000	-0.603680000
1		1.693261000	-3.193930000	-2.302579000
6		2.379610000	1.093833000	0.157771000
1		2.018690000	1.804864000	0.908539000
1		3.306764000	0.656135000	0.552245000
6		2.645329000	1.809835000	-1.157571000
1		1.720002000	2.171795000	-1.613685000
1		3.143954000	1.157147000	-1.880114000
1		3.291790000	2.677530000	-1.002316000
6		1.528637000	-1.258448000	1.531355000
1		0.857495000	-2.125870000	1.532093000
1		2.550562000	-1.648777000	1.426014000
6		1.374720000	-0.474786000	2.824677000
1		0.372572000	-0.039641000	2.901364000
1		2.092434000	0.349067000	2.884375000
1		1.535478000	-1.112310000	3.698281000
1		-2.030524000	-0.963527000	2.218527000
1		-1.116634000	-2.455245000	0.172174000
1		-1.959978000	-1.363933000	-2.152491000
1		-3.241363000	0.931948000	-1.533782000
1		-3.284599000	1.181728000	1.142788000
CpNiNEt ₃ Cl				
6		2.230428000	-0.142872000	1.394117000
6		1.588951000	1.115220000	1.264732000
6		1.842463000	1.666885000	-0.049591000
6		2.536694000	0.693863000	-0.771687000
6		2.716710000	-0.447976000	0.100626000
28		0.754110000	-0.102346000	-0.109772000
17		0.503875000	-1.849792000	-1.459800000
7		-1.205630000	0.249478000	0.273528000
6		-2.127742000	-0.460085000	-0.667789000
1		-1.824652000	-0.178715000	-1.678310000
1		-1.895092000	-1.521873000	-0.598572000
6		-3.606736000	-0.208848000	-0.447743000
1		-3.946585000	-0.522756000	0.544091000
1		-4.173404000	-0.791271000	-1.178142000
1		-3.890629000	0.839640000	-0.582675000
6		-1.455919000	1.719478000	0.215678000
1		-2.445931000	1.929331000	0.648268000
1		-0.725430000	2.189258000	0.880013000
6		-1.359382000	2.297538000	-1.178558000
1		-0.458573000	1.936873000	-1.686415000
1		-1.308062000	3.387918000	-1.127190000
1		-2.223786000	2.037777000	-1.795573000
6		-1.452200000	-0.195669000	1.678162000
1		-0.740410000	0.353320000	2.302204000
1		-2.456146000	0.133809000	1.987797000
6		-1.293579000	-1.685747000	1.880922000
1		-2.126702000	-2.253655000	1.458493000
1		-1.250754000	-1.911101000	2.949180000
1		-0.370966000	-2.044275000	1.412811000
1		3.157666000	-1.386163000	-0.208460000
1		2.835161000	0.735398000	-1.810001000
1		1.537014000	2.647225000	-0.391952000
1		1.066792000	1.638240000	2.059543000
1		2.280809000	-0.763893000	2.277181000
CpNiPMe ₃ Cl				
6		2.127091000	-0.587710000	-1.206900000
6		1.392527000	-1.608964000	-0.559432000
6		1.508888000	-1.431376000	0.879263000
6		2.270162000	-0.276865000	1.109230000
6		2.573556000	0.284833000	-0.177986000
28		0.557633000	0.120630000	-0.019226000
17		0.083188000	2.295559000	0.000269000
15		-1.523991000	-0.318787000	-0.004683000
6		-2.399863000	0.338343000	1.451708000
1		-2.011559000	-0.123751000	2.362224000
1		-2.208414000	1.412435000	1.504518000
6		-2.016583000	-2.078388000	-0.028722000
1		-3.103089000	-2.186202000	0.043450000
1		-1.683506000	-2.549595000	-0.956552000
6		-2.461532000	0.395926000	-1.393115000
CpCuNMe ₃				
29		0.227714000	0.127234000	0.005176000
7		-1.724901000	0.003491000	-0.000052000
6		-2.171939000	-0.573845000	1.278333000
1		-1.687059000	-1.541352000	1.423412000
1		-1.877242000	0.086511000	2.096090000
6		-2.366230000	1.313874000	-0.188017000
1		-2.036062000	1.746254000	-1.134325000
1		-3.465657000	1.222245000	-0.195832000
6		-2.128284000	-0.893028000	-1.096294000
1		-3.222012000	-1.033048000	-1.117501000
1		-1.641740000	-1.861563000	-0.964081000
1		-1.801116000	-0.469699000	-2.047880000
1		-3.266622000	-0.707597000	1.296143000
1		-2.068452000	1.982439000	0.621776000
6		1.866951000	-0.357627000	1.175173000

1	-2.110973000	-0.024649000	-2.338191000	6	1.983957000	0.963472000	0.643295000
1	-3.535117000	0.207051000	-1.292648000	6	1.969754000	0.865549000	-0.783842000
1	-1.558208000	-2.611374000	0.808004000	6	1.845032000	-0.515110000	-1.128216000
1	-3.477717000	0.157339000	1.389102000	6	1.784528000	-1.268115000	0.080716000
1	-2.275191000	1.472019000	-1.406963000	1	2.117590000	1.682773000	-1.477864000
1	1.093080000	-2.094865000	1.626865000	1	2.143641000	1.867555000	1.216421000
1	2.525803000	0.158599000	2.064519000	1	1.924674000	-0.626941000	2.222091000
1	0.878417000	-2.431883000	-1.041206000	1	1.765748000	-2.348303000	0.154674000
1	2.265796000	-0.455771000	-2.269870000	1	1.882300000	-0.924511000	-2.129749000
1	3.067154000	1.235516000	-0.333545000				
CpCuNMe ₃				CpCuCO			
29	0.812840000	0.034940000	0.067624000	29	0.329719000	-0.001933000	-0.000865000
15	-1.278890000	-0.009791000	-0.023510000	8	3.226737000	0.001097000	0.000561000
6	2.528652000	-0.410148000	1.166163000	6	2.069285000	-0.001189000	-0.000465000
6	2.530984000	0.966301000	0.797389000	6	-1.359993000	1.068721000	0.574966000
6	2.510475000	1.040474000	-0.625711000	6	-1.362159000	-0.214826000	1.192947000
6	2.492488000	-0.289633000	-1.135462000	6	-1.365128000	-1.199396000	0.163326000
6	2.504359000	-1.186360000	-0.028945000	6	-1.364934000	-0.524200000	-1.091067000
6	-2.215708000	0.140008000	1.558145000	6	-1.361600000	0.877436000	-0.836834000
1	-2.105903000	1.177735000	1.894219000	1	-1.385991000	-0.993185000	-2.065158000
1	-3.285331000	-0.017278000	1.363956000	1	-1.387044000	-2.270660000	0.308438000
6	-1.700146000	-0.812273000	2.623845000	1	-1.380669000	-0.407800000	2.256733000
1	-0.628330000	-0.658609000	2.789991000	1	-1.375869000	2.020778000	1.087337000
1	-1.834520000	-1.858674000	2.330907000	1	-1.378979000	1.658864000	-1.583995000
1	-2.217506000	-0.670669000	3.576491000				
6	-2.072262000	1.294580000	-1.059080000				
1	-1.810031000	1.072470000	-2.100257000				
1	-3.164519000	1.208775000	-0.982342000				
6	-1.597186000	2.688426000	-0.684175000				
1	-0.503490000	2.742371000	-0.722367000				
1	-1.898187000	2.957715000	0.333473000				
1	-2.001741000	3.449139000	-1.357172000				
6	-1.982696000	-1.554786000	-0.746009000				
1	-1.867655000	-2.339132000	0.011483000				
1	-3.061134000	-1.428649000	-0.910301000				
6	-1.263245000	-1.954320000	-2.023400000				
1	-0.184122000	-2.017003000	-1.841783000				
1	-1.412434000	-1.216719000	-2.818931000				
1	-1.608849000	-2.920179000	-2.401285000				
1	2.586721000	-0.797928000	2.174728000				
1	2.538967000	-2.266481000	-0.086348000				
1	2.511920000	-0.570060000	-2.180675000				
1	2.548719000	1.947165000	-1.215485000				
1	2.594128000	1.806008000	1.476701000				

10. Cartesian coordinates of optimized geometry of (C₆₀)ML_n complexes at Mo6L/6-31G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

(C ₆₀)ScNMe ₃ (CO) ₂				(C ₆₀)ScPMe ₃ (CO) ₂			
21	4.303208000	-0.320936000	0.000010000	21	4.099981000	0.931549000	-0.597391000
7	5.724179000	1.458180000	-0.000299000	15	5.663338000	-1.295651000	-0.267677000
8	5.242952000	-2.522955000	-2.375561000	8	4.587462000	1.525837000	2.654163000
8	5.243111000	-2.522483000	2.375955000	8	4.120682000	4.285905000	-0.953054000
6	4.940228000	-1.747885000	-1.574754000	6	4.523375000	1.352583000	1.511392000
6	4.940328000	-1.747572000	1.575017000	6	4.194039000	3.136092000	-0.885347000
6	7.144319000	1.058427000	-0.000349000	6	7.356476000	-0.985829000	0.355675000
1	7.364811000	0.463891000	0.890235000	1	7.959533000	-0.467359000	-0.393048000
1	7.364692000	0.463695000	-0.890832000	1	7.318789000	-0.365394000	1.254563000
6	5.411376000	2.244139000	-1.211454000	6	4.924339000	-2.304198000	1.065131000

1	4.355418000	2.531646000	-1.197399000	1	3.935526000	-2.661602000	0.764824000
1	6.021907000	3.154643000	-1.262551000	1	5.553470000	-3.169813000	1.292337000
6	5.411538000	2.244422000	1.210714000	6	5.933230000	-2.517117000	-1.604033000
1	6.022055000	3.154952000	1.261504000	1	6.502441000	-3.376332000	-1.237751000
1	5.609093000	1.644509000	2.103839000	1	6.481732000	-2.066993000	-2.434309000
1	4.355571000	2.531902000	1.196744000	1	4.972828000	-2.874533000	-1.984040000
1	7.802554000	1.936631000	-0.000490000	1	7.853887000	-1.926965000	0.606827000
1	5.608786000	1.644007000	-2.104464000	1	4.806662000	-1.701040000	1.968836000
6	-3.500545000	2.312051000	1.420496000	6	-3.718587000	-2.288446000	-1.247959000
6	-2.798041000	1.829486000	2.588607000	6	-3.235723000	-1.669567000	-2.460421000
6	-4.358209000	1.461963000	0.722640000	6	-4.463669000	-1.542848000	-0.335124000
6	-2.985285000	0.516171000	3.023095000	6	-3.518099000	-0.326559000	-2.719745000
6	-1.851042000	-0.260057000	3.465600000	6	-2.491922000	0.532171000	-3.265527000
6	-1.476367000	2.412051000	2.590248000	6	-1.918323000	-2.194605000	-2.737677000
6	-0.382544000	1.664338000	3.023362000	6	-0.933215000	-1.368334000	-3.275293000
6	-0.576045000	0.303383000	3.469696000	6	-1.225628000	0.021282000	-3.544021000
6	-3.500548000	2.311730000	-1.420970000	6	-3.240996000	-2.563365000	1.540742000
6	-2.610810000	3.191233000	-0.697848000	6	-2.464062000	-3.333472000	0.593816000
6	-4.358211000	1.461800000	-0.722919000	6	-4.220899000	-1.682905000	1.083931000
6	-2.610809000	3.191391000	0.697175000	6	-2.700046000	-3.200662000	-0.774753000
6	-1.358800000	3.254886000	1.417377000	6	-1.586621000	-3.142007000	-1.693299000
6	-1.358802000	3.254565000	-1.418069000	6	-1.109694000	-3.419841000	1.089748000
6	-0.156233000	3.325405000	-0.721269000	6	-0.035877000	-3.369897000	0.201340000
6	-0.156232000	3.325569000	0.720558000	6	-0.280129000	-3.228687000	-1.215172000
6	-3.874935000	-0.365038000	-2.298654000	6	-3.514117000	0.001312000	2.732031000
6	-2.985293000	0.515485000	-3.023163000	6	-2.495980000	-0.910126000	3.202794000
6	-4.548545000	0.099141000	-1.169621000	6	-4.361083000	-0.378331000	1.690956000
6	-2.798049000	1.828900000	-2.588974000	6	-2.364408000	-2.171417000	2.620391000
6	-1.476374000	2.411464000	-2.590750000	6	-1.047143000	-2.697844000	2.342930000
6	-1.851053000	-0.260842000	-3.465495000	6	-1.319066000	-0.137816000	3.530950000
6	-0.576056000	0.302597000	-3.469725000	6	-0.053196000	-0.650072000	3.269677000
6	-0.382553000	1.663653000	-3.023698000	6	0.082899000	-1.951328000	2.665857000
6	-4.106556000	-2.020928000	0.000255000	6	-4.170922000	1.859372000	0.686404000
6	-3.404681000	-2.500019000	-1.168507000	6	-3.295894000	2.254748000	1.766301000
6	-4.665184000	-0.742158000	0.000111000	6	-4.694135000	0.567193000	0.648656000
6	-3.292487000	-1.688054000	-2.297973000	6	-2.967863000	1.339236000	2.767900000
6	-2.040149000	-1.624662000	-3.016760000	6	-1.612935000	1.258226000	3.263290000
6	-2.270632000	-3.278495000	-0.723411000	6	-2.269073000	3.112416000	1.220403000
6	-1.067009000	-3.224206000	-1.423776000	6	-0.963947000	3.033277000	1.701994000
6	-0.950100000	-2.382130000	-2.591821000	6	-0.626481000	2.089154000	2.740861000
6	-3.874928000	-0.364517000	2.298787000	6	-4.294581000	0.444110000	-1.777192000
6	-3.292479000	-1.687532000	2.298405000	6	-3.747974000	1.782569000	-1.736757000
6	-4.548541000	0.099405000	1.169652000	6	-4.755378000	-0.152819000	-0.603543000
6	-3.404678000	-2.499755000	1.169123000	6	-3.687989000	2.477287000	-0.529132000
6	-2.270630000	-3.278331000	0.724201000	6	-2.511779000	3.251334000	-0.200414000
6	-2.040139000	-1.623977000	3.017173000	6	-2.634233000	1.838416000	-2.656667000
6	-0.950092000	-2.381543000	2.592405000	6	-1.505363000	2.591600000	-2.342251000
6	-1.067005000	-3.223884000	1.424550000	6	-1.442702000	3.312201000	-1.092416000
6	1.072459000	-2.282677000	-1.424343000	6	1.166835000	2.176509000	1.256901000
6	0.183996000	-3.156906000	-0.698414000	6	0.145627000	3.075212000	0.775996000
6	0.183998000	-3.156747000	0.699169000	6	-0.086989000	3.219482000	-0.593097000
6	1.930222000	-1.421596000	-0.722848000	6	1.975481000	1.465201000	0.343728000
6	1.443883000	0.406381000	-2.302708000	6	1.752966000	-0.560321000	1.792973000
6	0.552980000	-0.475967000	-3.016544000	6	0.981718000	0.208189000	2.715933000
6	0.371318000	-1.793258000	-2.584968000	6	0.698304000	1.564773000	2.461814000
6	2.146958000	-0.064927000	-1.183869000	6	2.317824000	0.036238000	0.626580000
6	1.684795000	2.080542000	-0.000217000	6	1.619946000	-1.977429000	-0.684309000
6	0.981880000	2.539420000	-1.161807000	6	1.139829000	-2.593653000	0.532089000
6	0.871566000	1.728494000	-2.303117000	6	1.192718000	-1.883597000	1.736626000
6	2.328519000	0.804315000	-0.000073000	6	2.155952000	-0.681729000	-0.644620000
6	1.443891000	0.406902000	2.302653000	6	0.963668000	-0.115856000	-2.740058000
6	0.871571000	1.729017000	2.302762000	6	0.421077000	-1.448601000	-2.772200000
6	0.981880000	2.539681000	1.161271000	6	0.741363000	-2.360644000	-1.759726000
6	2.146959000	-0.064658000	1.183917000	6	1.811559000	0.264136000	-1.683371000

6	1.072463000	-2.282356000	1.424899000	6	0.685063000	2.453593000	-1.542016000
6	0.371326000	-1.792674000	2.585415000	6	-0.188158000	2.055657000	-2.615449000
6	0.552990000	-0.475283000	3.016690000	6	-0.050983000	0.795668000	-3.206374000
6	1.930226000	-1.421433000	0.723207000	6	1.671624000	1.572071000	-1.078974000
$(C_{60})Sc(CO)_4$				$(C_{60})Ti(CO)_2Cl$			
6	0.705436000	1.849894000	2.453644000	6	2.858817000	1.181349000	-2.737479000
6	1.447023000	2.179632000	1.262681000	6	3.611406000	0.010754000	-2.347099000
6	0.759082000	0.555866000	2.982935000	6	2.840081000	2.306732000	-1.912574000
6	2.222703000	1.193610000	0.630536000	6	4.313797000	0.004846000	-1.142834000
6	2.220276000	1.084277000	-0.809781000	6	4.293710000	-1.169027000	-0.298773000
6	0.645876000	3.074197000	0.467033000	6	2.858413000	-1.155757000	-2.748732000
6	0.644400000	2.968836000	-0.927910000	6	2.839243000	-2.289007000	-1.934688000
6	1.443520000	1.964114000	-1.581451000	6	3.571974000	-2.296502000	-0.688462000
6	-1.655482000	0.608695000	3.430687000	6	0.435403000	2.605285000	-2.336609000
6	-1.712369000	1.947214000	2.880452000	6	0.455562000	1.441147000	-3.190290000
6	-0.443180000	-0.073963000	3.488621000	6	1.604354000	3.026496000	-1.705902000
6	-0.554981000	2.561494000	2.406889000	6	1.643624000	0.740327000	-3.383408000
6	-0.591753000	3.318414000	1.177702000	6	1.643357000	-0.708105000	-3.390326000
6	-2.952633000	2.074906000	2.149203000	6	-0.779810000	0.714688000	-2.982567000
6	-2.988072000	2.806808000	0.962058000	6	-0.780048000	-0.685476000	-2.989225000
6	-1.784217000	3.435152000	0.466931000	6	0.455047000	-1.410324000	-3.203923000
6	-1.544147000	-2.144257000	2.759703000	6	0.371820000	3.471446000	0.378901000
6	-2.805646000	-1.440045000	2.706949000	6	-0.842092000	3.018206000	-0.268145000
6	-0.385771000	-1.475687000	3.148171000	6	1.571992000	3.467995000	-0.326806000
6	-2.860801000	-0.086156000	3.037265000	6	-0.811824000	2.595101000	-1.601758000
6	-3.662865000	0.819344000	2.246070000	6	-1.563440000	1.436850000	-2.015875000
6	-3.552089000	-1.939208000	1.574038000	6	-1.627751000	2.306514000	0.704114000
6	-4.323713000	-1.065230000	0.809074000	6	-2.390734000	1.187571000	0.309907000
6	-4.380070000	0.338635000	1.151223000	6	-2.313242000	0.725194000	-1.064717000
6	0.883557000	-2.614126000	1.365093000	6	2.754377000	2.580987000	1.637279000
6	-0.320544000	-3.320061000	0.974341000	6	1.504903000	2.578218000	2.364105000
6	0.852840000	-1.709417000	2.433212000	6	2.787937000	3.018940000	0.313300000
6	-1.510965000	-3.081944000	1.655743000	6	0.336482000	3.019919000	1.748937000
6	-2.752061000	-2.952785000	0.924627000	6	-0.900957000	2.290433000	1.945106000
6	-0.322176000	-3.428892000	-0.465170000	6	1.485137000	1.401478000	3.210494000
6	-1.514175000	-3.295965000	-1.172035000	6	0.298153000	0.705025000	3.414694000
6	-2.753554000	-3.058019000	-0.466175000	6	-0.917949000	1.150970000	2.761787000
6	2.299658000	-0.143228000	1.191256000	6	4.294129000	1.170598000	-0.287564000
6	2.342916000	-1.095298000	0.078960000	6	4.260889000	0.717199000	1.085060000
6	1.557492000	-0.457148000	2.345037000	6	3.572841000	2.302067000	-0.666401000
6	1.620595000	-2.301157000	0.171127000	6	3.506567000	1.410608000	2.030999000
6	0.881091000	-2.790548000	-0.960434000	6	2.722240000	0.682804000	3.001995000
6	2.295567000	-0.321158000	-1.163014000	6	4.260610000	-0.728724000	1.078153000
6	1.551937000	-0.805240000	-2.254976000	6	3.506016000	-1.430876000	2.017350000
6	0.847613000	-2.056814000	-2.152478000	6	2.722001000	-0.712163000	2.995342000
6	-2.811705000	-1.831229000	-2.455951000	6	-0.918351000	-1.176712000	2.750579000
6	-1.550113000	-2.535757000	-2.405102000	6	0.297891000	-0.737503000	3.407803000
6	-0.392745000	-1.932756000	-2.891625000	6	1.484628000	-1.432380000	3.196932000
6	-2.867610000	-0.542035000	-2.985674000	6	-0.901787000	-2.308282000	1.922969000
6	-4.382754000	0.162064000	-1.181635000	6	-2.391288000	-1.189328000	0.298562000
6	-4.325477000	-1.174460000	-0.632616000	6	-2.426261000	-0.005019000	1.179595000
6	-3.555498000	-2.154023000	-1.259109000	6	-1.664843000	-0.010901000	2.374850000
6	-3.668441000	0.472349000	-2.338246000	6	-1.628603000	-2.312269000	0.681975000
6	-2.990505000	2.629911000	-1.369077000	6	-0.812796000	-2.579081000	-1.626615000
6	-3.734568000	2.309777000	-0.171764000	6	-1.563994000	-1.416618000	-2.029554000
6	-4.416414000	1.097004000	-0.079189000	6	-2.313552000	-0.713841000	-1.071583000
6	-2.957915000	1.727834000	-2.432655000	6	-0.843142000	-3.014836000	-0.297078000
6	-0.561007000	2.169574000	-2.765368000	6	1.570748000	-3.464951000	-0.360058000
6	-0.594986000	3.103472000	-1.664768000	6	1.603255000	-3.010297000	-1.734878000
6	-1.785859000	3.325962000	-0.976988000	6	0.434443000	-2.582700000	-2.361577000
6	-1.719399000	1.491672000	-3.139209000	6	0.370576000	-3.474729000	0.345590000
6	-0.451173000	-0.598185000	-3.438988000	6	1.503946000	-2.600854000	2.339158000

6	0.752188000	0.100304000	-3.036550000	6	2.753415000	-2.597151000	1.612394000
6	0.699232000	1.458913000	-2.707436000	6	2.786881000	-3.022493000	0.284312000
6	-1.663487000	0.085614000	-3.481846000	6	0.335387000	-3.036308000	1.719874000
21	4.504957000	0.019075000	-0.002284000	22	-4.417363000	-0.000896000	0.295550000
6	4.902986000	-1.698844000	-1.418376000	17	-6.058799000	-0.008384000	1.744315000
8	4.935629000	-2.596162000	-2.136067000	8	-5.467135000	-2.337384000	-1.681004000
6	5.100658000	1.626609000	1.483087000	8	-5.467133000	2.352508000	-1.660914000
8	5.316618000	2.447540000	2.256909000	6	-5.093509000	-1.494313000	-0.994767000
6	4.902600000	-1.491853000	1.632859000	6	-5.093463000	1.503653000	-0.981869000
8	4.933564000	-2.283835000	2.465430000				
6	5.105323000	1.414891000	-1.686889000				
8	5.325891000	2.126220000	-2.561316000				
(C ₆₀)TiCl ₃				(C ₆₀)V(CO) ₂			
22	4.472257000	-0.001078000	0.000383000	6	1.192665000	-2.583309000	1.417615000
17	5.355541000	-0.573738000	1.909112000	6	1.986620000	-1.431079000	1.745012000
17	5.347898000	-1.370504000	-1.453058000	6	1.084776000	-3.021515000	0.093297000
17	5.332460000	1.949915000	-0.460562000	6	2.700183000	-0.745073000	0.732947000
6	-1.619106000	-2.868707000	1.980544000	6	2.699879000	0.744375000	0.733436000
6	-1.619272000	-1.815644000	2.975384000	6	1.313724000	-0.702652000	2.783227000
6	-0.435539000	-3.229110000	1.340064000	6	1.313713000	0.700543000	2.783766000
6	-0.436354000	-1.156012000	3.299922000	6	1.986650000	1.429787000	1.746121000
6	-0.436666000	0.276554000	3.485367000	6	-1.311724000	-3.466450000	0.414963000
6	-2.850240000	-1.071424000	2.835173000	6	-1.196964000	-3.018863000	1.787655000
6	-2.850378000	0.312337000	3.014369000	6	-0.193603000	-3.474412000	-0.415854000
6	-1.619624000	0.996724000	3.339850000	6	0.031130000	-2.592828000	2.284664000
6	-1.620040000	-3.391247000	-0.806421000	6	0.104496000	-1.426558000	3.129789000
6	-2.850571000	-3.027597000	-0.141337000	6	-2.404725000	-2.298803000	2.124186000
6	-0.436038000	-3.495109000	-0.079522000	6	-2.334249000	-1.170358000	2.941025000
6	-2.850057000	-2.770416000	1.229729000	6	-1.055057000	-0.726343000	3.447996000
6	-3.611975000	-1.661137000	1.757671000	6	-1.538302000	-2.589261000	-2.272022000
6	-3.613272000	-2.185102000	-1.034892000	6	-2.701281000	-2.588706000	-1.413419000
6	-4.344530000	-1.112543000	-0.525729000	6	-0.310019000	-3.026284000	-1.782964000
6	-4.343733000	-0.845966000	0.895474000	6	-2.589848000	-3.020670000	-0.091804000
6	0.790752000	-2.366012000	-1.898127000	6	-3.265724000	-2.299455000	0.963671000
6	-0.438532000	-2.272955000	-2.657201000	6	-3.491768000	-1.420314000	-1.728817000
6	0.793627000	-2.967533000	-0.632975000	6	-4.140209000	-0.722738000	-0.710440000
6	-1.621335000	-2.770545000	-2.115338000	6	-4.025040000	-1.170104000	0.659735000
6	-2.852242000	-2.025660000	-2.253202000	6	0.828414000	-1.165149000	-2.938358000
6	-0.439230000	-1.004765000	-3.348853000	6	-0.449453000	-0.720668000	-3.454675000
6	-1.622179000	-0.280666000	-3.473228000	6	0.895276000	-2.295446000	-2.115208000
6	-2.852373000	-0.800462000	-2.920988000	6	-1.608915000	-1.416852000	-3.119626000
6	2.284464000	-1.210540000	0.226395000	6	-2.815116000	-0.697026000	-2.781566000
6	2.269255000	-0.587156000	-1.080787000	6	-0.449471000	0.723270000	-3.454122000
6	1.552083000	-2.389921000	0.447387000	6	-1.608956000	1.419183000	-3.118566000
6	1.548065000	-1.164423000	-2.137180000	6	-2.815136000	0.699082000	-2.781046000
6	0.790049000	-0.315110000	-3.017123000	6	2.538812000	-1.177971000	-0.664456000
6	2.275477000	0.844187000	-0.896821000	6	2.433750000	0.000598000	-1.492208000
6	1.549277000	1.670664000	-1.769489000	6	1.756903000	-2.307936000	-0.963731000
6	0.790807000	1.074365000	-2.837686000	6	1.618143000	0.001001000	-2.638927000
6	0.792335000	-1.517502000	2.624882000	6	0.828381000	1.167379000	-2.937477000
6	1.549788000	-0.311627000	2.412645000	6	2.538490000	1.178376000	-0.663427000
6	0.794260000	-2.536614000	1.663741000	6	1.756831000	2.308692000	-0.961969000
6	2.269581000	-0.156361000	1.218109000	6	0.895231000	2.297073000	-2.113497000
6	2.278974000	1.112224000	0.528238000	6	-2.701322000	2.589714000	-1.411444000
6	0.791896000	0.798873000	2.924989000	6	-1.538350000	2.590954000	-2.270064000
6	0.793127000	2.029390000	2.254999000	6	-0.310072000	3.027630000	-1.780680000
6	1.550821000	2.198025000	1.042775000	6	-2.589913000	3.020689000	-0.089506000
6	-0.438484000	2.874818000	-1.990089000	6	-4.025057000	1.169507000	0.660624000
6	0.791205000	2.772504000	-1.232652000	6	-4.140219000	0.723192000	-0.709886000
6	0.791980000	3.030761000	0.143959000	6	-3.491791000	1.421556000	-1.727738000
6	-1.621907000	3.217331000	-1.339551000	6	-3.265768000	2.298651000	0.965417000
6	-2.852514000	1.517561000	-2.620761000	6	-2.334257000	1.168053000	2.941896000

6	-1.62222000	1.15622000	-3.287295000	6	-3.124084000	-0.001038000	2.628372000
6	-0.439068000	1.824849000	-2.981920000	6	-3.953289000	-0.000624000	1.506864000
6	-2.852524000	2.531768000	-1.662895000	6	-2.404755000	2.297115000	2.125913000
6	-4.344538000	1.207841000	-0.225172000	6	0.031097000	2.591067000	2.286628000
6	-4.344877000	0.156971000	-1.218301000	6	0.104475000	1.424170000	3.130876000
6	-3.614178000	0.309731000	-2.395852000	6	-1.055069000	0.723680000	3.448533000
6	-3.613627000	2.374761000	-0.444047000	6	-1.197008000	3.017462000	1.789940000
6	-2.850819000	2.364672000	1.894788000	6	-0.193674000	3.474710000	-0.413210000
6	-3.612152000	1.157019000	2.122641000	6	1.084699000	3.021434000	0.095599000
6	-4.343872000	0.588029000	1.081155000	6	1.192641000	2.582236000	1.419582000
6	-2.851834000	2.962929000	0.634503000	6	-1.311789000	3.466105000	0.417600000
6	-0.437378000	3.400425000	0.813596000	23	4.466552000	-0.000140000	-0.177592000
6	-0.436840000	2.781400000	2.118572000	6	5.619307000	1.570585000	0.021482000
6	-1.619799000	2.268643000	2.645893000	8	6.247968000	2.529572000	0.167828000
6	-1.621230000	3.484166000	0.083983000	6	5.620303000	-1.570125000	0.021546000
				8	6.249737000	-2.528616000	0.167794000
$(C_{60})V(CO)_3$				$(C_{60})V(CO)_4$			
6	0.897181000	3.021387000	0.016736000	6	0.661846000	2.966016000	-0.737263000
6	1.523925000	2.312430000	-1.069934000	6	1.409588000	1.993797000	-1.490963000
6	1.063817000	2.584247000	1.336261000	6	0.697710000	2.959328000	0.663127000
6	2.309868000	1.175522000	-0.801616000	6	2.165048000	1.022717000	-0.808098000
6	2.178665000	0.000815000	-1.632724000	6	2.162498000	-0.348975000	-1.259522000
6	0.613893000	2.300144000	-2.183736000	6	0.622097000	1.601827000	-2.630171000
6	0.509860000	1.168843000	-3.002206000	6	0.620454000	0.271444000	-3.068119000
6	1.310929000	0.001297000	-2.737419000	6	1.406490000	-0.722446000	-2.385695000
6	-1.307464000	3.017568000	1.809364000	6	-1.717091000	3.401948000	0.752395000
6	-1.482024000	3.465813000	0.442998000	6	-1.754736000	3.407790000	-0.695904000
6	-0.058708000	2.592570000	2.253260000	6	-0.515097000	3.189794000	1.422014000
6	-0.401572000	3.475689000	-0.436041000	6	-0.588830000	3.201750000	-1.429485000
6	-0.576873000	3.029471000	-1.797547000	6	-0.613525000	2.357449000	-2.600304000
6	-2.780912000	3.020198000	-0.007717000	6	-2.992421000	2.786851000	-1.110401000
6	-2.949483000	2.589340000	-1.323624000	6	-3.015752000	1.971052000	-2.241953000
6	-1.824994000	2.591455000	-2.232315000	6	-1.802602000	1.750091000	-2.995824000
6	-1.094665000	0.723434000	3.460592000	6	-1.644631000	1.726181000	3.037843000
6	-2.394373000	1.167797000	3.009952000	6	-2.896197000	1.953126000	2.350945000
6	0.050129000	1.425233000	3.094235000	6	-0.477739000	2.337003000	2.585974000
6	-2.499250000	2.296610000	2.197380000	6	-2.931878000	2.777442000	1.226221000
6	-3.410140000	2.298365000	1.075550000	6	-3.720656000	2.398025000	0.076267000
6	-3.197215000	-0.001284000	2.730623000	6	-3.648602000	0.718893000	2.367364000
6	-4.074043000	-0.000810000	1.646335000	6	-4.406435000	0.351032000	1.256260000
6	-4.182216000	1.169415000	0.804058000	6	-4.443123000	1.205430000	0.090360000
6	1.240346000	-0.702013000	2.693386000	6	0.777967000	0.246747000	2.970454000
6	0.050184000	-1.428000000	3.092941000	6	-0.435581000	-0.379255000	3.455611000
6	1.240324000	0.699658000	2.694024000	6	0.757913000	1.581114000	2.543734000
6	-1.094637000	-0.726580000	3.459936000	6	-1.623104000	0.346499000	3.479617000
6	-2.394327000	-1.170586000	3.008890000	6	-2.861473000	-0.273156000	3.063894000
6	-0.058602000	-2.594580000	2.250905000	6	-0.437234000	-1.750219000	3.004175000
6	-1.307339000	-3.019221000	1.806619000	6	-1.626214000	-2.346058000	2.593170000
6	-2.499155000	-2.298665000	2.195292000	6	-2.863080000	-1.598130000	2.627716000
6	2.506747000	0.734493000	0.575410000	6	2.217993000	1.024220000	0.640280000
6	2.506794000	-0.734875000	0.574759000	6	2.245881000	-0.362376000	1.088885000
6	1.867384000	1.428069000	1.625816000	6	1.483473000	1.981993000	1.367525000
6	1.867438000	-1.429429000	1.624521000	6	1.524907000	-0.740935000	2.239491000
6	1.063925000	-2.585375000	1.333912000	6	0.775215000	-1.968026000	2.240854000
6	2.309981000	-1.174673000	-0.802702000	6	2.214564000	-1.210342000	-0.095882000
6	1.524024000	-2.311347000	-1.072035000	6	1.478611000	-2.412026000	-0.080000000
6	0.897311000	-3.021319000	0.013987000	6	0.753007000	-2.787639000	1.104924000
6	-2.780787000	-3.020258000	-0.010465000	6	-2.901813000	-2.964691000	0.731296000
6	-1.481881000	-3.466233000	0.439844000	6	-1.650272000	-3.193093000	1.417758000
6	-0.401430000	-3.475261000	-0.439202000	6	-0.484265000	-3.418217000	0.690433000
6	-2.949376000	-2.588212000	-1.325979000	6	-2.938367000	-2.959178000	-0.663271000
6	-4.356927000	-0.722759000	-0.560653000	6	-4.445482000	-1.016632000	-0.641638000

6	-4.182167000	-1.170272000	0.802994000	6	-4.407937000	-1.022370000	0.803704000
6	-3.410042000	-2.299434000	1.073458000	6	-3.651599000	-1.980242000	1.478162000
6	-3.753153000	-1.420083000	-1.606419000	6	-3.725638000	-1.968912000	-1.362052000
6	-3.122862000	0.699116000	-2.686651000	6	-3.018436000	-0.248847000	-2.973164000
6	-3.753215000	1.421439000	-1.605128000	6	-3.768478000	0.737190000	-2.228672000
6	-4.356957000	0.723137000	-0.559996000	6	-4.467135000	0.360250000	-1.082581000
6	-3.122833000	-0.696752000	-2.687282000	6	-2.997393000	-1.577611000	-2.547740000
6	-0.788802000	-0.720592000	-3.462544000	6	-0.594560000	-1.726389000	-3.052522000
6	-0.788833000	0.723755000	-3.461889000	6	-0.616640000	-0.351656000	-3.492297000
6	-1.932660000	1.419862000	-3.076784000	6	-1.804256000	0.374160000	-3.448869000
6	-1.932600000	-1.417095000	-3.078071000	6	-1.761345000	-2.325712000	-2.584269000
6	-0.576747000	-3.027812000	-1.800300000	6	-0.522525000	-3.411779000	-0.752518000
6	0.613991000	-2.298082000	-2.185821000	6	0.691157000	-2.777651000	-1.226643000
6	0.509910000	-1.166044000	-3.003266000	6	0.656083000	-1.950846000	-2.356681000
6	-1.824886000	-2.589450000	-2.234667000	6	-1.724568000	-3.182147000	-1.416339000
23	4.318871000	0.000125000	-0.461855000	23	4.199322000	0.005813000	-0.019817000
6	5.425202000	-1.608888000	-0.568741000	6	5.131139000	-1.520209000	0.752693000
8	6.054860000	-2.577178000	-0.602461000	8	5.651197000	-2.439195000	1.222005000
6	5.425507000	1.609008000	-0.568276000	6	5.195470000	1.527558000	-0.736934000
8	6.055097000	2.577338000	-0.602012000	8	5.756550000	2.442504000	-1.163640000
6	5.226838000	-0.000192000	1.232626000	6	5.127430000	0.738513000	1.527271000
8	5.750770000	-0.000522000	2.266122000	8	5.644667000	1.177733000	2.462607000
				6	5.200157000	-0.753045000	-1.518700000
				8	5.764544000	-1.211571000	-2.415956000
$(C_{60})Cr(CO)_2Cl$				$(C_{60})Cr(CO)_2H$			
6	2.651642000	-1.754418000	-2.570890000	6	2.443137000	-2.775134000	1.424158000
6	3.377530000	-2.190965000	-1.398143000	6	3.064349000	-1.670763000	2.121088000
6	2.768370000	-0.436236000	-3.013734000	6	2.686801000	-2.967445000	0.064273000
6	4.189416000	-1.292070000	-0.707644000	6	3.903556000	-0.796352000	1.431590000
6	4.187661000	-1.278940000	0.738655000	6	3.821264000	0.626987000	1.672928000
6	2.533400000	-3.107397000	-0.667512000	6	2.109893000	-1.153095000	3.074681000
6	2.531651000	-3.094750000	0.727178000	6	2.029099000	0.219929000	3.306166000
6	3.374068000	-2.165254000	1.443265000	6	2.901692000	1.126175000	2.594633000
6	0.353240000	-0.351282000	-3.472052000	6	0.315569000	-3.501629000	-0.311481000
6	0.232779000	-1.714074000	-3.015437000	6	0.062250000	-3.302362000	1.095344000
6	1.596506000	0.276617000	-3.466973000	6	1.601331000	-3.333259000	-0.817774000
6	1.360048000	-2.399985000	-2.568285000	6	1.105335000	-2.940863000	1.945382000
6	1.286358000	-3.239325000	-1.388243000	6	0.899049000	-1.936105000	2.968091000
6	-1.015440000	-1.828659000	-2.288209000	6	-1.227597000	-2.657291000	1.226640000
6	-1.079608000	-2.635858000	-1.144075000	6	-1.423794000	-1.683268000	2.212430000
6	0.088534000	-3.365730000	-0.692738000	6	-0.342936000	-1.323454000	3.107206000
6	0.590843000	2.358652000	-2.614116000	6	0.715132000	-2.161984000	-2.797225000
6	-0.699395000	1.704871000	-2.602380000	6	-0.623028000	-2.323843000	-2.268219000
6	1.717473000	1.652656000	-3.030780000	6	1.804127000	-2.651742000	-2.079848000
6	-0.820210000	0.372152000	-3.024480000	6	-0.820149000	-2.981503000	-1.047065000
6	-1.668271000	-0.545794000	-2.315203000	6	-1.773396000	-2.478373000	-0.096387000
6	-1.424089000	2.177383000	-1.450802000	6	-1.372927000	-1.137121000	-2.587383000
6	-2.221651000	1.277245000	-0.734038000	6	-2.280589000	-0.626416000	-1.644155000
6	-2.389458000	-0.094256000	-1.180016000	6	-2.508164000	-1.313892000	-0.394791000
6	3.032707000	2.610138000	-1.188740000	6	3.086036000	-0.613908000	-2.580147000
6	1.862413000	3.338505000	-0.752640000	6	1.951553000	-0.102982000	-3.315041000
6	2.963380000	1.783893000	-2.311755000	6	3.013184000	-1.868380000	-1.972218000
6	0.664860000	3.217749000	-1.454373000	6	0.790157000	-0.864245000	-3.426322000
6	-0.582109000	3.097992000	-0.729466000	6	-0.501511000	-0.225619000	-3.283849000
6	1.860710000	3.351575000	0.694464000	6	1.870549000	1.322901000	-3.074182000
6	0.661497000	3.243467000	1.395412000	6	0.630075000	1.942534000	-2.948926000
6	-0.583680000	3.110577000	0.669408000	6	-0.580468000	1.152629000	-3.049958000
6	4.309332000	0.073994000	-1.166582000	6	4.156418000	-0.996231000	0.022067000
6	4.382644000	0.930730000	-0.004300000	6	4.231078000	0.303267000	-0.607398000
6	3.614214000	0.493714000	-2.300450000	6	3.560713000	-2.063555000	-0.649020000
6	3.758083000	2.177271000	-0.016266000	6	3.708115000	0.490530000	-1.886239000
6	3.029880000	2.631088000	1.146485000	6	2.955139000	1.686740000	-2.190573000

6	4.306450000	0.095087000	1.173024000	6	4.024060000	1.306633000	0.412839000
6	3.608590000	0.535112000	2.297561000	6	3.301079000	2.462148000	0.118652000
6	2.957679000	1.825237000	2.283920000	6	2.754880000	2.654561000	-1.206466000
6	-0.705778000	1.751423000	2.566810000	6	-0.917214000	2.770888000	-1.403947000
6	0.584558000	2.405225000	2.570031000	6	0.421701000	2.943897000	-1.930660000
6	1.710089000	1.706923000	3.002299000	6	1.463396000	3.289424000	-1.073219000
6	-0.827527000	0.426506000	3.012541000	6	-1.160452000	2.958998000	-0.036975000
6	-2.392477000	-0.073132000	1.173172000	6	-2.667200000	1.007686000	-0.000245000
6	-2.223408000	1.290419000	0.702629000	6	-2.392152000	0.796348000	-1.423163000
6	-1.427440000	2.203173000	1.405149000	6	-1.533566000	1.677427000	-2.109870000
6	-1.673881000	-0.504231000	2.318077000	6	-2.038011000	2.076544000	0.681593000
6	-1.082593000	-2.614884000	1.186111000	6	-1.563194000	0.608326000	2.605381000
6	-1.801596000	-2.197751000	0.016282000	6	-2.181166000	-0.494539000	1.926180000
6	-2.448815000	-0.946785000	0.004067000	6	-2.744149000	-0.313825000	0.643646000
6	-1.021206000	-1.787169000	2.315846000	6	-1.490343000	1.868276000	1.992384000
6	1.353706000	-2.353425000	2.612078000	6	0.810980000	2.156759000	2.808383000
6	1.282868000	-3.213723000	1.446950000	6	0.736456000	0.853803000	3.440984000
6	0.086745000	-3.352679000	0.750887000	6	-0.426821000	0.096497000	3.348950000
6	0.225370000	-1.659500000	3.043906000	6	-0.279882000	2.659749000	2.105842000
6	1.588033000	0.339058000	3.463104000	6	1.209608000	3.489066000	0.339051000
6	2.761001000	-0.381834000	3.025592000	6	2.345903000	2.977651000	1.072300000
6	2.645309000	-1.707757000	2.606224000	6	2.149115000	2.321570000	2.287724000
6	0.344739000	-0.288754000	3.476019000	6	-0.076463000	3.336554000	0.848668000
24	-4.264375000	0.204770000	-0.002281000	24	-4.377921000	-0.007478000	-0.677753000
17	-5.566981000	1.923318000	0.000949000	1	-5.160022000	1.282114000	-1.235274000
8	-5.703515000	-1.619176000	1.891850000	8	-6.073846000	1.943823000	0.776971000
8	-5.711845000	-1.624569000	-1.885743000	8	-6.217780000	-1.977353000	0.663688000
6	-5.144763000	-0.911033000	1.169710000	6	-5.429638000	1.169020000	0.188008000
6	-5.149888000	-0.914271000	-1.168243000	6	-5.517447000	-1.233409000	0.121500000
$(C_{60})Mn(CO)_2NMe_3$				$(C_{60})Mn(CO)_2PMe_3$			
25	-3.963474000	-0.392835000	-0.000050000	25	3.796033000	-0.663560000	-0.000016000
7	-5.357224000	1.192095000	0.000040000	15	5.255106000	1.047949000	-0.000135000
8	-5.362061000	-1.893357000	2.091085000	8	5.352223000	-1.974874000	-2.112969000
8	-5.361866000	-1.893091000	-2.091493000	8	5.352148000	-1.973948000	2.113563000
6	-4.824871000	-1.291123000	1.253979000	6	4.742903000	-1.461534000	-1.265410000
6	-4.824768000	-1.290953000	-1.254258000	6	4.742957000	-1.461211000	1.265545000
6	-6.761282000	0.714080000	-0.000143000	6	7.010213000	0.570758000	-0.000653000
1	-6.946909000	0.109317000	-0.888709000	1	7.233798000	-0.029760000	0.884253000
1	-6.947048000	0.109043000	0.888208000	1	7.233388000	-0.029356000	-0.885935000
6	-5.161584000	2.029067000	1.206057000	6	5.110638000	2.156857000	-1.441303000
1	-4.156270000	2.455639000	1.205154000	1	4.113972000	2.604669000	-1.479191000
1	-5.890847000	2.848871000	1.226204000	1	5.852384000	2.959229000	-1.394205000
6	-5.161387000	2.029409000	-1.205706000	6	5.111347000	2.156274000	1.441552000
1	-5.890688000	2.849181000	-1.225769000	1	5.852982000	2.958743000	1.394358000
1	-5.292605000	1.419218000	-2.101935000	1	5.269291000	1.587809000	2.361551000
1	-4.156096000	2.456034000	-1.204485000	1	4.114656000	2.603967000	1.480199000
1	-7.450627000	1.567392000	-0.000065000	1	7.658462000	1.451059000	-0.000598000
1	-5.293012000	1.418635000	2.102092000	1	5.268000000	1.588753000	-2.361624000
6	3.733028000	2.041389000	-1.420673000	6	-3.640518000	2.268685000	1.421239000
6	2.984559000	1.638340000	-2.590524000	6	-2.931698000	1.797807000	2.590079000
6	4.492726000	1.103299000	-0.722708000	6	-4.483355000	1.404401000	0.723110000
6	3.024929000	0.312966000	-3.021887000	6	-3.093434000	0.481550000	3.021012000
6	1.813116000	-0.336764000	-3.468396000	6	-1.945955000	-0.276213000	3.467186000
6	1.730978000	2.358932000	-2.590883000	6	-1.617273000	2.400413000	2.591163000
6	0.566005000	1.734639000	-3.029044000	6	-0.514586000	1.672219000	3.029243000
6	0.607082000	0.361466000	-3.475310000	6	-0.682018000	0.308659000	3.474892000
6	3.733062000	2.040838000	1.421415000	6	-3.640481000	2.269035000	-1.420746000
6	2.940969000	3.009172000	0.698604000	6	-2.762776000	3.160465000	-0.697365000
6	4.492743000	1.103020000	0.723068000	6	-4.483334000	1.404578000	-0.722853000
6	2.940952000	3.009442000	-0.697466000	6	-2.762793000	3.160291000	0.698101000
6	1.704274000	3.207919000	-1.417521000	6	-1.512438000	3.243668000	1.418211000
6	1.704309000	3.207371000	1.418769000	6	-1.512401000	3.244018000	-1.417418000

6	0.513848000	3.409258000	0.722712000	6	-0.309197000	3.335395000	-0.721085000
6	0.513831000	3.409536000	-0.721355000	6	-0.309215000	3.335217000	0.721936000
6	3.815681000	-0.660368000	2.299525000	6	-3.969612000	-0.413260000	-2.299217000
6	3.025006000	0.311794000	3.021981000	6	-3.093349000	0.482297000	-3.020946000
6	4.534637000	-0.271740000	1.169845000	6	-4.650817000	0.039498000	-1.169918000
6	2.984622000	1.637334000	2.591128000	6	-2.931628000	1.798447000	-2.589683000
6	1.731041000	2.357923000	2.591796000	6	-1.617203000	2.401054000	-2.590581000
6	1.813203000	-0.338109000	3.468267000	6	-1.945855000	-0.275355000	-3.467275000
6	0.607169000	0.360120000	3.475482000	6	-0.681919000	0.309517000	-3.474798000
6	0.566080000	1.733464000	3.029749000	6	-0.514503000	1.672968000	-3.028809000
6	3.860987000	-2.328157000	-0.000475000	6	-4.169525000	-2.070804000	-0.000296000
6	3.111669000	-2.728563000	1.168699000	6	-3.459640000	-2.538274000	-1.169191000
6	4.559021000	-1.120930000	-0.000249000	6	-4.753310000	-0.804049000	-0.000148000
6	3.091295000	-1.910952000	2.298919000	6	-3.362816000	-1.725084000	-2.298586000
6	1.853940000	-1.713730000	3.019346000	6	-2.112223000	-1.642020000	-3.018614000
6	1.898727000	-3.377570000	0.724370000	6	-2.311473000	-3.296734000	-0.725105000
6	0.710581000	-3.194591000	1.424483000	6	-1.111178000	-3.222939000	-1.425505000
6	0.688862000	-2.346619000	2.591628000	6	-1.010294000	-2.379868000	-2.592062000
6	3.815624000	-0.659477000	-2.299829000	6	-3.969679000	-0.413828000	2.299040000
6	3.091237000	-1.910058000	-2.299687000	6	-3.362885000	-1.725654000	2.298103000
6	4.534607000	-0.271287000	-1.170015000	6	-4.650852000	0.039209000	1.169834000
6	3.111639000	-2.728107000	-1.169785000	6	-3.459674000	-2.538563000	1.168504000
6	1.898709000	-3.377290000	-0.725677000	6	-2.311494000	-3.296915000	0.724263000
6	1.853863000	-1.712558000	-3.020006000	6	-2.112312000	-1.642767000	3.018188000
6	0.688798000	-2.345611000	-2.592501000	6	-1.010370000	-2.380508000	2.591482000
6	0.710545000	-3.194039000	-1.425690000	6	-1.111220000	-3.223292000	1.424714000
6	-1.318261000	-2.039882000	1.428459000	6	1.015771000	-2.257296000	-1.428556000
6	-0.532464000	-2.993002000	0.701804000	6	0.143962000	-3.136346000	-0.701831000
6	-0.532481000	-2.992728000	-0.702900000	6	0.143941000	-3.136524000	0.701097000
6	-2.110877000	-1.096739000	0.733941000	6	1.877282000	-1.385784000	-0.728839000
6	-1.390601000	0.685248000	2.309123000	6	1.338001000	0.448821000	-2.310897000
6	-0.602732000	-0.291925000	3.021989000	6	0.463439000	-0.450583000	-3.020598000
6	-0.561703000	-1.618434000	2.581971000	6	0.302470000	-1.769520000	-2.582944000
6	-2.118841000	0.293181000	1.175815000	6	2.028068000	-0.010635000	-1.177240000
6	-1.447212000	2.363555000	0.000502000	6	1.552695000	2.117853000	0.000305000
6	-0.696719000	2.751423000	1.167769000	6	0.837360000	2.568718000	-1.165346000
6	-0.671863000	1.930862000	2.302639000	6	0.737143000	1.755247000	-2.302220000
6	-2.130522000	1.132572000	0.000271000	6	2.134794000	0.830487000	0.000151000
6	-1.390654000	0.686139000	-2.308771000	6	1.337941000	0.448255000	2.311083000
6	-0.671918000	1.931755000	-2.301824000	6	0.737086000	1.754679000	2.302714000
6	-0.696746000	2.751873000	-1.166634000	6	0.837336000	2.568437000	1.166043000
6	-2.118877000	0.293638000	-1.175602000	6	2.028029000	-0.010929000	1.177324000
6	-1.318297000	-2.039330000	-1.429167000	6	1.015722000	-2.257643000	1.428060000
6	-0.561769000	-1.617432000	-2.582531000	6	0.302391000	-1.770155000	2.582553000
6	-0.602811000	-0.290754000	-3.022042000	6	0.463351000	-0.451328000	3.020532000
6	-2.110893000	-1.096456000	-0.734257000	6	1.877247000	-1.385961000	0.728589000
$(C_{60})Mn(CO)_3$				$(C_{60})Fe(CO)_2Cl$			
25	4.230551000	0.002095000	-0.003117000	6	-2.710630000	-1.167091000	-2.856600000
6	5.235479000	1.439362000	-0.387520000	6	-3.484740000	0.001704000	-2.504911000
8	5.849353000	2.384804000	-0.638174000	6	-2.740867000	-2.297482000	-2.038587000
6	5.240380000	-0.381596000	1.430161000	6	-4.256422000	0.000944000	-1.343951000
8	5.860154000	-0.635488000	2.370762000	6	-4.285955000	1.170307000	-0.493697000
6	5.239839000	-1.055788000	-1.044914000	6	-2.710594000	1.170940000	-2.855041000
8	5.857822000	-1.754292000	-1.725798000	6	-2.740793000	2.300242000	-2.035524000
6	2.369976000	-0.540388000	-1.110895000	6	-3.544045000	2.300466000	-0.834400000
6	2.371537000	0.887595000	-0.865701000	6	-0.316103000	-2.593744000	-2.323790000
6	2.376478000	1.096903000	0.572003000	6	-0.285469000	-1.425883000	-3.170720000
6	2.371787000	-0.206867000	1.206935000	6	-1.518989000	-3.018536000	-1.764260000
6	2.378181000	-1.222380000	0.170841000	6	-1.459111000	-0.723192000	-3.425959000
6	1.635216000	-2.406120000	0.343382000	6	-1.459090000	0.727757000	-3.424989000
6	0.875765000	-2.934288000	-0.759455000	6	0.938890000	-0.701293000	-2.886956000
6	0.872777000	-2.276951000	-1.996229000				

6	1.635700000	-1.070407000	-2.191548000	6	0.938906000	0.705063000	-2.886015000
6	0.874104000	-0.186263000	-3.029149000	6	-0.285428000	1.430071000	-3.168817000
6	0.873431000	1.196128000	-2.791366000	6	-0.407715000	-3.477028000	0.386080000
6	1.632511000	1.746738000	-1.703763000	6	0.841366000	-3.021230000	-0.186525000
6	0.869228000	2.817760000	-1.114773000	6	-1.565839000	-3.467958000	-0.388330000
6	0.871239000	3.018841000	0.270999000	6	0.885499000	-2.585751000	-1.516721000
6	1.634229000	2.154175000	1.134150000	6	1.662668000	-1.430895000	-1.888395000
6	0.880096000	1.933561000	2.336658000	6	1.567154000	-2.314080000	0.840038000
6	0.881707000	0.673354000	2.951524000	6	2.317343000	-1.173823000	0.497484000
6	1.644125000	-0.412585000	2.397865000	6	2.372197000	-0.727305000	-0.888163000
6	0.881411000	-1.623228000	2.552702000	6	-2.860426000	-2.591168000	1.507547000
6	0.880994000	-2.603597000	1.551150000	6	-1.655547000	-2.593416000	2.307060000
6	-0.350737000	-3.282722000	1.200403000	6	-2.817048000	-3.022501000	0.182199000
6	-0.353241000	-3.488025000	-0.228647000	6	-0.453683000	-3.031921000	1.758927000
6	-1.537357000	-3.354812000	-0.949077000	6	0.770279000	-2.305373000	2.034792000
6	-1.539325000	-2.677476000	-2.229426000	6	-1.683603000	-1.420288000	3.156907000
6	-0.357551000	-2.155563000	-2.750243000	6	-0.509094000	-0.724339000	3.434640000
6	-0.358658000	-0.860949000	-3.387938000	6	0.740828000	-1.168623000	2.855430000
6	-1.541673000	-0.133379000	-3.480059000	6	-4.285992000	-1.169550000	-0.495257000
6	-1.542726000	1.295063000	-3.233646000	6	-4.332084000	-0.723380000	0.879201000
6	-0.360515000	1.950534000	-2.902043000	6	-3.544119000	-2.299277000	-0.837464000
6	-0.360921000	2.955661000	-1.866195000	6	-3.633670000	-1.422330000	1.862967000
6	-1.543226000	3.270644000	-1.200438000	6	-2.904761000	-0.700323000	2.880194000
6	-1.541576000	3.477739000	0.233077000	6	-4.332060000	0.722311000	0.880165000
6	-0.357277000	3.362235000	0.956860000	6	-3.633624000	1.419928000	1.864859000
6	-0.353507000	2.689236000	2.233926000	6	-2.904741000	0.696545000	2.881126000
6	-1.534645000	2.154363000	2.739824000	6	0.740862000	1.164760000	2.856979000
6	-1.531636000	0.853237000	3.377997000	6	-0.509072000	0.719749000	3.435603000
6	-0.348401000	0.128338000	3.491238000	6	-1.683561000	1.416103000	3.158798000
6	-0.347958000	-1.293618000	3.245149000	6	0.770351000	2.302600000	2.037855000
6	-1.530650000	-1.940239000	2.894867000	6	2.317391000	1.173052000	0.499048000
6	-1.532506000	-2.951346000	1.857055000	6	2.259276000	-0.000944000	1.334281000
6	-2.765328000	-2.821936000	1.112657000	6	1.514868000	-0.001723000	2.522473000
6	-2.768010000	-3.020979000	-0.267712000	6	1.567228000	2.312874000	0.843112000
6	-3.531590000	-2.140887000	-1.123822000	6	0.885579000	2.587699000	-1.513280000
6	-2.771320000	-1.929139000	-2.334527000	6	1.662711000	1.433317000	-1.886490000
6	-2.771645000	-0.676503000	-2.949202000	6	2.372195000	0.728362000	-0.887190000
6	-3.533808000	0.409835000	-2.377071000	6	0.841465000	3.021414000	-0.182506000
6	-2.773256000	1.626728000	-2.551081000	6	-1.565727000	3.468487000	-0.383714000
6	-2.774356000	2.599782000	-1.551404000	6	-1.518893000	3.020896000	-1.760242000
6	-3.534164000	2.390516000	-0.339694000	6	-0.316021000	2.596810000	-2.320341000
6	-2.771689000	2.933299000	0.762375000	6	-0.407603000	3.476490000	0.390706000
6	-2.767428000	2.281333000	1.995306000	6	-1.655464000	2.590355000	2.310506000
6	-3.527321000	1.064102000	2.172726000	6	-2.860346000	2.589218000	1.510996000
6	-2.762860000	0.182996000	3.025642000	6	-2.816953000	3.022313000	0.186223000
6	-2.762628000	-1.192124000	2.788259000	6	-0.453586000	3.029551000	1.762957000
6	-3.526564000	-1.736119000	1.688715000	26	4.170556000	0.000013000	-0.046765000
6	-4.260215000	-0.885206000	0.862796000	17	5.412558000	-0.000793000	1.794403000
6	-4.262573000	-1.091182000	-0.568670000	8	5.784891000	2.117663000	-1.223618000
6	-4.263782000	0.206632000	-1.206504000	8	5.785201000	-2.116473000	-1.225325000
6	-4.263400000	1.214330000	-0.169693000	6	5.153766000	1.276415000	-0.762704000
6	-4.260567000	0.539549000	1.109096000	6	5.153865000	-1.275692000	-0.763851000
$(C_{60})Fe(CO)_2Br$				$(C_{60})CoCONMe_3$			
6	-3.150493000	-2.704772000	1.168043000	27	-3.976614000	0.419537000	-0.000034000
6	-3.895398000	-2.295109000	-0.000726000	7	-5.476278000	-0.910893000	-0.000018000
6	-3.118081000	-1.886750000	2.298242000	8	-5.608660000	2.795410000	-0.000016000
6	-4.576285000	-1.078715000	-0.000380000	6	-4.977786000	1.824322000	-0.000029000
6	-4.540864000	-0.229208000	-1.170165000	6	-6.841827000	-0.330160000	-0.000358000
6	-3.150453000	-2.704085000	-1.169710000	1	-6.981128000	0.286582000	0.888473000
6	-3.118001000	-1.885397000	-2.299426000	1	-6.980817000	0.286269000	-0.889455000
6	-3.827230000	-0.626251000	-2.300204000	6	-5.339214000	-1.757986000	-1.210329000
6	-0.722192000	-2.356422000	2.594693000	1	-4.375733000	-2.270177000	-1.198317000

6	-0.756567000	-3.203686000	1.427052000	1	-6.141194000	-2.506318000	-1.238805000
6	-1.878822000	-1.706459000	3.019323000	6	-5.339563000	-1.757436000	1.210718000
6	-1.946308000	-3.368638000	0.724393000	1	-6.141524000	-2.505786000	1.239285000
6	-1.946282000	-3.368209000	-0.726409000	1	-5.404268000	-1.131447000	2.102446000
6	0.485695000	-3.014726000	0.702155000	1	-4.376056000	-2.269593000	1.199233000
6	0.485718000	-3.014310000	-0.703878000	1	-7.588256000	-1.133271000	-0.000343000
6	-0.756518000	-3.202844000	-1.428930000	1	-5.403620000	-1.132399000	-2.102362000
6	-0.605984000	0.352709000	3.476508000	6	3.508959000	-2.119861000	1.421627000
6	0.595505000	-0.314078000	3.021013000	6	2.776380000	-1.692017000	2.592378000
6	-1.820188000	-0.330900000	3.467812000	6	4.299476000	-1.207936000	0.723052000
6	0.537687000	-1.644016000	2.586507000	6	2.860231000	-0.368824000	3.022682000
6	1.284219000	-2.074743000	1.431514000	6	1.671338000	0.321833000	3.471498000
6	1.398615000	0.653760000	2.314592000	6	1.498689000	-2.369959000	2.591027000
6	2.118634000	0.253678000	1.173865000	6	0.355785000	-1.708309000	3.030561000
6	2.067289000	-1.131754000	0.727511000	6	0.443016000	-0.337157000	3.478241000
6	-2.965798000	1.658455000	2.590681000	6	3.508924000	-2.120626000	-1.420544000
6	-1.703275000	2.363215000	2.592591000	6	2.684140000	-3.061680000	-0.697722000
6	-3.023949000	0.333666000	3.022067000	6	4.299457000	-1.208323000	-0.722480000
6	-0.546739000	1.724883000	3.031299000	6	2.684155000	-3.061303000	0.699332000
6	0.694758000	1.905994000	2.304720000	6	1.442828000	-3.219505000	1.418643000
6	-1.666306000	3.212402000	1.419215000	6	1.442794000	-3.220265000	-1.416911000
6	-0.474008000	3.398918000	0.723023000	6	0.245114000	-3.380553000	-0.721006000
6	0.727986000	2.725617000	1.167422000	6	0.245131000	-3.380166000	0.722854000
6	-4.540905000	-0.229896000	1.169906000	6	3.681417000	0.575917000	-2.300370000
6	-4.481812000	1.144027000	0.723177000	6	2.860157000	-0.370454000	-3.022527000
6	-3.827309000	-0.627604000	2.299736000	6	4.386014000	0.164545000	-1.169831000
6	-3.709749000	2.071689000	1.421584000	6	2.776317000	-1.693416000	-2.591510000
6	-2.904941000	3.029288000	0.699170000	6	1.498626000	-2.371356000	-2.589760000
6	-4.481787000	1.144452000	-0.722626000	6	1.671255000	0.319962000	-3.471691000
6	-3.709700000	2.072525000	-1.420460000	6	0.442931000	-0.339031000	-3.478042000
6	-2.904917000	3.029699000	-0.697455000	6	0.355711000	-1.709940000	-3.029621000
6	0.728023000	2.726299000	-1.165758000	6	3.779114000	2.241983000	-0.000636000
6	-0.473984000	3.399343000	-0.721007000	6	3.043946000	2.666827000	-1.170331000
6	-1.666258000	3.213236000	-1.417349000	6	4.438260000	1.013147000	-0.000312000
6	0.694834000	1.907345000	-2.303537000	6	2.996159000	1.848570000	-2.299942000
6	2.118678000	0.254366000	-1.173607000	6	1.755343000	1.692625000	-3.024417000
6	2.127715000	1.092620000	0.000377000	6	1.851588000	3.350460000	-0.726364000
6	1.473725000	2.333536000	0.000731000	6	0.657960000	3.205868000	-1.426989000
6	1.398690000	0.655116000	-2.314121000	6	0.608913000	2.361789000	-2.596817000
6	0.537775000	-1.642493000	-2.587421000	6	3.681470000	0.577157000	2.299995000
6	1.284268000	-2.073900000	-1.432657000	6	2.996213000	1.849813000	2.298900000
6	2.067304000	-1.131324000	-0.728065000	6	4.386044000	0.165176000	1.169664000
6	0.595610000	-0.312302000	-3.021145000	6	3.043972000	2.667459000	1.168845000
6	-1.820068000	-0.328860000	-3.468037000	6	1.851605000	3.350853000	0.724539000
6	-1.878717000	-1.704683000	-3.020359000	6	1.755415000	1.694257000	3.023487000
6	-0.722102000	-2.354895000	-2.596071000	6	0.608974000	2.363191000	2.595557000
6	-0.605865000	0.354752000	-3.476287000	6	0.657991000	3.206637000	1.425269000
6	-1.703187000	2.364739000	-2.591226000	6	-1.408804000	2.124083000	-1.434514000
6	-2.965710000	1.659979000	-2.589775000	6	-0.590697000	3.045301000	-0.705546000
6	-3.023844000	0.335444000	-3.021941000	6	-0.590684000	3.045686000	0.703949000
6	-0.546636000	1.726663000	-3.030267000	6	-2.211281000	1.195304000	-0.734576000
26	3.922350000	-0.419018000	-0.000069000	6	-1.566122000	-0.600109000	-2.317132000
35	5.391873000	1.397754000	0.000196000	6	-0.743653000	0.353902000	-3.026890000
8	5.461438000	-1.690472000	-2.117799000	6	-0.665563000	1.679074000	-2.594570000
8	5.460967000	-1.691282000	2.117526000	6	-2.264581000	-0.180031000	-1.181354000
6	4.860892000	-1.189909000	-1.275645000	6	-1.683390000	-2.277053000	0.000649000
6	4.860960000	-1.190293000	1.275243000	6	-0.946762000	-2.690344000	-1.166305000
				6	-0.888260000	-1.865567000	-2.300868000
				6	-2.338219000	-1.020342000	0.000317000
				6	-1.566068000	-0.598864000	2.317522000
				6	-0.888203000	-1.864330000	2.301923000
				6	-0.946736000	-2.689722000	1.167813000
				6	-2.264552000	-0.179400000	1.181535000
				6	-1.408771000	2.124855000	1.433429000

	6	-0.665503000	1.680476000	2.593708000
	6	-0.743578000	0.355531000	3.026736000
	6	-2.211265000	1.195694000	0.734009000
(C₆₀)CoCOPeT₃				
27	3.494777000	0.803924000	-0.144018000	
8	5.206974000	3.114669000	-0.113503000	
6	4.530235000	2.173178000	-0.156717000	
6	-3.754550000	-2.389172000	-1.283645000	
6	-3.099717000	-1.928610000	-2.487293000	
6	-4.610500000	-1.536396000	-0.587479000	
6	-3.325448000	-0.634251000	-2.953118000	
6	-2.222803000	0.154432000	-3.458083000	
6	-1.762099000	-2.477894000	-2.506548000	
6	-0.702957000	-1.721372000	-3.000283000	
6	-0.937093000	-0.380685000	-3.484456000	
6	-3.673553000	-2.298848000	1.555646000	
6	-2.781639000	-3.178742000	0.834688000	
6	-4.569372000	-1.490584000	0.856649000	
6	-2.821666000	-3.223335000	-0.560239000	
6	-1.590405000	-3.280890000	-1.313133000	
6	-1.509658000	-3.190593000	1.518937000	
6	-0.323148000	-3.255028000	0.791248000	
6	-0.364546000	-3.300777000	-0.650654000	
6	-4.085630000	0.395049000	2.361417000	
6	-3.154450000	-0.442627000	3.083967000	
6	-4.778664000	-0.119285000	1.266390000	
6	-2.952986000	-1.764629000	2.689318000	
6	-1.615101000	-2.313148000	2.667292000	
6	-2.027014000	0.374342000	3.475349000	
6	-0.740603000	-0.160462000	3.462560000	
6	-0.531081000	-1.529056000	3.051494000	
6	-4.414448000	1.969702000	0.019175000	
6	-3.692093000	2.501831000	1.152430000	
6	-4.947889000	0.682244000	0.074981000	
6	-3.530141000	1.728330000	2.302397000	
6	-2.259664000	1.717828000	2.991678000	
6	-2.586365000	3.285675000	0.651048000	
6	-1.364777000	3.279885000	1.317880000	
6	-1.198221000	2.481976000	2.509136000	
6	-4.215120000	0.249372000	-2.233469000	
6	-3.659597000	1.582592000	-2.290468000	
6	-4.844627000	-0.193327000	-1.070758000	
6	-3.757798000	2.427901000	-1.184327000	
6	-2.627167000	3.240026000	-0.797576000	
6	-2.429774000	1.526411000	-3.047720000	
6	-1.344041000	2.318174000	-2.676466000	
6	-1.444598000	3.189781000	-1.530430000	
6	0.798007000	2.401378000	1.291329000	
6	-0.128385000	3.217646000	0.561686000	
6	-0.167453000	3.174105000	-0.843398000	
6	1.662181000	1.535447000	0.591621000	
6	1.253033000	-0.258269000	2.248341000	
6	0.360161000	0.629950000	2.953984000	
6	0.137662000	1.927084000	2.486675000	
6	1.887603000	0.191824000	1.081683000	
6	1.466442000	-1.991104000	-0.021744000	
6	0.807824000	-2.435699000	1.177661000	
6	0.701590000	-1.583408000	2.288951000	
6	2.011487000	-0.683509000	-0.079869000	
6	1.121208000	-0.404306000	-2.380920000	
6	0.569031000	-1.729693000	-2.305406000	
6	0.739821000	-2.509138000	-1.151833000	
(C₆₀)NiNeT₃Cl				
6	-3.225180000	0.222474000	3.041997000	
6	-2.085825000	1.074605000	3.306510000	
6	-3.055094000	-1.156747000	2.936338000	
6	-0.818541000	0.515737000	3.459711000	
6	0.325529000	1.157702000	2.849501000	
6	-2.253742000	2.294188000	2.548140000	
6	-1.148369000	2.915721000	1.966774000	
6	0.167749000	2.337636000	2.120063000	
6	-4.590119000	-1.225270000	1.016533000	
6	-4.767128000	0.205728000	1.126759000	
6	-3.749733000	-1.894287000	1.905195000	
6	-4.098491000	0.916658000	2.122198000	
6	-3.494733000	2.193360000	1.815079000	
6	-4.864757000	0.748315000	-0.209844000	
6	-4.286854000	1.982181000	-0.505704000	
6	-3.588689000	2.718028000	0.524276000	
6	-2.850065000	-3.255860000	0.060641000	
6	-3.728091000	-2.566474000	-0.857873000	
6	-2.860700000	-2.925277000	1.419340000	
6	-4.579484000	-1.567213000	-0.388552000	
6	-4.749882000	-0.347282000	-1.146486000	
6	-3.015767000	-2.382636000	-2.102104000	
6	-3.179169000	-1.206241000	-2.831980000	
6	-4.064373000	-0.170660000	-2.347532000	
6	-0.407611000	-3.074696000	1.498821000	
6	-0.396525000	-3.415745000	0.095581000	
6	-1.618834000	-2.831058000	2.146507000	
6	-1.596951000	-3.500117000	-0.609551000	
6	-1.697369000	-2.956556000	-1.949494000	
6	0.752136000	-2.777019000	-0.508686000	
6	0.648097000	-2.243258000	-1.805120000	
6	-0.595585000	-2.345947000	-2.542255000	
6	-0.641564000	-0.914374000	3.346785000	
6	0.612718000	-1.157867000	2.663217000	
6	-1.736843000	-1.732947000	3.084475000	
6	0.734210000	-2.226294000	1.759941000	
6	1.450520000	-2.055624000	0.521995000	
6	1.210031000	0.117063000	2.375557000	
6	1.883444000	0.295768000	1.165533000	
6	2.025548000	-0.796858000	0.220619000	
6	0.371338000	-0.274752000	-3.039765000	
6	1.245298000	-0.978186000	-2.126676000	
6	1.903882000	-0.259872000	-1.124291000	
6	0.205272000	1.106764000	-2.935056000	
6	-2.208942000	0.863985000	-3.332150000	
6	-2.033675000	-0.566967000	-3.442430000	
6	-0.765917000	-1.129100000	-3.303037000	
6	-1.110287000	1.686908000	-3.084255000	
6	-2.429090000	3.007586000	-1.487331000	
6	-3.571868000	2.165160000	-1.748640000	
6	-3.461276000	1.106898000	-2.652568000	
6	-1.223113000	2.778377000	-2.144605000	
6	0.014182000	3.203096000	-0.043321000	
6	-1.243862000	3.452543000	0.629244000	
6	-2.439742000	3.350726000	-0.077481000	
6	0.023884000	2.869507000	-1.413060000	
6	1.735472000	1.168653000	-1.009397000	
6	1.727435000	1.511792000	0.403979000	

6	1.816872000	0.116269000	-1.282347000	6	0.884519000	2.533418000	0.877637000
6	0.718487000	2.311408000	-1.570978000	6	0.904169000	1.854629000	-1.910491000
6	-0.007273000	1.764359000	-2.694990000	28	3.617618000	0.599830000	-0.121072000
6	0.189354000	0.438655000	-3.090279000	17	4.666092000	2.436704000	-0.475203000
6	1.624053000	1.489608000	-0.867033000	7	5.175496000	-0.611469000	0.124220000
15	5.188430000	-0.550892000	0.054262000	6	6.516017000	0.044480000	-0.063548000
6	5.516572000	-1.618642000	-1.402808000	1	6.508233000	0.498225000	-1.055078000
1	5.790114000	-0.954189000	-2.229249000	1	6.557811000	0.881038000	0.633903000
1	6.416245000	-2.200821000	-1.160299000	6	7.708144000	-0.873704000	0.109781000
6	4.371077000	-2.528749000	-1.807973000	1	7.774272000	-1.307630000	1.111208000
1	3.508934000	-1.951135000	-2.155397000	1	8.615241000	-0.284857000	-0.040983000
1	4.039076000	-3.170228000	-0.985714000	1	7.733617000	-1.688324000	-0.619052000
1	4.675318000	-3.181740000	-2.628654000	6	4.999633000	-1.733578000	-0.854976000
6	6.825056000	0.201773000	0.400508000	1	5.739042000	-2.509290000	-0.617069000
1	6.677556000	0.959062000	1.178005000	1	4.019087000	-2.175250000	-0.653741000
1	7.454395000	-0.579952000	0.845108000	6	5.119964000	-1.307006000	-2.299983000
6	7.504447000	0.802639000	-0.821562000	1	4.496273000	-0.432994000	-2.518796000
1	6.855143000	1.499593000	-1.358414000	1	4.788994000	-2.119834000	-2.949842000
1	7.822424000	0.030940000	-1.526871000	1	6.147499000	-1.063158000	-2.578750000
1	8.395719000	1.358339000	-0.524244000	6	5.049324000	-1.167626000	1.511532000
6	4.939009000	-1.713626000	1.454352000	1	4.067631000	-1.648239000	1.567033000
1	3.977736000	-2.217378000	1.298938000	1	5.790165000	-1.969921000	1.624010000
1	5.715145000	-2.486763000	1.378950000	6	5.211244000	-0.133846000	2.602306000
6	4.980107000	-1.030724000	2.813058000	1	6.242766000	0.211228000	2.700911000
1	4.238990000	-0.227910000	2.883630000	1	4.918767000	-0.566876000	3.561161000
1	5.961639000	-0.596208000	3.020408000	1	4.579745000	0.744508000	2.428064000
1	4.767133000	-1.747311000	3.609206000				
(C ₆₀)NiPMe ₃ Cl				(C ₆₀)CuNMe ₃			
6	-3.297816000	-1.216620000	-2.588247000	29	4.126931000	-0.253979000	-0.007392000
6	-2.220067000	-2.181635000	-2.585456000	7	6.046449000	0.077904000	0.001512000
6	-3.063668000	0.086698000	-3.022890000	6	6.379117000	0.844134000	1.223971000
6	-0.951656000	-0.813019000	-3.024390000	1	5.794820000	1.766664000	1.246963000
6	0.217358000	-2.259544000	-2.294167000	1	6.139952000	0.249442000	2.107659000
6	-2.368689000	-3.016085000	-1.411209000	6	6.836042000	-1.172563000	-0.021956000
6	-1.243287000	-3.454895000	-0.713974000	1	6.599764000	-1.740464000	-0.923528000
6	0.077693000	-3.070543000	-1.159731000	1	7.911278000	-0.949840000	-0.014157000
6	-4.415504000	0.975188000	-1.171189000	6	6.385922000	0.893652000	-1.186416000
6	-4.660261000	-0.376941000	-0.720583000	1	7.453809000	1.148879000	-1.189897000
6	-3.633616000	1.203107000	-2.302544000	1	5.800846000	1.815914000	-1.175200000
6	-4.111058000	-1.453453000	-1.416562000	1	6.152661000	0.335496000	-2.095140000
6	-3.535272000	-2.563046000	-0.691928000	1	7.447115000	1.098101000	1.244478000
6	-4.659801000	-0.373536000	0.724668000	1	6.594430000	-1.777354000	0.853845000
6	-4.110182000	-1.446778000	1.425367000	6	-3.546781000	-0.442324000	-2.354058000
6	-3.534817000	-2.559751000	0.705583000	6	-2.753574000	0.590653000	-2.981330000
6	-2.515284000	3.085123000	-1.176576000	6	-4.267719000	-0.158952000	-1.194686000
6	-3.331033000	2.851197000	-0.006000000	6	-2.711729000	1.870862000	-2.429017000
6	-2.663349000	2.274969000	-2.304095000	6	-1.457501000	2.586462000	-2.360689000
6	-4.262492000	1.814317000	-0.003250000	6	-1.542451000	-0.018204000	-3.483627000
6	-4.414734000	0.980700000	1.168730000	6	-0.334882000	0.674827000	-3.423230000
6	-2.514498000	3.090635000	1.162930000	6	-0.291558000	2.001111000	-2.851677000
6	-2.661831000	2.285798000	2.294362000	6	-3.603190000	-2.318244000	-0.220387000
6	-3.632093000	1.213943000	2.298470000	6	-2.853419000	-2.611157000	-1.421327000
6	-0.223286000	2.204091000	-2.604135000	6	-4.296286000	-1.113514000	-0.108875000
6	-0.069990000	3.037294000	-1.435663000	6	-2.825645000	-1.690403000	-2.468642000
6	-1.497030000	1.826310000	-3.028922000	6	-1.587373000	-1.429759000	-3.166864000
6	-1.194741000	3.463142000	-0.733926000	6	-1.643556000	-3.302046000	-1.036492000
6	-1.194254000	3.466559000	0.717647000	6	-0.451614000	-3.055671000	-1.715103000
6	1.101545000	2.581277000	-0.712406000	6	-0.423018000	-2.102178000	-2.799837000
6	1.102044000	2.584629000	0.698800000	6	-3.552746000	-0.869781000	2.223534000
6	-0.069019000	3.044016000	1.420637000	6	-2.831843000	-2.117868000	2.107367000
6	-0.708338000	-0.461558000	-3.475663000	6	-4.270794000	-0.376505000	1.134935000
6	0.609126000	-0.071292000	-3.023965000	6	-2.856869000	-2.829168000	0.907697000

6	-1.743354000	0.471739000	-3.472365000	6	-1.645589000	-3.436695000	0.404918000
6	0.851186000	1.237003000	-2.601606000	6	-1.595424000	-1.990918000	2.844926000
6	1.675952000	1.490593000	-1.441013000	6	-0.429978000	-2.584655000	2.363630000
6	1.178199000	-1.191159000	-2.307011000	6	-0.455570000	-3.320472000	1.120703000
6	1.955607000	-0.953049000	-1.174332000	6	-3.465374000	1.901047000	1.600418000
6	2.244507000	0.400794000	-0.740185000	6	-2.718547000	1.389069000	2.727660000
6	0.852909000	1.249236000	2.594442000	6	-4.226469000	1.033652000	0.817724000
6	1.676920000	1.497359000	1.432137000	6	-2.761817000	0.029037000	3.033717000
6	2.245100000	0.404221000	0.736070000	6	-1.551711000	-0.662416000	3.417914000
6	0.611093000	-0.057078000	3.023128000	6	-1.464460000	2.104514000	2.796219000
6	-1.741088000	0.488071000	3.470446000	6	-0.299674000	1.438620000	3.174352000
6	-1.495045000	1.840567000	3.020528000	6	-0.344185000	0.029486000	3.490089000
6	-0.221571000	2.216300000	2.593097000	6	-3.461639000	2.165565000	-1.228534000
6	-0.706082000	-0.445206000	3.477546000	6	-2.670339000	3.063153000	-0.417226000
6	-2.218406000	-2.169484000	2.596458000	6	-4.224673000	1.168278000	-0.621930000
6	-3.296151000	-1.204428000	2.595363000	6	-2.672365000	2.933423000	0.971597000
6	-3.061702000	0.100927000	3.023681000	6	-1.435630000	3.059875000	1.709913000
6	-0.949701000	-1.798767000	3.032775000	6	-1.431707000	3.323752000	-1.115808000
6	0.078438000	-3.065094000	1.173473000	6	-0.240972000	3.452297000	-0.402563000
6	-1.242820000	-3.451524000	0.730371000	6	-0.242990000	3.317898000	1.036104000
6	-2.367769000	-3.009427000	1.426261000	6	1.656817000	0.453705000	2.362580000
6	0.218827000	-2.248766000	2.303934000	6	0.937520000	1.699583000	2.471454000
6	1.956360000	-0.947529000	1.176854000	6	0.964988000	2.621051000	1.421435000
6	1.821609000	-1.781091000	0.003279000	6	2.391623000	0.170935000	1.204699000
6	0.893977000	-2.841331000	0.006060000	6	1.572866000	-2.168644000	1.236114000
6	1.179710000	-1.180292000	2.311120000	6	0.824004000	-1.865278000	2.430443000
28	3.836824000	-0.604220000	-0.000478000	6	0.865611000	-0.581072000	2.982018000
17	5.279767000	-2.181650000	0.000048000	6	2.346954000	-1.169178000	0.628641000
15	5.410244000	0.847705000	-0.000017000	6	1.576421000	-1.902210000	-1.609243000
6	6.480568000	0.695975000	1.451677000	6	0.784785000	-2.925824000	-0.973320000
1	5.901359000	0.828600000	2.367691000	6	0.782804000	-3.056056000	0.419430000
6	6.927439000	-0.299575000	1.463476000	6	2.348262000	-1.032852000	-0.825396000
6	4.833526000	2.568467000	-0.004329000	6	1.662467000	0.882343000	-2.230187000
1	5.691022000	3.247722000	-0.005500000	6	0.873733000	-0.019461000	-3.033601000
1	4.229939000	2.768698000	-0.892601000	6	0.830710000	-1.383184000	-2.729111000
6	6.487354000	0.691355000	-1.446156000	6	2.394107000	0.389913000	-1.143162000
1	5.912566000	0.821810000	-2.365255000	6	1.712532000	2.333225000	0.221224000
1	7.275887000	1.448991000	-1.411808000	6	0.968451000	2.839175000	-0.906990000
1	4.229001000	2.772874000	0.882333000	6	0.943632000	2.127468000	-2.109261000
1	7.268879000	1.453921000	1.419039000	6	2.418824000	1.130689000	0.109913000
1	6.933617000	-0.304497000	-1.453109000				
$(C_{60})CuPEt_3$				$(C_{60})CuCO$			
29	3.670247000	0.076939000	-0.120872000	29	-4.456395000	-0.001425000	-0.003183000
15	5.828730000	-0.015238000	0.031631000	8	-7.392880000	0.002444000	0.006817000
6	-3.992349000	1.608072000	1.827059000	6	-6.250458000	0.000496000	0.001675000
6	-3.200375000	1.019486000	2.883596000	6	3.212600000	-0.114277000	-2.412640000
6	-4.732093000	0.791221000	0.972849000	6	2.452177000	-1.300514000	-2.736093000
6	-3.177402000	-0.365360000	3.049180000	6	3.943415000	-0.057645000	-1.226686000
6	-1.930346000	-1.036450000	3.340717000	6	2.451992000	-2.388765000	-1.863566000
6	-1.976925000	1.780470000	3.002960000	6	1.221048000	-3.097680000	-1.596165000
6	-0.776448000	1.133420000	3.290725000	6	1.221518000	-0.885069000	-3.370300000
6	-0.752772000	-0.300828000	3.462406000	6	0.037756000	-1.575122000	-3.118792000
6	-4.062401000	2.158887000	-0.959822000	6	0.037578000	-2.701679000	-2.215294000
6	-3.293138000	3.004568000	-0.074518000	6	3.211378000	2.261373000	-0.853895000
6	-4.767941000	1.071471000	-0.445460000	6	2.451000000	2.201773000	-2.082026000
6	-3.258790000	2.733866000	1.293528000	6	3.942925000	1.151336000	-0.433457000
6	-2.013285000	2.841105000	2.019164000	6	2.451520000	1.035518000	-2.847096000
6	-2.082375000	3.390493000	-0.763527000	6	1.220975000	0.561305000	-3.438823000
6	-0.883403000	3.500761000	-0.061720000	6	1.219758000	2.932622000	-1.883258000
6	-0.848383000	3.221364000	1.355263000	6	0.036378000	2.479234000	-2.461877000
6	-4.057909000	-0.322679000	-2.344389000	6	0.037033000	1.271748000	-3.254075000
6	-3.324171000	0.803984000	-2.876353000	6	3.210180000	1.512876000	1.887179000

6	-4.765755000	-0.191599000	-1.149985000	6	2.449008000	2.661775000	1.450820000
6	-3.326327000	2.022125000	-2.196838000	6	3.942325000	0.770478000	0.961532000
6	-2.102965000	2.783171000	-2.077101000	6	2.449589000	3.029256000	0.105282000
6	-2.098709000	0.305496000	-3.459428000	6	1.218911000	3.444939000	-0.528912000
6	-0.921640000	1.043704000	-3.350460000	6	1.217619000	2.697470000	2.207031000
6	-0.923897000	2.305061000	-2.645831000	6	0.034143000	3.107133000	1.596894000
6	-3.986113000	-2.406070000	-0.413466000	6	0.034766000	3.487869000	0.203788000
6	-3.250140000	-2.540779000	-1.650626000	6	3.211000000	-1.325655000	2.022300000
6	-4.728600000	-1.251604000	-0.167537000	6	2.449060000	-0.556039000	2.979769000
6	-3.285319000	-1.518101000	-2.598332000	6	3.942564000	-0.674028000	1.030217000
6	-2.074938000	-1.131487000	-3.287670000	6	2.448615000	0.837216000	2.913498000
6	-2.003317000	-3.211589000	-1.359206000	6	1.217467000	1.567963000	3.112874000
6	-0.838348000	-2.842637000	-2.029393000	6	1.218189000	-1.265003000	3.247549000
6	-0.874693000	-1.784039000	-3.011577000	6	0.034248000	-0.558867000	3.448100000
6	-3.946174000	-1.212112000	2.164952000	6	0.033711000	0.883709000	3.379745000
6	-3.173967000	-2.407388000	1.909250000	6	3.212436000	-2.331161000	-0.635385000
6	-4.708166000	-0.643838000	1.144588000	6	2.450955000	-3.004809000	0.392290000
6	-3.193871000	-2.993542000	0.643620000	6	3.943245000	-1.185719000	-0.322165000
6	-1.968297000	-3.491585000	0.060270000	6	2.450088000	-2.511071000	1.696799000
6	-1.928070000	-2.300145000	2.634966000	6	1.218850000	-2.475658000	2.453280000
6	-0.748550000	-2.788021000	2.075108000	6	1.220429000	-3.479414000	-0.199396000
6	-0.769080000	-3.393963000	0.763722000	6	0.036288000	-3.452768000	0.534078000
6	1.138017000	-1.612381000	-1.838350000	6	0.035467000	-2.941793000	1.884874000
6	0.406229000	-2.732276000	-1.299313000	6	-1.953446000	0.114910000	2.424037000
6	0.440206000	-3.003051000	0.071663000	6	-1.194796000	-1.034144000	2.848738000
6	1.888038000	-0.794510000	-0.983429000	6	-1.194293000	-2.203539000	2.081599000
6	1.091663000	1.219810000	-2.178202000	6	-2.696992000	0.058184000	1.236478000
6	0.324795000	0.369536000	-3.054746000	6	-1.953327000	2.342038000	0.638518000
6	0.347802000	-1.018727000	-2.888625000	6	-1.195325000	2.390668000	1.862984000
6	1.864289000	0.650810000	-1.156880000	6	-1.195480000	1.299493000	2.737874000
6	1.131825000	2.418190000	0.411499000	6	-2.696854000	1.195019000	0.324915000
6	0.341164000	2.997256000	-0.646665000	6	-1.951854000	1.331943000	-2.031531000
6	0.321303000	2.410209000	-1.915246000	6	-1.193405000	2.511028000	-1.698614000
6	1.884460000	1.262789000	0.164769000	6	-1.194299000	3.006077000	-0.390572000
6	1.203318000	0.326065000	2.348769000	6	-2.696110000	0.679433000	-1.038001000
6	0.432684000	1.519964000	2.595740000	6	-1.951052000	-1.519775000	-1.895812000
6	0.397556000	2.545402000	1.646363000	6	-1.191917000	-0.839008000	-2.913821000
6	1.921831000	0.194794000	1.154119000	6	-1.192386000	0.558010000	-2.980287000
6	1.207540000	-2.164468000	0.959824000	6	-2.695844000	-0.776311000	-0.968816000
6	0.473704000	-2.021867000	2.193674000	6	-1.952250000	-2.271749000	0.858029000
6	0.471597000	-0.800850000	2.874368000	6	-1.192930000	-3.030179000	-0.103469000
6	1.922811000	-1.076605000	0.444739000	6	-1.192340000	-2.661691000	-1.452647000
6	6.700108000	-0.337459000	-1.548323000	6	-2.696427000	-1.160127000	0.437021000
1	6.627025000	0.577686000	-2.146356000				
1	7.765517000	-0.487390000	-1.335020000				
6	6.113814000	-1.518104000	-2.306722000				
1	5.047950000	-1.366160000	-2.510983000				
1	6.211837000	-2.453819000	-1.748449000				
1	6.618466000	-1.657964000	-3.264579000				
6	6.593526000	1.510365000	0.701140000				
1	6.310631000	1.572358000	1.758018000				
1	7.683808000	1.393447000	0.675647000				
6	6.150317000	2.759329000	-0.044919000				
1	5.060148000	2.867880000	-0.019562000				
1	6.454428000	2.738846000	-1.095476000				
1	6.583581000	3.656918000	0.400441000				
6	6.364945000	-1.356224000	1.162293000				
1	6.203409000	-2.303083000	0.635007000				
1	7.446192000	-1.269017000	1.323683000				
6	5.601212000	-1.341982000	2.477796000				
1	4.520941000	-1.414738000	2.303599000				
1	5.779637000	-0.423686000	3.045164000				
1	5.894441000	-2.179501000	3.113565000				

**ii. Cartesian coordinates of optimized geometry of $(\text{Cl}^-@C_{60})\text{ML}_n$ complexes at Mo6L/6-31G(d,p) level.
Atomic number followed by X, Y, Z coordinates in Å.**

$(\text{Cl}^-@C_{60})\text{ScNMe}_3(\text{CO})_2$				$(\text{Cl}^-@C_{60})\text{ScPMe}_3(\text{CO})_2$			
21	4.325985000	-0.358307000	-0.000172000	21	4.148142000	0.955801000	-0.578874000
7	5.664712000	1.515743000	-0.000165000	15	5.552011000	-1.364868000	-0.251128000
8	5.418243000	-2.493277000	-2.340335000	8	4.796067000	1.773916000	2.585100000
8	5.418012000	-2.492061000	2.341201000	8	4.081036000	4.268259000	-1.061912000
6	5.050211000	-1.737033000	-1.537048000	6	4.660126000	1.495841000	1.462635000
6	5.050073000	-1.736258000	1.537457000	6	4.191266000	3.116559000	-0.955153000
6	7.092595000	1.162733000	0.000032000	6	7.353538000	-1.235688000	0.075371000
1	7.330211000	0.573205000	0.890012000	1	7.883134000	-0.864986000	-0.805576000
1	7.330458000	0.573207000	-0.889884000	1	7.531478000	-0.538654000	0.898228000
6	5.326871000	2.288885000	-1.209441000	6	4.952629000	-2.182363000	1.271363000
1	4.265279000	2.552555000	-1.185977000	1	3.900794000	-2.458732000	1.157591000
1	5.921312000	3.211211000	-1.269810000	1	5.531983000	-3.086607000	1.483734000
6	5.326563000	2.288934000	1.208999000	6	5.478039000	-2.732300000	-1.472318000
1	5.921081000	3.211199000	1.269536000	1	5.997291000	-3.623641000	-1.106897000
1	5.522217000	1.684519000	2.099686000	1	5.929496000	-2.427535000	-2.419350000
1	4.265004000	2.552707000	1.185200000	1	4.432231000	-2.990104000	-1.661585000
1	7.725560000	2.061501000	0.000125000	1	7.774557000	-2.208188000	0.348007000
1	5.522879000	1.684489000	-2.100062000	1	5.029687000	-1.493781000	2.116104000
6	-3.468912000	2.286054000	1.419298000	6	-3.610797000	-2.392045000	-1.115648000
6	-2.764077000	1.810004000	2.586407000	6	-3.090770000	-1.880691000	-2.361941000
6	-4.318974000	1.429455000	0.722149000	6	-4.384798000	-1.573163000	-0.295981000
6	-2.938522000	0.495981000	3.018610000	6	-3.365848000	-0.568871000	-2.746589000
6	-1.799511000	-0.270935000	3.464034000	6	-2.326080000	0.242099000	-3.334608000
6	-1.446990000	2.401881000	2.587824000	6	-1.766767000	-2.424448000	-2.552710000
6	-0.350238000	1.664587000	3.026542000	6	-0.767910000	-1.643994000	-3.129208000
6	-0.531234000	0.303289000	3.472336000	6	-1.052355000	-0.286602000	-3.527968000
6	-3.469074000	2.285713000	-1.419577000	6	-3.218639000	-2.418020000	1.696586000
6	-2.586453000	3.170860000	-0.697318000	6	-2.413282000	-3.264245000	0.846897000
6	-4.319056000	1.429281000	-0.722126000	6	-4.185342000	-1.586272000	1.134721000
6	-2.586373000	3.171030000	0.696726000	6	-2.606116000	-3.251455000	-0.534064000
6	-1.336630000	3.245193000	1.416699000	6	-1.466830000	-3.273620000	-1.420518000
6	-1.336797000	3.244853000	-1.417456000	6	-1.074917000	-3.299774000	1.386997000
6	-0.134511000	3.328623000	-0.721699000	6	0.023330000	-3.331119000	0.530836000
6	-0.134426000	3.328793000	0.720779000	6	-0.176699000	-3.317021000	-0.897927000
6	-3.821230000	-0.391519000	-2.296392000	6	-3.535554000	0.237281000	2.649857000
6	-2.938868000	0.495259000	-3.018525000	6	-2.531509000	-0.623578000	3.229538000
6	-4.498594000	0.067133000	-1.168309000	6	-4.347106000	-0.235452000	1.619890000
6	-2.764375000	1.809383000	-2.586655000	6	-2.377173000	-1.927837000	2.762450000
6	-1.447292000	2.401262000	-2.588367000	6	-1.052115000	-2.471208000	2.573217000
6	-1.799908000	-0.271762000	-3.463902000	6	-1.367790000	0.179440000	3.525161000
6	-0.531631000	0.302459000	-3.472484000	6	-0.092387000	-0.348966000	3.352850000
6	-0.350588000	1.663862000	-3.027033000	6	0.066130000	-1.696921000	2.866413000
6	-4.038127000	-2.046209000	0.000410000	6	-4.125232000	1.903362000	0.428842000
6	-3.333014000	-2.519737000	-1.167255000	6	-3.283928000	2.392328000	1.495248000
6	-4.608441000	-0.774202000	0.000291000	6	-4.646728000	0.612269000	0.489640000
6	-3.227815000	-1.707963000	-2.296085000	6	-2.993458000	1.573815000	2.585281000
6	-1.977917000	-1.635737000	-3.015826000	6	-1.654159000	1.541590000	3.126113000
6	-2.193922000	-3.288283000	-0.722859000	6	-2.243140000	3.204588000	0.908710000
6	-0.992704000	-3.225427000	-1.423962000	6	-0.956662000	3.177406000	1.436886000
6	-0.882930000	-2.384437000	-2.591500000	6	-0.656076000	2.331567000	2.565654000
6	-3.820968000	-0.390969000	2.296792000	6	-4.171292000	0.278315000	-1.898743000
6	-3.227552000	-1.707416000	2.296729000	6	-3.628250000	1.614797000	-1.961011000
6	-4.498464000	0.067412000	1.168678000	6	-4.669829000	-0.214549000	-0.694314000
6	-3.332883000	-2.519462000	1.168109000	6	-3.605262000	2.413047000	-0.818452000
6	-2.193839000	-3.288112000	0.723763000	6	-2.442188000	3.217437000	-0.524996000
6	-1.977570000	-1.635015000	3.016304000	6	-2.488656000	1.594775000	-2.847726000
6	-0.882630000	-2.383817000	2.592032000	6	-1.373004000	2.377972000	-2.567277000

6	-0.992538000	-3.225088000	1.424708000	6	-1.348501000	3.205550000	-1.386060000
6	1.136689000	-2.268818000	-1.424288000	6	1.179303000	2.291644000	1.128048000
6	0.256379000	-3.146721000	-0.698571000	6	0.182696000	3.144006000	0.544364000
6	0.256460000	-3.146553000	0.699151000	6	-0.007841000	3.162378000	-0.841223000
6	1.989289000	-1.404966000	-0.722051000	6	2.011765000	1.501752000	0.311521000
6	1.482773000	0.420307000	-2.303437000	6	1.745062000	-0.382663000	1.914405000
6	0.603114000	-0.467673000	-3.017595000	6	0.947938000	0.464088000	2.755563000
6	0.432886000	-1.785278000	-2.585043000	6	0.669563000	1.780871000	2.367783000
6	2.184088000	-0.045344000	-1.181829000	6	2.302014000	0.112011000	0.716388000
6	1.702356000	2.086293000	-0.000415000	6	1.700686000	-2.015113000	-0.421286000
6	1.003511000	2.549867000	-1.165165000	6	1.183447000	-2.518552000	0.825447000
6	0.899299000	1.735495000	-2.301281000	6	1.200949000	-1.710826000	1.968169000
6	2.324385000	0.813961000	-0.000305000	6	2.225964000	-0.713976000	-0.482178000
6	1.483037000	0.420861000	2.303025000	6	1.109945000	-0.342944000	-2.651003000
6	0.899569000	1.736044000	2.300628000	6	0.569628000	-1.674936000	-2.579608000
6	1.003649000	2.550145000	1.164300000	6	0.858955000	-2.495232000	-1.484808000
6	2.184240000	-0.045063000	1.181455000	6	1.921719000	0.133227000	-1.608996000
6	1.136848000	-2.268472000	1.424554000	6	0.789171000	2.319653000	-1.691289000
6	0.433183000	-1.784657000	2.585280000	6	-0.048550000	1.824291000	-2.748875000
6	0.603458000	-0.466950000	3.017493000	6	0.109756000	0.519272000	-3.224674000
6	1.989374000	-1.404796000	0.722016000	6	1.781298000	1.494124000	-1.135642000
17	-1.115567000	0.012062000	0.000009000	17	-1.163935000	-0.045968000	-0.006636000
$(Cl^-@C_{60})Sc(CO)_4$				$(Cl^-@C_{60})Ti(CO)_2Cl$			
6	0.861287000	-1.911126000	2.300064000	6	2.779966000	1.563158000	-2.561494000
6	1.579201000	-0.665607000	2.307665000	6	3.536933000	0.351539000	-2.352452000
6	0.884252000	-2.734244000	1.168073000	6	2.771650000	2.557695000	-1.584002000
6	2.316446000	-0.274572000	1.176289000	6	4.254895000	0.174457000	-1.171612000
6	2.264322000	1.099418000	0.721329000	6	4.245441000	-1.106730000	-0.504911000
6	0.795021000	0.306585000	3.018175000	6	2.779323000	-0.745198000	-2.906862000
6	0.757871000	1.637381000	2.586571000	6	2.769790000	-1.982225000	-2.263003000
6	1.503164000	2.046208000	1.425681000	6	3.518598000	-2.167051000	-1.042040000
6	-1.513106000	-3.190939000	1.419183000	6	0.364726000	2.912486000	-1.932370000
6	-1.537412000	-2.339344000	2.589710000	6	0.373815000	1.883235000	-2.943302000
6	-0.325077000	-3.394340000	0.723921000	6	1.540410000	3.237882000	-1.261243000
6	-0.373102000	-1.716767000	3.030331000	6	1.557919000	1.217824000	-3.247560000
6	-0.413787000	-0.344699000	3.474621000	6	1.557641000	-0.213541000	-3.461773000
6	-2.788525000	-1.618237000	2.587704000	6	-0.856531000	1.131596000	-2.823950000
6	-2.827547000	-0.292549000	3.017501000	6	-0.856685000	-0.254049000	-3.030916000
6	-1.616504000	0.355488000	3.463495000	6	0.373208000	-0.938262000	-3.365032000
6	-1.512882000	-3.193045000	-1.414552000	6	0.336942000	3.380828000	0.881409000
6	-2.748934000	-2.992862000	-0.694992000	6	-0.883556000	3.021992000	0.191608000
6	-0.324966000	-3.395413000	-0.718782000	6	1.526181000	3.476684000	0.166196000
6	-2.749031000	-2.991811000	0.699135000	6	-0.871063000	2.793935000	-1.189905000
6	-3.537414000	-2.021161000	1.420672000	6	-1.625786000	1.708252000	-1.756273000
6	-3.537191000	-2.023261000	-1.418083000	6	-1.652175000	2.177294000	1.061666000
6	-4.296115000	-1.084659000	-0.721649000	6	-2.405523000	1.117814000	0.518957000
6	-4.296224000	-1.083588000	0.722727000	6	-2.357656000	0.862866000	-0.905523000
6	0.861663000	-1.914537000	-2.296924000	6	2.733148000	2.319970000	1.965909000
6	-0.372623000	-1.721253000	-3.027660000	6	1.494933000	2.211352000	2.700352000
6	0.884412000	-2.735950000	-1.163698000	6	2.748657000	2.942503000	0.718524000
6	-1.537008000	-2.343209000	-2.586361000	6	0.320124000	2.738213000	2.172593000
6	-2.788114000	-1.622070000	-2.585600000	6	-0.910755000	1.983451000	2.276760000
6	-0.413227000	-0.349850000	-3.473999000	6	1.486226000	0.927207000	3.369709000
6	-1.615945000	0.350353000	-3.464119000	6	0.302931000	0.206630000	3.490859000
6	-2.827073000	-0.297023000	-3.017368000	6	-0.918384000	0.739936000	2.923235000
6	2.346784000	-1.135018000	0.001137000	6	4.246082000	1.204386000	-0.159128000
6	2.316678000	-0.276322000	-1.175324000	6	4.230707000	0.559754000	1.133234000
6	1.625695000	-2.342608000	0.001963000	6	3.519938000	2.375967000	-0.362379000
6	1.579539000	-0.669018000	-2.306201000	6	3.489554000	1.108669000	2.177964000
6	0.795497000	0.302111000	-3.018302000	6	2.718828000	0.248911000	3.044154000
6	2.264477000	1.098363000	-0.722382000	6	4.230343000	-0.868436000	0.919508000
6	1.503384000	2.044075000	-1.428262000	6	3.489117000	-1.698868000	1.757816000

6	0.758303000	1.633550000	-2.588680000	6	2.718635000	-1.129928000	2.837794000
6	-2.890879000	1.923370000	-2.296927000	6	-0.918999000	-1.562599000	2.578929000
6	-1.655408000	1.726261000	-3.017390000	6	0.302751000	-1.219404000	3.277455000
6	-0.491126000	2.362632000	-2.595615000	6	1.485720000	-1.873459000	2.950629000
6	-2.915000000	2.743439000	-1.169650000	6	-0.912074000	-2.562095000	1.596639000
6	-4.360806000	1.137588000	-0.001117000	6	-2.406810000	-1.218833000	0.169500000
6	-4.336061000	0.288001000	-1.168927000	6	-2.425705000	-0.178587000	1.201254000
6	-3.616008000	0.674701000	-2.297457000	6	-1.667007000	-0.355608000	2.381266000
6	-3.664584000	2.344433000	-0.001943000	6	-1.653130000	-2.390847000	0.378167000
6	-2.891280000	1.926783000	2.293816000	6	-0.872607000	-2.321959000	-1.955387000
6	-3.616385000	0.678103000	2.296039000	6	-1.626456000	-1.117692000	-2.179026000
6	-4.336244000	0.289730000	1.167960000	6	-2.358746000	-0.558105000	-1.118218000
6	-2.915176000	2.745156000	1.165302000	6	-0.884954000	-2.944211000	-0.701071000
6	-0.516373000	3.213006000	1.423597000	6	1.524380000	-3.373781000	-0.858671000
6	-0.491546000	2.366493000	2.592244000	6	1.538765000	-2.727085000	-2.153651000
6	-1.655904000	1.730736000	3.014744000	6	0.363384000	-2.218315000	-2.699730000
6	-1.704370000	3.393774000	0.720864000	6	0.335129000	-3.490048000	-0.146606000
6	-0.516145000	3.210872000	-1.428227000	6	1.493964000	-2.905953000	1.935068000
6	0.717492000	3.004925000	-0.701760000	6	2.732102000	-2.795226000	1.200797000
6	0.717398000	3.005999000	0.697634000	6	2.747334000	-3.025243000	-0.174267000
6	-1.704257000	3.392704000	-0.725969000	6	0.318787000	-3.253486000	1.275897000
21	4.509857000	0.012716000	0.000000000	17	0.875057000	-0.002391000	0.007106000
17	-0.961384000	0.005619000	-0.000155000	22	-4.436033000	-0.043869000	0.297105000
6	5.109179000	1.521694000	-1.568358000	17	-6.123996000	-0.253987000	1.719687000
8	5.338312000	2.300096000	-2.387118000	8	-5.441100000	-2.051387000	-2.010518000
6	4.962424000	-1.577815000	1.530372000	8	-5.441312000	2.544677000	-1.332481000
8	5.046011000	-2.414838000	2.318826000	6	-5.073578000	-1.316726000	-1.198418000
6	4.962618000	-1.581245000	-1.526723000	6	-5.073467000	1.606605000	-0.767709000
8	5.046221000	-2.420010000	-2.313320000				
6	5.109353000	1.525317000	1.564796000				
8	5.338695000	2.305598000	2.381708000				
(Cl ⁻ @C ₆₀)TiCl ₃				(Cl ⁻ @C ₆₀)V(CO) ₂			
22	4.461259000	0.000588000	-0.000840000	6	1.122753000	-2.394650000	1.833505000
17	5.374052000	-0.810947000	1.834769000	6	1.929124000	-1.219864000	2.018693000
17	5.371528000	-1.189726000	-1.617880000	6	1.042711000	-3.009495000	0.579900000
17	5.355952000	2.005088000	-0.217960000	6	2.656217000	-0.686795000	0.930642000
6	-1.569537000	-3.061621000	1.663150000	6	2.700517000	0.769961000	0.735814000
6	-1.571145000	-2.121504000	2.763718000	6	1.240290000	-0.339900000	2.921438000
6	-0.387307000	-3.352537000	0.988005000	6	1.265230000	1.047121000	2.720188000
6	-0.390608000	-1.499139000	3.158876000	6	1.983523000	1.609499000	1.615146000
6	-0.393502000	-0.095418000	3.495299000	6	-1.366159000	-3.362271000	0.878447000
6	-2.801625000	-1.369368000	2.702973000	6	-1.283722000	-2.727674000	2.175934000
6	-2.804096000	-0.013317000	3.027972000	6	-0.225030000	-3.509290000	0.096004000
6	-1.576437000	0.634026000	3.424616000	6	-0.063773000	-2.258459000	2.650881000
6	-1.571301000	-3.284201000	-1.161817000	6	0.009000000	-0.986874000	3.326858000
6	-2.799985000	-2.994878000	-0.461941000	6	-2.483118000	-1.945885000	2.364183000
6	-0.388172000	-3.465959000	-0.450931000	6	-2.414191000	-0.716132000	3.016443000
6	-2.799259000	-2.885448000	0.928195000	6	-1.143830000	-0.227832000	3.497955000
6	-3.562351000	-1.841695000	1.570619000	6	-1.489345000	-2.871057000	-1.908862000
6	-3.563967000	-2.064638000	-1.259099000	6	-2.675848000	-2.726713000	-1.099095000
6	-4.296722000	-1.054809000	-0.639095000	6	-0.288237000	-3.258719000	-1.323642000
6	-4.295805000	-0.941265000	0.800719000	6	-2.616177000	-2.970117000	0.271423000
6	0.833260000	-2.145527000	-2.139439000	6	-3.308984000	-2.096805000	1.189858000
6	-0.394352000	-1.975698000	-2.885103000	6	-3.429488000	-1.603318000	-1.602622000
6	0.837696000	-2.878499000	-0.945083000	6	-4.093672000	-0.758944000	-0.716493000
6	-1.574475000	-2.528233000	-2.396132000	6	-4.031981000	-1.009523000	0.703973000
6	-2.804972000	-1.775923000	-2.452709000	6	0.924615000	-1.600103000	-2.689610000
6	-0.397885000	-0.642251000	-3.437508000	6	-0.324662000	-1.210138000	-3.305242000
6	-1.580855000	0.089317000	-3.481119000	6	0.940577000	-2.604845000	-1.715352000
6	-2.808006000	-0.487569000	-2.986422000	6	-1.507172000	-1.830911000	-2.913776000
6	2.317010000	-1.218315000	0.094417000	6	-2.704877000	-1.049154000	-2.721008000
6	2.299203000	-0.461335000	-1.135154000	6	-0.292666000	0.217895000	-3.508975000

6	1.593498000	-2.419541000	0.189416000	6	-1.445210000	0.973357000	-3.313949000
6	1.586007000	-0.926053000	-2.250652000	6	-2.675424000	0.330478000	-2.918828000
6	0.827923000	0.010361000	-3.032739000	6	2.532157000	-1.310215000	-0.375951000
6	2.304660000	0.938664000	-0.800965000	6	2.513649000	-0.272204000	-1.372267000
6	1.582806000	1.854823000	-1.583161000	6	1.762405000	-2.469230000	-0.543400000
6	0.826555000	1.373322000	-2.706426000	6	1.728576000	-0.418022000	-2.530826000
6	0.836053000	-1.783738000	2.447390000	6	0.976732000	0.707905000	-3.016999000
6	1.588912000	-0.562211000	2.365293000	6	2.620063000	1.015826000	-0.714957000
6	0.839002000	-2.694848000	1.382428000	6	1.864142000	2.103278000	-1.192132000
6	2.300344000	-0.278182000	1.189641000	6	1.040365000	1.940931000	-2.356222000
6	2.307157000	1.052786000	0.640209000	6	-2.563597000	2.391832000	-1.828654000
6	0.831640000	0.485433000	2.991673000	6	-1.375563000	2.251046000	-2.636722000
6	0.830073000	1.780555000	2.455986000	6	-0.156394000	2.733680000	-2.174081000
6	1.584651000	2.079608000	1.269697000	6	-2.483192000	3.001174000	-0.578303000
6	-0.403170000	3.070709000	-1.673579000	6	-3.979847000	1.304019000	0.375608000
6	0.825113000	2.889234000	-0.931657000	6	-4.062479000	0.670517000	-0.920006000
6	0.826204000	2.999725000	0.465302000	6	-3.368753000	1.205879000	-2.003085000
6	-1.585267000	3.338032000	-0.988600000	6	-3.207037000	2.450399000	0.543063000
6	-2.811789000	1.782580000	-2.441644000	6	-2.364510000	1.596211000	2.688261000
6	-1.583187000	1.497164000	-3.143247000	6	-3.167629000	0.408963000	2.515256000
6	-0.402462000	2.133212000	-2.770850000	6	-3.960490000	0.265653000	1.379284000
6	-2.812950000	2.688497000	-1.381425000	6	-2.383529000	2.598196000	1.719820000
6	-4.301050000	1.217568000	-0.093967000	6	0.048815000	2.873505000	1.922283000
6	-4.299750000	0.279443000	-1.191873000	6	0.067923000	1.836792000	2.923309000
6	-3.570364000	0.557770000	-2.345942000	6	-1.113685000	1.206228000	3.294577000
6	-3.572769000	2.401724000	-0.187749000	6	-1.152008000	3.242741000	1.327606000
6	-2.808977000	2.143566000	2.134462000	6	-0.072860000	3.368156000	-0.881843000
6	-3.567119000	0.918674000	2.232406000	6	1.177435000	2.968232000	-0.270717000
6	-4.298351000	0.463109000	1.137476000	6	1.234522000	2.721434000	1.104710000
6	-2.811516000	2.872054000	0.945477000	6	-1.213945000	3.492871000	-0.096607000
6	-0.401222000	3.295156000	1.171184000	23	4.490451000	-0.019853000	-0.093688000
6	-0.399004000	2.541067000	2.401794000	17	-0.699003000	-0.002839000	0.001523000
6	-1.579366000	1.971416000	2.870448000	6	5.541172000	1.593783000	0.010695000
6	-1.584299000	3.451848000	0.454242000	8	6.102880000	2.609422000	0.091055000
17	-0.928852000	-0.000843000	-0.000332000	6	5.699137000	-1.537674000	0.012394000
				8	6.373030000	-2.482370000	0.089617000
$(Cl^-@C_{60})V(CO)_3$				$(Cl^-@C_{60})V(CO)_4$			
6	0.932813000	3.020690000	0.015672000	6	0.765905000	1.418306000	-2.661226000
6	1.557309000	2.312623000	-1.070797000	6	1.500880000	0.206281000	-2.425498000
6	1.097717000	2.583755000	1.334818000	6	0.786835000	2.457381000	-1.721493000
6	2.341080000	1.173933000	-0.803121000	6	2.233643000	0.063679000	-1.231435000
6	2.209760000	0.000927000	-1.633904000	6	2.201082000	-1.184978000	-0.507850000
6	0.649028000	2.299477000	-2.183562000	6	0.720190000	-0.898788000	-2.907331000
6	0.544491000	1.168064000	-3.000841000	6	0.698762000	-2.113362000	-2.208980000
6	1.347794000	0.001671000	-2.741462000	6	1.457436000	-2.273380000	-0.999061000
6	-1.267403000	3.013961000	1.808239000	6	-1.616273000	2.829790000	-2.041656000
6	-1.442629000	3.463072000	0.443283000	6	-1.638787000	1.755198000	-3.011658000
6	-0.020470000	2.592237000	2.254025000	6	-0.426687000	3.184107000	-1.413621000
6	-0.364117000	3.475159000	-0.435765000	6	-0.470896000	1.066783000	-3.325941000
6	-0.540361000	3.027582000	-1.795909000	6	-0.499207000	-0.367242000	-3.477978000
6	-2.740338000	3.018364000	-0.005642000	6	-2.881923000	1.039076000	-2.850909000
6	-2.907742000	2.586880000	-1.319860000	6	-2.909012000	-0.347153000	-2.998438000
6	-1.786244000	2.588869000	-2.229156000	6	-1.693729000	-1.060851000	-3.311465000
6	-1.054111000	0.722092000	3.457013000	6	-1.598477000	3.415036000	0.729661000
6	-2.352166000	1.165653000	3.007669000	6	-2.836968000	3.060079000	0.077609000
6	0.089312000	1.424714000	3.093607000	6	-0.417529000	3.482564000	-0.002680000
6	-2.457520000	2.294171000	2.197077000	6	-2.845766000	2.772238000	-1.286553000
6	-3.367907000	2.296501000	1.076628000	6	-3.628518000	1.666846000	-1.786271000
6	-3.156198000	-0.001673000	2.730323000	6	-3.611532000	2.253820000	0.991285000
6	-4.030173000	-0.000917000	1.645591000	6	-4.363228000	1.184232000	0.508882000
6	-4.139918000	1.168702000	0.805486000	6	-4.372337000	0.886026000	-0.904105000
6	1.275192000	-0.702573000	2.688999000	6	0.794176000	2.367844000	1.837273000

6	0.089188000	-1.428906000	3.091726000	6	-0.433320000	2.318481000	2.602954000
6	1.275258000	0.698789000	2.689931000	6	0.801797000	2.939294000	0.557904000
6	-1.054174000	-0.726635000	3.456070000	6	-1.606432000	2.824126000	2.051395000
6	-2.352256000	-1.169438000	3.006099000	6	-2.849881000	2.107524000	2.209101000
6	-0.020710000	-2.595321000	2.250617000	6	-0.455898000	1.068361000	3.321849000
6	-1.267692000	-3.016246000	1.804213000	6	-1.650357000	0.369761000	3.464411000
6	-2.457747000	-2.296881000	2.194037000	6	-2.871461000	0.899449000	2.904762000
6	2.520412000	0.728550000	0.569180000	6	2.264782000	1.142369000	-0.263347000
6	2.520379000	-0.729719000	0.568215000	6	2.254390000	0.548753000	1.061587000
6	1.897163000	1.426813000	1.622591000	6	1.544141000	2.328255000	-0.508670000
6	1.897079000	-1.429281000	1.620725000	6	1.529029000	1.162216000	2.102173000
6	1.097505000	-2.585741000	1.331415000	6	0.757754000	0.348523000	2.999164000
6	2.340924000	-1.173213000	-0.804688000	6	2.214869000	-0.888855000	0.903128000
6	1.557061000	-2.311460000	-1.073858000	6	1.475262000	-1.681830000	1.800283000
6	0.932495000	-3.020855000	0.011678000	6	0.731690000	-1.044756000	2.852310000
6	-2.740672000	-3.018176000	-0.009623000	6	-2.916105000	-1.421821000	2.657741000
6	-1.442979000	-3.463567000	0.438701000	6	-1.677996000	-1.069469000	3.311123000
6	-0.364466000	-3.474665000	-0.440364000	6	-0.510177000	-1.768635000	3.020846000
6	-2.907985000	-2.584884000	-1.323256000	6	-2.938034000	-2.456299000	1.723144000
6	-4.314169000	-0.721597000	-0.557716000	6	-4.408475000	-1.138903000	0.261655000
6	-4.140043000	-1.169415000	0.803928000	6	-4.385509000	-0.067131000	1.229439000
6	-3.368153000	-2.297660000	1.073595000	6	-3.654526000	-0.206629000	2.407289000
6	-3.711933000	-1.418442000	-1.602259000	6	-3.699548000	-2.313427000	0.504972000
6	-3.083538000	0.699240000	-2.680846000	6	-2.944772000	-2.370093000	-1.833778000
6	-3.711813000	1.420879000	-1.600386000	6	-3.683478000	-1.155602000	-2.086834000
6	-4.314106000	0.722712000	-0.556769000	6	-4.400245000	-0.549733000	-1.056998000
6	-3.083584000	-0.695443000	-2.681745000	6	-2.952832000	-2.938928000	-0.560658000
6	-0.752579000	-0.719175000	-3.460585000	6	-0.551345000	-3.428373000	-0.737871000
6	-0.752509000	0.723754000	-3.459669000	6	-0.543089000	-2.840066000	-2.054963000
6	-1.895163000	1.418019000	-3.072099000	6	-1.716016000	-2.315236000	-2.589360000
6	-1.895285000	-1.413832000	-3.073943000	6	-1.732179000	-3.470993000	-0.002781000
6	-0.540662000	-3.025296000	-1.799930000	6	-0.533417000	-2.838852000	2.053926000
6	0.648795000	-2.296792000	-2.186624000	6	0.694260000	-2.774551000	1.290187000
6	0.544389000	-1.164269000	-3.002394000	6	0.685505000	-3.064396000	-0.080672000
6	-1.786486000	-2.585791000	-2.232536000	6	-1.723016000	-3.171534000	1.413278000
23	4.346349000	0.000092000	-0.466701000	23	4.223263000	-0.011307000	-0.001081000
17	-0.879023000	-0.000071000	-0.001600000	17	-1.020708000	0.000625000	-0.001310000
6	5.443307000	-1.594220000	-0.566871000	6	5.185369000	-0.792312000	1.498581000
8	6.078852000	-2.565951000	-0.582284000	8	5.741964000	-1.258231000	2.402186000
6	5.443455000	1.594320000	-0.566630000	6	5.165477000	0.803508000	-1.491450000
8	6.079009000	2.566045000	-0.582140000	8	5.709553000	1.298171000	-2.387631000
6	5.246369000	0.000034000	1.221427000	6	5.150413000	1.495587000	0.794760000
8	5.780104000	-0.000303000	2.254764000	8	5.684552000	2.406293000	1.273783000
				6	5.200661000	-1.494039000	-0.800922000
				8	5.767057000	-2.383008000	-1.282609000
$(Cl^-@C_{60})Cr(CO)_2Cl$				$(Cl^-@C_{60})Cr(CO)_2H$			
6	-2.519182000	-3.085189000	-0.696930000	6	-1.468779000	1.233627000	0.409958000
6	-3.353739000	-2.156368000	-1.419376000	6	-0.927038000	0.304906000	1.353577000
6	-2.519157000	-3.085161000	0.697167000	6	-1.949434000	-0.885743000	-0.338826000
6	-4.158208000	-1.257808000	-0.722182000	6	-2.098235000	0.489810000	-0.617599000
6	-4.265107000	0.111793000	-1.168122000	6	-1.220063000	-1.007453000	0.882353000
6	-2.623898000	-1.716074000	-2.586653000	24	0.058809000	-0.015164000	-0.484412000
6	-2.729206000	-0.394003000	-3.017909000	1	0.292754000	-1.286827000	-1.436611000
6	-3.566252000	0.535437000	-2.297245000	8	2.202659000	-1.949275000	0.210918000
6	-0.078747000	-3.366487000	0.721451000	8	2.221185000	1.988076000	0.109384000
6	-0.078776000	-3.366528000	-0.721300000	6	1.385644000	-1.160818000	-0.071053000
6	-1.273624000	-3.220429000	1.416334000	6	1.374440000	1.226917000	-0.147403000
6	-1.273680000	-3.220495000	-1.416137000	1	-1.424381000	2.312043000	0.478244000
6	-1.339221000	-2.371422000	-2.588772000	1	-2.564770000	0.904954000	-1.503317000
6	1.092664000	-2.640161000	-1.164174000	1	-2.315280000	-1.702018000	-0.945752000
6	1.036150000	-1.822161000	-2.301137000	1	-0.957730000	-1.934354000	1.373767000
6	-0.207206000	-1.692113000	-3.030881000	1	-0.411972000	0.552265000	2.271103000

6	-0.207076000	-1.691956000	3.030952000				
6	1.036246000	-1.822042000	2.301163000				
6	-1.339114000	-2.371288000	2.588919000				
6	1.092708000	-2.640097000	1.164236000				
6	1.814184000	-2.217563000	0.000005000				
6	1.696374000	-0.546117000	2.315691000				
6	2.412340000	-0.110215000	1.172100000				
6	2.456776000	-0.966093000	-0.000050000				
6	-2.729082000	-0.393840000	3.018001000				
6	-1.552159000	0.312707000	3.463794000				
6	-2.623790000	-1.715941000	2.586824000				
6	-0.315465000	-0.325350000	3.475478000				
6	0.861315000	0.384701000	3.018761000				
6	-1.661634000	1.683942000	3.014504000				
6	-0.530433000	2.378150000	2.592106000				
6	0.751983000	1.714408000	2.584532000				
6	-4.158185000	-1.257773000	0.722388000				
6	-4.265055000	0.111854000	1.168257000				
6	-3.353674000	-2.156288000	1.419595000				
6	-3.566158000	0.535561000	2.297331000				
6	-2.905270000	1.818698000	2.296577000				
6	-4.333023000	0.957708000	0.000047000				
6	-3.698952000	2.198330000	0.000000000				
6	-2.968322000	2.634141000	1.165900000				
6	0.645128000	3.089234000	0.699607000				
6	-0.598838000	3.225502000	1.424417000				
6	-1.794578000	3.348936000	0.722903000				
6	0.645102000	3.089201000	-0.699841000				
6	2.263072000	1.257698000	-0.717307000				
6	2.263094000	1.257733000	0.717103000				
6	1.478873000	2.171788000	1.428742000				
6	1.478813000	2.171713000	-1.428963000				
6	0.861190000	0.384541000	-3.018855000				
6	1.696280000	-0.546242000	-2.315772000				
6	2.412282000	-0.110271000	-1.172232000				
6	0.751875000	1.714269000	-2.584695000				
6	-1.661764000	1.683787000	-3.014571000				
6	-1.552303000	0.312526000	-3.463784000				
6	-0.315608000	-0.325530000	-3.475489000				
6	-0.530545000	2.378013000	-2.592251000				
6	-1.794610000	3.348897000	-0.723050000				
6	-2.968370000	2.634079000	-1.165957000				
6	-2.905371000	1.818578000	-2.296597000				
6	-0.598896000	3.225428000	-1.424607000				
17	-0.881189000	0.000178000	-0.000007000				
24	4.285048000	0.187550000	-0.000050000				
17	5.585381000	1.944449000	-0.000002000				
8	5.754425000	-1.624282000	-1.870536000				
8	5.754396000	-1.624060000	1.870657000				
6	5.177008000	-0.913665000	-1.156844000				
6	5.176991000	-0.913537000	1.156859000				
$(Cl^-@C_{60})Mn(CO)_2NMe_3$				$(Cl^-@C_{60})Mn(CO)_2PMe_3$			
25	-3.989658000	-0.434150000	0.000046000	25	3.842905000	-0.691943000	-0.000059000
7	-5.334045000	1.215560000	-0.000144000	15	5.222046000	1.054412000	-0.000178000
8	-5.438056000	-1.866017000	2.102246000	8	5.422056000	-1.965114000	-2.116008000
8	-5.437610000	-1.866616000	-2.102035000	8	5.421880000	-1.963881000	2.116746000
6	-4.872581000	-1.289814000	1.257865000	6	4.795668000	-1.465562000	-1.265932000
6	-4.872369000	-1.290153000	-1.257673000	6	4.795501000	-1.464823000	1.266369000
6	-6.743912000	0.769338000	-0.000342000	6	6.999918000	0.649242000	-0.000813000
1	-6.940539000	0.166598000	-0.888189000	1	7.241062000	0.054128000	0.883404000
1	-6.940749000	0.166489000	0.887386000	1	7.240581000	0.055106000	-0.885816000
6	-5.119556000	2.046352000	1.203759000	6	5.058119000	2.173853000	-1.434674000

1	-4.105422000	2.450494000	1.200151000	1	4.046570000	2.587782000	-1.470120000
1	-5.834234000	2.880911000	1.226906000	1	5.775480000	2.998221000	-1.380467000
6	-5.119251000	2.046446000	-1.203929000	6	5.058784000	2.172814000	1.435212000
1	-5.834039000	2.880906000	-1.227270000	1	5.775884000	2.997420000	1.381183000
1	-5.256487000	1.434491000	-2.098053000	1	5.231911000	1.611962000	2.357239000
1	-4.105181000	2.450739000	-1.199948000	1	4.047137000	2.586443000	1.471609000
1	-7.417351000	1.637597000	-0.000369000	1	7.617736000	1.551750000	-0.000489000
1	-5.257189000	1.434365000	2.097802000	1	5.230536000	1.613648000	-2.357219000
6	3.636023000	2.092030000	-1.419484000	6	-3.553131000	2.295161000	1.420082000
6	2.896823000	1.673154000	-2.587662000	6	-2.851041000	1.815524000	2.587432000
6	4.415361000	1.171163000	-0.722059000	6	-4.406393000	1.442611000	0.722319000
6	2.965760000	0.349840000	-3.019312000	6	-3.030228000	0.502343000	3.018478000
6	1.769357000	-0.324705000	-3.465386000	6	-1.894094000	-0.269455000	3.464429000
6	1.629710000	2.366599000	-2.589250000	6	-1.530276000	2.400039000	2.589120000
6	0.479865000	1.718154000	-3.028732000	6	-0.438602000	1.658818000	3.029859000
6	0.550094000	0.347720000	-3.475253000	6	-0.623808000	0.298844000	3.475245000
6	3.636083000	2.091370000	1.420151000	6	-3.553113000	2.295492000	-1.419620000
6	2.824111000	3.041553000	0.698287000	6	-2.664583000	3.174190000	-0.697024000
6	4.415466000	1.170866000	0.722299000	6	-4.406387000	1.442783000	-0.722058000
6	2.824052000	3.041841000	-0.697115000	6	-2.664589000	3.174017000	0.697688000
6	1.584822000	3.213904000	-1.416580000	6	-1.414946000	3.241408000	1.417114000
6	1.584933000	3.213301000	1.417942000	6	-1.414927000	3.241732000	-1.416420000
6	0.391676000	3.391571000	0.722187000	6	-0.211655000	3.320917000	-0.720800000
6	0.391615000	3.391900000	-0.720655000	6	-0.211665000	3.320763000	0.721533000
6	3.776242000	-0.604926000	2.297135000	6	-3.917258000	-0.379677000	-2.297236000
6	2.965996000	0.348528000	3.019277000	6	-3.030177000	0.503014000	-3.018383000
6	4.486538000	-0.201072000	1.168460000	6	-4.591808000	0.081740000	-1.168602000
6	2.897025000	1.672033000	2.588243000	6	-2.851006000	1.816108000	-2.587064000
6	1.629910000	2.365473000	2.590231000	6	-1.530231000	2.400612000	-2.588604000
6	1.769635000	-0.326199000	3.465157000	6	-1.894040000	-0.268686000	-3.464483000
6	0.550373000	0.346227000	3.475492000	6	-0.623756000	0.299612000	-3.475201000
6	0.480102000	1.716868000	3.029568000	6	-0.438549000	1.659500000	-3.029526000
6	3.858510000	-2.270144000	-0.000601000	6	-4.140204000	-2.033466000	-0.000251000
6	3.118531000	-2.686117000	1.166928000	6	-3.436760000	-2.509433000	-1.167753000
6	4.529230000	-1.048530000	-0.000368000	6	-4.705326000	-0.759405000	-0.000110000
6	3.079783000	-1.869409000	2.296233000	6	-3.328827000	-1.698097000	-2.296659000
6	1.839755000	-1.699473000	3.016034000	6	-2.078650000	-1.632008000	-3.016001000
6	1.921427000	-3.361117000	0.723607000	6	-2.300516000	-3.282880000	-0.724474000
6	0.731122000	-3.206793000	1.425414000	6	-1.100926000	-3.226929000	-1.426008000
6	0.690089000	-2.359787000	2.591617000	6	-0.988211000	-2.385982000	-2.591693000
6	3.776037000	-0.603923000	-2.297609000	6	-3.917293000	-0.380188000	2.297113000
6	3.079593000	-1.868412000	-2.297204000	6	-3.328865000	-1.698606000	2.296252000
6	4.486460000	-0.200565000	-1.168835000	6	-4.591821000	0.081477000	1.168567000
6	3.118428000	-2.685603000	-1.168240000	6	-3.436777000	-2.509687000	1.167153000
6	1.921365000	-3.360799000	-0.725111000	6	-2.300531000	-3.283042000	0.723719000
6	1.839501000	-1.698163000	-3.016813000	6	-2.078706000	-1.632686000	3.015652000
6	0.689873000	-2.358675000	-2.592600000	6	-0.988257000	-2.386546000	2.591153000
6	0.731005000	-3.206174000	-1.426760000	6	-1.100950000	-3.227234000	1.425280000
6	-1.317693000	-2.094007000	1.427519000	6	1.034820000	-2.289205000	-1.428564000
6	-0.512718000	-3.029788000	0.701281000	6	0.152322000	-3.154850000	-0.701465000
6	-0.512775000	-3.029474000	-0.702442000	6	0.152304000	-3.154999000	0.700763000
6	-2.117571000	-1.164090000	0.728099000	6	1.897035000	-1.424773000	-0.724327000
6	-1.449542000	0.627306000	2.309501000	6	1.393871000	0.411401000	-2.311484000
6	-0.643983000	-0.331299000	3.021220000	6	0.510162000	-0.475193000	-3.019937000
6	-0.573769000	-1.656971000	2.580343000	6	0.330719000	-1.792113000	-2.581562000
6	-2.169076000	0.219323000	1.174104000	6	2.075909000	-0.057850000	-1.174574000
6	-1.544126000	2.306376000	0.000625000	6	1.628716000	2.078949000	0.000246000
6	-0.802215000	2.706467000	1.166661000	6	0.920982000	2.536575000	-1.164547000
6	-0.760308000	1.886697000	2.301886000	6	0.811949000	1.724095000	-2.301675000
6	-2.186446000	1.055021000	0.000378000	6	2.178027000	0.779810000	0.000093000
6	-1.449720000	0.628287000	-2.308988000	6	1.393833000	0.410903000	2.311575000
6	-0.760485000	1.887678000	-2.300882000	6	0.811908000	1.723585000	2.302053000
6	-0.802307000	2.706960000	-1.165310000	6	0.920970000	2.536326000	1.165123000
6	-2.169204000	0.219831000	-1.173726000	6	2.075867000	-0.058106000	1.174563000

6	-1.317829000	-2.093405000	-1.428220000	6	1.034788000	-2.289526000	1.428067000
6	-0.573987000	-1.655855000	-2.580899000	6	0.330676000	-1.792684000	2.581172000
6	-0.644245000	-0.329999000	-3.021215000	6	0.510108000	-0.475854000	3.019818000
6	-2.117611000	-1.163768000	-0.728309000	6	1.897008000	-1.424935000	0.724040000
17	1.113074000	0.008090000	0.000008000	17	-1.209894000	0.010543000	0.000021000
(Cl ⁻ @C ₆₀)Mn(CO) ₃				(Cl ⁻ @C ₆₀)Fe(CO) ₂ Cl			
25	4.253580000	0.005445000	-0.003785000	6	2.691210000	1.167798000	-2.837403000
6	5.240554000	1.483220000	-0.192781000	6	3.461861000	0.000259000	-2.480760000
8	5.855386000	2.457958000	-0.317893000	6	2.714145000	2.296693000	-2.018326000
6	5.244155000	-0.569955000	1.366418000	6	4.222898000	0.000061000	-1.314158000
8	5.865581000	-0.952169000	2.267249000	6	4.245277000	-1.168806000	-0.465655000
6	5.249142000	-0.907721000	-1.173111000	6	2.691111000	-1.167104000	-2.837731000
8	5.873760000	-1.515147000	-1.937773000	6	2.713955000	-2.296250000	-2.018991000
6	2.393865000	-0.384357000	-1.167971000	6	3.506888000	-2.298146000	-0.813204000
6	2.397378000	0.992082000	-0.735530000	6	0.294953000	2.595763000	-2.326847000
6	2.404780000	1.006593000	0.713832000	6	0.271883000	1.429460000	-3.174605000
6	2.390520000	-0.364875000	1.165009000	6	1.491657000	3.017160000	-1.754586000
6	2.409534000	-1.230671000	0.007168000	6	1.446246000	0.725411000	-3.417419000
6	1.670117000	-2.430767000	0.018807000	6	1.446192000	-0.724449000	-3.417628000
6	0.913110000	-2.803949000	-1.143574000	6	-0.951399000	0.703674000	-2.899034000
6	0.909830000	-1.986343000	-2.281588000	6	-0.951445000	-0.702662000	-2.899231000
6	1.670758000	-0.767007000	-2.315143000	6	0.271772000	-1.428480000	-3.175031000
6	0.910705000	0.221152000	-3.024261000	6	0.363867000	3.476672000	0.385891000
6	0.909721000	1.559501000	-2.602942000	6	-0.879002000	3.020057000	-0.196578000
6	1.666675000	1.960276000	-1.453251000	6	1.526964000	3.465429000	-0.379010000
6	0.905104000	2.939702000	-0.726167000	6	-0.910659000	2.584758000	-1.528036000
6	0.906839000	2.952928000	0.674745000	6	-1.682202000	1.432502000	-1.907965000
6	1.666792000	1.982429000	1.414067000	6	-1.611562000	2.314813000	0.822404000
6	0.914068000	1.602325000	2.574112000	6	-2.357619000	1.171384000	0.472757000
6	0.914971000	0.270834000	3.014803000	6	-2.386269000	0.723931000	-0.909018000
6	1.676530000	-0.730687000	2.323314000	6	2.804092000	2.586913000	1.524598000
6	0.915520000	-1.948852000	2.311774000	6	1.594401000	2.589438000	2.313333000
6	0.917014000	-2.786489000	1.187341000	6	2.771967000	3.019606000	0.200203000
6	-0.312529000	-3.413697000	0.748825000	6	0.398676000	3.030445000	1.757137000
6	-0.314197000	-3.425157000	-0.693363000	6	-0.825957000	2.302736000	2.021023000
6	-1.496597000	-3.194061000	-1.389277000	6	1.615334000	1.416201000	3.161521000
6	-1.498086000	-2.351973000	-2.566471000	6	0.440065000	0.720906000	3.431633000
6	-0.317692000	-1.766676000	-3.014611000	6	-0.802963000	1.164484000	2.840867000
6	-0.318973000	-0.399361000	-3.472666000	6	4.245371000	1.168676000	-0.465315000
6	-1.500827000	0.334229000	-3.464704000	6	4.279565000	0.721775000	0.907355000
6	-1.502276000	1.715337000	-3.028699000	6	3.507081000	2.298180000	-0.812537000
6	-0.321798000	2.322466000	-2.613473000	6	3.574113000	1.419630000	1.885426000
6	-0.322495000	3.178689000	-1.452940000	6	2.837199000	0.697628000	2.894397000
6	-1.503762000	3.398695000	-0.750760000	6	4.279504000	-0.722306000	0.907146000
6	-1.502678000	3.411138000	0.696370000	6	3.574000000	-1.420387000	1.885014000
6	-0.320151000	3.202480000	1.399602000	6	2.837140000	-0.698614000	2.894191000
6	-0.317416000	2.365058000	2.573871000	6	-0.803060000	-1.165158000	2.840533000
6	-1.497335000	1.765821000	3.001502000	6	0.440006000	-0.721855000	3.431430000
6	-1.494660000	0.392047000	3.459001000	6	1.615221000	-1.417162000	3.161100000
6	-0.312572000	-0.341601000	3.477437000	6	-0.826135000	-2.303152000	2.020343000
6	-0.311536000	-1.716599000	3.042807000	6	-2.357702000	-1.171219000	0.472410000
6	-1.492500000	-2.309262000	2.605911000	6	-2.297447000	-0.000042000	1.305957000
6	-1.493397000	-3.171197000	1.442625000	6	-1.575105000	-0.000250000	2.506483000
6	-2.724150000	-2.942753000	0.722675000	6	-1.611740000	-2.314816000	0.821718000
6	-2.725948000	-2.954480000	-0.671070000	6	-0.910862000	-2.584139000	-1.528784000
6	-3.487851000	-1.968414000	-1.400626000	6	-1.682309000	-1.431717000	-1.908382000
6	-2.728563000	-1.597418000	-2.570882000	6	-2.386276000	-0.723346000	-0.909224000
6	-2.729261000	-0.274499000	-3.011886000	6	-0.879247000	-3.019836000	-0.197458000
6	-3.491441000	0.723957000	-2.300171000	6	1.526683000	-3.465380000	-0.380021000
6	-2.731395000	1.951245000	-2.308780000	6	1.491414000	-3.016712000	-1.755476000
6	-2.733072000	2.781321000	-1.188438000	6	0.294745000	-2.595031000	-2.327612000
6	-3.492463000	2.411994000	-0.017429000	6	0.363584000	-3.476725000	0.384878000

6	-2.731371000	2.801012000	1.146326000	6	1.594195000	-2.590155000	2.312578000
6	-2.727939000	1.989993000	2.280021000	6	2.803881000	-2.587507000	1.523846000
6	-3.487440000	0.761971000	2.292582000	6	2.771720000	-3.019816000	0.199325000
6	-2.723663000	-0.224302000	3.018797000	6	0.398433000	-3.030891000	1.756247000
6	-2.722846000	-1.554357000	2.599303000	17	0.893586000	-0.000037000	-0.005026000
6	-3.485080000	-1.945223000	1.437682000	26	-4.181935000	0.000090000	-0.054839000
6	-4.217690000	-0.991914000	0.733451000	17	-5.453953000	-0.001053000	1.808635000
6	-4.219069000	-1.003814000	-0.710780000	8	-5.772338000	-2.124302000	-1.244494000
6	-4.220760000	0.366015000	-1.168092000	8	-5.772622000	2.125478000	-1.242380000
6	-4.221147000	1.224746000	-0.006944000	6	-5.147051000	-1.278906000	-0.771883000
6	-4.219004000	0.385251000	1.168245000	6	-5.147221000	1.279708000	-0.770595000
17	-0.850212000	-0.002219000	0.000100000				
$(Cl^-@C_{60})Fe(CO)_2Br$				$(Cl^-@C_{60})CoCONMe_3$			
6	3.131862000	-2.677396000	-1.167248000	27	4.006299000	0.459617000	-0.000004000
6	3.871526000	-2.260071000	-0.000023000	7	5.461612000	-0.941547000	-0.000008000
6	3.089324000	-1.859828000	-2.296573000	8	5.723423000	2.770205000	0.000252000
6	4.536257000	-1.035942000	0.000040000	6	5.042211000	1.825365000	0.000133000
6	4.490641000	-0.188312000	1.168834000	6	6.837578000	-0.399177000	-0.000712000
6	3.131803000	-2.677494000	1.167123000	1	6.989500000	0.216716000	-0.888397000
6	3.089208000	-1.860022000	2.296515000	1	6.990201000	0.217306000	0.886444000
6	3.782458000	-0.594021000	2.297968000	6	5.302901000	-1.784464000	1.207320000
6	0.702407000	-2.361107000	-2.595442000	1	4.323584000	-2.265553000	1.194923000
6	0.747437000	-3.207941000	-1.429091000	1	6.084361000	-2.556572000	1.235860000
6	1.849448000	-1.694797000	-3.016778000	6	5.302164000	-1.785518000	-1.206523000
6	1.937491000	-3.355793000	-0.724940000	1	6.083703000	-2.557552000	-1.234912000
6	1.937453000	-3.355841000	0.724688000	1	5.380065000	-1.161276000	-2.098535000
6	-0.494162000	-3.031904000	-0.703175000	1	4.322932000	-2.266737000	-1.193072000
6	-0.494178000	-3.031936000	0.702831000	1	7.566523000	-1.220749000	-0.000707000
6	0.747363000	-3.208079000	1.428807000	1	5.381456000	-1.159452000	2.098737000
6	0.553434000	0.348220000	-3.476183000	6	-3.428032000	-2.157858000	-1.418900000
6	-0.638740000	-0.332241000	-3.019770000	6	-2.702925000	-1.718847000	-2.587586000
6	1.774305000	-0.321018000	-3.465057000	6	-4.231805000	-1.258691000	-0.721364000
6	-0.563582000	-1.662000000	-2.584600000	6	-2.807259000	-0.398709000	-3.018207000
6	-1.302408000	-2.102848000	-1.432168000	6	-1.630869000	0.309894000	-3.467695000
6	-1.451145000	0.624650000	-2.315345000	6	-1.415350000	-2.374436000	-2.586828000
6	-2.164999000	0.215352000	-1.171502000	6	-0.284810000	-1.696280000	-3.029647000
6	-2.083842000	-1.163743000	-0.723701000	6	-0.394241000	-0.327103000	-3.476856000
6	2.894554000	1.679494000	-2.587272000	6	-3.428130000	-2.156881000	1.420401000
6	1.625445000	2.368663000	-2.590041000	6	-2.588374000	-3.083591000	0.698988000
6	2.968772000	0.356550000	-3.019523000	6	-4.231857000	-1.258192000	0.722192000
6	0.478129000	1.717707000	-3.030260000	6	-2.588328000	-3.084081000	-0.696814000
6	-0.763845000	1.882632000	-2.302775000	6	-1.345738000	-3.221598000	-1.415839000
6	1.578288000	3.215989000	-1.416846000	6	-1.345824000	-3.220603000	1.418145000
6	0.385277000	3.390230000	-0.721155000	6	-0.147791000	-3.363982000	0.722724000
6	-0.806792000	2.701697000	-1.164623000	6	-0.147739000	-3.364501000	-0.720270000
6	4.490711000	-0.188208000	-1.168682000	6	-3.643494000	0.534820000	2.297339000
6	4.415313000	1.182995000	-0.722022000	6	-2.807456000	-0.396577000	3.018479000
6	3.782565000	-0.593816000	-2.297874000	6	-4.340147000	0.111861000	1.168159000
6	3.633009000	2.101044000	-1.419701000	6	-2.703079000	-1.717010000	2.588786000
6	2.817617000	3.047451000	-0.697854000	6	-1.415516000	-2.372611000	2.588537000
6	4.415274000	1.182927000	0.722293000	6	-1.631075000	0.312330000	3.467461000
6	3.632943000	2.100924000	1.420005000	6	-0.394462000	-0.324662000	3.477125000
6	2.817588000	3.047399000	0.698201000	6	-0.285012000	-1.694150000	3.030928000
6	-0.806836000	2.701584000	1.164743000	6	-3.766582000	2.195232000	-0.000809000
6	0.385243000	3.390171000	0.721395000	6	-3.040514000	2.633550000	1.167441000
6	1.578219000	3.215867000	1.417137000	6	-4.406450000	0.958871000	-0.000369000
6	-0.763956000	1.882447000	2.302837000	6	-2.978729000	1.816651000	2.295806000
6	-2.165055000	0.215243000	1.171329000	6	-1.737550000	1.683088000	3.020898000
6	-2.174556000	1.051411000	-0.000047000	6	-1.861100000	3.335367000	0.723771000
6	-1.548461000	2.305672000	0.000030000	6	-0.667380000	3.212847000	1.425492000
6	-1.451190000	0.624441000	2.315188000	6	-0.603816000	2.371108000	2.593666000
6	-0.563724000	-1.662241000	2.584389000	6	-3.643338000	0.533192000	-2.297745000

6	-1.302492000	-2.102981000	1.431867000	6	-2.978583000	1.815032000	-2.297125000
6	-2.083911000	-1.163828000	0.723415000	6	-4.340075000	0.111041000	-1.168302000
6	-0.638863000	-0.332501000	3.019615000	6	-3.040473000	2.632749000	-1.169351000
6	1.774134000	-0.321311000	3.465057000	6	-1.861064000	3.334839000	-0.726110000
6	1.849291000	-1.695059000	3.016691000	6	-1.737375000	1.680978000	-3.022114000
6	0.702274000	-2.361322000	2.595212000	6	-0.603667000	2.369315000	-2.595312000
6	0.553261000	0.347929000	3.476203000	6	-0.667313000	3.211876000	-1.427718000
6	1.625307000	2.368413000	2.590241000	6	1.415036000	2.165472000	1.432938000
6	2.894421000	1.679274000	2.587504000	6	0.581165000	3.070375000	0.703212000
6	2.968624000	0.356292000	3.019649000	6	0.581188000	3.069895000	-0.705298000
6	0.477971000	1.717468000	3.030416000	6	2.226464000	1.247797000	0.730117000
17	1.110268000	0.001848000	-0.000042000	6	1.614833000	-0.552825000	2.316653000
26	-3.939360000	-0.435248000	-0.000031000	6	0.779579000	0.386916000	3.025032000
35	-5.422803000	1.407865000	0.000033000	6	0.681330000	1.709957000	2.591333000
8	-5.462608000	-1.705184000	2.126605000	6	2.302349000	-0.122579000	1.179197000
8	-5.462802000	-1.705225000	-2.126519000	6	1.757508000	-2.229973000	0.000886000
6	-4.864404000	-1.200502000	1.279211000	6	1.029910000	-2.652741000	1.167147000
6	-4.864476000	-1.200532000	-1.279218000	6	0.957937000	-1.827724000	2.300089000
				6	2.381474000	-0.960692000	0.000431000
				6	1.614990000	-0.554407000	-2.316129000
				6	0.958103000	-1.829321000	-2.298661000
				6	1.029981000	-2.653544000	-1.165122000
				6	2.302414000	-0.123363000	-1.178917000
				6	1.415140000	2.164510000	-1.434367000
				6	0.681492000	1.708167000	-2.592479000
				6	0.779793000	0.384819000	-3.025260000
				6	2.226431000	1.247301000	-0.730794000
				17	-0.993116000	-0.005750000	-0.000696000
$(Cl^- @ C_{60})CoCOPEt_3$				$(Cl^- @ C_{60})NiNET_3Cl$			
27	3.544865000	0.831124000	-0.144759000	6	-3.166796000	0.322070000	3.030654000
8	5.289176000	3.114908000	-0.112691000	6	-2.038384000	1.196331000	3.260732000
6	4.583312000	2.187802000	-0.158508000	6	-2.981569000	-1.057272000	2.979466000
6	-3.676559000	-2.412526000	-1.268839000	6	-0.766035000	0.658867000	3.436284000
6	-3.024936000	-1.955919000	-2.473862000	6	0.368390000	1.289091000	2.798831000
6	-4.538230000	-1.561951000	-0.578964000	6	-2.220605000	2.382270000	2.455795000
6	-3.259392000	-0.666617000	-2.947541000	6	-1.124203000	2.993315000	1.849335000
6	-2.163342000	0.125960000	-3.456538000	6	0.197669000	2.437978000	2.023991000
6	-1.684623000	-2.494517000	-2.488703000	6	-4.514426000	-1.217680000	1.066779000
6	-0.631795000	-1.734814000	-2.988660000	6	-4.708472000	0.212285000	1.120983000
6	-0.875200000	-0.399939000	-3.481072000	6	-3.667602000	-1.841733000	1.980041000
6	-3.598467000	-2.303002000	1.568186000	6	-4.048022000	0.968791000	2.086666000
6	-2.700111000	-3.179513000	0.854107000	6	-3.458621000	2.236717000	1.728357000
6	-4.498908000	-1.506509000	0.863473000	6	-4.813686000	0.700296000	-0.234579000
6	-2.738651000	-3.233560000	-0.539848000	6	-4.251227000	1.927440000	-0.579409000
6	-1.507925000	-3.287671000	-1.290688000	6	-3.560800000	2.709998000	0.418608000
6	-1.430087000	-3.177614000	1.538426000	6	-2.754525000	-3.262581000	0.188937000
6	-0.243491000	-3.241415000	0.812842000	6	-3.640777000	-2.621209000	-0.753710000
6	-0.283406000	-3.296899000	-0.627404000	6	-2.767459000	-2.878728000	1.533609000
6	-4.030499000	0.390720000	2.354900000	6	-4.501093000	-1.613951000	-0.322632000
6	-3.094428000	-0.434170000	3.082374000	6	-4.687617000	-0.428878000	-1.126639000
6	-4.718139000	-0.135661000	1.263351000	6	-2.933361000	-2.479324000	-2.004441000
6	-2.883434000	-1.756780000	2.697585000	6	-3.110548000	-1.334711000	-2.778710000
6	-1.542820000	-2.294267000	2.680034000	6	-4.006248000	-0.292406000	-2.334289000
6	-1.974521000	0.392810000	3.469447000	6	-0.315381000	-3.000216000	1.615853000
6	-0.685644000	-0.132491000	3.463938000	6	-0.301934000	-3.395638000	0.228060000
6	-0.465848000	-1.501418000	3.062990000	6	-1.528107000	-2.743003000	2.254048000
6	-4.369529000	1.946332000	0.004307000	6	-1.501453000	-3.518888000	-0.471620000
6	-3.652617000	2.490835000	1.133257000	6	-1.609500000	-3.029793000	-1.830940000
6	-4.892310000	0.655957000	0.068035000	6	0.836523000	-2.767574000	-0.401785000
6	-3.485217000	1.726208000	2.287490000	6	0.723503000	-2.284846000	-1.718572000
6	-2.216636000	1.730523000	2.977233000	6	-0.516479000	-2.433166000	-2.450981000
6	-2.553871000	3.278868000	0.628512000	6	-0.573054000	-0.771703000	3.378971000

6	-1.334333000	3.289360000	1.297406000	6	0.679868000	-1.026834000	2.700980000
6	-1.162286000	2.501045000	2.492734000	6	-1.657871000	-1.611345000	3.147444000
6	-4.155260000	0.213939000	-2.235229000	6	0.814897000	-2.129638000	1.841463000
6	-3.609723000	1.549240000	-2.299864000	6	1.527390000	-2.001834000	0.598215000
6	-4.781601000	-0.225426000	-1.070640000	6	1.262169000	0.241594000	2.366030000
6	-3.715736000	2.400862000	-1.200265000	6	1.922148000	0.378794000	1.145291000
6	-2.593110000	3.223269000	-0.818644000	6	2.076428000	-0.744643000	0.245578000
6	-2.380608000	1.498063000	-3.055647000	6	0.424905000	-0.373417000	-3.031022000
6	-1.302979000	2.301552000	-2.690486000	6	1.305882000	-1.030098000	-2.093064000
6	-1.411327000	3.178950000	-1.551383000	6	1.948620000	-0.264241000	-1.117099000
6	0.832003000	2.426018000	1.278441000	6	0.243652000	1.008889000	-2.980088000
6	-0.099580000	3.227587000	0.541955000	6	-2.165752000	0.722878000	-3.361921000
6	-0.137140000	3.173831000	-0.862439000	6	-1.974638000	-0.707983000	-3.416571000
6	1.696869000	1.558977000	0.581595000	6	-0.701521000	-1.250191000	-3.258612000
6	1.304782000	-0.222350000	2.251611000	6	-1.077664000	1.567460000	-3.148843000
6	0.408001000	0.662721000	2.950212000	6	-2.408239000	2.931805000	-1.602157000
6	0.176932000	1.955823000	2.474650000	6	-3.540394000	2.069062000	-1.828252000
6	1.929557000	0.224038000	1.079226000	6	-3.417603000	0.977110000	-2.688722000
6	1.532703000	-1.968715000	-0.006496000	6	-1.201865000	2.692537000	-2.253284000
6	0.877749000	-2.408314000	1.193969000	6	0.030408000	3.211813000	-0.170230000
6	0.764368000	-1.550348000	2.299780000	6	-1.227085000	3.475726000	0.492972000
6	2.063053000	-0.655040000	-0.072830000	6	-2.421210000	3.330017000	-0.207703000
6	1.177566000	-0.399847000	-2.375022000	6	0.042148000	2.824006000	-1.527001000
6	0.636454000	-1.727554000	-2.290759000	6	1.766725000	1.161133000	-1.058325000
6	0.812405000	-2.497943000	-1.132081000	6	1.756721000	1.558312000	0.338383000
6	1.863321000	0.133181000	-1.276953000	6	0.908731000	2.592695000	0.774888000
6	0.755635000	2.316661000	-1.585309000	6	0.932860000	1.803828000	-1.987603000
6	0.036982000	1.757508000	-2.704181000	17	-1.318310000	-0.019700000	0.006139000
6	0.243143000	0.430391000	-3.090503000	28	3.643051000	0.630794000	-0.145750000
6	1.661826000	1.504023000	-0.872150000	17	4.744702000	2.466245000	-0.522619000
17	-1.381729000	0.002729000	-0.004649000	7	5.184337000	-0.628805000	0.140997000
15	5.190755000	-0.546526000	0.051692000	6	6.525372000	0.005053000	-0.070057000
6	5.542582000	-1.628401000	-1.394693000	1	6.516831000	0.436790000	-1.071903000
1	5.832848000	-0.967243000	-2.218444000	1	6.578717000	0.862130000	0.601658000
1	6.432241000	-2.221419000	-1.138918000	6	7.715161000	-0.914337000	0.119866000
6	4.391457000	-2.522831000	-1.817797000	1	7.778328000	-1.327646000	1.130788000
1	3.538215000	-1.932457000	-2.165101000	1	8.628078000	-0.338138000	-0.047078000
1	4.041590000	-3.162463000	-1.001662000	1	7.729077000	-1.748178000	-0.588120000
1	4.693536000	-3.175641000	-2.640456000	6	4.996439000	-1.780515000	-0.795289000
6	6.847161000	0.167373000	0.412645000	1	5.721242000	-2.563700000	-0.531366000
1	6.706794000	0.925769000	1.190407000	1	4.006341000	-2.195682000	-0.586448000
1	7.463042000	-0.626240000	0.856054000	6	5.125901000	-1.404869000	-2.253925000
6	7.542365000	0.767152000	-0.800421000	1	4.519557000	-0.524707000	-2.493989000
1	6.902358000	1.477737000	-1.330400000	1	4.771701000	-2.228569000	-2.877779000
1	7.846890000	-0.004322000	-1.512801000	1	6.159147000	-1.192557000	-2.540558000
1	8.443029000	1.306936000	-0.499026000	6	5.057659000	-1.142268000	1.541070000
6	4.949039000	-1.727676000	1.441588000	1	4.067356000	-1.601490000	1.614581000
1	3.986206000	-2.226927000	1.281170000	1	5.786298000	-1.953360000	1.681339000
1	5.726487000	-2.499956000	1.363827000	6	5.234486000	-0.076614000	2.599130000
6	4.980597000	-1.054820000	2.805014000	1	6.272873000	0.250999000	2.693625000
1	4.231203000	-0.259754000	2.872371000	1	4.922107000	-0.469122000	3.569443000
1	5.958187000	-0.612019000	3.017923000	1	4.620919000	0.805141000	2.384573000
1	4.767426000	-1.776460000	3.597387000				
(Cl ⁻ @C ₆₀)NiPMe ₃ Cl				(Cl ⁻ @C ₆₀)CuNMe ₃			
6	-3.244653000	-1.183020000	-2.603013000	29	-4.143149000	-0.393764000	-0.005294000
6	-2.165021000	-2.143816000	-2.615748000	7	-6.028557000	0.119826000	0.001825000
6	-3.014223000	0.126462000	-3.017478000	6	-6.226898000	1.043325000	-1.134230000
6	-0.899786000	-1.766286000	-3.052042000	1	-5.522836000	1.874337000	-1.050991000
6	0.269209000	-2.219179000	-2.328279000	1	-6.036638000	0.517126000	-2.071690000
6	-2.309933000	-2.995764000	-1.455058000	6	-6.959497000	-1.016401000	-0.117351000
6	-1.183911000	-3.443354000	-0.765992000	1	-6.812133000	-1.700876000	0.719969000
6	0.134372000	-3.049330000	-1.206286000	1	-8.002920000	-0.667918000	-0.115170000

6	-4.365659000	0.981873000	-1.152537000	6	-6.289405000	0.843929000	1.262362000
6	-4.605494000	-0.375901000	-0.722885000	1	-7.316204000	1.237296000	1.283053000
6	-3.585793000	1.228741000	-2.280186000	1	-5.584198000	1.672958000	1.354882000
6	-4.054810000	-1.439506000	-1.435492000	1	-6.148668000	0.168933000	2.108732000
6	-3.475201000	-2.556895000	-0.729104000	1	-7.253614000	1.437151000	-1.144332000
6	-4.603733000	-0.394534000	0.721055000	1	-6.766355000	-1.552502000	-1.048300000
6	-4.051089000	-1.476050000	1.404547000	6	3.517195000	-0.607275000	2.294787000
6	-3.473571000	-2.574989000	0.668255000	6	2.705860000	0.342702000	3.019064000
6	-2.472794000	3.095496000	-1.126856000	6	4.228054000	-0.199453000	1.167737000
6	-3.286164000	2.841524000	0.039201000	6	2.634982000	1.667620000	2.591715000
6	-2.618675000	2.301081000	-2.265316000	6	1.367441000	2.359658000	2.594416000
6	-4.213647000	1.802633000	0.026837000	6	1.510785000	-0.336185000	3.462614000
6	-4.362810000	0.951706000	1.184994000	6	0.289810000	0.334112000	3.472700000
6	-2.470206000	3.065504000	1.209511000	6	0.216834000	1.706865000	3.030791000
6	-2.613266000	2.241838000	2.327297000	6	3.605630000	-2.267291000	-0.006440000
6	-3.580347000	1.169523000	2.316854000	6	2.867283000	-2.689530000	1.160868000
6	-0.181915000	2.245315000	-2.571426000	6	4.273117000	-1.044028000	-0.003174000
6	-0.030105000	3.061207000	-1.391462000	6	2.823803000	-1.874376000	2.290943000
6	-1.453791000	1.868836000	-2.999056000	6	1.584286000	-1.708637000	3.012640000
6	-1.154920000	3.470386000	-0.680681000	6	1.672533000	-3.365942000	0.714219000
6	-1.153307000	3.451425000	0.769823000	6	0.479411000	-3.212930000	1.415883000
6	1.138441000	2.594962000	-0.675359000	6	0.434448000	-2.369010000	2.586388000
6	1.139565000	2.576391000	0.736309000	6	3.517000000	-0.594492000	-2.298564000
6	-0.026929000	3.024388000	1.467406000	6	2.823288000	-1.861516000	-2.301205000
6	-0.660476000	-0.408718000	-3.482897000	6	4.228354000	-0.192931000	-1.169558000
6	0.654940000	-0.021907000	-3.026146000	6	2.866972000	-2.683086000	-1.175757000
6	-1.696617000	0.521407000	-3.462104000	6	1.672343000	-3.361949000	-0.732601000
6	0.893874000	1.281153000	-2.585207000	6	1.583971000	-1.691870000	-3.022010000
6	1.713368000	1.518095000	-1.421080000	6	0.434206000	-2.354448000	-2.599077000
6	1.226504000	-1.150412000	-2.329161000	6	0.479136000	-3.204788000	-1.433409000
6	1.998394000	-0.927706000	-1.190092000	6	3.373163000	2.098555000	-1.413301000
6	2.271233000	0.415827000	-0.733239000	6	2.634647000	1.681963000	-2.582498000
6	0.900000000	1.214088000	2.612835000	6	4.155595000	1.177614000	-0.719115000
6	1.716787000	1.480963000	1.453047000	6	2.705421000	0.359471000	-3.017406000
6	2.271299000	0.397185000	0.735528000	6	1.510343000	-0.316961000	-3.464762000
6	0.662601000	-0.099603000	3.021014000	6	1.367207000	2.374098000	-2.581395000
6	-1.688283000	0.432186000	3.476193000	6	0.216513000	1.723815000	-3.021429000
6	-1.446625000	1.790950000	3.047289000	6	0.289384000	0.353419000	-3.470387000
6	-0.175773000	2.178475000	2.626448000	6	3.373522000	2.090775000	1.424871000
6	-0.651984000	-0.498077000	3.470077000	6	2.561921000	3.044045000	0.705372000
6	-2.158583000	-2.210006000	2.561526000	6	4.155623000	1.173573000	0.725243000
6	-3.238266000	-1.249770000	2.576566000	6	2.561706000	3.047980000	-0.688548000
6	-3.006712000	0.048642000	3.024001000	6	1.321776000	3.219262000	-1.409295000
6	-0.892329000	-1.844012000	3.004658000	6	1.321981000	3.211005000	1.426960000
6	0.137149000	-3.078738000	1.123474000	6	0.127402000	3.384575000	0.731400000
6	-1.182144000	-3.461874000	0.676629000	6	0.127268000	3.388411000	-0.712739000
6	-2.306430000	-3.031977000	1.379588000	6	-1.711272000	0.625122000	-2.303064000
6	0.274827000	-2.277748000	2.266534000	6	-1.021663000	1.890201000	-2.294450000
6	2.000976000	-0.957455000	1.157837000	6	-1.065411000	2.706152000	-1.161263000
6	1.871422000	-1.773791000	-0.026802000	6	-2.432591000	0.218083000	-1.175672000
6	0.951213000	-2.841087000	-0.039418000	6	-1.568404000	-2.089646000	-1.434491000
6	1.232139000	-1.209656000	2.293021000	6	-0.832835000	-1.658012000	-2.594563000
17	-1.123064000	0.012946000	0.000309000	6	-0.903582000	-0.328354000	-3.020144000
28	3.860504000	-0.619831000	-0.013951000	6	-2.358544000	-1.167882000	-0.732601000
17	5.341585000	-2.208978000	0.005456000	6	-1.568089000	-2.097704000	1.423264000
15	5.389403000	0.863914000	-0.001430000	6	-0.759943000	-3.037474000	0.691210000
6	6.437039000	0.759833000	1.477626000	6	-0.760261000	-3.033698000	-0.707774000
1	5.835048000	0.923422000	2.374081000	6	-2.358593000	-1.172383000	0.727138000
1	6.868550000	-0.241788000	1.529019000	6	-1.711230000	0.612216000	2.307270000
6	4.824140000	2.590335000	-0.051038000	6	-0.903085000	-0.345198000	3.018840000
1	5.675474000	3.275666000	-0.003774000	6	-0.832569000	-1.672604000	2.585891000
1	4.268021000	2.777413000	-0.972659000	6	-2.432811000	0.211116000	1.178097000
6	6.537616000	0.712227000	-1.399042000	6	-1.800250000	2.288517000	0.006509000
1	5.999135000	0.837458000	-2.340749000	6	-1.065125000	2.699698000	1.176254000

1	7.327561000	1.466899000	-1.336794000	6	-1.021114000	1.877142000	2.304713000
1	4.158017000	2.793395000	0.791461000	6	-2.478873000	1.066127000	0.003427000
1	7.235591000	1.507200000	1.442760000	17	0.849753000	0.000196000	0.000750000
1	6.975795000	-0.287539000	-1.382246000				
(Cl ⁻ @C ₆₀)CuPMe ₃				(Cl ⁻ @C ₆₀)CuCO			
29	3.702285000	0.056375000	-0.173734000	29	-4.464002000	-0.003633000	-0.002729000
15	5.832660000	-0.008448000	0.039092000	8	-7.387735000	0.007778000	0.005406000
6	-3.922013000	1.874159000	1.568126000	6	-6.238898000	0.001795000	0.000848000
6	-3.121050000	1.461411000	2.696712000	6	3.183976000	-1.442134000	-1.933767000
6	-4.666056000	0.931838000	0.860723000	6	2.424373000	-2.605164000	-1.539271000
6	-3.093927000	0.121219000	3.079404000	6	3.914602000	-0.732465000	-0.982953000
6	-1.844836000	-0.493638000	3.463516000	6	2.423990000	-3.019125000	-0.208099000
6	-1.899912000	2.232335000	2.684953000	6	1.194648000	-3.458010000	0.409072000
6	-0.697295000	1.640841000	3.063904000	6	1.195594000	-2.616473000	-2.297369000
6	-0.669087000	0.252885000	3.460783000	6	0.013107000	-3.050311000	-1.704309000
6	-4.014149000	1.975006000	-1.267386000	6	0.012644000	-3.478967000	-0.326255000
6	-3.241223000	2.950431000	-0.534691000	6	3.182473000	1.396202000	-1.969988000
6	-4.713017000	0.983192000	-0.581947000	6	2.423126000	0.660841000	-2.953858000
6	-3.195947000	2.900869000	0.857835000	6	3.913767000	0.711754000	-1.001287000
6	-1.946416000	3.123558000	1.546673000	6	2.423973000	-0.733119000	-2.936158000
6	-2.038356000	3.223819000	-1.285431000	6	1.195247000	-1.456890000	-3.162478000
6	-0.835548000	3.447260000	-0.619980000	6	1.193499000	1.377063000	-3.198553000
6	-0.788712000	3.396175000	0.822016000	6	0.011629000	0.677830000	-3.427474000
6	-4.015856000	-0.692009000	-2.240333000	6	0.012502000	-0.765245000	-3.409128000
6	-3.289779000	0.335291000	-2.949711000	6	3.180437000	2.307582000	0.718326000
6	-4.713919000	-0.373824000	-1.076979000	6	2.420205000	3.015346000	-0.284777000
6	-3.288912000	1.644959000	-2.471952000	6	3.912730000	1.175472000	0.366520000
6	-2.067915000	2.415769000	-2.484778000	6	2.421238000	2.567833000	-1.605090000
6	-2.069643000	-0.247645000	-3.456389000	6	1.192379000	2.558275000	-2.363144000
6	-0.894685000	0.499519000	-3.476725000	6	1.190343000	3.468243000	0.321151000
6	-0.893799000	1.855772000	-2.982176000	6	0.008300000	3.468745000	-0.414396000
6	-3.925180000	-2.440985000	-0.006015000	6	0.009360000	3.005311000	-1.781087000
6	-3.199714000	-2.769785000	-1.210825000	6	3.181037000	0.032401000	2.415892000
6	-4.667811000	-1.263645000	0.059856000	6	2.419862000	1.204501000	2.779254000
6	-3.244313000	-1.910914000	-2.307987000	6	3.912916000	0.017833000	1.230223000
6	-2.041463000	-1.638213000	-3.059079000	6	2.419510000	2.321783000	1.945576000
6	-1.950738000	-3.385159000	-0.827680000	6	1.189876000	3.038583000	1.702639000
6	-0.793011000	-3.128744000	-1.558236000	6	1.190495000	0.767086000	3.397313000
6	-0.839284000	-2.239399000	-2.694675000	6	0.007721000	1.465626000	3.171036000
6	-3.867019000	-0.854837000	2.347710000	6	0.007349000	2.622345000	2.308104000
6	-3.095490000	-2.073787000	2.278781000	6	3.183236000	-2.285033000	0.776666000
6	-4.638214000	-0.456597000	1.257387000	6	2.422340000	-2.269098000	2.003807000
6	-3.124148000	-2.852673000	1.123007000	6	3.914172000	-1.161325000	0.396214000
6	-1.903816000	-3.436172000	0.616902000	6	2.421273000	-1.131031000	2.808845000
6	-1.845883000	-1.852279000	2.968130000	6	1.191359000	-0.679556000	3.415641000
6	-0.671033000	-2.423015000	2.484447000	6	1.193611000	-2.993359000	1.779148000
6	-0.700638000	-3.229445000	1.287188000	6	0.010596000	-2.563509000	2.374042000
6	1.178226000	-1.882035000	-1.579987000	6	0.009496000	-1.385179000	3.207302000
6	0.455172000	-2.901590000	-0.864554000	6	-1.975159000	1.450430000	1.944746000
6	0.500380000	-2.951040000	0.531685000	6	-1.219011000	0.735654000	2.938175000
6	1.930559000	-0.937020000	-0.870911000	6	-1.218179000	-0.662960000	2.955981000
6	1.122818000	0.860402000	-2.363567000	6	-2.713742000	0.737583000	0.989704000
6	0.353252000	-0.118446000	-3.086722000	6	-1.974296000	2.297856000	-0.780816000
6	0.380455000	-1.462517000	-2.702966000	6	-1.219078000	3.021817000	0.206648000
6	1.902756000	0.461298000	-1.270362000	6	-1.219596000	2.606712000	1.542361000
6	1.181022000	2.453906000	0.001928000	6	-2.713229000	1.169177000	-0.398636000
6	0.383272000	2.856910000	-1.127283000	6	-1.971942000	-0.032375000	-2.429031000
6	0.354619000	2.075948000	-2.286400000	6	-1.216351000	1.130497000	-2.811747000
6	1.931497000	1.273380000	-0.064227000	6	-1.217468000	2.272383000	-2.003989000
6	1.272005000	0.696059000	2.245493000	6	-2.711954000	-0.017731000	-1.238186000
6	0.503658000	1.912669000	2.305803000	6	-1.971370000	-2.320131000	-0.722145000
6	0.458951000	2.774294000	1.206070000	6	-1.214620000	-2.324739000	-1.945667000

6	1.978051000	0.377494000	1.079629000	6	-1.214876000	-1.203611000	-2.782027000
6	1.270277000	-1.982498000	1.268767000	6	-2.711755000	-1.183054000	-0.368779000
6	0.548476000	-1.646204000	2.469209000	6	-1.973473000	-1.403742000	1.981037000
6	0.549529000	-0.333104000	2.948146000	6	-1.216309000	-2.568793000	1.608087000
6	1.976196000	-0.988325000	0.581301000	6	-1.215271000	-3.017836000	0.283351000
17	-1.323171000	0.001985000	-0.004592000	6	-2.712828000	-0.716228000	1.008131000
6	6.775181000	-0.620068000	-1.413073000		0.542377000	-0.000064000	0.000215000
1	6.738670000	0.169684000	-2.172043000				
1	7.829179000	-0.735845000	-1.129533000				
6	6.202341000	-1.914722000	-1.967974000				
1	5.148699000	-1.792134000	-2.240837000				
1	6.256874000	-2.729557000	-1.239563000				
1	6.744472000	-2.237862000	-2.859533000				
6	6.618448000	1.602940000	0.438067000				
1	6.319859000	1.855950000	1.461848000				
1	7.708212000	1.473071000	0.450487000				
6	6.198049000	2.703671000	-0.522967000				
1	5.109046000	2.821187000	-0.530013000				
1	6.510028000	2.489380000	-1.549803000				
1	6.637019000	3.663836000	-0.242624000				
6	6.354582000	-1.111605000	1.413377000				
1	6.213253000	-2.141390000	1.065671000				
1	7.430541000	-0.981689000	1.586600000				
6	5.548363000	-0.867753000	2.680086000				
1	4.476703000	-0.994945000	2.489207000				
1	5.690722000	0.146907000	3.065019000				
1	5.834520000	-1.562022000	3.473210000				

**12. Cartesian coordinates of optimized geometry of (Cl⁻C₆₀)ML_n complexes at Mo6L/6-31G(d,p) level.
Atomic number followed by X, Y, Z coordinates in Å.**

(Cl ⁻ C ₆₀)ScNMe ₃ (CO) ₂				(Cl ⁻ C ₆₀)ScPMe ₃ (CO) ₂			
21	4.150186000	0.033600000	0.240518000	21	-4.030703000	0.783751000	-0.529902000
7	5.166361000	-1.775332000	-0.788468000	15	-5.333428000	-1.455184000	0.429932000
8	5.620808000	-0.290533000	3.242627000	8	-6.634314000	0.398642000	-2.595882000
8	6.486871000	2.360521000	-0.498794000	8	-6.308665000	2.196134000	1.478209000
6	5.094694000	-0.173745000	2.212691000	6	-5.692369000	0.601339000	-1.938691000
6	5.661186000	1.580938000	-0.264416000	6	-5.478836000	1.779043000	0.776089000
6	6.612919000	-1.495085000	-0.724854000	6	-7.141761000	-1.306300000	0.649194000
1	6.850375000	-0.623535000	-1.340355000	1	-7.365799000	-0.516575000	1.369900000
6	6.910328000	-1.290304000	0.308891000	1	-7.610270000	-1.035318000	-0.299804000
6	4.868893000	-2.999689000	-0.020154000	6	-5.158017000	-2.918416000	-0.651329000
1	3.803047000	-3.228281000	-0.094440000	1	-4.097545000	-3.153559000	-0.779937000
1	5.446667000	-3.851768000	-0.405397000	1	-5.667307000	-3.789817000	-0.229079000
6	4.749840000	-1.944603000	-2.192387000	6	-4.754822000	-2.047085000	2.059265000
1	5.328953000	-2.741017000	-2.680544000	1	-5.325265000	-2.920175000	2.389844000
1	4.907390000	-1.010325000	-2.739189000	1	-4.858331000	-1.253077000	2.803109000
1	3.688840000	-2.203371000	-2.229303000	1	-3.696802000	-2.318568000	1.998678000
1	7.197585000	-2.350003000	-1.092380000	1	-7.576498000	-2.244978000	1.005076000
1	5.126148000	-2.848072000	1.032500000	1	-5.582256000	-2.703307000	-1.635407000
6	-3.805912000	-1.237567000	-2.230342000	6	3.533844000	-2.306495000	1.828805000
6	-2.990217000	-0.420224000	-3.095270000	6	2.793628000	-1.654997000	2.885608000
6	-4.591103000	-0.638339000	-1.243249000	6	4.452474000	-1.580702000	1.067907000
6	-2.989259000	0.968985000	-2.953101000	6	2.997515000	-0.295679000	3.142911000
6	-1.748436000	1.701338000	-3.037933000	6	1.871295000	0.563035000	3.413068000
6	-1.748448000	-1.124880000	-3.331784000	6	1.456852000	-2.198177000	2.895350000
6	-0.551525000	-0.415104000	-3.414490000	6	0.367032000	-1.364182000	3.163182000
6	-0.548828000	1.021148000	-3.262101000	6	0.580482000	0.040473000	3.427139000
6	-3.955861000	-2.390037000	0.362728000	6	3.672245000	-2.691747000	-0.983518000
6	-3.144373000	-3.014746000	-0.658159000	6	2.717060000	-3.437313000	-0.197028000

6	-4.669429000	-1.225908000	0.076095000	6	4.522208000	-1.776108000	-0.362848000
6	-3.068079000	-2.447792000	-1.934034000	6	2.652159000	-3.254106000	1.186971000
6	-1.801950000	-2.384259000	-2.618885000	6	1.367073000	-3.185199000	1.842024000
6	-1.955665000	-3.533910000	-0.027189000	6	1.502625000	-3.567285000	-0.968146000
6	-0.728900000	-3.477217000	-0.687764000	6	0.261913000	-3.509290000	-0.333692000
6	-0.649437000	-2.887588000	-2.008389000	6	0.192774000	-3.316821000	1.097707000
6	-4.052083000	-0.280985000	2.264662000	6	4.180998000	-0.170808000	-2.197556000
6	-3.315029000	-1.490528000	2.563352000	6	3.301553000	-1.122084000	-2.843431000
6	-4.716690000	-0.151842000	1.042995000	6	4.785487000	-0.494461000	-0.980921000
6	-3.270056000	-2.528063000	1.628072000	6	3.047976000	-2.356561000	-2.244598000
6	-2.033044000	-3.232116000	1.390195000	6	1.707167000	-2.896567000	-2.235239000
6	-2.124943000	-1.125752000	3.290573000	6	2.220546000	-0.382267000	-3.453954000
6	-0.927463000	-1.806998000	3.061996000	6	0.926106000	-0.903574000	-3.445493000
6	-0.881473000	-2.882885000	2.094140000	6	0.663347000	-2.183219000	-2.823722000
6	-3.955117000	2.180254000	0.843907000	6	4.335981000	1.773810000	-0.135890000
6	-3.266183000	2.046607000	2.110232000	6	3.713734000	2.111531000	-1.398692000
6	-4.667726000	1.099027000	0.321986000	6	4.863184000	0.495044000	0.067565000
6	-3.312902000	0.835058000	2.803236000	6	3.647527000	1.152109000	-2.418661000
6	-2.118568000	0.315110000	3.433352000	6	2.435268000	1.022189000	-3.187446000
6	-2.024366000	2.775932000	2.018796000	6	2.597582000	2.979251000	-1.133711000
6	-0.869988000	2.271729000	2.622970000	6	1.418364000	2.833448000	-1.856509000
6	-0.920550000	1.021459000	3.343425000	6	1.345052000	1.852518000	-2.917363000
6	-3.803687000	1.590251000	-1.929816000	6	3.950343000	0.456723000	2.354010000
6	-3.064117000	2.704837000	-1.386921000	6	3.411848000	1.780302000	2.144591000
6	-4.590199000	0.798324000	-1.091067000	6	4.661615000	-0.174926000	1.333063000
6	-3.139128000	2.995185000	-0.024668000	6	3.595520000	2.423426000	0.915365000
6	-1.942328000	3.356696000	0.704160000	6	2.513829000	3.164506000	0.313214000
6	-1.790649000	2.766880000	-2.071637000	6	2.132634000	1.849817000	2.793036000
6	-0.630059000	3.102728000	-1.366218000	6	1.092635000	2.558089000	2.186511000
6	-0.708126000	3.403411000	0.048507000	6	1.289887000	3.254616000	0.950873000
6	1.147534000	1.139681000	2.274559000	6	-0.720660000	1.992992000	-1.834101000
6	0.398512000	2.344372000	1.939985000	6	0.125577000	2.925888000	-1.223492000
6	0.482804000	2.924057000	0.682431000	6	-0.018373000	3.329164000	0.192494000
6	1.876441000	0.531087000	1.248161000	6	-1.731402000	1.281125000	-1.110413000
6	1.124463000	-1.714906000	1.967543000	6	-1.155183000	-0.797565000	-2.385378000
6	0.317871000	-1.083865000	2.979683000	6	-0.195202000	-0.037632000	-3.162469000
6	0.325880000	0.315881000	3.112541000	6	0.012853000	1.312882000	-2.898154000
6	1.918239000	-0.911455000	1.120618000	6	-1.838902000	-0.148261000	-1.351315000
6	1.274393000	-2.311442000	-0.835214000	6	-1.564532000	-2.131678000	0.111374000
6	0.471063000	-3.121910000	0.040005000	6	-0.828882000	-2.773431000	-0.939680000
6	0.395282000	-2.823144000	1.414644000	6	-0.624209000	-2.111274000	-2.164594000
6	1.966210000	-1.202688000	-0.300890000	6	-2.066890000	-0.820985000	-0.091424000
6	1.395892000	0.173877000	-2.278628000	6	-1.381374000	-0.163421000	2.190622000
6	0.647541000	-0.937683000	-2.786462000	6	-0.846835000	-1.491637000	2.389705000
6	0.595007000	-2.164764000	-2.097710000	6	-0.933060000	-2.451336000	1.370113000
6	1.967379000	0.051017000	-1.007904000	6	-1.967954000	0.166301000	0.959116000
6	1.464244000	2.459662000	-0.371487000	6	-0.886322000	2.374159000	0.972154000
6	0.610271000	2.434585000	-1.622619000	6	-0.248138000	2.009036000	2.189682000
6	0.643503000	1.394391000	-2.540598000	6	-0.507130000	0.780327000	2.820801000
6	2.043562000	1.130432000	-0.056625000	6	-1.724879000	1.453611000	0.346798000
17	2.862966000	3.775835000	-0.559629000	17	-0.749546000	5.104421000	0.352756000
$(Cl^-C_{60})Sc(CO)_4$				$(Cl^-C_{60})Ti(CO)_2Cl$			
6	-0.991265000	2.504177000	-1.175831000	6	2.617345000	1.843597000	2.591310000
6	-1.889452000	2.183139000	-0.000067000	6	3.300493000	2.350602000	1.422015000
6	-0.874760000	1.691249000	-2.288059000	6	2.847300000	0.531641000	3.016361000
6	-2.339981000	0.760968000	0.000048000	6	4.190282000	1.532574000	0.724080000
6	-2.129507000	-0.085327000	1.159061000	6	4.190390000	1.532850000	-0.723077000
6	-0.991190000	2.504344000	1.175589000	6	2.376398000	3.193216000	0.696577000
6	-0.874623000	1.691582000	2.287931000	6	2.376501000	3.193488000	-0.695206000
6	-1.481116000	0.363709000	2.322367000	6	3.300695000	2.351138000	-1.420830000
6	1.472639000	2.372954000	-2.588819000	6	0.449116000	0.220383000	3.453247000
6	1.357431000	3.206239000	-1.421094000	6	0.209131000	1.572405000	3.011068000

6	0.371977000	1.623537000	-3.010824000	6	1.742630000	-0.290883000	3.457359000
6	0.148735000	3.249172000	-0.722645000	6	1.274843000	2.370713000	2.589683000
6	0.148780000	3.249275000	0.722225000	6	1.121860000	3.197075000	1.421176000
6	2.610557000	3.145061000	-0.696170000	6	-1.038545000	1.583261000	2.288173000
6	2.610599000	3.145162000	0.695617000	6	-1.191642000	2.387854000	1.175678000
6	1.357517000	3.206447000	1.420608000	6	-0.087602000	3.184577000	0.722724000
6	1.820820000	-0.306769000	-3.457762000	6	0.930962000	-2.452002000	2.588819000
6	2.961119000	0.465369000	-3.015735000	6	-0.420847000	-1.934381000	2.591513000
6	0.550729000	0.262475000	-3.453603000	6	1.990047000	-1.651511000	3.014880000
6	2.790598000	1.786112000	-2.590846000	6	-0.663499000	-0.605749000	3.012740000
6	3.495814000	2.261906000	-1.421467000	6	-1.582333000	0.228316000	2.322181000
6	3.846514000	-0.417720000	-2.298233000	6	-1.085918000	-2.446640000	1.438645000
6	4.527823000	0.042239000	-1.169748000	6	-1.953202000	-1.602353000	0.717045000
6	4.348751000	1.404859000	-0.723718000	6	-2.222612000	-0.250957000	1.164015000
6	-0.414764000	-1.848579000	-2.592070000	6	3.393275000	-2.467683000	1.168364000
6	0.912171000	-2.426355000	-2.589494000	6	2.297606000	-3.296282000	0.722967000
6	-0.597821000	-0.512356000	-3.013667000	6	3.239146000	-1.659263000	2.296347000
6	2.007272000	-1.676651000	-3.017425000	6	1.090092000	-3.291041000	1.421703000
6	3.254722000	-1.740555000	-2.296751000	6	-0.160889000	-3.279953000	0.696967000
6	1.033452000	-3.271580000	-1.422347000	6	2.297704000	-3.296008000	-0.724055000
6	2.239104000	-3.332233000	-0.723529000	6	1.090289000	-3.290492000	-1.422960000
6	3.372215000	-2.555197000	-1.168954000	6	-0.160801000	-3.279670000	-0.698394000
6	-2.129587000	-0.085495000	-1.158861000	6	4.430564000	0.179611000	1.169881000
6	-1.945141000	-1.455490000	-0.719093000	6	4.583366000	-0.656952000	0.000113000
6	-1.481250000	0.363368000	-2.322263000	6	3.770347000	-0.310578000	2.298008000
6	-1.101515000	-2.327311000	-1.435469000	6	4.073356000	-1.955319000	-0.000164000
6	-0.215838000	-3.203440000	-0.697393000	6	3.393436000	-2.467238000	-1.168981000
6	-1.945078000	-1.455374000	0.719489000	6	4.430729000	0.180056000	-1.169358000
6	-1.101426000	-2.327098000	1.435941000	6	3.770677000	-0.309708000	-2.297767000
6	-0.215795000	-3.203339000	0.697939000	6	3.239476000	-1.658394000	-2.296685000
6	3.372286000	-2.555027000	1.169189000	6	-0.420475000	-1.933399000	-2.592475000
6	2.239148000	-3.332127000	0.723948000	6	0.931327000	-2.451031000	-2.589791000
6	1.033537000	-3.271370000	1.422828000	6	1.990476000	-1.650369000	-3.015384000
6	3.254861000	-1.740219000	2.296874000	6	-0.663084000	-0.604626000	-3.013254000
6	4.527894000	0.042410000	1.169533000	6	-2.222670000	-0.250530000	-1.164686000
6	4.643567000	-0.800300000	-0.000050000	6	-1.953073000	-1.602055000	-0.718130000
6	4.073928000	-2.073829000	0.000061000	6	-1.085742000	-2.446112000	-1.439906000
6	3.846653000	-0.417384000	2.298126000	6	-1.581976000	0.229181000	-2.322444000
6	2.790753000	1.786489000	2.590479000	6	-1.191455000	2.388269000	-1.175092000
6	3.495900000	2.262113000	1.420990000	6	-2.087387000	2.038872000	0.000148000
6	4.348795000	1.404964000	0.723315000	6	-2.485827000	0.591087000	-0.000149000
6	2.961302000	0.465809000	3.015553000	6	-1.038203000	1.584101000	-2.287868000
6	0.550938000	0.262979000	3.453594000	6	1.275208000	2.371675000	-2.588763000
6	0.372159000	1.623976000	3.010628000	6	1.122062000	3.197603000	-1.419967000
6	1.472795000	2.373331000	2.588446000	6	-0.087493000	3.184847000	-0.721689000
6	1.821030000	-0.306264000	3.457760000	6	0.209563000	1.573528000	-3.010606000
6	0.912328000	-2.425975000	2.589860000	6	1.743122000	-0.289583000	-3.457401000
6	-0.414605000	-1.848198000	2.592433000	6	2.847731000	0.532780000	-3.015927000
6	-0.597637000	-0.511914000	3.013838000	6	2.617717000	1.844571000	-2.590411000
6	2.007456000	-1.676209000	3.017614000	6	0.449606000	0.221671000	-3.453259000
21	-4.310011000	-0.573984000	0.000080000	22	-4.188278000	-0.894271000	-0.000399000
6	-4.679901000	-2.172764000	1.546053000	17	-5.727606000	-2.512901000	0.000243000
8	-4.797758000	-2.990683000	2.351394000	8	-5.351099000	1.075866000	-2.244029000
6	-5.079383000	0.886661000	-1.552628000	8	-5.349384000	1.075017000	2.244814000
8	-5.382404000	1.632572000	-2.374619000	6	-4.941774000	0.369918000	-1.426210000
6	-4.679859000	-2.172543000	-1.546147000	6	-4.940856000	0.369372000	1.426334000
8	-4.797698000	-2.990065000	-2.351894000	17	-3.559206000	3.205046000	0.000176000
6	-5.079094000	0.886532000	1.553032000				
8	-5.381886000	1.632623000	2.374945000				
17	-3.346840000	3.418612000	-0.000090000				
$(Cl^-C_{60})TiCl_3$				$(Cl^-C_{60})V(CO)_2$			
22	-4.603922000	-0.581031000	-0.005179000	6	-0.505526000	-0.764754000	3.185426000

17	-4.981030000	-1.708584000	1.839628000	6	-1.219642000	-1.674872000	2.343575000
17	-5.516064000	1.399271000	0.023883000	6	-0.733510000	0.624967000	3.079406000
17	-5.166720000	-1.683772000	-1.816551000	6	-2.111515000	-1.158613000	1.385759000
6	0.538831000	0.064947000	3.495608000	6	-2.233045000	-1.741963000	0.068027000
6	0.926187000	-1.312874000	3.309243000	6	-0.322939000	-2.740334000	1.944279000
6	-0.674807000	0.520026000	2.974038000	6	-0.377948000	-3.264465000	0.650847000
6	0.084355000	-2.184922000	2.612506000	6	-1.339516000	-2.776427000	-0.314153000
6	0.641478000	-3.122932000	1.663487000	6	1.683652000	1.057842000	3.278447000
6	2.352906000	-1.349388000	3.079017000	6	1.917642000	-0.370698000	3.380060000
6	2.887644000	-2.255510000	2.164480000	6	0.389047000	1.545581000	3.130188000
6	2.017286000	-3.161309000	1.446522000	6	0.844105000	-1.261125000	3.330762000
6	0.384209000	2.589804000	2.208298000	6	0.957377000	-2.484638000	2.567892000
6	1.639116000	2.125475000	2.737468000	6	3.136810000	-0.667304000	2.672713000
6	-0.750990000	1.799395000	2.311393000	6	3.246171000	-1.846670000	1.933103000
6	1.720166000	0.882042000	3.376862000	6	2.136893000	-2.769399000	1.879688000
6	2.844658000	0.011789000	3.119658000	6	1.169920000	3.192101000	1.477368000
6	2.687634000	2.538511000	1.830096000	6	2.514033000	2.689391000	1.629676000
6	3.776961000	1.701440000	1.592059000	6	0.124713000	2.629134000	2.213238000
6	3.853984000	0.413115000	2.245196000	6	2.767072000	1.637195000	2.514941000
6	-1.578595000	2.553535000	-0.005201000	6	3.663734000	0.573738000	2.138780000
6	-0.211298000	3.206648000	-0.113483000	6	3.147621000	2.703607000	0.330356000
6	-1.673465000	1.680827000	1.198950000	6	4.012617000	1.670661000	-0.035027000
6	0.658616000	3.296866000	0.955062000	6	4.275692000	0.587940000	0.884542000
6	2.080480000	3.261796000	0.736639000	6	-1.354146000	2.702922000	0.259616000
6	0.305303000	3.034006000	-1.433772000	6	-0.270693000	3.249738000	-0.505643000
6	1.684315000	3.016339000	-1.667565000	6	-1.150255000	2.379954000	1.588468000
6	2.591414000	3.131686000	-0.558889000	6	0.966801000	3.511544000	0.089024000
6	-2.525946000	-0.293137000	-0.089859000	6	2.191789000	3.215530000	-0.625863000
6	-2.098193000	0.431951000	-1.322467000	6	-0.327579000	2.696076000	-1.839732000
6	-2.130541000	0.374302000	1.155804000	6	0.854556000	2.426121000	-2.534546000
6	-1.633268000	1.732168000	-1.280283000	6	2.136761000	2.683478000	-1.910465000
6	-0.562862000	2.121862000	-2.147358000	6	-2.337872000	0.258821000	1.286979000
6	-1.518207000	-0.514645000	-2.235923000	6	-2.648470000	0.592121000	-0.088864000
6	-0.509443000	-0.122238000	-3.120275000	6	-1.682945000	1.142728000	2.155253000
6	-0.021147000	1.227290000	-3.075187000	6	-2.288926000	1.928600000	-0.653958000
6	-1.165714000	-1.704799000	2.076297000	6	-1.447110000	1.800961000	-1.912480000
6	-1.386359000	-2.363114000	0.790621000	6	-2.476119000	-0.627451000	-0.867355000
6	-1.532839000	-0.379572000	2.252464000	6	-1.868222000	-0.634255000	-2.135615000
6	-1.976173000	-1.672440000	-0.260905000	6	-1.325638000	0.625736000	-2.631846000
6	-1.447460000	-1.802407000	-1.588766000	6	2.310412000	0.711471000	-3.155624000
6	-0.268770000	-3.231419000	0.543491000	6	0.966508000	1.214642000	-3.303724000
6	0.231731000	-3.385721000	-0.754747000	6	-0.110074000	0.326874000	-3.346326000
6	-0.370315000	-2.659654000	-1.840946000	6	2.526646000	-0.665960000	-3.054625000
6	1.798884000	-0.181120000	-3.485882000	6	4.183384000	-0.305369000	-1.275246000
6	0.611470000	-0.998712000	-3.369687000	6	3.956557000	1.118314000	-1.371330000
6	0.680849000	-2.244023000	-2.742731000	6	3.035846000	1.618043000	-2.293724000
6	3.013415000	-0.636826000	-2.969702000	6	3.480070000	-1.181396000	-2.104644000
6	3.501111000	1.605506000	-2.080421000	6	3.155882000	-2.739898000	-0.225097000
6	2.244580000	2.073990000	-2.613018000	6	3.878435000	-1.827861000	0.632685000
6	1.407741000	1.197251000	-3.302266000	6	4.384951000	-0.634044000	0.118156000
6	3.878844000	0.272469000	-2.252726000	6	2.953344000	-2.420601000	-1.568678000
6	4.688191000	0.177001000	0.070554000	6	0.637383000	-3.235572000	-1.449371000
6	4.296325000	1.555509000	0.249310000	6	0.846330000	-3.567187000	-0.058779000
6	3.715013000	2.259692000	-0.805681000	6	2.079687000	-3.321650000	0.542990000
6	4.482715000	-0.454331000	-1.159540000	6	1.676869000	-2.674667000	-2.189246000
6	3.719878000	-2.490906000	-0.009814000	6	0.115286000	-1.094743000	-3.249972000
6	3.938533000	-1.840349000	1.261083000	6	-0.980853000	-1.680885000	-2.491197000
6	4.413479000	-0.529009000	1.300783000	6	-0.719717000	-2.748809000	-1.597848000
6	3.990797000	-1.811016000	-1.200752000	6	1.408792000	-1.582970000	-3.108122000
6	1.937031000	-2.715571000	-2.210346000	23	-4.245604000	-0.738646000	0.334159000
6	1.658364000	-3.421157000	-0.976694000	6	-5.146468000	-2.048493000	-0.770953000
6	2.534486000	-3.308712000	0.102607000	8	-5.608200000	-2.855839000	-1.469865000
6	3.082500000	-1.925300000	-2.319088000	6	-5.614923000	0.324273000	1.216383000
17	-2.895259000	3.880023000	0.007168000	8	-6.393192000	1.017411000	1.731855000

				17	-3.834024000	2.949063000	-1.012531000
(Cl ⁻ C ₆₀)V(CO) ₃				(Cl ⁻ C ₆₀)V(CO) ₄			
6	-0.457683000	-0.482498000	-3.150482000	6	-0.904190000	2.526691000	-1.176791000
6	-1.359794000	0.446933000	-2.557813000	6	-1.818117000	2.228926000	-0.000222000
6	-0.381094000	-1.820725000	-2.704110000	6	-0.799757000	1.712153000	-2.289422000
6	-2.104854000	0.043086000	-1.438575000	6	-2.268520000	0.800415000	-0.000124000
6	-2.399256000	0.912436000	-0.320041000	6	-2.072733000	-0.046066000	1.157345000
6	-0.690443000	1.743762000	-2.473527000	6	-0.904235000	2.526903000	1.176298000
6	-0.866280000	2.573875000	-1.381828000	6	-0.799755000	1.712523000	2.289042000
6	-1.893402000	2.321558000	-0.291853000	6	-1.428285000	0.394766000	2.328161000
6	2.073797000	-1.776122000	-2.905432000	6	1.558374000	2.355365000	-2.588941000
6	1.997473000	-0.404448000	-3.370849000	6	1.456005000	3.189817000	-1.421137000
6	0.906938000	-2.464778000	-2.573578000	6	0.445841000	1.623990000	-3.011339000
6	0.763241000	0.228593000	-3.489308000	6	0.247945000	3.252133000	-0.722859000
6	0.612756000	1.602751000	-3.074801000	6	0.247936000	3.252254000	0.722252000
6	3.130701000	0.315354000	-2.833219000	6	2.708214000	3.108189000	-0.695980000
6	2.987156000	1.647981000	-2.434561000	6	2.708198000	3.108300000	0.695405000
6	1.707201000	2.301731000	-2.559635000	6	1.455986000	3.190072000	1.420546000
6	2.009439000	-3.412351000	-0.587092000	6	1.862321000	-0.329651000	-3.456533000
6	3.215350000	-2.697753000	-0.932662000	6	3.015616000	0.423384000	-3.015394000
6	0.876256000	-3.301025000	-1.393256000	6	0.602955000	0.260527000	-3.453869000
6	3.244542000	-1.893150000	-2.073424000	6	2.865907000	1.746514000	-2.590087000
6	3.900454000	-0.600906000	-2.030201000	6	3.579258000	2.211119000	-1.420893000
6	3.831491000	-2.237481000	0.292085000	6	3.886342000	-0.473832000	-2.298078000
6	4.461955000	-0.993950000	0.334375000	6	4.575069000	-0.024923000	-1.169791000
6	4.498071000	-0.161419000	-0.847676000	6	4.418288000	1.340250000	-0.723756000
6	-0.557248000	-3.141420000	0.602442000	6	-0.397601000	-1.836311000	-2.589917000
6	0.617341000	-3.264809000	1.438971000	6	0.920205000	-2.436131000	-2.588607000
6	-0.428702000	-3.164289000	-0.787063000	6	-0.559325000	-0.496019000	-3.013544000
6	1.876288000	-3.393327000	0.854109000	6	2.026254000	-1.702895000	-3.015369000
6	3.002299000	-2.667618000	1.395175000	6	3.272998000	-1.786947000	-2.296329000
6	0.433129000	-2.399670000	2.581380000	6	1.027366000	-3.283611000	-1.422327000
6	1.519022000	-1.698644000	3.100024000	6	2.231715000	-3.362609000	-0.723422000
6	2.823622000	-1.833828000	2.499947000	6	3.376780000	-2.603164000	-1.168513000
6	-2.043971000	-1.323349000	-0.983218000	6	-2.072816000	-0.046276000	-1.157446000
6	-2.208566000	-1.316820000	0.450103000	6	-1.914768000	-1.415810000	-0.719247000
6	-1.194857000	-2.250528000	-1.611923000	6	-1.428268000	0.394365000	-2.328277000
6	-1.465692000	-2.220188000	1.251296000	6	-1.094035000	-2.309602000	-1.438832000
6	-0.859910000	-1.755381000	2.452794000	6	-0.221627000	-3.196856000	-0.697654000
6	-2.344831000	0.075507000	0.862366000	6	-1.914662000	-1.415658000	0.719395000
6	-1.775194000	0.504597000	2.076722000	6	-1.094041000	-2.309336000	1.439203000
6	-1.012018000	-0.404672000	2.852202000	6	-0.221619000	-3.196736000	0.698178000
6	2.578504000	0.393426000	3.172459000	6	3.376776000	-2.602962000	1.168962000
6	1.364320000	-0.314029000	3.513371000	6	2.231714000	-3.362482000	0.723997000
6	0.132339000	0.317650000	3.389450000	6	1.027354000	-3.283368000	1.422882000
6	2.516161000	1.715935000	2.723727000	6	3.272982000	-1.786547000	2.296635000
6	4.215888000	1.232429000	1.010239000	6	4.575060000	-0.024715000	1.169785000
6	4.283498000	-0.131653000	1.481585000	6	4.676157000	-0.869266000	0.000072000
6	3.478785000	-0.542735000	2.545692000	6	4.086871000	-2.133511000	0.000184000
6	3.347880000	2.139923000	1.619256000	6	3.886324000	-0.473426000	2.298147000
6	2.704485000	3.038419000	-0.576806000	6	2.865890000	1.746968000	2.589758000
6	3.606838000	2.103094000	-1.210369000	6	3.579242000	2.211366000	1.420485000
6	4.347718000	1.213473000	-0.430713000	6	4.418281000	1.340376000	0.723506000
6	2.578434000	3.057189000	0.808971000	6	3.015594000	0.423911000	3.015300000
6	0.132178000	3.284988000	0.608115000	6	0.602931000	0.261131000	3.453796000
6	0.263972000	3.264807000	-0.830927000	6	0.445825000	1.624512000	3.011008000
6	1.528336000	3.154480000	-1.414870000	6	1.558356000	2.355815000	2.588493000
6	1.269069000	3.190181000	1.414676000	6	1.862298000	-0.329049000	3.456576000
6	0.065459000	1.679931000	2.921376000	6	0.920189000	-2.435682000	2.589016000
6	-1.103295000	1.799386000	2.085258000	6	-0.397615000	-1.835858000	2.590219000
6	-1.080860000	2.604449000	0.961076000	6	-0.559343000	-0.495499000	3.013596000
6	1.235960000	2.368357000	2.596150000	6	2.026240000	-1.702373000	3.015664000

23	-4.163125000	-0.399001000	-0.317341000	23	-4.029504000	-0.505877000	-0.000009000
6	-5.366545000	0.952668000	0.377211000	6	-4.889793000	-1.777434000	1.204372000
8	-6.087272000	1.743826000	0.824052000	8	-5.384064000	-2.530183000	1.934779000
6	-5.179790000	-1.804807000	-1.217862000	6	-5.064988000	0.633368000	-1.188303000
8	-5.759986000	-2.667822000	-1.733850000	8	-5.668707000	1.321168000	-1.898345000
6	-4.996780000	-1.302760000	1.155505000	6	-4.889953000	-1.776950000	-1.204825000
8	-5.497702000	-1.838730000	2.058903000	8	-5.384358000	-2.529189000	-1.935667000
17	-3.276007000	3.586349000	-0.443330000	6	-5.063774000	0.633376000	1.189489000
				8	-5.666589000	1.321221000	1.900221000
				17	-3.254042000	3.435500000	-0.000430000
$(Cl^-C_{60})Cr(CO)_2Cl$				$(Cl^-C_{60})Cr(CO)_2H$			
6	2.592831000	2.001476000	2.508987000	6	-1.468779000	1.233627000	0.409958000
6	3.286485000	2.451822000	1.321797000	6	-0.927038000	0.304906000	1.353577000
6	2.827786000	0.716801000	3.005956000	6	-1.949434000	-0.885743000	-0.338826000
6	4.189522000	1.604675000	0.678193000	6	-2.098235000	0.489810000	-0.617599000
6	4.205435000	1.528588000	-0.766756000	6	-1.220063000	-1.007453000	0.882353000
6	2.365890000	3.249297000	0.544140000	24	0.058809000	-0.015164000	-0.484412000
6	2.379159000	3.173293000	-0.846134000	1	0.292754000	-1.286827000	-1.436611000
6	3.317031000	2.301995000	-1.515234000	8	2.202659000	-1.949275000	0.210918000
6	0.425480000	0.414179000	3.433318000	8	2.221185000	1.988076000	0.109384000
6	0.180948000	1.739657000	2.920268000	6	1.385644000	-1.160818000	-0.071053000
6	1.722079000	-0.088293000	3.476123000	6	1.374440000	1.226917000	-0.147403000
6	1.247349000	2.519225000	2.465991000	1	-1.424381000	2.312043000	0.478244000
6	1.103420000	3.281759000	1.252864000	1	-2.564770000	0.904954000	-1.503317000
6	-1.059395000	1.706411000	2.184063000	1	-2.315280000	-1.702018000	-0.945752000
6	-1.196641000	2.444353000	1.023626000	1	-0.957730000	-1.934354000	1.373767000
6	-0.097597000	3.226483000	0.541640000	1	-0.411972000	0.552265000	2.271103000
6	0.932539000	-2.297494000	2.709253000				
6	-0.415784000	-1.782171000	2.661567000				
6	1.981731000	-1.466566000	3.104617000				
6	-0.675439000	-0.441001000	3.020265000				
6	-1.590395000	0.350483000	2.271656000				
6	-1.071603000	-2.368525000	1.531601000				
6	-1.926118000	-1.568545000	0.761620000				
6	-2.222543000	-0.200984000	1.136152000				
6	3.407233000	-2.369406000	1.319754000				
6	2.322099000	-3.229999000	0.906104000				
6	3.240172000	-1.505414000	2.404232000				
6	1.107347000	-3.197446000	1.589900000				
6	-0.135925000	-3.237747000	0.851662000				
6	2.339268000	-3.305948000	-0.538444000				
6	1.140528000	-3.345604000	-1.250747000				
6	-0.119630000	-3.308888000	-0.542495000				
6	4.432982000	0.278438000	1.197160000				
6	4.602786000	-0.616789000	0.073813000				
6	3.764537000	-0.156074000	2.342732000				
6	4.098815000	-1.916654000	0.134771000				
6	3.435415000	-2.493459000	-1.013194000				
6	4.459351000	0.156123000	-1.138845000				
6	3.813828000	-0.397155000	-2.247148000				
6	3.291014000	-1.746832000	-2.183532000				
6	-0.362792000	-2.061794000	-2.507479000				
6	0.990387000	-2.568592000	-2.462123000				
6	2.051166000	-1.785869000	-2.919236000				
6	-0.611408000	-0.761551000	-2.999971000				
6	-2.167362000	-0.318933000	-1.181503000				
6	-1.918026000	-1.644577000	-0.670702000				
6	-1.039656000	-2.517871000	-1.333446000				
6	-1.550346000	0.103278000	-2.366728000				
6	-1.180890000	2.326952000	-1.324874000				
6	-2.083084000	2.030836000	-0.138826000				
6	-2.454069000	0.575539000	-0.076033000				

6	-1.008572000	1.460587000	-2.388809000				
6	1.303998000	2.247788000	-2.705606000				
6	1.133442000	3.134449000	-1.585996000				
6	-0.083805000	3.149556000	-0.901668000				
6	0.248074000	1.419113000	-3.094852000				
6	1.799261000	-0.453543000	-3.430414000				
6	2.893011000	0.399189000	-3.018570000				
6	2.648563000	1.728528000	-2.663292000				
6	0.501208000	0.049024000	-3.467128000				
24	-4.095284000	-0.708059000	0.068834000				
17	-5.100184000	-2.637133000	-0.273803000				
8	-5.838235000	1.025963000	-1.643177000				
8	-5.846368000	0.657053000	2.059056000				
6	-5.131334000	0.378279000	-0.991600000				
6	-5.158678000	0.109279000	1.297492000				
17	-3.568218000	3.161069000	-0.160234000				
$(Cl^- C_{60})Mn(CO)_2NMe_3$				$(Cl^- C_{60})Mn(CO)_2PMe_3$			
25	-3.839176000	-0.020885000	0.165329000	25	-3.708370000	0.244129000	0.265659000
7	-5.063189000	-1.692157000	-0.395644000	15	-5.005432000	-1.477585000	-0.323706000
8	-5.634690000	1.864447000	-1.188358000	8	-5.474701000	2.060978000	-1.215714000
8	-5.184538000	0.428983000	2.719005000	8	-5.224936000	0.636378000	2.741100000
6	-4.910445000	1.126607000	-0.647679000	6	-4.765200000	1.352242000	-0.619655000
6	-4.666753000	0.249149000	1.686428000	6	-4.630141000	0.483862000	1.747125000
6	-6.478738000	-1.461525000	-0.036995000	6	-6.785361000	-1.272771000	0.018559000
1	-6.570725000	-1.344418000	1.043751000	1	-6.940209000	-1.142839000	1.092265000
1	-6.839965000	-0.553555000	-0.522453000	1	-7.152617000	-0.375809000	-0.486640000
6	-4.988351000	-1.873425000	-1.860511000	6	-4.983030000	-1.844630000	-2.115256000
1	-3.957724000	-2.081974000	-2.156278000	1	-3.965258000	-2.088264000	-2.433461000
1	-5.625010000	-2.711094000	-2.179379000	1	-5.640508000	-2.683877000	-2.361796000
6	-4.625813000	-2.939447000	0.262988000	6	-4.629245000	-3.098076000	0.434909000
1	-5.295688000	-3.770127000	-0.001561000	1	-5.326095000	-3.869260000	0.092950000
1	-4.634658000	-2.802412000	1.346269000	1	-4.692431000	-3.019632000	1.523041000
1	-3.612353000	-3.192027000	-0.055186000	1	-3.611891000	-3.403610000	0.174273000
1	-7.097076000	-2.311061000	-0.359976000	1	-7.364697000	-2.134982000	-0.324030000
1	-5.325771000	-0.962225000	-2.359276000	1	-5.311431000	-0.962053000	-2.670515000
6	3.928534000	-2.428633000	0.170768000	6	3.858066000	-2.608426000	0.209672000
6	3.185218000	-2.731221000	1.373260000	6	3.145310000	-2.792778000	1.454013000
6	4.642960000	-1.234710000	0.069482000	6	4.645409000	-1.473730000	0.014247000
6	3.169704000	-1.820036000	2.430677000	6	3.234440000	-1.827126000	2.458095000
6	1.944280000	-1.554302000	3.142724000	6	2.058412000	-1.439187000	3.197288000
6	1.964759000	-3.401911000	0.989199000	6	1.868723000	-3.399025000	1.154176000
6	0.779893000	-3.145197000	1.678281000	6	0.732373000	-3.024153000	1.870137000
6	0.765018000	-2.199497000	2.773285000	6	0.825764000	-2.022042000	2.909336000
6	3.881476000	-0.945552000	-2.254754000	6	3.810285000	-1.259344000	-2.292609000
6	3.137704000	-2.185221000	-2.147887000	6	2.990832000	-2.437205000	-2.087869000
6	4.618360000	-0.480216000	-1.163978000	6	4.620874000	-0.787273000	-1.258545000
6	3.166027000	-2.914866000	-0.957855000	6	3.019216000	-3.101528000	-0.860249000
6	1.953179000	-3.515258000	-0.453880000	6	1.791018000	-3.589982000	-0.278647000
6	1.901431000	-2.032727000	-2.873673000	6	1.738630000	-2.240269000	-2.774699000
6	0.729008000	-2.615230000	-2.391115000	6	0.551440000	-2.712604000	-2.215738000
6	0.757757000	-3.372092000	-1.159120000	6	0.580325000	-3.402316000	-0.945974000
6	3.852066000	1.817742000	-1.593917000	6	3.991716000	1.531130000	-1.790062000
6	3.088597000	1.336491000	-2.724109000	6	3.152746000	1.042950000	-2.862011000
6	4.603799000	0.924883000	-0.828572000	6	4.713268000	0.631681000	-1.003480000
6	3.101117000	-0.024737000	-3.042274000	6	3.061234000	-0.331262000	-3.101982000
6	1.874620000	-0.690711000	-3.424158000	6	1.778683000	-0.931044000	-3.399697000
6	1.848566000	2.071744000	-2.771104000	6	1.963451000	1.858191000	-2.905643000
6	0.664568000	1.426091000	-3.135603000	6	0.725736000	1.275934000	-3.188389000
6	0.680034000	0.021865000	-3.470080000	6	0.633659000	-0.141821000	-3.441976000
6	3.872309000	2.044314000	1.238397000	6	4.142359000	1.909108000	1.022145000
6	3.090094000	2.963895000	0.443166000	6	3.391600000	2.835684000	0.205283000
6	4.614241000	1.040418000	0.613861000	6	4.789436000	0.824085000	0.428819000

6	3.082181000	2.854769000	-0.944373000	6	3.319196000	2.651601000	-1.172028000
6	1.839045000	3.002548000	-1.673617000	6	2.060107000	2.845253000	-1.862369000
6	1.859513000	3.231744000	1.159480000	6	2.211038000	3.225792000	0.950102000
6	0.657301000	3.356301000	0.458412000	6	0.992650000	3.395542000	0.287892000
6	0.648000000	3.240762000	-0.982298000	6	0.916921000	3.202128000	-1.142461000
6	3.912153000	-0.579430000	2.327190000	6	4.052631000	-0.647900000	2.256807000
6	3.142081000	0.455768000	2.970185000	6	3.379409000	0.471053000	2.867618000
6	4.635759000	-0.293979000	1.167794000	6	4.745441000	-0.476219000	1.056779000
6	3.124530000	1.749418000	2.440640000	6	3.426026000	1.731943000	2.265818000
6	1.885536000	2.486101000	2.389971000	6	2.237400000	2.547749000	2.218902000
6	1.921647000	-0.139679000	3.468420000	6	2.143166000	-0.010731000	3.443534000
6	0.728851000	0.573135000	3.415278000	6	0.999061000	0.778471000	3.394777000
6	0.708457000	1.904558000	2.866286000	6	1.044491000	2.076751000	2.772004000
6	-1.508175000	2.496385000	-0.181789000	6	-1.249225000	2.650665000	-0.221574000
6	-0.560745000	2.794387000	0.968488000	6	-0.238371000	2.946509000	0.874194000
6	-0.528893000	2.058164000	2.139400000	6	-0.208356000	2.275908000	2.083967000
6	-2.098927000	1.125781000	-0.068802000	6	-1.912509000	1.328233000	-0.007249000
6	-1.313735000	0.448330000	-2.352995000	6	-1.281455000	0.481307000	-2.281601000
6	-0.558794000	1.697605000	-2.423325000	6	-0.447452000	1.668524000	-2.448057000
6	-0.573587000	2.602024000	-1.377087000	6	-0.359872000	2.627841000	-1.455104000
6	-1.985534000	0.175186000	-1.153213000	6	-1.920810000	0.320560000	-1.041277000
6	-1.254194000	-2.190956000	-1.254820000	6	-1.355351000	-2.097194000	-1.036451000
6	-0.520026000	-1.886368000	-2.443300000	6	-0.649500000	-1.904360000	-2.262271000
6	-0.548686000	-0.577922000	-2.976006000	6	-0.613028000	-0.626881000	-2.869796000
6	-1.960682000	-1.158830000	-0.604241000	6	-1.974005000	-0.985612000	-0.419682000
6	-1.229409000	-1.960227000	1.614713000	6	-1.196423000	-1.711062000	1.815735000
6	-0.458886000	-2.989897000	0.948617000	6	-0.522791000	-2.824628000	1.179747000
6	-0.469382000	-3.100192000	-0.443802000	6	-0.597007000	-3.008105000	-0.203087000
6	-1.983609000	-1.058878000	0.832039000	6	-1.915739000	-0.801084000	1.010202000
6	-1.294866000	0.826780000	2.291409000	6	-1.046528000	1.107641000	2.333000000
6	-0.511597000	-0.091481000	3.035700000	6	-0.296636000	0.180138000	3.100339000
6	-0.488280000	-1.476027000	2.731299000	6	-0.377343000	-1.216631000	2.870729000
6	-1.999403000	0.365618000	1.152943000	6	-1.818277000	0.631502000	1.248136000
17	-2.807216000	3.844680000	-0.292231000	17	-2.471785000	4.064951000	-0.360391000
$(Cl^-C_{60})Mn(CO)_3$				$(Cl^-C_{60})Fe(CO)_2Cl$			
25	-4.099375000	-0.593906000	-0.008136000	6	2.701024000	1.793134000	2.589066000
6	-5.005625000	-1.389389000	1.303129000	6	3.403179000	2.274281000	1.420006000
8	-5.566154000	-1.913178000	2.173131000	6	2.881446000	0.474149000	3.015310000
6	-5.225980000	0.797410000	0.002358000	6	4.261825000	1.422850000	0.723151000
8	-5.936800000	1.711706000	0.016859000	6	4.261702000	1.422729000	-0.723934000
6	-5.020971000	-1.473875000	-1.273794000	6	2.510680000	3.150793000	0.695415000
8	-5.605439000	-2.041938000	-2.098674000	6	2.510565000	3.150679000	-0.696190000
6	-2.218746000	-0.525156000	-1.269176000	6	3.402938000	2.274043000	-1.420786000
6	-2.134513000	-1.619662000	-0.325996000	6	0.473544000	0.255516000	3.458181000
6	-2.191578000	-1.046057000	1.002582000	6	0.285157000	1.615448000	3.011193000
6	-2.414994000	0.381460000	0.897446000	6	1.746635000	-0.305482000	3.458197000
6	-2.349520000	0.703520000	-0.520566000	6	1.380253000	2.372426000	2.587964000
6	-1.762416000	1.884772000	-0.988234000	6	1.257494000	3.203898000	1.420464000
6	-0.963632000	1.826881000	-2.153189000	6	-0.959756000	1.676372000	2.288688000
6	-0.837944000	0.641108000	-2.907533000	6	-1.088201000	2.490910000	1.177926000
6	-1.480296000	-0.552214000	-2.470052000	6	0.046878000	3.239555000	0.722713000
6	-0.593240000	-1.667139000	-2.716691000	6	0.851810000	-2.432817000	2.589440000
6	-0.496670000	-2.721355000	-1.803514000	6	-0.477536000	-1.862460000	2.592836000
6	-1.282778000	-2.718555000	-0.586184000	6	1.941347000	-1.673792000	3.015914000
6	-0.491157000	-3.259476000	0.468078000	6	-0.669013000	-0.529227000	3.020845000
6	-0.563159000	-2.701123000	1.764382000	6	-1.555329000	0.342969000	2.329508000
6	-1.438541000	-1.614630000	2.051659000	6	-1.165533000	-2.351277000	1.440120000
6	-0.766558000	-0.717180000	2.973510000	6	-1.996860000	-1.474400000	0.721982000
6	-0.903811000	0.662188000	2.856421000	6	-2.169336000	-0.112216000	1.156356000
6	-1.712431000	1.250625000	1.795551000	6	3.310495000	-2.543812000	1.168750000
6	-1.089365000	2.415518000	1.345616000	6	2.182776000	-3.329263000	0.723470000
6	-1.237562000	2.937896000	-0.038200000	6	3.189173000	-1.729997000	2.296416000

6	0.101941000	3.279533000	-0.665706000	6	0.976232000	-3.277540000	1.422046000
6	0.186007000	2.696590000	-1.968797000	6	-0.274391000	-3.221289000	0.698437000
6	1.416348000	2.347378000	-2.526834000	6	2.182650000	-3.329382000	-0.723078000
6	1.549990000	1.110888000	-3.278743000	6	0.975992000	-3.277785000	-1.421460000
6	0.450950000	0.279866000	-3.469982000	6	-0.274506000	-3.221397000	-0.697640000
6	0.599087000	-1.150137000	-3.354374000	6	4.450052000	0.061697000	1.169367000
6	1.845229000	-1.702065000	-3.051092000	6	4.569104000	-0.780415000	-0.000231000
6	1.943054000	-2.790179000	-2.105543000	6	3.771746000	-0.402905000	2.297439000
6	0.791735000	-3.295740000	-1.496991000	6	4.009419000	-2.058313000	-0.000073000
6	0.800486000	-3.617970000	-0.087399000	6	3.310293000	-2.544004000	-1.168691000
6	1.959441000	-3.427178000	0.659065000	6	4.449849000	0.061500000	-1.169951000
6	1.883228000	-2.868004000	1.996094000	6	3.771350000	-0.403292000	-2.297829000
6	0.651365000	-2.515948000	2.539705000	6	3.188777000	-1.730380000	-2.296474000
6	0.521236000	-1.291754000	3.293871000	6	-0.477968000	-1.862882000	-2.592212000
6	1.628100000	-0.462652000	3.479331000	6	0.851371000	-2.433259000	-2.588975000
6	1.484375000	0.970690000	3.359980000	6	1.940824000	-1.674296000	-3.015763000
6	0.238855000	1.518395000	3.054339000	6	-0.669537000	-0.529736000	-3.020452000
6	0.130362000	2.595255000	2.097995000	6	-2.169550000	-0.112408000	-1.155718000
6	1.276478000	3.114484000	1.508111000	6	-1.996916000	-1.474504000	-0.721158000
6	1.254907000	3.435430000	0.081246000	6	-1.165774000	-2.351524000	-1.439320000
6	2.534761000	3.066743000	-0.470728000	6	-1.555677000	0.342568000	-2.329051000
6	2.617524000	2.535462000	-1.763513000	6	-1.088387000	2.490694000	-1.177950000
6	3.501301000	1.426220000	-2.032254000	6	-1.998728000	2.169996000	0.000092000
6	2.841642000	0.545537000	-2.974435000	6	-2.416390000	0.726050000	0.000289000
6	2.987725000	-0.838348000	-2.859195000	6	-0.960136000	1.675985000	-2.288609000
6	3.794537000	-1.392976000	-1.796035000	6	1.379813000	2.371991000	-2.588418000
6	3.147239000	-2.598434000	-1.332111000	6	1.257252000	3.203650000	-1.421026000
6	3.152501000	-2.909605000	0.030151000	6	0.046757000	3.239434000	-0.723068000
6	3.814988000	-2.036888000	0.971466000	6	0.284645000	1.614947000	-3.011334000
6	3.031730000	-2.012723000	2.187369000	6	1.746038000	-0.306059000	-3.458258000
6	2.906001000	-0.828575000	2.914957000	6	2.880927000	0.473644000	-3.015696000
6	3.552538000	0.379700000	2.448561000	6	2.700588000	1.792704000	-2.589652000
6	2.672374000	1.489253000	2.726662000	6	0.472950000	0.254938000	-3.458125000
6	2.560559000	2.540985000	1.808710000	26	-4.017803000	-0.543881000	-0.000003000
6	3.340295000	2.513537000	0.588049000	17	-5.027200000	-2.561767000	-0.000941000
6	4.199281000	1.443579000	0.328640000	8	-5.676543000	0.615754000	-2.075833000
6	4.276197000	0.888123000	-1.004734000	8	-5.676818000	0.613527000	2.076907000
6	4.426835000	-0.544578000	-0.885211000	6	-5.025861000	0.145653000	-1.247548000
6	4.438673000	-0.872763000	0.522856000	6	-5.026071000	0.144309000	1.248178000
6	4.306973000	0.356713000	1.274077000	17	-3.473670000	3.311547000	0.000055000
17	-2.380038000	4.444381000	-0.085771000				
$(Cl^-C_{60})Fe(CO)_2Br$				$(Cl^-C_{60})CoCONMe_3$			
6	3.085583000	1.583859000	2.589560000	27	-3.785588000	-0.803498000	-0.099644000
6	3.834492000	1.987227000	1.419968000	7	-5.417358000	0.160755000	0.574673000
6	3.124913000	0.253068000	3.015832000	8	-5.195702000	-3.040150000	-1.247043000
6	4.597878000	1.049528000	0.723185000	6	-4.644970000	-2.167738000	-0.706031000
6	4.597789000	1.049443000	-0.723906000	6	-6.068834000	0.811625000	-0.583267000
6	3.040406000	2.953657000	0.695428000	1	-5.369002000	1.511793000	-1.043136000
6	3.040322000	2.953575000	-0.696184000	1	-6.357341000	0.051599000	-1.311861000
6	3.834318000	1.987058000	-1.420706000	6	-6.377314000	-0.768228000	1.209499000
6	0.707123000	0.291862000	3.458582000	1	-5.889893000	-1.290238000	2.035100000
6	0.664436000	1.663896000	3.011452000	1	-7.241163000	-0.209825000	1.595600000
6	1.913537000	-0.401618000	3.458501000	6	-5.069042000	1.191615000	1.578744000
6	1.833772000	2.300159000	2.588245000	1	-5.983062000	1.685839000	1.935107000
6	1.800200000	3.139913000	1.420472000	1	-4.413446000	1.939151000	1.131427000
6	-0.567245000	1.856687000	2.289111000	1	-4.562061000	0.720910000	2.423446000
6	-0.608434000	2.680402000	1.178106000	1	-6.966056000	1.357445000	-0.257374000
6	0.600170000	3.303148000	0.722632000	1	-6.725453000	-1.503406000	0.483234000
6	0.797483000	-2.421616000	2.589788000	6	3.434655000	2.503105000	1.053967000
6	-0.463976000	-1.713560000	2.593727000	6	2.557410000	3.232216000	0.165823000
6	1.961637000	-1.782920000	3.016366000	6	4.313397000	1.548906000	0.537637000
6	-0.512793000	-0.367000000	3.021587000	6	2.592420000	2.987808000	-1.204778000

6	-1.301654000	0.594728000	2.331303000	6	1.356426000	2.903057000	-1.954827000
6	-1.199588000	-2.126574000	1.440931000	6	1.288073000	3.404349000	0.841817000
6	-1.932905000	-1.166400000	0.721906000	6	0.094414000	3.303042000	0.122958000
6	-1.957036000	0.206990000	1.155629000	6	0.130382000	3.052168000	-1.300383000
6	3.230093000	-2.792855000	1.168738000	6	3.795246000	0.028532000	2.401304000
6	2.025425000	-3.453744000	0.723378000	6	2.884970000	1.011841000	2.932687000
6	3.196393000	-1.971145000	2.296642000	6	4.495567000	0.289931000	1.222555000
6	0.831231000	-3.274788000	1.422055000	6	2.709176000	2.232277000	2.274787000
6	-0.406090000	-3.085568000	0.698462000	6	1.384777000	2.789698000	2.139521000
6	2.025337000	-3.453829000	-0.723251000	6	1.745105000	0.313422000	3.486766000
6	0.831059000	-3.274955000	-1.421804000	6	0.466827000	0.854931000	3.353278000
6	-0.406175000	-3.085650000	-0.698084000	6	0.283119000	2.111467000	2.665796000
6	4.640330000	-0.323853000	1.169378000	6	4.085326000	-2.006040000	0.439346000
6	4.669146000	-1.173988000	-0.000234000	6	3.364174000	-2.281654000	1.662168000
6	3.917045000	-0.713733000	2.297818000	6	4.643211000	-0.745857000	0.223684000
6	3.976667000	-2.384710000	-0.000119000	6	3.215505000	-1.281623000	2.624589000
6	3.229950000	-2.792994000	-1.168836000	6	1.954794000	-1.106320000	3.302346000
6	4.640187000	-0.323992000	-1.169942000	6	2.246513000	-3.136626000	1.337139000
6	3.916766000	-0.714005000	-2.298248000	6	1.025063000	-2.967228000	1.988353000
6	3.196114000	-1.971418000	-2.296835000	6	0.872697000	-1.932580000	2.988554000
6	-0.464290000	-1.713868000	-2.593507000	6	3.896389000	-0.787750000	-2.121830000
6	0.797169000	-2.421924000	-2.589637000	6	3.316697000	-2.096378000	-1.897651000
6	1.961271000	-1.783277000	-3.016431000	6	4.546842000	-0.125895000	-1.079097000
6	-0.513159000	-0.367360000	-3.021522000	6	3.413647000	-2.696023000	-0.639637000
6	-1.957178000	0.206849000	-1.155459000	6	2.278238000	-3.395320000	-0.087148000
6	-1.932982000	-1.166482000	-0.721571000	6	2.084300000	-2.176151000	-2.640432000
6	-1.199765000	-2.126745000	-1.440572000	6	0.986865000	-2.851245000	-2.109211000
6	-1.301936000	0.594448000	-2.331249000	6	1.086724000	-3.474412000	-0.808659000
6	-0.608577000	2.680262000	-1.178386000	6	3.502620000	2.002226000	-1.742042000
6	-1.547705000	2.457512000	-0.000069000	6	2.829972000	1.316729000	-2.824726000
6	-2.109753000	1.065246000	0.000045000	6	4.345608000	1.292449000	-0.885735000
6	-0.567525000	1.856416000	-2.289299000	6	3.021466000	-0.055577000	-3.004821000
6	1.833456000	2.299851000	-2.588776000	6	1.896966000	-0.907950000	-3.323581000
6	1.800026000	3.139745000	-1.421100000	6	1.507382000	1.878123000	-2.954408000
6	0.600081000	3.303063000	-0.723134000	6	0.424137000	1.051325000	-3.261696000
6	0.664068000	1.663539000	-3.011766000	6	0.623663000	-0.364088000	-3.449467000
6	1.913117000	-0.402028000	-3.458725000	6	-1.060644000	-2.589190000	-1.039444000
6	3.124547000	0.252711000	-3.016280000	6	-0.347109000	-2.302964000	-2.241384000
6	3.085267000	1.583552000	-2.590159000	6	-0.530593000	-1.063518000	-2.900941000
6	0.706703000	0.291451000	-3.458741000	6	-1.929309000	-1.604098000	-0.503766000
26	-3.831310000	-0.042869000	0.000327000	6	-1.117910000	-2.072441000	1.797581000
35	-5.137734000	-2.010515000	0.000351000	6	-0.209707000	-3.046966000	1.238496000
8	-5.381044000	1.255850000	-2.077934000	6	-0.182655000	-3.302115000	-0.138200000
8	-5.380568000	1.255647000	2.079052000	6	-1.939508000	-1.345091000	0.922394000
6	-4.773512000	0.732839000	-1.248118000	6	-1.549815000	0.733696000	2.189667000
6	-4.773253000	0.732702000	1.249033000	6	-0.662039000	-0.000423000	3.041778000
17	-2.900719000	3.741993000	-0.000059000	6	-0.457332000	-1.382795000	2.869595000
				6	-2.122221000	0.073176000	1.098624000
				6	-1.906008000	2.095897000	-0.441639000
				6	-1.053434000	2.642697000	0.676640000
				6	-0.950033000	2.034178000	1.919888000
				6	-2.341864000	0.691694000	-0.194367000
				6	-1.434837000	-0.089165000	-2.402285000
				6	-0.837942000	1.229440000	-2.587573000
				6	-0.988021000	2.222718000	-1.639559000
				6	-2.108664000	-0.331834000	-1.191049000
				17	-3.391779000	3.314867000	-0.766917000
$(Cl^- C_{60})CoCOPeT_3$				$(Cl^- C_{60})NiNEt_3Cl$			
27	-3.354801000	-0.717297000	-0.546241000	6	3.394881000	-1.972276000	-2.317699000
8	-4.930255000	-2.761353000	-1.814775000	6	2.254350000	-1.599023000	-3.114022000
6	-4.287939000	-1.953020000	-1.272307000	6	3.257804000	-2.894972000	-1.278334000
6	3.753844000	2.358814000	1.466954000	6	0.999259000	-2.153774000	-2.842538000

6	2.972535000	3.171817000	0.562269000	6	-0.184727000	-1.333312000	-2.883953000
6	4.668833000	1.434224000	0.959761000	6	2.367993000	-0.188166000	-3.416150000
6	3.137720000	3.039153000	-0.813691000	6	1.229393000	0.615547000	-3.434256000
6	1.978405000	3.036462000	-1.682519000	6	-0.073983000	0.041159000	-3.166508000
6	1.645044000	3.310675000	1.126363000	6	4.726966000	-1.536259000	0.156447000
6	0.525169000	3.289422000	0.291426000	6	4.878284000	-0.583698000	-0.921230000
6	0.697026000	3.153184000	-1.137152000	6	3.930903000	-2.668359000	-0.019145000
6	3.959106000	-0.223058000	2.633984000	6	4.223339000	-0.795263000	-2.135600000
6	3.010818000	0.729542000	3.154942000	6	3.589008000	0.305151000	-2.815502000
6	4.772686000	0.121056000	1.552972000	6	4.920543000	0.740717000	-0.345490000
6	2.911264000	2.002548000	2.586445000	6	4.306681000	1.807542000	-1.003608000
6	1.611530000	2.591942000	2.372398000	6	3.630943000	1.587953000	-2.262760000
6	1.815973000	0.008809000	3.537935000	6	2.995580000	-2.391937000	2.241492000
6	0.562670000	0.581678000	3.328230000	6	3.824323000	-1.216640000	2.424060000
6	0.458624000	1.891764000	2.732780000	6	3.051769000	-3.106585000	1.041981000
6	4.417974000	-2.095969000	0.548243000	6	4.673892000	-0.798203000	1.399110000
6	3.580004000	-2.457491000	1.669895000	6	4.795263000	0.608486000	1.089758000
6	5.006617000	-0.832393000	0.490730000	6	3.067657000	-0.245466000	3.174588000
6	3.348699000	-1.536706000	2.692997000	6	3.186455000	1.115746000	2.881761000
6	2.029379000	-1.395788000	3.259032000	6	4.063848000	1.548953000	1.815827000
6	2.490657000	-3.265125000	1.171177000	6	0.606419000	-3.371212000	1.059622000
6	1.214228000	-3.127946000	1.714912000	6	0.549673000	-2.629050000	2.300175000
6	0.975546000	-2.174686000	2.776626000	6	1.836901000	-3.601764000	0.441427000
6	4.487849000	-0.671359000	-1.910646000	6	1.727069000	-2.149268000	2.877094000
6	3.876658000	-1.983174000	-1.850330000	6	1.767774000	-0.816180000	3.452826000
6	5.041668000	-0.107484000	-0.759862000	6	-0.637312000	-1.804884000	2.276488000
6	3.846047000	-2.683995000	-0.642661000	6	-0.598700000	-0.505823000	2.834239000
6	2.656355000	-3.407184000	-0.259968000	6	0.633850000	-0.011811000	3.428123000
6	2.719990000	-1.981289000	-2.711117000	6	0.854948000	-3.107802000	-1.761868000
6	1.570822000	-2.678469000	-2.343814000	6	-0.417829000	-2.867770000	-1.121501000
6	1.539409000	-3.406471000	-1.095870000	6	1.963483000	-3.468440000	-0.994372000
6	4.085806000	2.084769000	-1.341654000	6	-0.543595000	-3.001168000	0.266978000
6	3.513212000	1.501190000	-2.535828000	6	-1.307187000	-2.040150000	1.032513000
6	4.836106000	1.293568000	-0.470454000	6	-1.051012000	-1.771447000	-1.821913000
6	3.708228000	0.144576000	-2.809116000	6	-1.745564000	-0.812868000	-1.078017000
6	2.611307000	-0.659178000	-3.302427000	6	-1.887560000	-0.943707000	0.355179000
6	2.215165000	2.094200000	-2.744628000	6	-0.385277000	1.774208000	2.328324000
6	1.158273000	1.314230000	-3.220661000	6	-1.222782000	0.588586000	2.175543000
6	1.361158000	-0.084694000	-3.503622000	6	-1.834414000	0.382852000	0.933747000
6	-0.567903000	-2.466515000	-1.455311000	6	-0.256185000	2.686898000	1.299946000
6	0.260980000	-2.096312000	-2.554690000	6	2.150102000	2.888777000	1.773333000
6	0.152768000	-0.805483000	-3.126496000	6	2.009207000	1.949085000	2.854062000
6	-1.472711000	-1.513153000	-0.925437000	6	0.754710000	1.395149000	3.121132000
6	-0.893367000	-2.182865000	1.395477000	6	1.032136000	3.229973000	1.002681000
6	0.056051000	-3.124366000	0.846716000	6	2.393029000	3.149523000	-1.048308000
6	0.213075000	-3.266042000	-0.536306000	6	3.541331000	2.776501000	-0.250697000
6	-1.629176000	-1.377125000	0.508748000	6	3.424793000	2.650792000	1.131861000
6	-1.335333000	0.588762000	1.975644000	6	1.153215000	3.359881000	-0.433297000
6	-0.541311000	-0.225466000	2.840728000	6	0.001434000	2.188493000	-2.219130000
6	-0.333025000	-1.594989000	2.575972000	6	1.269412000	1.940553000	-2.855834000
6	-1.819980000	0.030317000	0.783199000	6	2.451610000	2.419813000	-2.285311000
6	-1.432555000	2.174145000	-0.563290000	6	-0.062247000	2.910057000	-1.039558000
6	-0.679811000	2.607903000	0.676527000	6	-1.806535000	1.342608000	-0.152200000
6	-0.697545000	1.894985000	1.867938000	6	-1.619177000	0.586527000	-1.376994000
6	-1.892996000	0.757168000	-0.469786000	6	-0.835664000	1.012273000	-2.440431000
6	-0.784893000	0.140457000	-2.634854000	6	-1.119122000	2.675545000	0.036617000
6	-0.161195000	1.459937000	-2.658648000	28	-3.535209000	0.334379000	-0.179996000
6	-0.390034000	2.371614000	-1.647900000	17	-4.771829000	1.917787000	-0.990892000
6	-1.570239000	-0.186394000	-1.514456000	7	-5.001166000	-1.036118000	0.225728000
15	-5.135542000	0.031780000	0.447802000	6	-6.379481000	-0.539581000	-0.081824000
6	-5.372193000	1.820212000	0.799565000	1	-6.502413000	0.403437000	0.452105000
1	-5.227304000	2.355562000	-0.143492000	1	-6.387364000	-0.261319000	-1.136615000
1	-6.426963000	1.941184000	1.083917000	6	-7.507884000	-1.499316000	0.240090000
6	-4.459400000	2.389478000	1.870198000	1	-7.455540000	-2.429160000	-0.334074000

1	-3.406127000	2.259429000	1.612379000	1	-8.455939000	-1.019848000	-0.014404000
1	-4.627763000	1.924351000	2.846156000	1	-7.556613000	-1.760867000	1.301420000
1	-4.626349000	3.463684000	1.980192000	6	-4.864739000	-1.328896000	1.684401000
6	-6.731329000	-0.392240000	-0.357551000	1	-5.535679000	-2.160461000	1.944484000
1	-6.787167000	-1.481827000	-0.445494000	1	-3.846525000	-1.701076000	1.834114000
1	-7.537986000	-0.085343000	0.320814000	6	-5.130647000	-0.132806000	2.571685000
6	-6.887213000	0.257822000	-1.723451000	1	-4.580202000	0.749330000	2.225561000
1	-6.084093000	-0.047249000	-2.401548000	1	-4.802370000	-0.349497000	3.590838000
1	-6.864918000	1.349679000	-1.659402000	1	-6.190618000	0.130228000	2.613910000
1	-7.835873000	-0.026031000	-2.185193000	6	-4.721296000	-2.293790000	-0.527889000
6	-5.277639000	-0.742982000	2.112866000	1	-3.714796000	-2.614463000	-0.242516000
1	-4.409585000	-0.402492000	2.690626000	1	-5.403811000	-3.079302000	-0.172443000
1	-6.168616000	-0.324396000	2.601204000	6	-4.828440000	-2.132541000	-2.027693000
6	-5.325596000	-2.262160000	2.083426000	1	-5.864378000	-2.037665000	-2.363354000
1	-4.404894000	-2.676889000	1.661196000	1	-4.396778000	-3.003628000	-2.525920000
1	-6.160511000	-2.636889000	1.482916000	1	-4.281364000	-1.247801000	-2.372482000
1	-5.440840000	-2.666827000	3.091934000	17	-2.277867000	4.110534000	0.125144000
17	-2.847503000	3.407415000	-0.960586000				
(Cl ⁻ C ₆₀)NiPMe ₃ Cl				(Cl ⁻ C ₆₀)CuNMe ₃			
6	3.334595000	2.730047000	0.696695000	29	4.054865000	-0.412083000	-0.614777000
6	2.121390000	3.043420000	1.421938000	7	5.781875000	-0.790868000	0.195084000
6	3.334708000	2.730152000	-0.695948000	6	5.761103000	-2.160168000	0.748777000
6	0.942224000	3.328084000	0.723611000	1	4.903964000	-2.264223000	1.418198000
6	-0.322053000	2.835903000	1.179645000	1	5.661411000	-2.883774000	-0.062727000
6	2.069221000	2.205725000	2.589982000	6	6.922309000	-0.646203000	-0.727972000
6	0.839854000	1.694280000	3.012623000	1	6.940381000	0.366761000	-1.133769000
6	-0.365018000	2.015829000	2.292318000	1	7.870885000	-0.839505000	-0.206143000
6	4.685802000	0.673821000	-0.723024000	6	5.919042000	0.175222000	1.307440000
6	4.685690000	0.673713000	0.723674000	1	6.846436000	-0.007631000	1.868510000
6	4.024454000	1.685798000	-1.420415000	1	5.062812000	0.074033000	1.978552000
6	4.024229000	1.685586000	1.421113000	1	5.933231000	1.193095000	0.912778000
6	3.240852000	1.362827000	2.592756000	1	6.685863000	-2.369331000	1.305401000
6	4.584033000	-0.697072000	1.169641000	1	6.820063000	-1.354028000	-1.552514000
6	3.824870000	-1.008795000	2.298301000	6	-3.352354000	1.315539000	2.267792000
6	3.141224000	0.035612000	3.018468000	6	-2.620988000	0.407812000	3.126932000
6	3.141700000	0.036064000	-3.018159000	6	-4.192845000	0.807043000	1.276461000
6	3.825232000	-1.008451000	-2.298042000	6	-2.763801000	-0.972068000	2.968763000
6	3.241261000	1.363214000	-2.592229000	6	-1.603051000	-1.830943000	3.046697000
6	4.584215000	-0.696897000	-1.169213000	6	-1.315388000	0.976395000	3.365781000
6	4.523294000	-1.545933000	0.000146000	6	-0.197782000	0.148838000	3.443787000
6	2.976201000	-2.184671000	-2.297508000	6	-0.342671000	-1.279222000	3.282911000
6	2.924401000	-3.007236000	-1.169546000	6	-3.380318000	2.497860000	-0.316526000
6	3.708554000	-2.678006000	-0.000020000	6	-2.506624000	3.019255000	0.704654000
6	0.840327000	1.694724000	-3.012418000	6	-4.212915000	1.412284000	-0.038219000
6	0.740245000	0.323206000	-3.456854000	6	-2.496618000	2.441949000	1.978439000
6	2.069628000	2.206106000	-2.589506000	6	-1.242470000	2.235506000	2.650103000
6	1.868246000	-0.490966000	-3.460549000	6	-1.270714000	3.418479000	0.074889000
6	1.770760000	-1.868914000	-3.017897000	6	-0.065181000	3.243044000	0.730694000
6	-0.541241000	-0.206256000	-3.021144000	6	-0.055048000	2.613775000	2.018517000
6	-0.638163000	-1.550837000	-2.599055000	6	-3.709480000	0.433592000	-2.235520000
6	0.543576000	-2.380851000	-2.589954000	6	-2.860045000	1.561358000	-2.536295000
6	0.942341000	3.328184000	-0.723137000	6	-4.382177000	0.360418000	-1.014398000
6	-0.321851000	2.836050000	-1.179437000	6	-2.687383000	2.578893000	-1.587051000
6	2.121613000	3.043621000	-1.421328000	6	-1.392920000	3.157454000	-1.357077000
6	-0.364652000	2.016159000	-2.292251000	6	-1.715456000	1.076034000	-3.264783000
6	-1.222429000	0.835130000	-2.328836000	6	-0.453332000	1.622246000	-3.026442000
6	-1.283967000	2.710068000	0.000015000	6	-0.282402000	2.667533000	-2.040084000
6	-1.966601000	1.367419000	-0.000135000	6	-3.855618000	-2.038984000	-0.835522000
6	-1.916891000	0.518553000	-1.161931000	6	-3.160756000	-1.963737000	-2.102584000
6	-0.727030000	-2.921011000	-0.701683000	6	-4.451570000	-0.896686000	-0.301005000
6	-1.418881000	-1.891174000	-1.446438000	6	-3.091312000	-0.752626000	-2.790625000
6	-2.052313000	-0.853264000	-0.728961000	6	-1.856711000	-0.354144000	-3.426845000

6	-0.727140000	-2.921124000	0.700939000	6	-1.997622000	-2.818469000	-2.024078000
6	1.657826000	-3.536437000	0.723711000	6	-0.806538000	-2.433113000	-2.636891000
6	1.657938000	-3.536327000	-0.724165000	6	-0.734744000	-1.180262000	-3.350559000
6	0.488008000	-3.232088000	-1.421663000	6	-3.638542000	-1.495490000	1.944538000
6	0.487789000	-3.232303000	1.421068000	6	-3.020576000	-2.678692000	1.392153000
6	1.770288000	-1.869368000	3.017712000	6	-4.343690000	-0.620400000	1.114419000
6	2.975842000	-2.185014000	2.297459000	6	-3.122027000	-2.940171000	0.023358000
6	2.924222000	-3.007413000	1.169371000	6	-1.975521000	-3.426069000	-0.710064000
6	0.543174000	-2.381235000	2.589493000	6	-1.760709000	-2.884938000	2.069475000
6	-0.541715000	-0.206694000	3.020837000	6	-0.652624000	-3.356007000	1.362004000
6	0.739701000	0.322693000	3.456834000	6	-0.760602000	-3.627948000	-0.056132000
6	1.867702000	-0.491484000	3.460579000	6	1.312931000	-1.526990000	-2.265260000
6	-0.638573000	-1.551225000	2.598535000	6	0.457810000	-2.636578000	-1.957076000
6	-2.052435000	-0.853377000	0.728317000	6	0.479865000	-3.237666000	-0.688767000
6	-1.917022000	0.518367000	1.161525000	6	2.159667000	-1.003920000	-1.270572000
6	-1.222815000	0.834809000	2.328609000	6	1.577540000	1.326142000	-1.919942000
6	-1.419079000	-1.891386000	1.445722000	6	0.703279000	0.770664000	-2.943112000
28	-3.705633000	0.199204000	-0.000218000	6	0.571563000	-0.607280000	-3.102208000
17	-5.292047000	1.690479000	0.000124000	6	2.361725000	0.441331000	-1.124612000
15	-5.186056000	-1.386357000	-0.000033000	6	1.816734000	1.846583000	0.859033000
6	-6.296528000	-1.311877000	1.435879000	6	1.217023000	2.923390000	-0.001550000
1	-5.726264000	-1.441766000	2.358243000	6	0.988416000	2.483550000	-1.388104000
1	-6.765503000	-0.325903000	1.456609000	6	2.403440000	0.708189000	0.321551000
6	-4.550028000	-3.092554000	-0.000367000	6	1.654348000	-0.632367000	2.256631000
1	-5.368417000	-3.818274000	-0.000462000	6	1.040911000	0.544172000	2.804500000
1	-3.929069000	-3.259240000	-0.884387000	6	1.103114000	1.748075000	2.090846000
6	-6.297651000	-1.311693000	-1.435058000	6	2.325797000	-0.556250000	1.029852000
1	-5.728225000	-1.442118000	-2.357863000	6	1.343145000	-2.708499000	0.332945000
1	-7.067134000	-2.087430000	-1.378097000	6	0.649586000	-2.780627000	1.600554000
1	-3.929012000	-3.259523000	0.883563000	6	0.805071000	-1.762884000	2.545154000
1	-7.065678000	-2.088005000	1.379770000	6	2.168348000	-1.611050000	0.055144000
1	-6.766187000	-0.325509000	-1.455647000	17	2.396522000	4.489295000	0.082655000
17	-2.472944000	4.129875000	-0.000070000				
(Cl ⁻ C ₆₀)CuPEt ₃				(Cl ⁻ C ₆₀)CuCO			
29	3.494551000	-0.772831000	-0.068112000	29	-4.217770000	-0.813159000	-0.000237000
15	5.619788000	-0.384859000	-0.015858000	8	-7.068716000	-1.450877000	0.000615000
6	-4.187153000	-0.420245000	2.314004000	6	-5.942465000	-1.221716000	0.000101000
6	-3.637222000	-1.758393000	2.270011000	6	3.745888000	-1.964771000	0.000003000
6	-4.860482000	0.093040000	1.204667000	6	3.063958000	-2.473094000	1.169269000
6	-3.785528000	-2.535677000	1.120593000	6	4.266317000	-0.670137000	0.000383000
6	-2.677617000	-3.331206000	0.641794000	6	2.915862000	-1.664708000	2.297440000
6	-2.380670000	-1.752350000	2.982719000	6	1.666987000	-1.650755000	3.020004000
6	-1.312028000	-2.521452000	2.520786000	6	1.960605000	-3.292550000	0.723387000
6	-1.465315000	-3.327203000	1.330178000	6	0.754355000	-3.280937000	1.422306000
6	-3.751087000	2.269316000	1.505632000	6	0.601120000	-2.441718000	2.590272000
6	-3.051831000	1.736950000	2.654869000	6	3.456576000	-0.319214000	-2.298701000
6	-4.639219000	1.461400000	0.794113000	6	2.916555000	-1.663630000	-2.297542000
6	-3.266432000	0.414894000	3.049579000	6	4.117731000	0.167118000	-1.169308000
6	-2.149149000	-0.405763000	3.461240000	6	3.064312000	-2.472548000	-1.169708000
6	-1.715242000	2.284089000	2.658558000	6	1.960821000	-3.292210000	-0.724545000
6	-0.637580000	1.490587000	3.054945000	6	1.667898000	-1.649339000	-3.020477000
6	-0.860039000	0.124170000	3.464296000	6	0.601900000	-2.440508000	-2.591445000
6	-3.776852000	2.349122000	-1.332362000	6	0.754779000	-3.280264000	-1.423820000
6	-2.857447000	3.184989000	-0.594093000	6	2.997099000	2.343664000	-1.419340000
6	-4.652420000	1.502109000	-0.651384000	6	2.311090000	1.839582000	-2.589186000
6	-2.844773000	3.145566000	0.798865000	6	3.883987000	1.521303000	-0.722586000
6	-1.584476000	3.151988000	1.512130000	6	2.536098000	0.528396000	-3.015904000
6	-1.610111000	3.232039000	-1.328387000	6	1.427423000	-0.289031000	-3.458617000
6	-0.396335000	3.229725000	-0.641205000	6	0.971143000	2.374502000	-2.587134000
6	-0.383227000	3.189122000	0.804070000	6	-0.098442000	1.581527000	-3.009468000
6	-4.228668000	-0.290674000	-2.282758000	6	0.135394000	0.230478000	-3.454564000
6	-3.321272000	0.584942000	-2.986862000	6	2.996671000	2.343000000	1.421136000

6	-4.881672000	0.158925000	-1.134379000	6	2.077104000	3.190511000	0.696860000
6	-3.098548000	1.882432000	-2.521891000	6	3.883767000	1.520964000	0.724265000
6	-1.762008000	2.429634000	-2.519093000	6	2.077316000	3.190842000	-0.694946000
6	-2.211943000	-0.210797000	-3.464264000	6	0.822425000	3.202817000	-1.419956000
6	-0.922861000	0.319058000	-3.460760000	6	0.821995000	3.202151000	1.421502000
6	-0.692244000	1.660500000	-2.979528000	6	-0.387742000	3.196127000	0.723207000
6	-4.482855000	-2.002205000	-0.028279000	6	-0.387519000	3.196463000	-0.722028000
6	-3.806946000	-2.470062000	-1.217955000	6	3.455884000	-0.320294000	2.299389000
6	-5.012190000	-0.711981000	0.012815000	6	2.535188000	0.526983000	3.016709000
6	-3.678898000	-1.628965000	-2.324188000	6	4.117376000	0.166570000	1.170423000
6	-2.435374000	-1.582178000	-3.058013000	6	2.310318000	1.838375000	2.590546000
6	-2.690794000	-3.290529000	-0.805123000	6	0.970369000	2.373298000	2.588341000
6	-1.491039000	-3.247086000	-1.513985000	6	1.426380000	-0.290647000	3.458707000
6	-1.358846000	-2.375717000	-2.660066000	6	0.134355000	0.228869000	3.454518000
6	1.119411000	0.331538000	-2.333504000	6	-0.099342000	1.580127000	3.009981000
6	0.197989000	-0.503963000	-3.048318000	6	-2.385948000	2.054659000	0.000009000
6	-0.017780000	-1.834981000	-2.659148000	6	-1.500304000	2.410910000	1.176755000
6	1.771490000	-0.177739000	-1.203044000	6	-1.348908000	1.599590000	2.287950000
6	1.475576000	1.966745000	0.029512000	6	-2.750545000	0.614064000	-0.000408000
6	0.716294000	2.446247000	-1.121565000	6	-1.903467000	0.252820000	-2.327379000
6	0.566340000	1.668997000	-2.267897000	6	-1.348230000	1.600650000	-2.287811000
6	1.934655000	0.628880000	-0.012375000	6	-1.499931000	2.411455000	-1.176284000
6	1.161081000	0.201129000	2.302096000	6	-2.522324000	-0.219967000	-1.161238000
6	0.607924000	1.540001000	2.322379000	6	-1.414565000	-2.421113000	-1.434540000
6	0.737544000	2.380554000	1.219138000	6	-0.745344000	-1.915422000	-2.594529000
6	1.791496000	-0.243092000	1.133166000	6	-0.980601000	-0.589828000	-3.013512000
6	0.700112000	-2.452205000	1.342990000	6	-2.299306000	-1.591114000	-0.724583000
6	0.028822000	-1.980487000	2.525762000	6	-1.414987000	-2.421785000	1.432762000
6	0.252625000	-0.673884000	2.985818000	6	-0.497589000	-3.263281000	0.697219000
6	1.577276000	-1.600773000	0.654517000	6	-0.497382000	-3.262942000	-0.699099000
6	0.674335000	-2.372190000	-1.516928000	6	-2.299502000	-1.591461000	0.722879000
6	-0.231253000	-3.239857000	-0.801051000	6	-1.904163000	0.251744000	2.326729000
6	-0.218530000	-3.279257000	0.596189000	6	-0.981508000	-0.591231000	3.012732000
6	1.564284000	-1.560283000	-0.797326000	6	-0.746124000	-1.916625000	2.593186000
6	6.019331000	1.105498000	-1.005326000	6	-2.522555000	-0.220470000	1.160101000
1	5.699969000	1.968776000	-0.407889000	17	-3.923791000	3.179477000	-0.000031000
1	7.109848000	1.153053000	-1.122259000				
6	5.296531000	1.140958000	-2.340631000				
1	4.214232000	1.183248000	-2.176856000				
1	5.517909000	0.267230000	-2.964294000				
1	5.569875000	2.035236000	-2.904849000				
6	6.225383000	0.030842000	1.666728000				
1	6.398857000	-0.908520000	2.204865000				
1	7.203780000	0.515982000	1.555484000				
6	5.247406000	0.921157000	2.420373000				
1	4.314359000	0.385502000	2.627524000				
1	4.976122000	1.817177000	1.849346000				
1	5.666749000	1.240741000	3.377406000				
6	6.779796000	-1.670756000	-0.625147000				
1	6.644001000	-1.732349000	-1.711000000				
1	7.804395000	-1.313543000	-0.459700000				
6	6.560715000	-3.028186000	0.021396000				
1	5.545867000	-3.395074000	-0.162771000				
1	6.701604000	-2.989074000	1.106022000				
1	7.259544000	-3.771325000	-0.370280000				
17	3.520666000	3.356818000	0.055166000				
(Cl ⁻ C ₆₀)ScPMe ₃ (CO) ₂ _α-posiion				(Cl ⁻ C ₆₀)TiCl ₃ _α-posiion			
21	4.020399000	0.944728000	-0.251926000	22	-5.523060000	0.001342000	0.003569000
15	5.030915000	-1.737438000	-0.155521000	17	-4.930052000	0.006054000	-2.098750000
8	5.578439000	0.620560000	2.733865000	17	-7.701499000	-0.023519000	0.022063000
8	7.190951000	1.103792000	-1.472336000	17	-4.922423000	1.830652000	1.036297000
6	5.008345000	0.744906000	1.736158000	6	3.186277000	-0.751762000	-2.958014000

6	6.099208000	1.019239000	-1.103879000	6	3.192765000	0.694222000	-2.968113000
6	6.852495000	-1.934848000	-0.145441000	6	1.995264000	-1.445359000	-3.173017000
1	7.282302000	-1.597467000	-1.090723000	6	2.008058000	1.395744000	-3.193257000
1	7.288005000	-1.329775000	0.654429000	6	1.704470000	2.572412000	-2.409604000
6	4.567012000	-2.629560000	1.375244000	6	4.117265000	1.143869000	-1.951240000
1	3.480541000	-2.704365000	1.461573000	6	3.824070000	2.279058000	-1.195074000
1	4.989076000	-3.639026000	1.375511000	6	2.596250000	3.006187000	-1.428610000
6	4.525686000	-2.897025000	-1.480193000	6	2.569353000	-3.037094000	-1.386313000
1	4.942072000	-3.894388000	-1.309079000	6	3.803796000	-2.317703000	-1.163175000
1	4.877771000	-2.532322000	-2.448122000	6	1.681352000	-2.608821000	-2.373499000
1	3.436121000	-2.974732000	-1.519248000	6	4.106905000	-1.195704000	-1.934857000
1	7.130342000	-2.981056000	0.012930000	6	4.681839000	-0.024074000	-1.312342000
1	4.943813000	-2.093760000	2.249809000	6	4.065322000	-2.308623000	0.259287000
6	-4.238702000	0.276044000	-2.263514000	6	4.620194000	-1.178398000	0.859736000
6	-3.682953000	1.609033000	-2.298195000	6	4.934274000	-0.015573000	0.059757000
6	-4.875402000	-0.181868000	-1.107354000	6	-0.224616000	-3.020712000	-0.872913000
6	-3.783738000	2.438539000	-1.178884000	6	0.695745000	-3.464890000	0.150361000
6	-2.655457000	3.241711000	-0.769120000	6	0.259113000	-2.600768000	-2.112077000
6	-2.448136000	1.558624000	-3.046596000	6	2.067726000	-3.472538000	-0.101653000
6	-1.361278000	2.341169000	-2.653140000	6	2.992287000	-3.022103000	0.915409000
6	-1.465657000	3.198237000	-1.492552000	6	0.197914000	-3.006918000	1.428565000
6	-3.785911000	-2.376499000	-1.338698000	6	1.089738000	-2.571633000	2.409063000
6	-3.124310000	-1.903018000	-2.535839000	6	2.512141000	-2.580342000	2.148753000
6	-4.646463000	-1.530506000	-0.639505000	6	-1.334857000	-0.726010000	-2.128322000
6	-3.345270000	-0.598910000	-2.987014000	6	-1.834044000	-1.162028000	-0.844524000
6	-2.240678000	0.193356000	-3.474487000	6	-0.305851000	-1.433101000	-2.751457000
6	-1.790023000	-2.451293000	-2.546375000	6	-1.291793000	-2.289232000	-0.227777000
6	-0.721047000	-1.691607000	-3.021668000	6	-1.029305000	-2.278711000	1.194597000
6	-0.950609000	-0.342135000	-3.493349000	6	-2.141685000	0.015492000	-0.060846000
6	-3.732863000	-2.330055000	1.503035000	6	-1.878988000	0.024217000	1.311974000
6	-2.840405000	-3.205549000	0.780950000	6	-1.322109000	-1.144132000	1.952701000
6	-4.618965000	-1.505365000	0.807277000	6	0.773300000	0.676681000	-3.416049000
6	-2.868470000	-3.232819000	-0.621047000	6	-0.293316000	1.409464000	-2.771602000
6	-1.633877000	-3.273934000	-1.360618000	6	0.767010000	-0.718717000	-3.406316000
6	-1.579555000	-3.231441000	1.478096000	6	-1.329127000	0.720387000	-2.139231000
6	-0.381028000	-3.279194000	0.760903000	6	-1.823323000	1.179115000	-0.860998000
6	-0.409391000	-3.301927000	-0.688771000	6	0.281919000	2.581026000	-2.148977000
6	-4.140988000	0.359607000	2.340829000	6	-0.198618000	3.023578000	-0.916052000
6	-3.221089000	-0.493685000	3.061535000	6	-1.271428000	2.309931000	-0.260031000
6	-4.827668000	-0.141028000	1.233312000	6	-0.392150000	0.752357000	2.960253000
6	-3.021433000	-1.811357000	2.651427000	6	-1.312103000	1.196680000	1.936212000
6	-1.687238000	-2.366498000	2.634629000	6	-1.009240000	2.317809000	1.162589000
6	-2.095194000	0.314853000	3.471230000	6	0.798991000	1.445472000	3.173830000
6	-0.809944000	-0.223622000	3.460430000	6	2.021020000	-0.676252000	3.416805000
6	-0.602808000	-1.587654000	3.035474000	6	0.786319000	-1.395134000	3.194186000
6	-4.445264000	1.963967000	0.017047000	6	-0.398462000	-0.693917000	2.970373000
6	-3.735361000	2.485056000	1.163642000	6	2.027173000	0.718864000	3.406890000
6	-4.983299000	0.677203000	0.049664000	6	4.128683000	0.725724000	2.127845000
6	-3.585385000	1.692338000	2.310170000	6	4.122665000	-0.720336000	2.138287000
6	-2.324165000	1.666730000	3.005947000	6	3.087654000	-1.408930000	2.771365000
6	-2.627986000	3.269262000	0.681392000	6	3.099857000	1.432696000	2.750566000
6	-1.403188000	3.246496000	1.352675000	6	3.018215000	3.019519000	0.872139000
6	-1.248648000	2.427836000	2.539994000	6	4.085596000	2.287924000	0.227136000
6	1.207606000	-0.311816000	2.280188000	6	4.630743000	1.161029000	0.843548000
6	0.304076000	0.565972000	2.974125000	6	2.534822000	2.600452000	2.111521000
6	0.081516000	1.876611000	2.531543000	6	0.224664000	3.038291000	1.386108000
6	1.866295000	0.157220000	1.113739000	6	0.726150000	3.473317000	0.101322000
6	1.394601000	-1.999606000	-0.026597000	6	2.098129000	3.464508000	-0.150661000
6	0.743487000	-2.479966000	1.175407000	6	1.112761000	2.608605000	2.372739000
6	0.638669000	-1.632851000	2.288450000	17	-4.887987000	-1.816729000	1.036719000
6	1.929949000	-0.704489000	-0.055584000				
6	1.099589000	-0.396795000	-2.372570000				
6	0.548761000	-1.719137000	-2.329678000				
6	0.695212000	-2.514332000	-1.173768000				

6	1.771511000	0.111223000	-1.244861000
6	0.687912000	2.320674000	-1.524756000
6	-0.029396000	1.781728000	-2.664352000
6	0.172523000	0.466743000	-3.084264000
6	1.563757000	1.475493000	-0.815677000
6	0.739347000	2.354213000	1.331790000
6	-0.167657000	3.206433000	0.611239000
6	-0.193877000	3.178950000	-0.798465000
6	1.591644000	1.494800000	0.631788000
17	4.413657000	3.268888000	-0.127713000
((Cl ⁻ C ₆₀)CuNMe ₃ _α-posiion			
29	4.203005000	0.448376000	0.000121000
7	5.531152000	-1.140640000	0.000000000
6	6.357634000	-0.947603000	1.201686000
1	6.763794000	0.067079000	1.198907000
1	5.736288000	-1.075796000	2.092850000
6	4.964214000	-2.490401000	0.000180000
1	4.340247000	-2.627732000	-0.886681000
1	5.754570000	-3.257342000	0.000080000
6	6.357190000	-0.947783000	-1.202042000
1	7.181260000	-1.676609000	-1.238999000
1	6.763256000	0.066938000	-1.199608000
1	5.735520000	-1.076232000	-2.092939000
1	7.181663000	-1.676486000	1.238521000
1	4.340561000	-2.627644000	0.887282000
6	-3.320913000	-1.596533000	-2.298703000
6	-2.947618000	-0.401193000	-3.022180000
6	-4.134441000	-1.503086000	-1.169501000
6	-3.401912000	0.845494000	-2.590659000
6	-2.506416000	1.981113000	-2.590153000
6	-1.581735000	-0.558161000	-3.468885000
6	-0.716710000	0.537207000	-3.467673000
6	-1.187660000	1.828918000	-3.019842000
6	-2.747663000	-3.165761000	0.000540000
6	-1.903686000	-3.262305000	-1.169834000
6	-3.842735000	-2.301679000	0.000504000
6	-2.185186000	-2.491972000	-2.299058000
6	-1.110760000	-1.850428000	-3.022445000
6	-0.537957000	-3.414928000	-0.723119000
6	0.498034000	-2.794161000	-1.420458000
6	0.207183000	-1.999910000	-2.590358000
6	-3.320574000	-1.595908000	2.299439000
6	-2.184863000	-2.491366000	2.299887000
6	-4.134276000	-1.502774000	1.170342000
6	-1.903526000	-3.262004000	1.170827000
6	-0.537859000	-3.414754000	0.723964000
6	-1.110332000	-1.849623000	3.022952000
6	0.207543000	-1.999222000	2.590711000
6	0.498235000	-2.793801000	1.420986000
6	-4.245976000	0.942784000	1.420754000
6	-3.401530000	0.846204000	2.590744000
6	-4.606191000	-0.210841000	0.723078000
6	-2.947178000	-0.400370000	3.022540000
6	-1.581231000	-0.557217000	3.469082000
6	-2.506044000	1.981830000	2.589814000
6	-1.187224000	1.829746000	3.019357000
6	-0.716207000	0.538158000	3.467461000
6	-4.246181000	0.942397000	-1.420567000
6	-3.873225000	2.138147000	-0.697947000
6	-4.606301000	-0.211037000	-0.722526000
6	-3.873122000	2.138332000	0.697756000
6	-2.798013000	2.780766000	1.420601000

6	-2.798217000	2.780376000	-1.421116000
6	-1.760771000	3.399957000	-0.723560000
6	-1.760667000	3.400150000	0.722724000
6	1.023359000	1.576169000	2.293763000
6	-0.112978000	2.469401000	2.294379000
6	-0.394314000	3.241060000	1.167802000
6	1.836678000	1.479749000	1.168790000
6	1.952053000	-0.961274000	1.425335000
6	1.105119000	-0.865151000	2.589412000
6	0.648402000	0.381254000	3.018300000
6	2.404176000	0.198447000	0.752429000
6	1.951954000	-0.961661000	-1.425540000
6	1.572905000	-2.145700000	-0.699891000
6	1.573004000	-2.145540000	0.700085000
6	2.404133000	0.198264000	-0.753016000
6	1.023017000	1.575524000	-2.294551000
6	0.647978000	0.380416000	-3.018718000
6	1.104766000	-0.865850000	-2.589501000
6	1.836612000	1.479447000	-1.169753000
6	0.448421000	3.138753000	-0.000516000
6	-0.394478000	3.240743000	-1.168778000
6	-0.113308000	2.468768000	-2.295182000
6	1.541021000	2.268875000	-0.000602000
17	5.415043000	2.269099000	-0.000012000

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