Supplementary Materials

Preference of C_{2v} symmetry in low-spin hexacarbonyls of rare-earth and f elements

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Table S1. Theoretical $<\hat{S}^2>$ eigenvalues (au) compared with the calculated ones (before annihilation) of the minimum structures from B3LYP geometry optimizations, relative energies (kJ/mol) from PBE0 geometry optimizations and CASPT2 single-point calculations.[a]

			B3LYP	PBE0	CASPT2
Complex	Spin	$<\hat{S}^2>_{theor}$	$<\hat{S}^2>$	ΔE	ΔE
$Sc(CO)_6$	2	0.75	0.76	2.0	0.0
	4	3.75	3.75	0.0	1.2
$Lu(CO)_6$	2	0.75	0.76	0.0	0.0
	4	3.75	3.75	9.4	27.1
$Y(CO)_6$	2	0.75	0.76	0.0	0.0
	4	3.75	3.75	14.2	22.9
$U(CO)_6$	5	6.00	6.02	0.0	0.0
	7	12.00	12.01	34.7	44.6
$La(CO)_6$	2	0.75	0.75	0.0	0.0
	4	3.75	3.75	36.0	35.2
$Ac(CO)_6$	2	0.75	0.75	0.0	0.0
	4	3.75	3.75	41.1	65.0

[a]For computational details, see this section in the main manuscript.

Table S2. Computed (B3LYP) M-C bond distances (Å) of the $M(CO)_6$ complexes, empirical radii of neutral M [1] and the effective ionic radii of hexa-coordinated M^{3+} [2].

M	r_M	r_{M3+}	Structure[a]				
			$^{H}O_h$	$^{L}C_{2v}$ (eq)	$^{L}C_{2v}$ (ax)	$^{L}D_{4h}$ (eq)	$^{L}D_{4h}$ (ax)
Sc	1.60	0.745	2.295	2.281	2.251	2.296	2.292
Lu	1.75	0.861	2.382	2.375	2.334	2.384	2.379
Y	1.80	0.9	2.467	2.457	2.408	2.467	2.462
U	1.75	1.025	2.501	2.481	2.377	2.552	2.513
La	1.95	1.032	2.677	2.663	2.552	2.678	2.671
Ac	1.95	1.12	2.767	2.767/ 2.746	2.631	2.758	2.756

[a]The high- and low-spin states of the structures are indicated by the superscripts H and L, respectively. Here, they mean the spin multiplicities 7 and 5, respectively, for $U(CO)_6$, whereas 4 and 2 are for the other complexes. The low-spin structure of $Ac(CO)_6$ is a distorted C_{2v} (to C_s), hence the two equatorial Ac-C bond distances.

Table S3. Selected C-M-C bond angles (deg) of the optimized $M(CO)_6$ C_{2v} structures. For the numbering of C atoms see Figure 1b.

Complex	C_3-M-C_5	C_1-M-C_2
$Sc(CO)_6$	154.3	75.7
$Lu(CO)_6$	157.1	75.0
$Y(CO)_6$	162.8	73.8
$U(CO)_6$	186.6[a]	67.1
$La(CO)_6$	181.4[a]	68.6
$Ac(CO)_6$	186.4[a]	66.9

[a]In these complexes with large metals, the equatorial CO groups are slightly bent towards the axial ones.

Table S4. DFT steric energies from Shubin Liu's energy decomposition analysis [3].

Structure	**$Sc(CO)_6$**	**$Lu(CO)_6$**	**$Y(CO)_6$**	**$La(CO)_6$**
$^2C_{2v}$ (hartree)	948.287364	10003.84775	2296.810474	5348.494464
$^2D_{4h}$ (hartree)	948.537476	10004.07965	2297.067027	5348.87106
^4O_h (hartree)	948.546654	10004.08852	2297.076154	5348.885153
$\Delta E_{2D4h\text{-}2C2v}$ (kJ/mol)	656.7	608.8	673.6	988.8
$\Delta E_{4Oh\text{-}2C2v}$ (kJ/mol)	680.8	632.1	697.5	1025.8

Structure	**$U(CO)_6$**	**Structure**	**$Ac(CO)_6$**
$^5C_{2v}$ (hartree)	30824.97396	^2C_s (au)	24265.53268
$^5D_{4h}$ (hartree)	30825.73744	$^2C_{2h}$ (au)	24265.75592
^7O_h (hartree)	30825.73659	^4O_h (au)	24265.91645
$^7C_{3v}$ (hartree)	30825.50125		
^3C_s (hartree)	30824.64677		
$\Delta E_{5D4h\text{-}5C2v}$ (kJ/mol)	2004.5	$\Delta E_{2C2h\text{-}2Cs}$ (kJ/mol)	586.1
$\Delta E_{7Oh\text{-}5C2v}$ (kJ/mol)	2002.3	$\Delta E_{4Oh\text{-}2Cs}$ (kJ/mol)	1007.6
$\Delta E_{7C3v\text{-}5C2v}$ (kJ/mol)	1384.4		
$\Delta E_{3Cs\text{-}5C2v}$ (kJ/mol)	-859.0		

Table S5. Compilation of selected calculated[a] and experimental vibrational data.

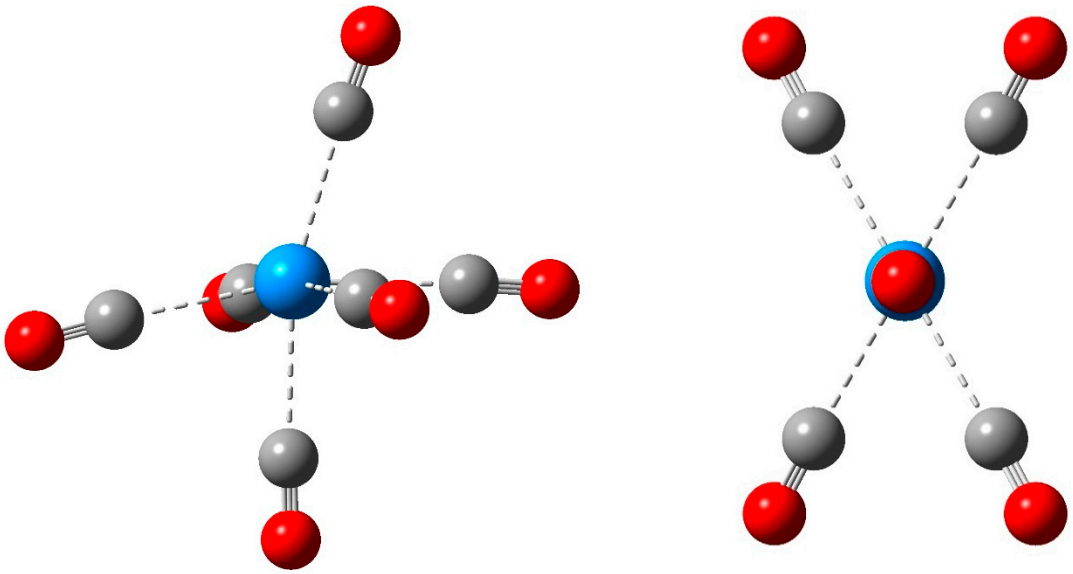
Structure	$Sc(CO)_8$	$Sc(CO)_7$	$Sc(CO)_6$	$Sc(CO)_5$	$Sc(CO)_4$	$Sc(CO)_3$
Spin state/symmetry	$^2D_{4h}$	$^2C_{2v}$	^4O_h	$^4C_{4v}$	$^4C_{2v}$	$^4C_{3v}$
Calculated frequency (cm^{-1})	1979, 1976	1996, 1980, 1972, 1967, 1964	1960	2x1939, 1917	1920, 1893	2x1864
IR intensity (km/mol)	2838, 2×2723	930, 964, 2942, 1582, 1423	3×2974	2×3747, 1270	3642, 2158	2×2052
Deposition CO/Ar = 1/10	1984 w	1998 w, 1966 m	1955 s	1930 w	1930 w, 1890 w	1866 w
UV irrad at 404 nm	incr	-	incr	-	-	-
UV irrad at 289 nm	-	loss	incr	-	-	loss
Annealed to 25 K	incr	incr	incr	loss	loss	loss
Deposition Neat CO (1)	1982 s	~2000 br, ~1960 sh	1952 s	1940 m		
Annealed to 22 K	slight decr	growth of 2002 w, 1978 w, 1971 w, 1966 w, 1961 w	slight decr	slight growth		
UV irrad at 495 nm at 10 K	-	--	-	-		
Deposition Neat CO (2)	1982 s	~2000 br, ~1960 sh	1952 s	1940 m		
UV irrad at 420 nm	-		loss	loss		
Literature exp. data						
IR gas [4]		2082 w, 1992 m, 1978 sh, 1970 s				
IR Ar or Ne matrix [5]					1893, 1884	1865

[a]Calculated at the B3LYP-D3/TZP level (for details see section Computational Details in the text). The calculated frequencies are scaled by 0.96, and the IR intensities are unscaled.

Comments:

The calculated (scaled) vibrational data are generally in good agreement with the experimental observations and thus support the presence of all Sc(CO)x species with x= 3-8 in the matrix with 10% CO in argon. As expected, upon irradiation and annealing, the species with x=8-6 generally increase, and the lower coordinated species vanish. In neat CO, the spectrum is dominated by the $ScCO)_6$ feature, but minor amounts of $Sc(CO)_8$ and $Sc(CO)_5$ are clearly present.

The UV–vis spectrum exhibits in neat and diluted CO matrices a band centred at 380 nm, which we assign mostly to $Sc(CO)_6$.



$^{7}C_2$ $^{1}C_{2h}$

Figure S1. Structures of the heptet C_2 and singlet C_{2h} species of the $U(CO)_6$ complex.

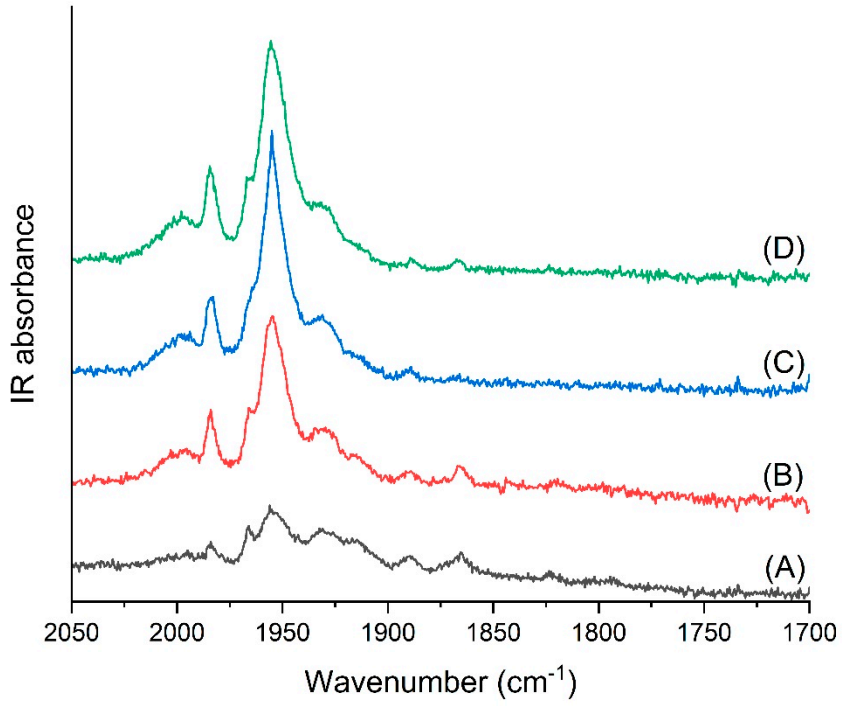


Figure S2. Infrared spectrum of the matrix obtained after cocondensation of Sc atoms with a CO:Ar = 1:10 mixture at 10K: (A) deposition; (B) result of 5 min irradiation at 404 nm; (C) spectrum after a subsequent 7 min irradiation at 289 nm; (D) spectrum after a further 5 min broadband irradiation.

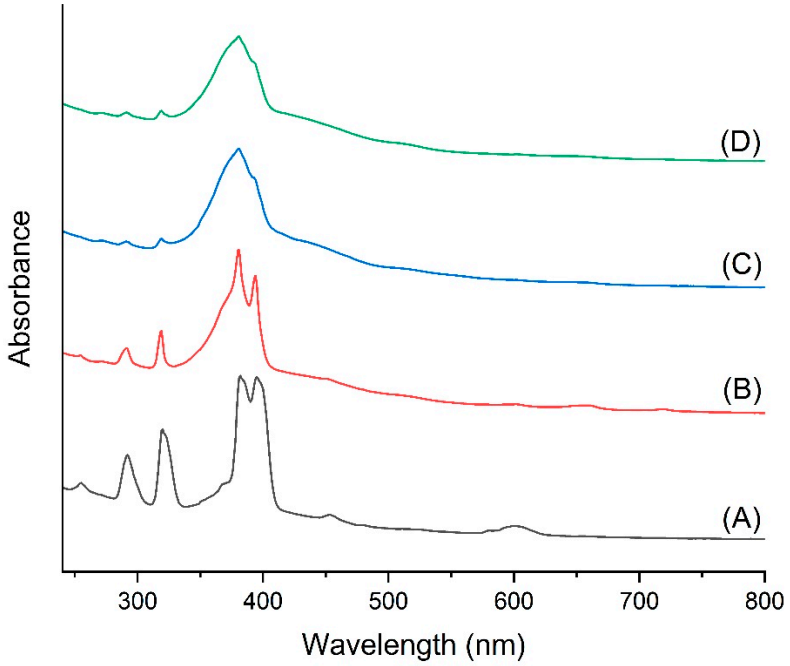


Figure S3. UV–vis spectrum of the matrix obtained after cocondensation of Sc atoms with a CO:Ar = 1:10 mixture at 10K: (A) deposition, indicating the presence of both isolated and coordinated Sc atoms; (B) result of 5 min irradiation at 404 nm, demonstrating loss of the isolated Sc atoms and growth of coordinated species; (C) spectrum after a subsequent 7 min irradiation at 289 nm; (D) spectrum after a further 5 min broad band irradiation.

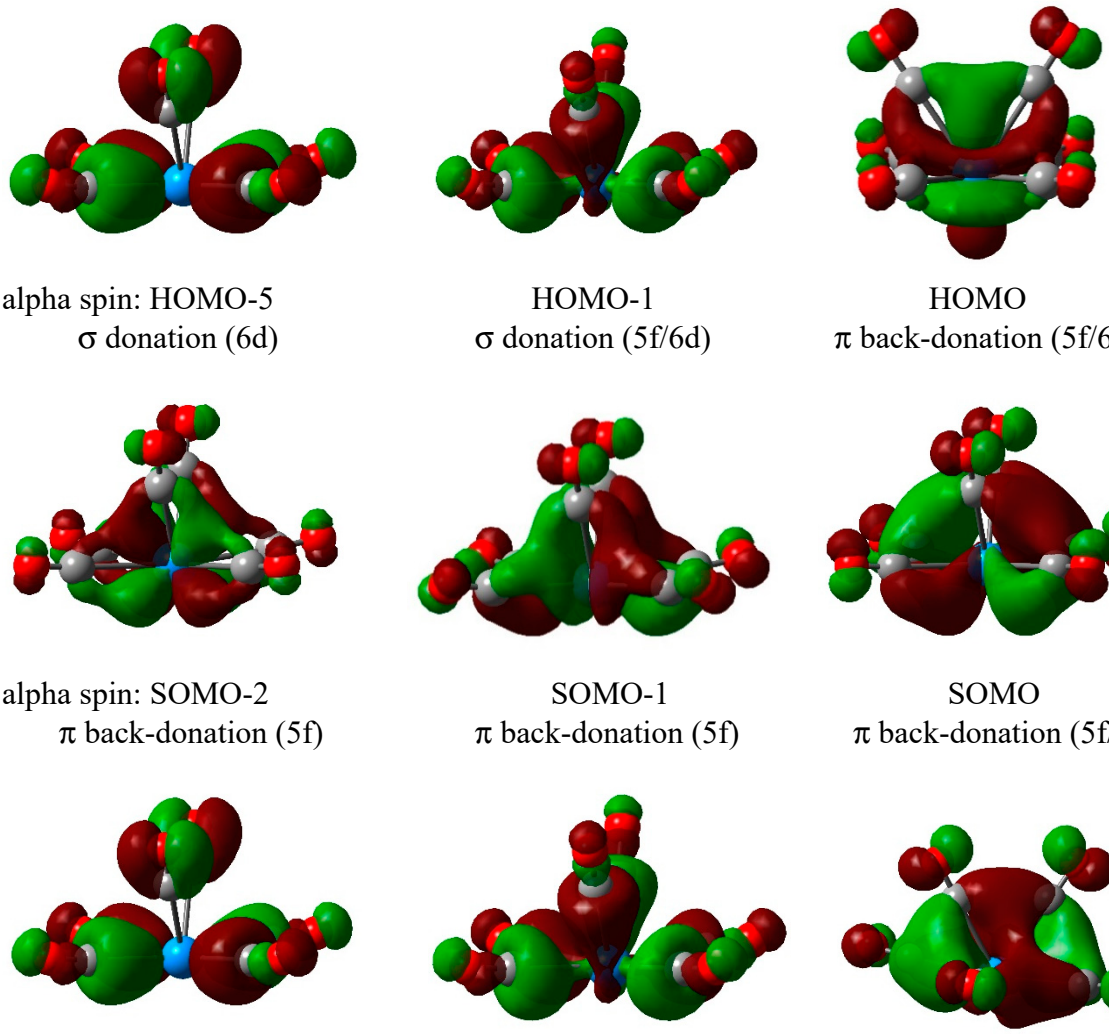


Figure S4. Bonding molecular orbitals of the quintet C_{2v} global minimum of $U(CO)_6$ using an isovalue of 0.03 $(electrons/(Bohr)^3)^{1/2}$.

Cartesian coordinates (Å) of the optimized structures and B3LYP-D3/TZP electronic energies

$Sc(CO)_6$ ^4O_h

E= -1440.998345 hartree

Sc	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.29505400
C	0.00000000	2.29505400	0.00000000
C	-2.29505400	0.00000000	0.00000000
C	2.29505400	0.00000000	0.00000000
C	0.00000000	-2.29505400	0.00000000
C	0.00000000	0.00000000	-2.29505400
O	0.00000000	0.00000000	3.43358100
O	0.00000000	3.43358100	0.00000000
O	3.43358100	0.00000000	0.00000000
O	0.00000000	-3.43358100	0.00000000
O	-3.43358100	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.43358100

$Sc(CO)_6$ $^2D_{4h}$

E= -1440.994172 hartree

Sc	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.29166800
C	0.00000000	2.29571000	0.00000000
C	-2.29571000	0.00000000	0.00000000
C	2.29571000	0.00000000	0.00000000
C	0.00000000	-2.29571000	0.00000000
C	0.00000000	0.00000000	-2.29166800
O	0.00000000	0.00000000	3.43048400
O	0.00000000	3.43431800	0.00000000
O	3.43431800	0.00000000	0.00000000
O	0.00000000	-3.43431800	0.00000000
O	-3.43431800	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.43048400

$Sc(CO)_6$ $^2C_{2v}$

E= -1440.995090 hartree

Sc	0.00000000	0.00000000	-0.27586701
C	-1.50387093	-1.63891379	-0.78243531
C	-1.50387093	1.63891379	-0.78243531
C	1.50387093	1.63891379	-0.78243531
C	-1.38078015	0.00000000	1.50127185
C	1.50387093	-1.63891379	-0.78243531
C	1.38078015	0.00000000	1.50127185
O	-2.27040591	-2.45034876	-1.00876746
O	-2.27040591	2.45034876	-1.00876746
O	-2.10272224	0.00000000	2.38653977
O	2.27040591	-2.45034876	-1.00876746
O	2.27040591	2.45034876	-1.00876746
O	2.10272224	0.00000000	2.38653977

$Lu(CO)_6$ ^4O_h

E= -1916.543809 hartree

Lu	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.38180600
C	0.00000000	2.38180600	0.00000000
C	-2.38180600	0.00000000	0.00000000
C	2.38180600	0.00000000	0.00000000
C	0.00000000	-2.38180600	0.00000000
C	0.00000000	0.00000000	-2.38180600
O	0.00000000	0.00000000	3.52124300
O	0.00000000	3.52124300	0.00000000
O	3.52124300	0.00000000	0.00000000
O	0.00000000	-3.52124300	0.00000000
O	-3.52124300	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.52124300

$Lu(CO)_6$ $^2D_{4h}$

E= -1916.540312 hartree

Lu	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.37925800
C	0.00000000	2.38391300	0.00000000
C	-2.38391300	0.00000000	0.00000000
C	2.38391300	0.00000000	0.00000000
C	0.00000000	-2.38391300	0.00000000
C	0.00000000	0.00000000	-2.37925800
O	0.00000000	0.00000000	3.51920900
O	0.00000000	3.52336400	0.00000000
O	3.52336400	0.00000000	0.00000000
O	0.00000000	-3.52336400	0.00000000
O	-3.52336400	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.51920900

$Lu(CO)_6$ $^2C_{2v}$

E= -1916.544859 hartree

Lu	0.00000000	0.00000000	0.21416100
C	1.72554500	1.56271500	0.68591000
C	-1.72554500	1.56271500	0.68591000
C	-1.72554500	-1.56271500	0.68591000
C	0.00000000	1.42079600	-1.63789600
C	1.72554500	-1.56271500	0.68591000
C	0.00000000	-1.42079600	-1.63789600
O	2.55409800	2.31767600	0.89216700
O	-2.55409800	2.31767600	0.89216700
O	0.00000000	2.12893000	-2.53511500
O	2.55409800	-2.31767600	0.89216700
O	-2.55409800	-2.31767600	0.89216700
O	0.00000000	-2.12893000	-2.53511500

$Y(CO)_6$ ^4O_h

E= -718.574517 hartree

Y	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.46644500
C	0.00000000	2.46644500	0.00000000
C	-2.46644500	0.00000000	0.00000000
C	2.46644500	0.00000000	0.00000000
C	0.00000000	-2.46644500	0.00000000
C	0.00000000	0.00000000	-2.46644500
O	0.00000000	0.00000000	3.60519800
O	0.00000000	3.60519800	0.00000000
O	3.60519800	0.00000000	0.00000000
O	0.00000000	-3.60519800	0.00000000
O	-3.60519800	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.60519800

$Y(CO)_6$ $^2C_{2v}$

E= -718.576748 hartree

Y	0.00000000	0.00000000	-0.34925909
C	-1.59429175	-1.83331055	-0.71653843
C	-1.59429175	1.83331055	-0.71653843
C	1.59429175	1.83331055	-0.71653843
C	-1.44496831	0.00000000	1.57681938
C	1.59429175	-1.83331055	-0.71653843
C	1.44496831	0.00000000	1.57681938
O	-2.34066812	-2.68145628	-0.86404712
O	-2.34066812	2.68145628	-0.86404712
O	-2.15169902	0.00000000	2.47406361
O	2.34066812	-2.68145628	-0.86404712
O	2.34066812	2.68145628	-0.86404712
O	2.15169902	0.00000000	2.47406361

$U(CO)_6$ $^7C_2$

E= -1157.193274 hartree

U	0.00000000	0.00000000	0.16548300
C	2.03269900	-0.72434700	1.47412300
C	0.00000000	2.48503700	-0.12035200
C	-2.03269900	0.72434700	1.47412300
C	1.69330900	-0.37551600	-1.60590400
C	0.00000000	-2.48503700	-0.12035200
C	-1.69330900	0.37551600	-1.60590400
O	2.97520200	-1.07576800	2.01176500
O	-0.00137900	3.60981100	-0.31406000
O	2.43663500	-0.52460900	-2.46013200
O	0.00137900	-3.60981100	-0.31406000
O	-2.97520200	1.07576800	2.01176500
O	-2.43663500	0.52460900	-2.46013200

$U(CO)_6$ $^5C_{2v}$

E= -1157.201765 hartree

U	0.00000000	0.00000000	0.47348600
C	1.98650600	1.47954900	0.32996700
C	-1.98650600	1.47954900	0.32996700
C	-1.98650600	-1.47954900	0.32996700
C	0.00000000	1.31338700	-1.50725100
C	1.98650600	-1.47954900	0.32996700
C	0.00000000	-1.31338700	-1.50725100
O	2.89361800	2.15952300	0.18786000
O	-2.89361800	2.15952300	0.18786000
O	0.00000000	1.94800900	-2.46277400
O	2.89361800	-2.15952300	0.18786000
O	-2.89361800	-2.15952300	0.18786000
O	0.00000000	-1.94800900	-2.46277400

$U(CO)_6$ ^3C_s

E= -1157.197049 hartree

U	-0.52130777	0.00911187	0.00000000
C	-0.30331320	-1.97545136	1.36359464
C	-0.24857506	2.05536663	1.43501032
C	-0.24857506	2.05536663	-1.43501032
C	1.44311892	-0.06280340	1.19355241
C	-0.30331320	-1.97545136	-1.36359464
C	1.44311892	-0.06280340	-1.19355241
O	-0.10021440	-2.91718447	1.98073754
O	0.00110081	2.96354351	2.07637253
O	2.43018276	-0.11010754	1.78572065
O	-0.10021440	-2.91718447	-1.98073754
O	0.00110081	2.96354351	-2.07637253
O	2.43018276	-0.11010754	-1.78572065

$U(CO)_6$ $^1C_{C2h}$

E= -1157.166108 hartree

U	0.00000000	0.00000000	0.00000000
C	-0.97377469	-0.92278984	2.06885679
C	-0.74936383	2.40349399	0.00000000
C	-0.97377469	-0.92278984	-2.06885679
C	0.97377469	0.92278984	2.06885679
C	0.74936383	-2.40349399	0.00000000
C	0.97377469	0.92278984	-2.06885679
O	-1.38353328	-1.34658651	3.05035086
O	-1.06105503	3.49930452	0.00000000
O	1.38353328	1.34658651	3.05035086
O	1.06105503	-3.49930452	0.00000000
O	-1.38353328	-1.34658651	-3.05035086
O	1.38353328	1.34658651	-3.05035086

$La(CO)_6$ ^4O_h

E= -1115.879512 hartree

La	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.67677300
C	0.00000000	2.67677300	0.00000000
C	-2.67677300	0.00000000	0.00000000
C	2.67677300	0.00000000	0.00000000
C	0.00000000	-2.67677300	0.00000000
C	0.00000000	0.00000000	-2.67677300
O	0.00000000	0.00000000	3.81465900
O	0.00000000	3.81465900	0.00000000
O	3.81465900	0.00000000	0.00000000
O	0.00000000	-3.81465900	0.00000000
O	-3.81465900	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.81465900

$La(CO)_6$ $^2C_{2v}$

E= -1115.887798 hartree

La	0.00000000	0.00000000	0.55861400
C	2.09038400	1.64876100	0.52483600
C	-2.09038400	1.64876100	0.52483600
C	-2.09038400	-1.64876100	0.52483600
C	0.00000000	1.43773300	-1.54977200
C	2.09038400	-1.64876100	0.52483600
C	0.00000000	-1.43773300	-1.54977200
O	2.98085900	2.35234700	0.43551000
O	-2.98085900	2.35234700	0.43551000
O	0.00000000	2.09352000	-2.48600600
O	2.98085900	-2.35234700	0.43551000
O	-2.98085900	-2.35234700	0.43551000
O	0.00000000	-2.09352000	-2.48600600

$Ac(CO)_6$ ^4O_h

E= -1055.907118 hartree

Ac	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.76733700
C	0.00000000	2.76733700	0.00000000
C	-2.76733700	0.00000000	0.00000000
C	2.76733700	0.00000000	0.00000000
C	0.00000000	-2.76733700	0.00000000
C	0.00000000	0.00000000	-2.76733700
O	0.00000000	0.00000000	3.90613500
O	0.00000000	3.90613500	0.00000000
O	3.90613500	0.00000000	0.00000000
O	0.00000000	-3.90613500	0.00000000
O	-3.90613500	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.90613500

$Ac(CO)_6$ $^2C_{2h}$

E= -1055.907000 hartree

Ac	0.00000000	0.00000000	0.00000000
C	0.00000000	1.82884200	2.06418800
C	0.00000000	-1.82884200	2.06418800
C	2.33672300	-1.46067100	0.00000000
C	-2.33672300	1.46067100	0.00000000
C	0.00000000	1.82884200	-2.06418800
C	0.00000000	-1.82884200	-2.06418800
O	-0.07633900	2.57275300	2.92344500
O	0.07633900	-2.57275300	2.92344500
O	-3.24478100	2.14967300	0.00000000
O	-0.07633900	2.57275300	-2.92344500
O	3.24478100	-2.14967300	0.00000000
O	0.07633900	-2.57275300	-2.92344500

$Ac(CO)_6$ ^2C_s

E= -1055.916678 hartree

Ac	0.52328300	0.08079100	0.00000000
C	0.21661900	2.31095300	1.60841000
C	0.51607300	-2.17266300	1.56949800
C	0.51607300	-2.17266300	-1.56949800
C	-1.66766700	-0.28004700	1.41121900
C	0.21661900	2.31095300	-1.60841000
C	-1.66766700	-0.28004700	-1.41121900
O	0.00220800	3.22491600	2.25238100
O	0.41085600	-3.12662700	2.18362700
O	-2.62259400	-0.44137000	2.02023800
O	0.00220800	3.22491600	-2.25238100
O	0.41085600	-3.12662700	-2.18362700
O	-2.62259400	-0.44137000	-2.02023800

$Sc(CO)_8$ $^2D_{4h}$

E= -1667.739721 hartree

Sc	0.00000000	0.00000000	0.00000000
C	0.00000000	1.91083600	1.39540100
C	1.91083600	0.00000000	-1.39540100
C	0.00000000	1.91083600	-1.39540100
C	1.91083600	0.00000000	1.39540100
C	0.00000000	-1.91083600	-1.39540100
C	-1.91083600	0.00000000	1.39540100
C	0.00000000	-1.91083600	1.39540100
C	-1.91083600	0.00000000	-1.39540100
O	2.81815500	0.00000000	-2.08140400
O	0.00000000	2.81815500	2.08140400
O	2.81815500	0.00000000	2.08140400
O	0.00000000	2.81815500	-2.08140400
O	-2.81815500	0.00000000	2.08140400
O	0.00000000	-2.81815500	-2.08140400
O	-2.81815500	0.00000000	-2.08140400
O	0.00000000	-2.81815500	2.08140400

$Sc(CO)_7$ $^2C_{2v}$

E= -1554.377505 hartree

Sc	0.00000000	0.00000000	0.02723900
C	0.00000000	0.00000000	2.34393300
C	-1.83184300	1.37270300	0.31814400
C	-1.83184300	-1.37270300	0.31814400
C	0.00000000	-1.34874100	-1.81460000
C	1.83184300	1.37270300	0.31814400
C	1.83184300	-1.37270300	0.31814400
C	0.00000000	1.34874100	-1.81460000
O	0.00000000	-2.02775600	-2.73036900
O	2.75609700	-2.01667100	0.47973300
O	2.75609700	2.01667100	0.47973300
O	-2.75609700	2.01667100	0.47973300
O	-2.75609700	-2.01667100	0.47973300
O	0.00000000	0.00000000	3.47982400
O	0.00000000	2.02775600	-2.73036900

$Sc(CO)_5$ $^4C_{4v}$

E= -1327.605496 hartree

Sc	0.00000000	0.00000000	0.46764800
O	0.00000000	0.00000000	-2.88870100
O	0.00000000	3.42206800	0.39001200
O	0.00000000	-3.42206800	0.39001200
O	3.42206800	0.00000000	0.39001200
O	-3.42206800	0.00000000	0.39001200
C	-2.28481800	0.00000000	0.46940800
C	0.00000000	-2.28481800	0.46940800
C	2.28481800	0.00000000	0.46940800
C	0.00000000	0.00000000	-1.74286400
C	0.00000000	2.28481800	0.46940800

$Sc(CO)_4$ $^4C_{2v}$

E= -1214.214106 hartree

Sc	0.00000000	0.00000000	0.79428000
C	0.00000000	2.25480500	0.67617600
C	0.00000000	-2.25480500	0.67617600
C	-1.59673600	0.00000000	-0.71817800
C	1.59673600	0.00000000	-0.71817800
O	0.00000000	3.38396000	0.49569700
O	0.00000000	-3.38396000	0.49569700
O	-2.43005600	0.00000000	-1.50668800
O	2.43005600	0.00000000	-1.50668800

$Sc(CO)_3$ $^4C_{3v}$

E= -1100.819670 hartree

Sc	0.00000000	0.00000000	1.08581500
C	0.00000000	1.77741800	-0.16069000
C	-1.53928900	-0.88870900	-0.16069000
C	1.53928900	-0.88870900	-0.16069000
O	0.00000000	2.71508500	-0.82957000
O	-2.35133300	-1.35754300	-0.82957000
O	2.35133300	-1.35754300	-0.82957000