Supplementary Material

A DFT and matrix-isolation IR/UV-visible study of high-coordinated lanthanide-CO complexes

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Table S1. Relative stability of the significant high-spin and low-spin states of neutral Ln atoms.

Ln	m	Term	Config	$\Delta E(cm^{-1})$	$\Delta E(kJ/mol)$
La	2	$^2D_{3/2}$	$6s^25d^1$	0.0	0.0
	4	$^4F_{3/2}$	$6s^15d^2$	2668.188	31.9
Ce	1	$^1G_4$	$6s^25d^14f^1$	0.0	0.0
	3	$^3F_2$	$6s^25d^14f^1$	228.849	2.7
	5	$^5H_3$	$6s^15d^24f^1$	2369.068	28.3
Pr	2	$^2H_{9/2}$	$6s^25d^14f^2$	5822.87	69.7
	4	$^4I_{9/2}$	$6s^24f^3$	0.0	0.0
	6	$^6L_{11/2}$	$6s^15d^24f^2$	6714.22	80.3
Nd	5	$^5I_4$	$6s^24f^4$	0.0	0.0
	7	$^7L_5$	$6s^15d^14f^4$	8475.355	101.4
Sm	7	$^7F_0$	$6s^24f^6$	0.0	0.0
	9	$^9H_1$	$6s^15d^14f^6$	10801.10	129.2
Eu	6	$^6D_{9/2}$	$6s^15d^14f^7$	19273.24	230.6
	8	$^8S_{7/2}$	$6s^24f^7$	0.0	0.0
	10	$^{10}D_{5/2}$	$6s^15d^14f^7$	12923.72	154.6
Gd	7	$^7D_5$	$6s^25d^14f^7$	6976.508	83.5
	9	$^9D_2$	$6s^25d^14f^7$	0.0	0.0
	11	$^{11}F_2$	$6s^15d^24f^7$	6378.146	76.3
Tb	6	$^6H_{15/2}$	$6s^24f^9$	0.0	0.0
	8	$^8G_{13/2}$	$6s^25d^14f^8$	285.500	3.4
	10	$^{10}G_{15/2}$	$6s^15d^24f^8$	8190.465	98.0
Dy	5	$^5I_8$	$6s^24f^{10}$	0.0	0.0
	7	$^7H_8$	$6s^25d^14f^9$	7565.60	90.5
	9	[b]			
Ho	4	$^4I_{15/2}$	$6s^24f^{11}$		
	6	[b]			
	8	[b]			
Er	3	$^3H_6$	$6s^24f^{12}$		
	5	[b]			
	7	[b]			
Tm	2	$^2F_{7/2}$	$6s^24f^{13}$		
	4	[b]			
	6	[b]			
Yb	1	$^1S_0$	$6s^24f^{14}$	0.0	0.0
	3	$^3D_1$	$6s^15d^14f^{14}$	24489.102	193.0
Lu	2	$^2D_{3/2}$	$6s^25d^14f^{14}$	0.0	0.0
	4	$^4F_{3/2}$	$6s^15d^24f^{14}$	18851.31	225.5

[a]From Martin, W.C.; Zalubas, R.; Hagan, L. *Atomic energy levels— The rare-earth elements. The spectra of Lanthanum, Cerium, Praseodymium, Neodymium, Promethium, Samarium, Europium, Gadolinium, Terbium, Dysprosium, Holmium, Erbium, Thulium, Ytterbium, and Lutetium*; National Bureau of Standards, U.S. Department of Commerce: Washington, US, 1978.

[b]The character of these (lowest-energy) high-spin states of Dy, Ho, Er and Tm is not available because in their atomic spectra numerous low-energy lines are left unassigned.

Table S2. Selected computed properties[a] of $Ln(CO)_8$ complexes.

Ln	m	$<S^2>$	Sym	ΔE	Ln-C	C≡O	$<S^2>_{theor}$
La	2	0.75	D_{4h}	0.0	2.703	1.136	0.75
	4	3.75	D_{4d}	82.8	2.719	1.138	3.75
Ce	1	1.00	D_{4h}	5.7	2.654	1.136	0.00
	3	2.00	D_{4h}	0.0	2.651	1.136	2.00
	5	6.00	C_2	78.6	2.672-2.679	1.137-1.138	6.00
Pr	2	1.75	D_{4h}	10.2	2.628	1.136	0.75
	4	3.75	D_{4h}	0.0	2.627	1.136	3.75
	6	8.75	O_h	49.1	2.683	1.136	8.75
Nd	5	6.00	D_{4h}	0.0	2.606	1.136	6.00
	7	12.00	C_{2h}	43.2	2.667, 2.726	1.137, 1.132	12.00
Sm	7	12.39	C_1	18.5	2.608-2.647	1.135-1.137	12.00
	9	20.00	O_h	0.0	2.692	1.135	20.00
Eu	6	10.76	O_h	28.7	2.721	1.135	8.75
	8	16.76	D_{4d}	15.3	2.673	1.135	15.75
	10	24.76	O_h	0.0	2.704	1.135	24.75
Gd	7	13.07	C_2	14.0	2.608-2.609	1.136	12.00
	9	20.32	D_{4h}	0.0	2.607	1.136	20.00
	11	30.21	C_1	179.0	2.445-2.749	1.132-1.146	30.00
Tb	6	10.37	C_1	SCF	-	-	8.75
	8	16.37	D_{2d}	0.0	2.543	1.137	15.75
	10	24.75	D_{2d}	125.7	2.518	1.137	24.75
Dy	5	7.55	C_2	10.1	2.514-2.520	1.137	6.00
	7	12.55	C_s	0.0	2.511, 2.515	1.137	12.00
	9	20.54	C_1	105.3	2.510-2.575	1.138-1.140	20.00
Ho	4	4.76	C_{4h}	0.4	2.494	1.138	3.75
	6	8.76	D_{4h}	0.0	2.494	1.137	8.75
	8	15.76	C_2	99.0	2.515-2.518	1.139	15.75
Er	3	3.01	C_1	-8.3	2.478-2.489	1.137	2.00
	5	6.01	D_{4h}	0.0	2.479	1.138	6.01
	7	12.01	C_1	89.7	2.496-2.505	1.139-1.140	12.01
Tm	2	1.75	D_{4h}	0.2	2.464	1.137	0.75
	4	3.75	D_{4h}	0.0	2.464	1.137	3.75
	6	8.75	C_1	95.4	2.480-2.486	1.139-1.140	8.75
Yb	1	-	D_{4d}	0.0	2.528	1.136	-
	3	2.01	O_h	10.0	2.584	1.136	2.00
Lu	2	0.75	D_{2h}	0.0	2.447	1.138	0.75
	4	3.75	D_{4d}	99.5	2.454	1.140	3.75

[a]The properties include: spin multiplicity (m); total spin ($<S^2>$) after annihilation, symmetry of the structure; relative energy of the spin states (kJ/mol); Ln-C and C≡O bond distances (Å), theoretical total spin $<S^2>_{theor}$.

Table S3. Main computed properties[a] of selected $Ln(CO)_8$, $Ln(CO)_7$ and $Ln(CO)_6$ complexes.

$Ln(CO)_x$	m	Sym	ΔE	Ln-C	C≡O	Unscaled frequencies (significant IR intensities)
$La(CO)_8$	4	D_{4d}	82.8	2.719	1.138	2x2038 (4485), 2091 (2373)
$La(CO)_8$	*4*	*D_{4d}*	*73.1*	*2.687*	*1.151*	*2x1962 (3193), 2001 (2089)*
$La(CO)_7$	2	C_s	0.0	2.590-2.715	1.136-1.141	2038 (1082), 2051 (1564), 2054 (1510), 2064 (1214), 2072 (2316), 2075 (1886)
	4	C_{3v}	59.3	2.639-2.844	1.133-1.142	2x1995 (1836), 2043 (2044), 2x2064 (2231), 2081 (1518)
$La(CO)_7$	*2*	*C_1*	*0.0*	*2.540-2.689*	*1.149-1.155*	*1949 (689), 1959 (1118), 1961 (1028), 1967 (1122), 1976 (2225), 1983 (1762)*
	4	*C_{3v}*	*62.3*	*2.623-2.769*	*1.148-1.155*	*2x1929 (1150), 1957 (1057), 2x1972 (1948), 1983 (2001)*
$La(CO)_6$	2	C_2	0.0	2.587-2.729	1.136-1.142	2017 (1731), 2024 (1856), 2055 (3065), 2070 (2150)
	4	O_h	12.1	2.677	1.138	3x2041 (3816)
$La(CO)_6$	*2*	*C_2*	*0.0*	*2.519-2.725*	*1.149-1.157*	*1922 (1368), 1927 (1159), 1956 (2351), 1981 (2156)*
	4	*O_h*	*27.5*	*2.652*	*1.152*	*3x1958 (3028)*
Ce	5	C_2	78.6	2.672-2.679	1.137-1.138	2006 (304), 2040 (3948), 2042 (3872), 2090 (2315)
$Pr(CO)_8$	6	O_h	49.1	2.683	1.136	3x2074 (3194)
$Pr(CO)_7$	4	C_s	0.0	2.516-2.646	1.136-1.141	2037 (1051), 2050 (1453), 2051 (1616), 2065 (1299), 2072 (1549), 2075 (2104)
	6	C_1	40.2	2.628-2.677	1.136-1.139	2x2008 (127), 2038 (371), 2x2057 (3441), 2058 (1808)
$Pr(CO)_6$	4	C_2	0.0	2.511-2.678	1.135-1.142	2014 (1598), 2020 (1871), 2053 (2891), 2074 (2089)
	6	D_{4h}	8.3	2.600-2.606	1.138	2040 (3620), 2040 (3713), 2040 (3715)
$Nd(CO)_8$	7	C_{2h}	43.2	2.667-2.726	1.132-1.137	2053 (658), 2x2065 (3345), 2102 (2490)
$Nd(CO)_7$	5	C_1	0.0	2.502-2.618	1.136-1.141	2074 (1636), 2071 (2063), 2063 (1143), 2052 (1527), 2050 (1640), 2037 (1085)
	7	C_{3v}	34.7	2.642-2.681	1.136-1.139	2x2024 (214), 2047 (513), 2x2062 (3367), 2063 (1618)
$Nd(CO)_6$	5	C_s	0.0	2.463-2.573	1.139-1.144	2053 (1941), 2049 (3535), 2017 (1372), 2011 (904)
	7	O_h	14.7	2.580	1.138	3x2040 (3704)
$Sm(CO)_8$	7	C_1	18.5	2.608-2.647	1.135-1.137	2066 (2393), 2070 (1508), 2072 (2502), 2075 (472, 2076 (1760), 2079 (1345)
$Sm(CO)_7$	9	C_{3v}	0.0	2.625-2.689	1.134-1.137	2x2072 (2972), 2068 (1914), 2054 (643), 2x2052 (777)
	7	C_1	19.2	2.614-2.655	1.136-1.137	2x2069 (2655), 2066 (2313), 2060 (316), 2x2055 (937)

$Sm(CO)_6$	9	C_{2v}	0.0	2.593-2.654	1.137-1.140	2x2050 (3593), 2036 (1641), 2030 (819)
	7	C_{2v}	12.1	2.626-2.643	1.137-1.138	2062 (4305), 2052 (2207), 2050 (2391)
$Eu(CO)_8$	8	D_{4d}	15.3	2.673	1.135	2x2084 (3205), 2087 (3566)
$Eu(CO)_8$	*8*	*D_{4d}*	*0.0*	*2.570*	*1.149*	*1996 (2778), 2x1995 (2457)*
$Eu(CO)_7$	8	C_1	18.5	2.639-2.691	1.135-1.137	2050 (1226), 2055 (812), 2057 (2612), 2059 (2207), 2067 (1945), 2072 (2479)
	10	C_{3v}	0.0	2.634-2.683	1.135-1.137	2x2073 (2589), 2068 (2321), 2057 (615), 2x2055 (1206)
$Eu(CO)_7$	*8*	*C_s*	*13.2*	*2.532-2.569*	*1.150-1.152*	*1966 (393), 1974 (1329), 1982 (2498), 1984 (28149*
	10	*C_{3v}*	*0.0*	*2.546-2.606*	*1.149-1.151*	*2x1988 (2300), 1983 (2083), 2x1972 (470)*
$Eu(CO)_6$	8	C_{2v}	10.6	2.594-2.667	1.137-1.140	2026 (952), 2029 (1864), 2049 (4580), 2054 (2505)
	10	D_{3d}	0.0	2.651	1.137	2x2049 (4400), 2043 (1771)
$Eu(CO)_6$	*8*	C_s	3.4	2.480-2.585	1.152-1.156	1964 (2060), 1962 (3252), 1946 (718), 1936 (830)
	10	C_{3v}	0.0	2.570, 2.582	1.151, 1.152	2x1970 (2717), 1957 (1289), 2x1947 (321)
$Gd(CO)_8$	11	C_1	179.0	2.445-2.749	1.132-1.146	1922 (1063), 1950 (1209), 2000 (2642), 2021 (1763), 2062 (1889), 2077 (833), 2096 (1110)
$Gd(CO)_8$	*11*	*C_1*	*209.7*	*2.463-2.640*	*1.149-1.159*	*1832 (818), 1862 (943), 1902 (1492), 1929 (1401), 1958 (1267), 1961 (680), 1985 (1139)*
$Gd(CO)_7$	9	C_s	0.0	2.527-2.611	1.134-1.139	2086 (1303), 2079 (1369), 2060 (1192, 2056 (2258), 2050 (1434), 2047 (1303)
	11	C_{3v}	140.3	2.439-2.822	1.131-1.146	2x1922 (2137), 2015 (2099), 2069 (1615), 2109 (569), 2158 (270)
$Gd(CO)_7$	*9*	*C_s*	*0.0*	*2.479-2.581*	*1.148-1.153*	*1995 (1152), 1988 (1223), 1971 (1588), 1968 (1242), 1962 (1072), 1957 (904)*
	11	*C_s*	*177.7*	*2.366-2.696*	*1.146-1.167*	*1816 (750), 1904 (2386), 1905 (2419), 1982 (1356), 1999 (820)*
$Gd(CO)_6$	9	C_s	0.0	2.490-2.604	1.136-1.142	2x2025 (1500), 2051 (3801), 2073 (1056)
	11	O_h	88.3	2.498	1.139	3x2001 (3452)
$Gd(CO)_6$	*9*	*C_s*	*0.0*	*2.442-2.574*	*1.150-1.157*	*1978 (858), 1961 (3131), 1956 (456), 1938 (654), 1934 (1142)*
	11	*O_h*	*133.0*	*2.481*	*1.154*	*3x1894 (2465)*
$Tb(CO)_8$	10	D_{2d}	125.7	2.518	1.137	2x2049 (999), 2x2065 (1967), 2077 (2834)
$Dy(CO)_8$	9	C_1	105.3	2.510-2.575	1.138-1.140	2026 (3637), 2027 (3746), 2039 (615), 2042 (667), 2089 (1804)
$Ho(CO)_8$	8	C_2	99.0	2.515-2.518	1.139	2024 (4285), 2025 (4273), 2087 (1797)
$Ho(CO)_7$	6	C_1	0.0	2.426-2.481	1.136-1.140	2074 (1435), 2061 (1382), 2057 (2944), 2049 (1424), 2048 (1154)
	8	C_3	68.6	2.433-2.622	1.134-1.145	2080 (1267), 2x2067 (1830), 2044 (1512), 2x1978 (1920)

$Ho(CO)_6$	6	C_s	0.0	2.381-2.440	1.139-1.143	2049 (2264), 2046 (3282), 2027 (1609)
	8	D_{3d}	9.7	2.448	1.139	3x2038 (3425)
$Er(CO)_8$	7	C_1	89.7	2.496-2.505	1.139-1.140	2021 (4363), 2021 (4373) 2083 (1807)
$Tm(CO)_8$	6	C_1	95.4	2.480-2.486	1.139-1.140	2022 (4272), 2022 (4268), 2084 (1784)
$Tm(CO)_7$	4	C_1	0.0	2.404-2.441	1.137-1.140	2070 (1505), 2059 (1461), 2054 (3196), 2048 (1289), 2047 (1306)
	6	C_s	74.9	2.400-2.558	1.135-1.146	1966 (1852), 1977 (1954), 2043 (1375), 2064 (1948), 2065 (1750), 2069 (1423)
$Tm(CO)_6$	4	C_s	0.0	2.361-2.409	1.140-1.143	2046 (2359), 2043 (2809), 2028 (1707), 2018 (904)
	6	C_{2h}	5.5	2.411-2.417	1.139	2x2034 (3372), 2035 (3385)
$Yb(CO)_8$	3	O_h	10.0	2.584	1.136	3x2067 (3529)
$Yb(CO)_8$	*3*	*D_4*	*29.9*	*2.478*	*1.150*	*2x1982 (2586), 1976 (2625)*
$Yb(CO)_7$	1	C_s	5.0	2.504-2.531	1.136-1.138	2049 (809), 2049 (1433), 2052 (862), 2060 (2668), 2064 (2387), 2067 (1974)
	3	C_{3v}	0.0	2.503-2.530	1.136-1.138	2x2065 (2120), 2062 (2537), 2050 (677), 2x2047 (1415)
$Yb(CO)_7$	*1*	*C_s*	*6.0*	*2.423-2.446*	*1.150-1.152*	*1983 (1531), 1982 (2217), 1979 (2166), 1966 (833)*
	3	*C_{3v}*	*0.0*	*2.423-2.444*	*1.150-1.152*	*2x1984 (1588), 1982 (2207), 2x1967 (941)*
$Yb(CO)_6$	1	D_{3h}	0.0	2.488	1.138	2061 (3841), 2x2050 (2199)
	3	D_{3d}	16.7	2.508	1.138	2035 (2238), 2x2040 (4238)
$Yb(CO)_6$	*1*	D_{3h}	0.0	2.417	1.153	1975 (2941), 2x1964 (1675)
	3	C_{3v}	16.9	2.424, 2.437	1.152, 1.154	2x1964 (2439), 1956 (1392), 2x1942 (418)
$Lu(CO)_8$	4	D_{4d}	99.5	2.454	1.140	2085 (1727), 2x2019 (4309)
$Lu(CO)_7$	2	C_{2v}	0.0	2.373-2.407	1.136-1.140	2074 (1290), 2059 (1391), 2054 (3216), 2047 (1459), 2047 (1182)
	4	C_{3v}	77.1	2.376-2.525	1.135-1.145	2x1967 (1877), 2043 (1290), 2064 (1824), 2067 (1436)
$Lu(CO)_6$	2	C_{2v}	0.0	2.334-2.376	1.140-1.143	2049 (2276), 2043 (3176), 2028 (1739), 2015 (1032)
	4	O_h	2.8	2.382	1.140	3x2034 (3329)

[a]The majority of the presented data have been computed at the B3LYP/TZP level. ***BP86/TZP results are given in italics.***

Table S4. Absorption bands (nm) of $Ln(CO)_x$ species isolated in pure CO or CO/Ar (noted) matrix observed in the UV-visible spectra.[a]

Ln	At deposition	After irradiation
La	450 s, br HW = 70 nm	-
Ce	418 s, br HW = 120 nm (576, 653, 719w)	375-465 vbr
Pr	412 s, br HW = 70 nm	vanished
Pr CO/Ar	406 m, br HW = 110 nm (450-550 atomic features)	406 s
Nd	415 s, br HW = 100 nm	vanished
Sm	408 s, br HW = 70 nm (320 – 580 atomic features)	408 w
Eu	532 m, br HW = 180 nm	vanished
Eu CO/Ar	529 m, br; 485 m, br 529 remains upon tempering	
Gd	399 s, br HW = 50 nm	vanished
Tb	393 s, br HW = 50 nm	393 w
Dy	387 s, vbr HW = 100 nm	
Dy CO/Ar	387 (240 - 475 atomic features)	387 m
Ho	387 s, br HW = 80 nm	387 m, br
Er	388 s, br HW = 70 nm (330 – 485 atomic features)	388 m, br, 544 w
Tm	382 m, br HW = 80 nm (330 – 550 atomic features)	vanished
Yb	(Only strong atomic features)	468 m, br
Lu	385 s, br HW = 80 nm 521 m, br; 582 w, br (No atomic features !)	vanished

[a]All molecular UV spectra are fairly broad. The abbreviations s, br, vbr, w and sh mean strong, broad, very broad, weak and shoulder, respectively. HW = indicative half-width

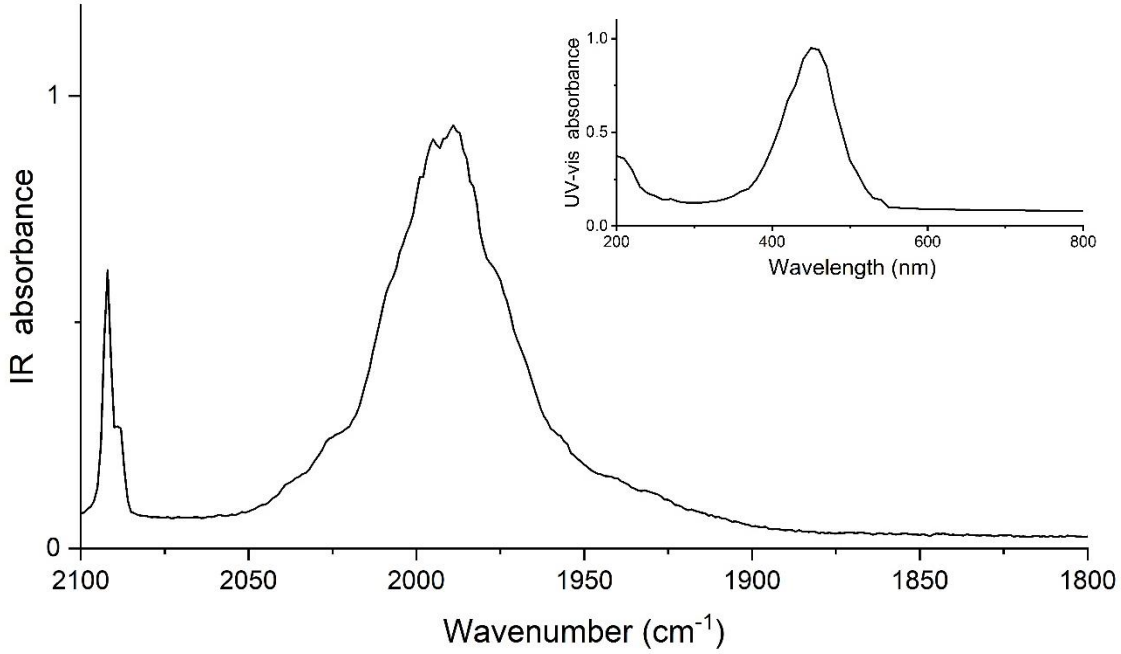


Figure S1. Characteristic UV-visible and FT-IR spectra of all the deposited Ln atoms: FT-IR spectrum of the cocondensation of lanthanum atoms with neat CO at 10 K with strong, splitted band centered at 1992 cm^{-1}. Note the band of isotopic CO at 2091/2088 cm^{-1}. Insert: UV-vis spectrum showing a strong single band centered at 450 nm with half-width of 70 nm.

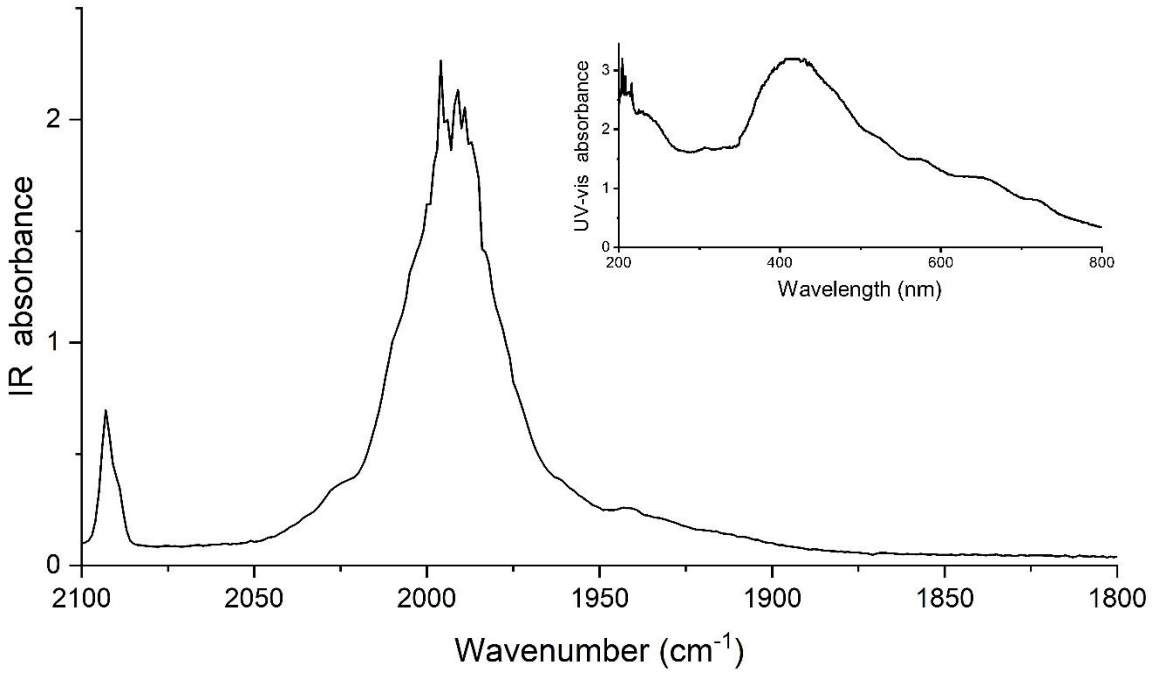
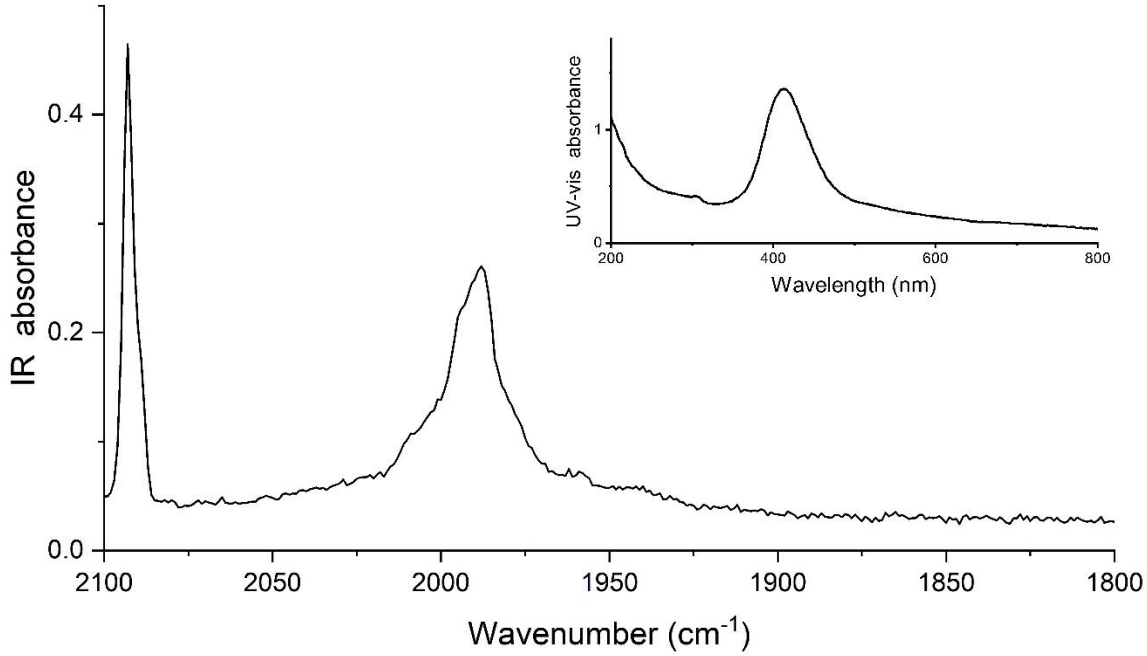
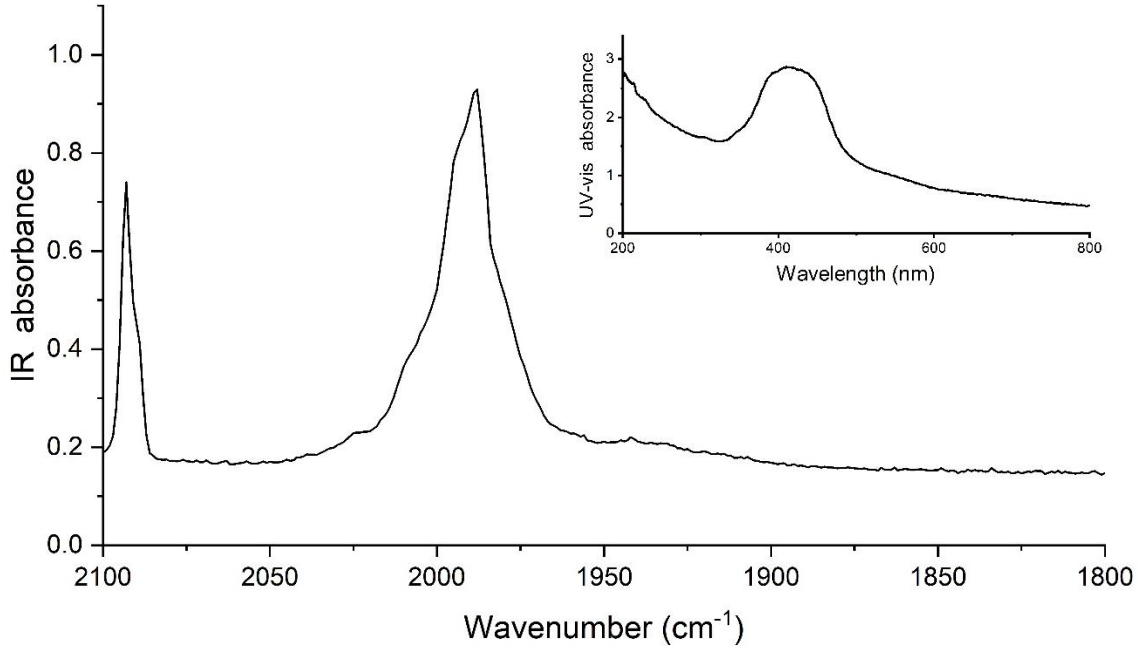


Figure S2. FT-IR spectrum of the cocondensation of cerium atoms with neat CO at 10 K with strong, splitted band centered at 1992 cm^{-1}.
Insert: UV-vis spectrum of the condensation of cerium atoms with neat CO at 10 K, with strong band centered at 418 nm.



(**a**)



(**b**)

Figure S3. (a) FT-IR spectrum of the cocondensation of praseodymium atoms with neat CO at 10 K with medium band centered at 1988 cm^{-1}.
Insert: UV-vis spectrum of the condensation of praseodymium atoms with neat CO at 10 K, with strong band centered at 412 nm.
(**b**) FT-IR spectrum of the cocondensation of neodymium atoms with neat CO at 10 K with strong band centered at 1987 cm^{-1}.
Insert: UV-vis spectrum of the condensation of neodymium atoms with neat CO at 10 K, with strong band centered at 415 nm.

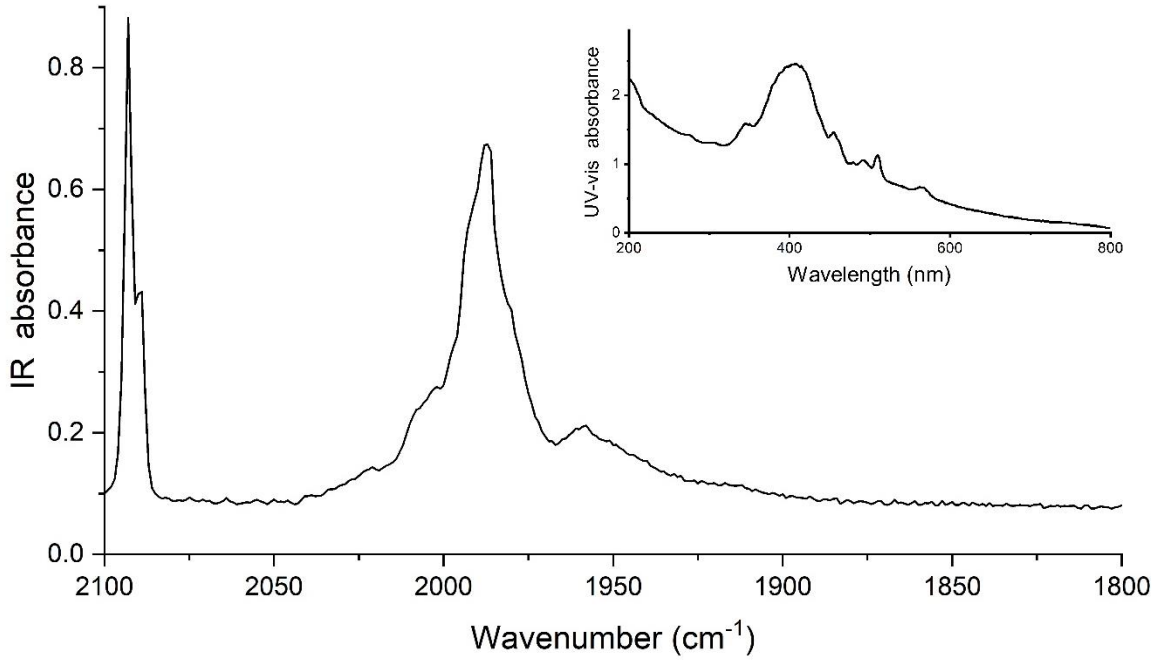


Figure S4. FT-IR spectrum of the cocondensation of samarium atoms with neat CO at 10 K with strong band centered at 1988 cm^{-1} and weak further features.
Insert: UV-vis spectrum of the condensation of samarium atoms with neat CO at 10 K, with weak atomic features and strong band centered at 408 nm.

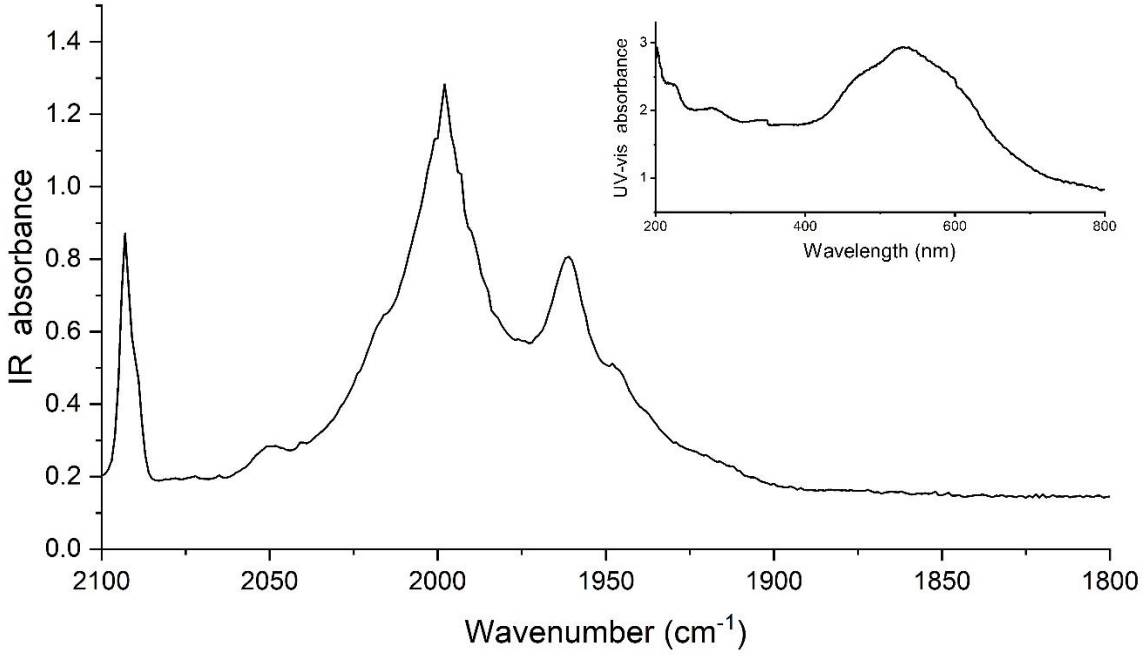


Figure S5. FT-IR spectrum of the cocondensation of europium atoms with neat CO at 10 K with two strong bands centered at 1999 and 1960 cm^{-1} as well as weaker features.
Insert: UV-vis spectrum of the condensation of europium atoms with neat CO at 10 K, with broad band centered at 532 nm.

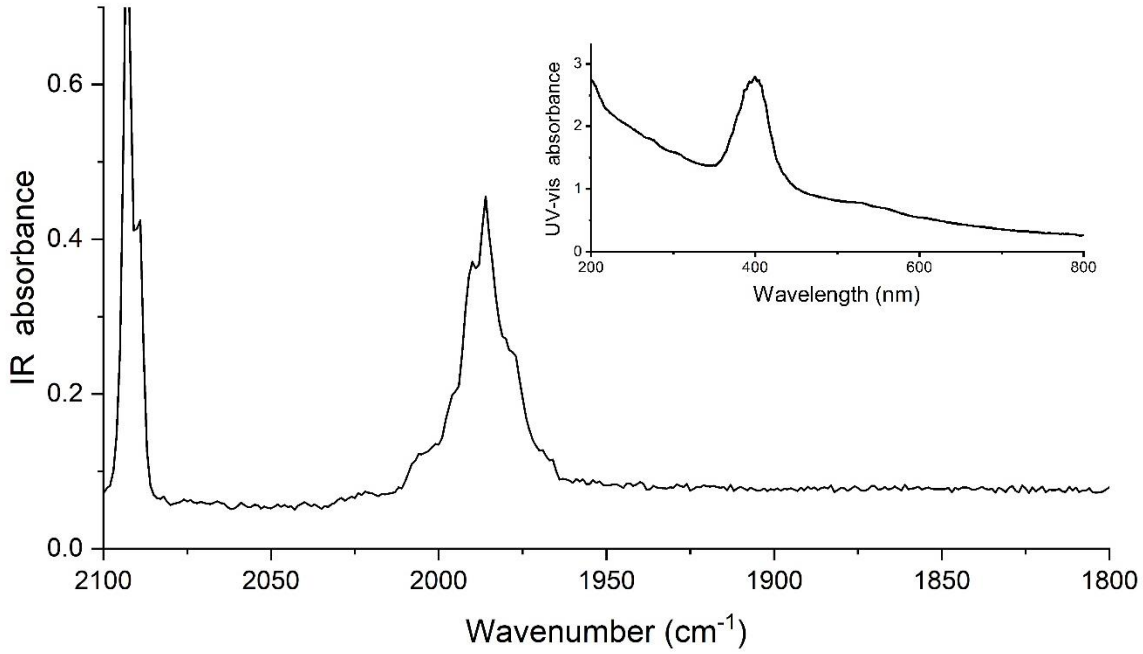


Figure S6. FT-IR spectrum of the cocondensation of gadolinium atoms with neat CO at 10 K with strong splitted band centered at 1986 cm^{-1}.
Insert: UV-vis spectrum of the condensation of gadolinium atoms with neat CO at 10 K, with broad band centered at 399 nm.

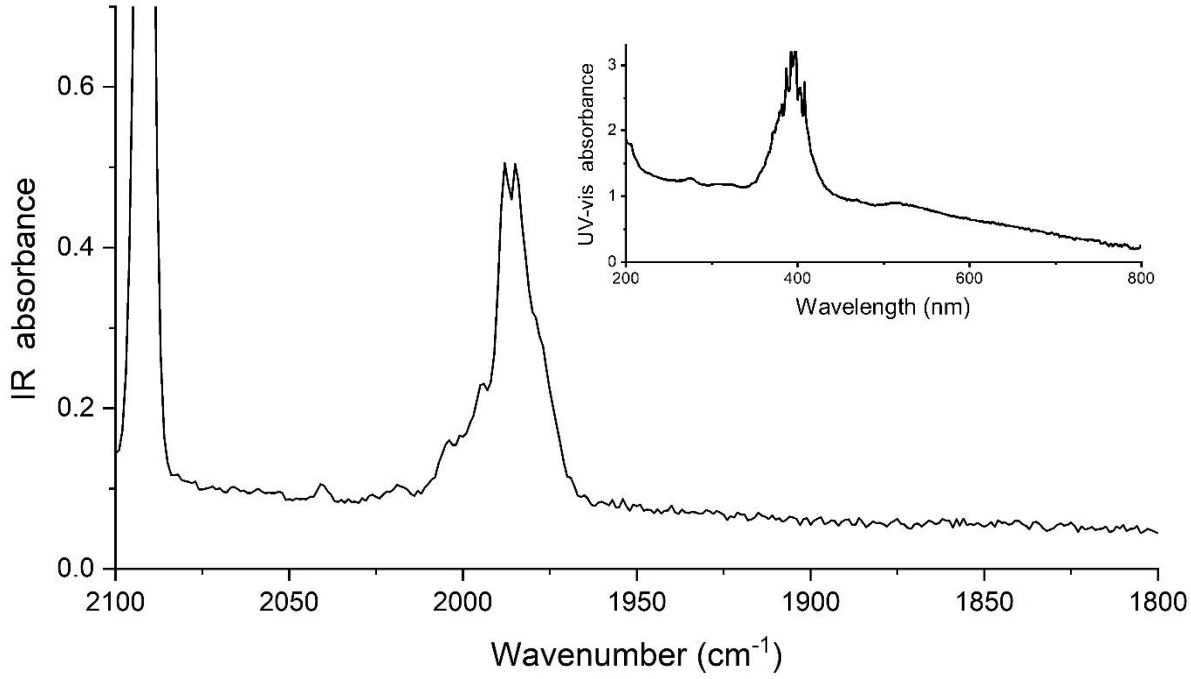


Figure S7. FT-IR spectrum of the cocondensation of terbium atoms with neat CO at 10 K with strong splitted band centered at 1985 cm^{-1}.
Insert: UV-vis spectrum of the condensation of terbium atoms with neat CO at 10 K, with broad band centered at 393 nm overlapping with spectral features of unreacted metal atoms.

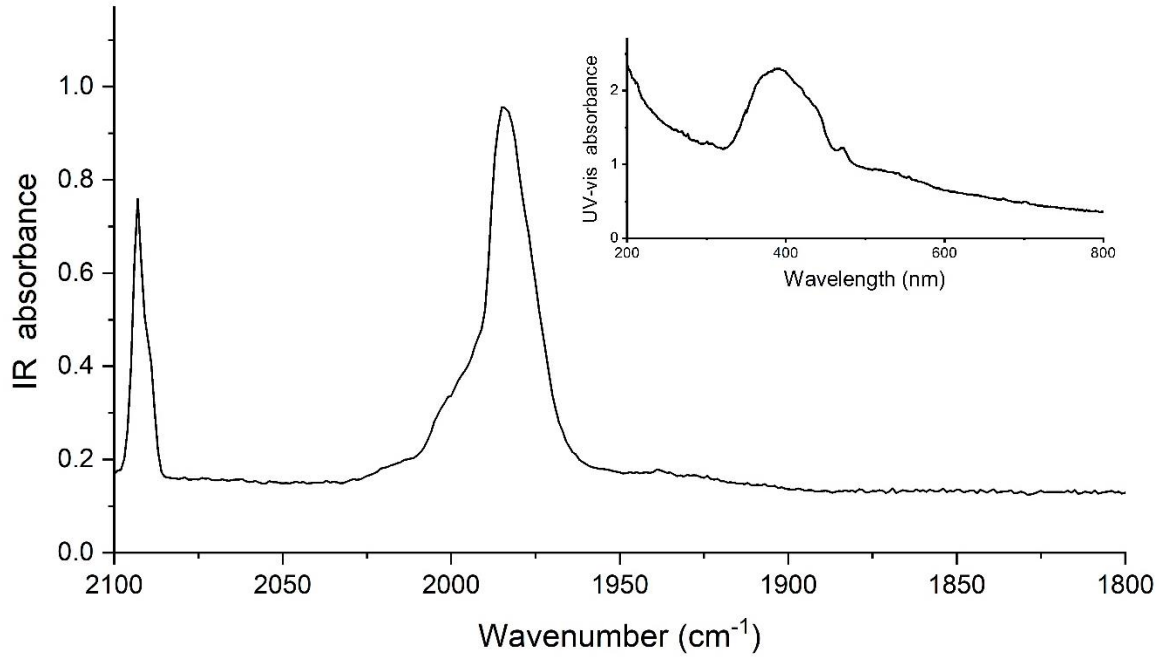


Figure S8. FT-IR spectrum of the cocondensation of dysprosium atoms with neat CO at 10 K with strong band centered at 1983 cm^{-1}.
Insert: UV-vis spectrum of the condensation of dysprosium atoms with neat CO at 10 K, with broad band centered at 387 nm overlappimg with weak spectral features of unreacted metal atoms.

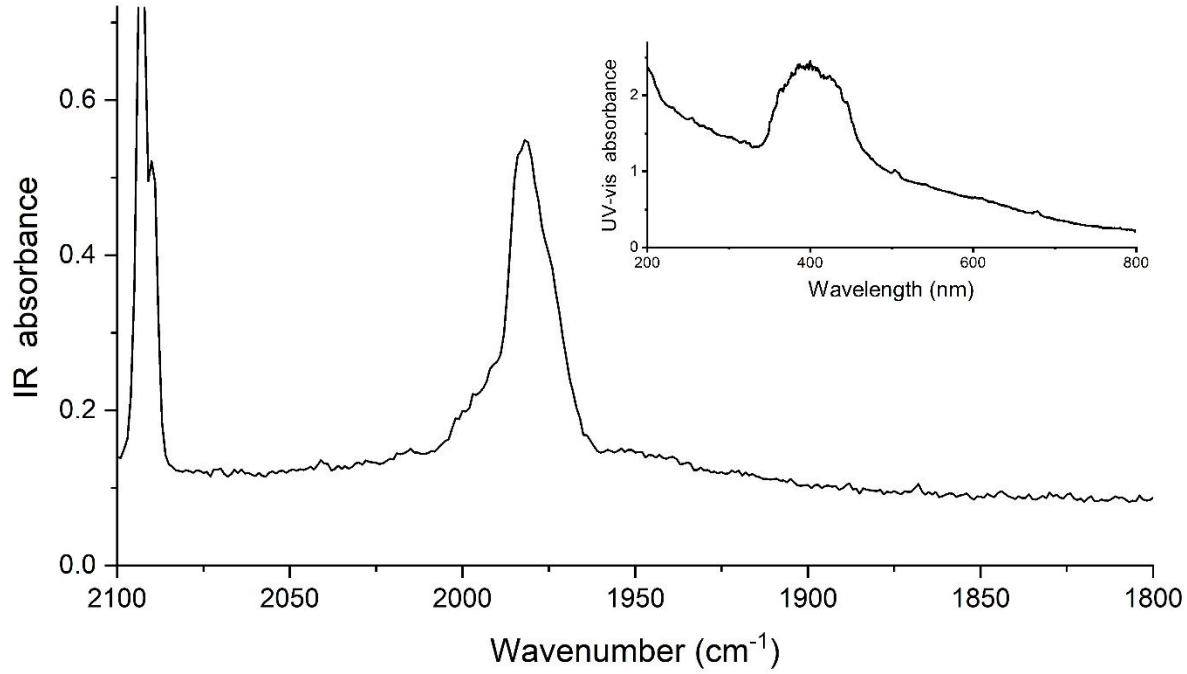


Figure S9. FT-IR spectrum of the cocondensation of holmium atoms with neat CO at 10 K with strong band centered at 1980 cm^{-1}.
Insert: UV-vis spectrum of the condensation of holmium atoms with neat CO at 10 K, with broad band centered at 387 nm.

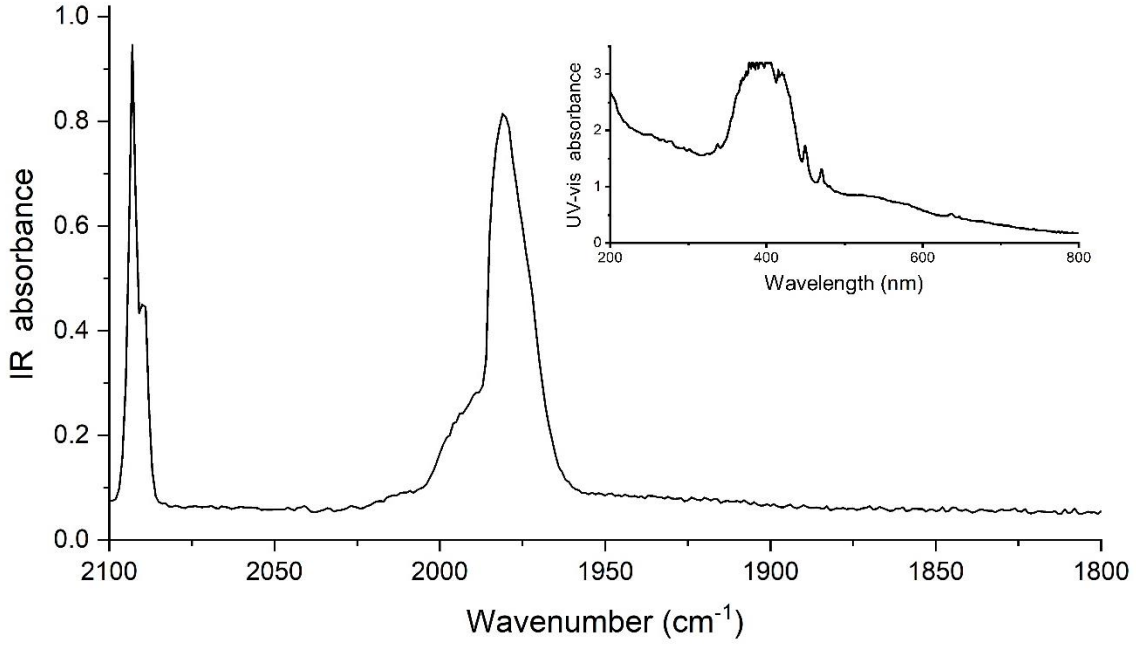


Figure S10. FT-IR spectrum of the cocondensation of erbium atoms with neat CO at 10 K with strong band centered at 1980 cm^{-1}.
Insert: UV-vis spectrum of the condensation of erbium atoms with neat CO at 10 K, with broad band centered at 388 nm overlapping with spectral features of unreacted metal atoms.

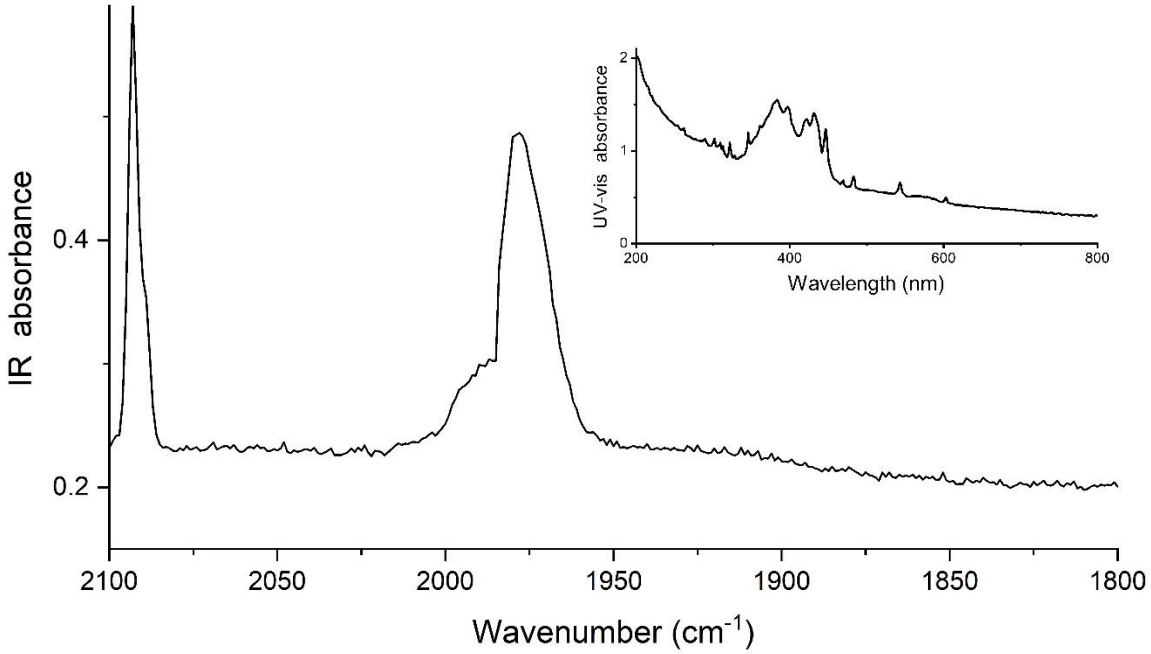


Figure S11. FT-IR spectrum of the cocondensation of thulium atoms with neat CO at 10 K with strong band centered at 1977 cm^{-1}.
Insert: UV-vis spectrum of the condensation of thulium atoms with neat CO at 10 K, with broad band centered at 382 nm overlapping with strong spectral features of unreacted metal atoms.

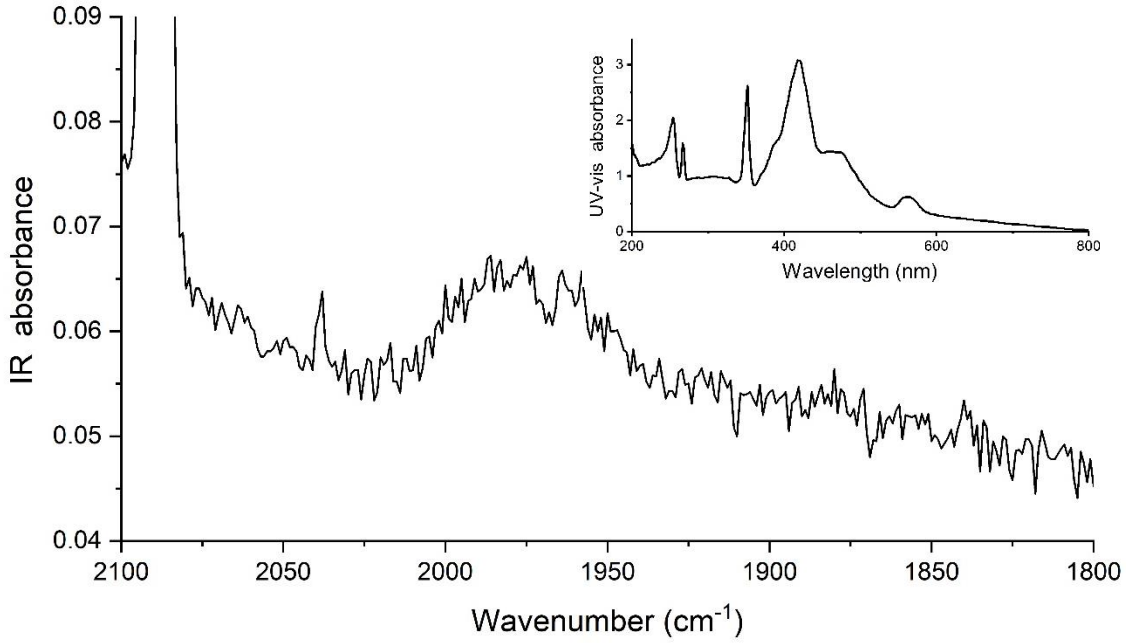


Figure S12. FT-IR spectrum of the cocondensation of ytterbium atoms with neat CO at 10 K with weak band centered at 1975 cm^{-1}.
Insert: UV-vis spectrum of the condensation of ytterbium atoms with neat CO at 10 K, with broad band centered at 368 nm overlapping with strong spectral features of unreacted metal atoms.

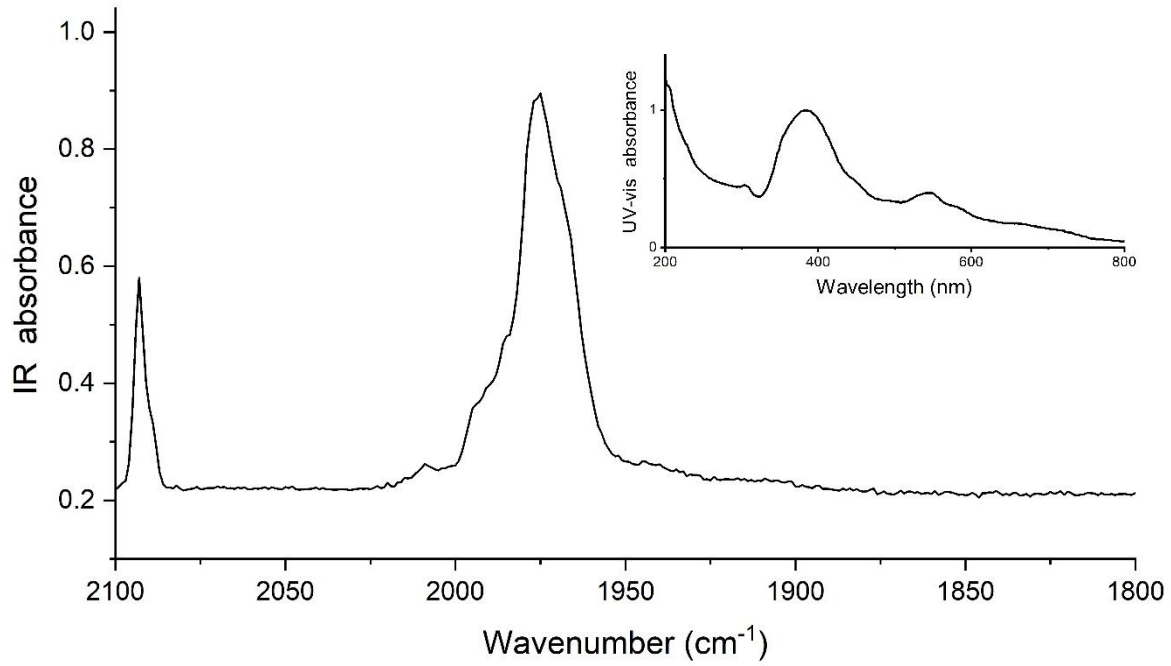


Figure S13. FT-IR spectrum of the cocondensation of lutetium atoms with neat CO at 10 K with strong band centered at 1974 cm^{-1}.
Insert: UV-vis spectrum of the condensation of lutetium atoms with neat CO at 10 K, with broad band centered at 385 nm and weak further features.

Cartesian coordinates of the optimized structures

$^2La(CO)_8$ BP86

La	0.00000000	0.00000000	0.00000000
C	0.00000000	2.23604900	1.45265000
C	0.00000000	-2.23604900	1.45265000
C	2.23604900	0.00000000	1.45265000
C	-2.23604900	0.00000000	1.45265000
C	0.00000000	-2.23604900	-1.45265000
C	0.00000000	2.23604900	-1.45265000
C	-2.23604900	0.00000000	-1.45265000
C	2.23604900	0.00000000	-1.45265000
O	0.00000000	-3.21470900	2.05578600
O	0.00000000	3.21470900	2.05578600
O	-3.21470900	0.00000000	2.05578600
O	3.21470900	0.00000000	2.05578600
O	0.00000000	3.21470900	-2.05578600
O	0.00000000	-3.21470900	-2.05578600
O	3.21470900	0.00000000	-2.05578600
O	-3.21470900	0.00000000	-2.05578600

$^2La(CO)_8$ B3LYP

La	0.00000000	0.00000000	0.00000000
C	0.00000000	2.24584000	1.50348600
C	0.00000000	-2.24584000	1.50348600
C	2.24584000	0.00000000	1.50348600
C	-2.24584000	0.00000000	1.50348600
C	0.00000000	-2.24584000	-1.50348600
C	0.00000000	2.24584000	-1.50348600
C	-2.24584000	0.00000000	-1.50348600
C	2.24584000	0.00000000	-1.50348600
O	0.00000000	-3.20097700	2.11826000
O	0.00000000	3.20097700	2.11826000
O	-3.20097700	0.00000000	2.11826000
O	3.20097700	0.00000000	2.11826000
O	0.00000000	3.20097700	-2.11826000
O	0.00000000	-3.20097700	-2.11826000
O	3.20097700	0.00000000	-2.11826000
O	-3.20097700	0.00000000	-2.11826000

$^2La(CO)_8^-$ BP86

La	0.00000000	0.00000000	0.00000000
C	0.00000000	2.14867000	1.52005800
C	0.00000000	-2.14867000	1.52005800
C	2.14867000	0.00000000	1.52005800
C	-2.14867000	0.00000000	1.52005800
C	0.00000000	-2.14867000	-1.52005800
C	0.00000000	2.14867000	-1.52005800
C	-2.14867000	0.00000000	-1.52005800
C	2.14867000	0.00000000	-1.52005800
O	0.00000000	-3.09648700	2.19080900
O	0.00000000	3.09648700	2.19080900
O	-3.09648700	0.00000000	2.19080900
O	3.09648700	0.00000000	2.19080900
O	0.00000000	3.09648700	-2.19080900
O	0.00000000	-3.09648700	-2.19080900
O	3.09648700	0.00000000	-2.19080900
O	-3.09648700	0.00000000	-2.19080900

$^2La(CO)_8Ar_8$ BP86

La	-0.00000000	-0.00000000	0.00000000
C	0.00000000	-2.23813861	1.44860732
C	-0.00000000	2.23813861	1.44860732
C	-2.23813861	-0.00000000	1.44860732
C	2.23813861	0.00000000	1.44860732
C	0.00000000	2.23813861	-1.44860732
C	-0.00000000	-2.23813861	-1.44860732
C	2.23813861	-0.00000000	-1.44860732
C	-2.23813861	0.00000000	-1.44860732
O	0.00000000	3.21930341	2.04743353
O	0.00000000	-3.21930341	2.04743353
O	3.21930341	0.00000000	2.04743353
O	-3.21930341	-0.00000000	2.04743353
O	-0.00000000	-3.21930341	-2.04743353
O	-0.00000000	3.21930341	-2.04743353
O	-3.21930341	0.00000000	-2.04743353
O	3.21930341	-0.00000000	-2.04743353
Ar	-6.40815387	0.00000000	-3.96961816
Ar	6.40815387	0.00000000	3.96961816
Ar	6.40815387	0.00000000	-3.96961816
Ar	-6.40815387	0.00000000	3.96961816
Ar	-0.00000000	6.40815387	-3.96961816
Ar	-0.00000000	-6.40815387	3.96961816
Ar	0.00000000	6.40815387	3.96961816
Ar	0.00000000	-6.40815387	-3.96961816

$^2La(CO)_8(CO)_8$ BP86

La	-0.00000000	-0.00000000	0.00000000
C	0.00000000	-2.24233081	1.44296509
C	-0.00000000	2.24233081	1.44296509
C	-2.24233081	-0.00000000	1.44296509
C	2.24233081	0.00000000	1.44296509
C	0.00000000	2.24233081	-1.44296509
C	-0.00000000	-2.24233081	-1.44296509
C	2.24233081	-0.00000000	-1.44296509
C	-2.24233081	0.00000000	-1.44296509
O	0.00000000	3.22387568	2.04092014
O	0.00000000	-3.22387568	2.04092014
O	3.22387568	0.00000000	2.04092014
O	-3.22387568	-0.00000000	2.04092014
O	-0.00000000	-3.22387568	-2.04092014
O	-0.00000000	3.22387568	-2.04092014
O	-3.22387568	0.00000000	-2.04092014
O	3.22387568	-0.00000000	-2.04092014
C	-7.41131516	0.00000000	4.50170891
C	7.41131516	0.00000000	-4.50170891
C	7.41131516	0.00000000	4.50170891
C	-0.00000000	7.41131516	4.50170891
C	-7.41131516	-0.00000000	-4.50170891
C	-0.00000000	-7.41131516	-4.50170891
C	0.00000000	-7.41131516	4.50170891
C	0.00000000	7.41131516	-4.50170891
O	8.43839034	-0.00000000	4.99519835
O	-0.00000000	8.43839034	4.99519835
O	8.43839034	-0.00000000	-4.99519835
O	-0.00000000	-8.43839034	-4.99519835
O	-8.43839034	-0.00000000	-4.99519835
O	-8.43839034	-0.00000000	4.99519835
O	0.00000000	8.43839034	-4.99519835
O	-0.00000000	-8.43839034	4.99519835

$^4La(CO)_8$ BP86

La	0.00000000	0.00000000	0.00000000
C	0.00000000	2.08821300	1.69135200
C	0.00000000	-2.08821300	1.69135200
C	2.08821300	0.00000000	1.69135200
C	-2.08821300	0.00000000	1.69135200
C	1.47659000	-1.47659000	-1.69135200
C	-1.47659000	1.47659000	-1.69135200
C	-1.47659000	-1.47659000	-1.69135200
C	1.47659000	1.47659000	-1.69135200
O	0.00000000	-2.99045800	2.40625000
O	0.00000000	2.99045800	2.40625000
O	-2.99045800	0.00000000	2.40625000
O	2.99045800	0.00000000	2.40625000
O	-2.11457300	2.11457300	-2.40625000
O	2.11457300	-2.11457300	-2.40625000
O	2.11457300	2.11457300	-2.40625000
O	-2.11457300	-2.11457300	-2.40625000

$^4La(CO)_8$ B3LYP

La	0.00000000	0.00000000	0.00000000
C	0.00000000	2.14875800	1.66651400
C	0.00000000	-2.14875800	1.66651400
C	2.14875800	0.00000000	1.66651400
C	-2.14875800	0.00000000	1.66651400
C	1.51940200	-1.51940200	-1.66651400
C	-1.51940200	1.51940200	-1.66651400
C	-1.51940200	-1.51940200	-1.66651400
C	1.51940200	1.51940200	-1.66651400
O	0.00000000	-3.07304400	2.32986700
O	0.00000000	3.07304400	2.32986700
O	-3.07304400	0.00000000	2.32986700
O	3.07304400	0.00000000	2.32986700
O	-2.17297000	2.17297000	-2.32986700
O	2.17297000	-2.17297000	-2.32986700
O	2.17297000	2.17297000	-2.32986700
O	-2.17297000	-2.17297000	-2.32986700

$^2La(CO)_7$ BP86

La	-0.00292600	0.06352600	0.29773700
C	-0.12192900	2.70668700	0.77565200
C	2.27876300	-0.82451000	1.38588500
C	2.16968000	1.09424100	-0.74705100
C	0.03711500	-0.52236400	-2.17330500
C	-2.22217700	-0.99064800	1.36570500
C	-2.23586600	0.93257900	-0.76715600
C	0.10126700	-2.48798700	-0.24271300
O	0.05785600	-0.81080200	-3.29103100
O	-3.23194800	1.30018800	-1.21560200
O	-3.21154500	-1.44164500	1.74080600
O	3.29447600	-1.20573000	1.76790000
O	3.13993200	1.53018000	-1.19086700
O	-0.17968700	3.84721800	0.90133400
O	0.14662700	-3.60302800	-0.53168200

$^4La(CO)_7$ BP86

La	0.00000000	0.00000000	0.09664000
C	1.57295400	0.90814500	-1.79601200
C	-1.57295400	0.90814500	-1.79601200
C	0.00000000	2.56793500	0.90774500
C	0.00000000	0.00000000	2.86574500
C	0.00000000	-1.81629000	-1.79601200
C	2.22389700	-1.28396700	0.90774500
C	-2.22389700	-1.28396700	0.90774500
O	0.00000000	0.00000000	4.01375700
O	3.20530300	-1.85058300	1.10144000
O	0.00000000	-2.50987000	-2.71911600
O	-2.17361100	1.25493500	-2.71911600
O	0.00000000	3.70116600	1.10144000
O	2.17361100	1.25493500	-2.71911600
O	-3.20530300	-1.85058300	1.10144000

$^2La(CO)_7$ B3LYP

La	-0.24642200	0.12791000	0.00000000
C	-2.52659500	-1.34494500	0.00000000
C	-0.39729500	1.63190300	-2.25383400
C	-0.09855600	-1.34686000	-2.21006300
C	2.00923100	-1.14529100	0.00000000
C	-0.39729500	1.63190300	2.25383400
C	-0.09855600	-1.34686000	2.21006300
C	1.87075000	1.72486800	0.00000000
O	3.00984000	-1.69248300	0.00000000
O	-0.02852700	-1.96074700	3.16595600
O	-0.39729500	2.21919800	3.22588300
O	-0.39729500	2.21919800	-3.22588300
O	-0.02852700	-1.96074700	-3.16595600
O	-3.46512700	-1.98415000	0.00000000
O	2.79142600	2.39483600	0.00000000

$^4La(CO)_7$ B3LYP

La	0.00000000	0.00000000	0.04585300
O	0.00000000	0.00000000	4.02357500
O	3.20125800	-1.84824700	1.14212600
O	0.00000000	-2.62537200	-2.66750700
O	-2.27363900	1.31268600	-2.66750700
O	0.00000000	3.69649400	1.14212600
O	2.27363900	1.31268600	-2.66750700
O	-3.20125800	-1.84824700	1.14212600
C	1.64356900	0.94891500	-1.78766200
C	-1.64356900	0.94891500	-1.78766200
C	0.00000000	2.58205800	0.92463700
C	0.00000000	0.00000000	2.89022500
C	0.00000000	-1.89783000	-1.78766200
C	2.23612800	-1.29102900	0.92463700
C	-2.23612800	-1.29102900	0.92463700

$^{2}La(CO)_{6}$ BP86

La	0.00000000	0.00000000	0.49000700
C	0.00000000	1.93556300	-1.12212900
C	-2.23158800	0.55661900	1.95107300
C	2.23158800	-0.55661900	1.95107300
C	-1.92046400	0.17623900	-1.16651000
C	1.92046400	-0.17623900	-1.16651000
C	0.00000000	-1.93556300	-1.12212900
O	-0.00375900	2.75987300	-1.93452100
O	-3.24083900	0.86567000	2.40572100
O	-2.75628800	0.24807600	-1.96367400
O	2.75628800	-0.24807600	-1.96367400
O	3.24083900	-0.86567000	2.40572100
O	0.00375900	-2.75987300	-1.93452100

$^{4}La(CO)_{6}$ BP86

La	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.65241400
C	0.00000000	2.65241400	0.00000000
C	-2.65241400	0.00000000	0.00000000
C	2.65241400	0.00000000	0.00000000
C	0.00000000	-2.65241400	0.00000000
C	0.00000000	0.00000000	-2.65241400
O	0.00000000	0.00000000	3.80413700
O	0.00000000	3.80413700	0.00000000
O	3.80413700	0.00000000	0.00000000
O	0.00000000	-3.80413700	0.00000000
O	-3.80413700	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.80413700

$^{2}La(CO)_{6}$ B3LYP

La	0.00000000	0.00000000	0.35762100
C	0.00000000	2.07504700	-1.18623800
C	-1.97560400	0.66576500	2.11825700
C	1.97560400	-0.66576500	2.11825700
C	-2.05339300	0.15497000	-1.22935300
C	2.05339300	-0.15497000	-1.22935300
C	0.00000000	-2.07504700	-1.18623800
O	-0.01058600	2.94952300	-1.91947800
O	-2.81392600	1.00714100	2.80418600
O	-2.94787400	0.22304900	-1.93573200
O	2.94787400	-0.22304900	-1.93573200
O	2.81392600	-1.00714100	2.80418600
O	0.01058600	-2.94952300	-1.91947800

$^{4}La(CO)_{6}$ B3LYP

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

$^{3}Ce(CO)_{8}$ B3LYP

Ce	0.00000000	0.00000000	0.00000000
C	0.00000000	2.11647013	-1.59606072
C	-2.11647013	0.00000000	1.59606072
C	0.00000000	2.11647013	1.59606072
C	-2.11647013	-0.00000000	-1.59606072
C	2.11647013	-0.00000000	1.59606072
C	0.00000000	-2.11647013	-1.59606072
C	-0.00000000	-2.11647013	1.59606072
C	2.11647013	0.00000000	-1.59606072
O	-3.00748763	0.00000000	2.30092374
O	0.00000000	3.00748763	-2.30092374
O	-3.00748763	-0.00000000	-2.30092374
O	-0.00000000	3.00748763	2.30092374
O	-0.00000000	-3.00748763	-2.30092374
O	3.00748763	0.00000000	2.30092374
O	3.00748763	0.00000000	-2.30092374
O	0.00000000	-3.00748763	2.30092374

$^{5}Ce(CO)_{8}$ B3LYP

Ce	0.00000000	0.00000000	0.00011306
C	1.18227958	1.74927750	-1.63844112
C	1.17586358	-1.75523396	1.63612639
C	1.76015259	-1.20836657	-1.61797565
C	1.76886755	1.20022583	1.61537099
C	-1.18227958	-1.74927750	-1.63844112
C	-1.17586358	1.75523396	1.63612639
C	-1.76886755	-1.20022583	1.61537099
C	-1.76015259	1.20836657	-1.61797565
O	1.68025994	-2.50669229	2.32587454
O	1.68967619	2.49752594	-2.32946820
O	2.52323609	1.72216930	2.28784596
O	2.51059802	-1.73425726	-2.29179053
O	-1.68025994	2.50669229	2.32587454
O	-1.68967619	-2.49752594	-2.32946820
O	-2.51059802	1.73425726	-2.29179053
O	-2.52323609	-1.72216930	2.28784596

$^{4}Pr(CO)_{8}$ B3LYP

Pr	0.00000000	0.00000000	0.00000000
C	0.00000000	-2.18355419	1.46113103
C	-0.00000000	2.18355419	1.46113103
C	-2.18355419	-0.00000000	1.46113103
C	2.18355419	0.00000000	1.46113103
C	-2.18355419	0.00000000	-1.46113103
C	2.18355419	-0.00000000	-1.46113103
C	0.00000000	2.18355419	-1.46113103
C	-0.00000000	-2.18355419	-1.46113103
O	0.00000000	3.13814002	2.07727042
O	0.00000000	-3.13814002	2.07727042
O	3.13814002	0.00000000	2.07727042
O	-3.13814002	-0.00000000	2.07727042
O	3.13814002	-0.00000000	-2.07727042
O	-3.13814002	0.00000000	-2.07727042
O	-0.00000000	-3.13814002	-2.07727042
O	-0.00000000	3.13814002	-2.07727042

$^{6}Pr(CO)_{8}$ B3LYP

Pr	0.00000000	0.00000000	0.00000000
C	0.00000000	2.18985900	1.54925100
C	0.00000000	-2.18985900	1.54925100
C	2.18985900	0.00000000	1.54925100
C	-2.18985900	0.00000000	1.54925100
C	2.18985900	0.00000000	-1.54925100
C	-2.18985900	0.00000000	-1.54925100
C	0.00000000	-2.18985900	-1.54925100
C	0.00000000	2.18985900	-1.54925100
O	0.00000000	-3.11743100	2.20534200
O	0.00000000	3.11743100	2.20534200
O	-3.11743100	0.00000000	2.20534200
O	3.11743100	0.00000000	2.20534200
O	-3.11743100	0.00000000	-2.20534200
O	3.11743100	0.00000000	-2.20534200
O	0.00000000	3.11743100	-2.20534200
O	0.00000000	-3.11743100	-2.20534200

$^{4}Pr(CO)_{7}$ B3LYP

Pr	0.00002300	0.05764100	-0.25389500
O	-0.00116100	-3.62088900	0.37923900
O	-0.00038500	-0.81894800	3.29677600
O	3.06239200	1.45266800	1.32962900
O	3.19122800	-1.25912700	-1.79242400
O	-3.19186200	-1.25743100	-1.79247000
O	-3.06163100	1.45454800	1.32933900
O	0.00128500	3.70546600	-1.16512700
C	0.00088500	2.59882800	-0.90771000
C	-2.20893500	-0.86344600	-1.38264200
C	-2.12051900	1.03216000	0.84683800
C	-0.00026300	-0.54050000	2.19038700
C	2.20850700	-0.86464900	-1.38257300
C	2.12106800	1.03087200	0.84702600
C	-0.00079000	-2.50178300	0.17202800

$^{6}Pr(CO)_{7}$ B3LYP

Pr	0.00003800	-0.00002800	0.27950600
O	3.49321700	-0.88225500	-0.87381700
O	0.00002200	0.00000300	-3.48530900
O	-2.51121700	-2.58354600	-0.87356600
O	0.98616300	-3.48651500	1.46288200
O	2.52623300	2.59719500	1.46302100
O	-0.98249900	3.46624600	-0.87374100
O	-3.51233600	0.88919900	1.46272800
C	-2.44683100	0.62177800	1.16768400
C	1.76194400	1.80815300	1.16783100
C	-0.68262700	2.42002600	-0.53741100
C	0.00005300	-0.00003200	-2.34935200
C	0.68500500	-2.43003600	1.16789200
C	-1.75461200	-1.80118100	-0.53731300
C	2.43724900	-0.61887100	-0.53740600

$^{4}Pr(CO)_{6}$ B3LYP

Pr	0.00000000	0.00000000	0.31535900
C	0.00000000	2.04993100	-1.13499000
C	-1.84472700	0.84737000	2.06115000
C	1.84472700	-0.84737000	2.06115000
C	-2.02263400	0.15832900	-1.18938300
C	2.02263400	-0.15832900	-1.18938300
C	0.00000000	-2.04993100	-1.13499000
O	-0.01307500	2.95088400	-1.83644900
O	-2.64531300	1.27298600	2.74413600
O	-2.93473100	0.23238600	-1.87315500
O	2.93473100	-0.23238600	-1.87315500
O	2.64531300	-1.27298600	2.74413600
O	0.01307500	-2.95088400	-1.83644900

$^{6}Pr(CO)_{6}$ B3LYP

Pr	0.00000000	0.00000000	0.00000000
C	-0.00000100	0.00000100	2.60083300
C	-2.35287100	1.12152700	0.00000000
C	-1.12152700	-2.35287000	0.00000000
C	1.12152700	2.35287000	0.00000000
C	2.35287100	-1.12152600	0.00000000
C	0.00000100	-0.00000100	-2.60083300
O	0.00000100	-0.00000100	3.73899600
O	-3.38011700	1.61117900	0.00000000
O	1.61117800	3.38011700	0.00000000
O	3.38011700	-1.61117800	0.00000000
O	-1.61117900	-3.38011700	0.00000000
O	-0.00000100	0.00000000	-3.73899600

$^{5}Nd(CO)_{8}$ B3LYP

Nd	0.00000000	0.00000000	0.00000000
C	0.00000000	2.16082300	1.45690400
C	0.00000000	-2.16082300	1.45690400
C	2.16082300	0.00000000	1.45690400
C	-2.16082300	0.00000000	1.45690400
C	2.16082300	0.00000000	-1.45690400
C	-2.16082300	0.00000000	-1.45690400
C	0.00000000	-2.16082300	-1.45690400
C	0.00000000	2.16082300	-1.45690400
O	0.00000000	-3.11301700	2.07697400
O	0.00000000	3.11301700	2.07697400
O	-3.11301700	0.00000000	2.07697400
O	3.11301700	0.00000000	2.07697400
O	-3.11301700	0.00000000	-2.07697400
O	3.11301700	0.00000000	-2.07697400
O	0.00000000	3.11301700	-2.07697400
O	0.00000000	-3.11301700	-2.07697400

$^{7}Nd(CO)_{8}$ B3LYP

Nd	-0.00000000	0.00000000	0.00000000
C	-2.72643289	0.00788803	0.00000000
C	0.76228189	-2.55617492	0.00000000
C	-0.77230082	-1.27571599	2.21111993
C	-0.77230082	-1.27571599	-2.21111993
C	0.77230082	1.27571599	2.21111993
C	0.77230082	1.27571599	-2.21111993
C	2.72643289	-0.00788803	0.00000000
C	-0.76228189	2.55617492	0.00000000
O	1.05758622	-3.65443784	0.00000000
O	-3.85868589	0.01157169	0.00000000
O	-1.07111286	-1.81861534	-3.16479085
O	-1.07111286	-1.81861534	3.16479085
O	1.07111286	1.81861534	-3.16479085
O	1.07111286	1.81861534	3.16479085
O	-1.05758622	3.65443784	0.00000000
O	3.85868589	-0.01157169	0.00000000

$^{5}Nd(CO)_{7}$ B3LYP

Nd	-0.00263100	-0.05708300	-0.22893700
C	-0.12253700	-2.57612100	-0.92181200
C	2.19783800	0.74656800	-1.39763500
C	2.07147600	-1.10612300	0.86132800
C	0.04315300	0.57215800	2.19266100
C	-2.14623500	0.91336400	-1.37668700
C	-2.14554000	-0.93116000	0.88502500
C	0.10789800	2.47927000	0.12203600
O	0.16104100	3.60425400	0.29073100
O	0.06518400	0.86709000	3.29451600
O	-3.10463500	-1.30615000	1.37064500
O	-3.11037900	1.33048300	-1.80854600
O	3.18241800	1.10048500	-1.83977000
O	2.99575000	-1.56669100	1.34097200
O	-0.17418900	-3.67481500	-1.20520800

$^{7}Nd(CO)_{7}$ B3LYP

Nd	-0.00000000	-0.00000000	-0.28875104
C	2.19967254	1.26998153	-1.14774321
C	-2.19967254	1.26998153	-1.14774321
C	0.00000000	2.51374076	0.52569243
C	0.00000000	0.00000000	2.35444596
C	0.00000000	-2.53996306	-1.14774321
C	2.17696335	-1.25687038	0.52569243
C	-2.17696335	-1.25687038	0.52569243
O	-3.11860555	-1.80052775	0.86407546
O	-0.00000000	0.00000000	3.49007596
O	3.11860555	-1.80052775	0.86407546
O	0.00000000	-3.64167882	-1.42766512
O	-3.15378637	1.82083941	-1.42766512
O	0.00000000	3.60105550	0.86407546
O	3.15378637	1.82083941	-1.42766512

$^{5}Nd(CO)_{6}$ B3LYP

Nd	0.50640988	-0.01878825	0.00000000
C	0.54903188	1.99260689	1.59421904
C	0.49464098	-2.02507812	1.61150088
C	0.49464098	-2.02507812	-1.61150088
C	-1.52656808	0.04774095	1.38893906
C	0.54903188	1.99260689	-1.59421904
C	-1.52656808	0.04774095	-1.38893906
O	0.49898688	2.88662051	2.29779252
O	0.42479302	-2.90089951	2.33546341
O	-2.46387006	0.07495158	2.04376611
O	0.49898688	2.88662051	-2.29779252
O	0.42479302	-2.90089951	-2.33546341
O	-2.46387006	0.07495158	-2.04376611

$^{7}Nd(CO)_{6}$ B3LYP

Nd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.57945600
C	0.00000000	-2.57945600	-0.00000000
C	2.57945600	0.00000000	-0.00000000
C	-2.57945600	0.00000000	0.00000000
C	0.00000000	2.57945600	0.00000000
C	-0.00000000	0.00000000	-2.57945600
O	0.00000000	0.00000000	3.71749100
O	0.00000000	-3.71749100	-0.00000000
O	-3.71749100	0.00000000	0.00000000
O	0.00000000	3.71749100	0.00000000
O	3.71749100	0.00000000	-0.00000000
O	-0.00000000	0.00000000	-3.71749100

$^{7}Sm(CO)_{8}$ B3LYP

Sm	-0.05268200	-0.00057200	-0.00003600
C	0.11702000	2.13348500	1.50987200
C	-0.03031300	-2.18062800	1.46399500
C	2.13021000	-0.07383400	1.42430100
C	-2.19817200	0.04369400	1.54978400
C	2.12756200	0.10690800	-1.42620700
C	-2.19814800	-0.07729000	-1.54865400
C	0.14890800	-2.13202000	-1.50982100
C	-0.06524100	2.18000100	-1.46324200
O	-0.01899800	-3.12938500	2.08801300
O	0.22315600	3.06179700	2.15611700
O	-3.10695900	0.06040400	2.22945200
O	3.09897900	-0.09883200	2.01839500
O	-3.10688400	-0.10748200	-2.22792400
O	3.09529400	0.14722900	-2.02114800
O	-0.06908300	3.12918500	-2.08670900
O	0.26891300	-3.05872400	-2.15594000

$^{9}Sm(CO)_{8}$ B3LYP

Sm	0.00000000	0.00000000	0.00000000
C	0.00000000	2.19768400	1.55417400
C	0.00000000	-2.19768400	1.55417400
C	2.19768400	0.00000000	1.55417400
C	-2.19768400	0.00000000	1.55417400
C	2.19768400	0.00000000	-1.55417400
C	-2.19768400	0.00000000	-1.55417400
C	0.00000000	-2.19768400	-1.55417400
C	0.00000000	2.19768400	-1.55417400
O	0.00000000	-3.12411800	2.20963700
O	0.00000000	3.12411800	2.20963700
O	-3.12411800	0.00000000	2.20963700
O	3.12411800	0.00000000	2.20963700
O	-3.12411800	0.00000000	-2.20963700
O	3.12411800	0.00000000	-2.20963700
O	0.00000000	3.12411800	-2.20963700
O	0.00000000	-3.12411800	-2.20963700

$^{7}Sm(CO)_{7}$ B3LYP

Sm	-0.06785500	0.02065700	-0.08347300
C	1.50354100	-1.72935000	1.06256000
C	-2.01774400	-1.38716400	-1.20715000
C	1.42697300	-1.17278100	-1.86455900
C	1.43137700	1.88771000	-1.13199100
C	-1.67210100	-0.47021800	1.94909900
C	1.50792900	1.05776900	1.73015500
C	-2.01460300	1.78974800	-0.44131700
O	-2.90006500	2.49012100	-0.56324100
O	2.11045700	2.70061400	-1.54596500
O	2.19435300	1.48162800	2.53171400
O	-2.39057900	-0.67663300	2.80415200
O	-2.90427600	-1.95334200	-1.63489500
O	2.10413400	-1.71173900	-2.60235500
O	2.18782300	-2.47252400	1.58490500

$^{9}Sm(CO)_{7}$ B3LYP

Sm	0.00000000	0.00000000	-0.19165915
O	0.00000000	3.59837797	0.99749313
O	0.00000000	0.00000000	3.57062185
O	-3.11628673	-1.79918898	0.99749313
O	-3.00943238	1.73749660	-1.78336450
O	3.00943238	1.73749660	-1.78336450
O	3.11628673	-1.79918898	0.99749313
O	0.00000000	-3.47499319	-1.78336450
C	0.00000000	-2.43032816	-1.34117501
C	2.10472593	1.21516408	-1.34117501
C	2.17889089	-1.25798324	0.65106512
C	0.00000000	0.00000000	2.43346385
C	-2.10472593	1.21516408	-1.34117501
C	-2.17889089	-1.25798324	0.65106512
C	-0.00000000	2.51596648	0.65106512

$^{7}Sm(CO)_{6}$ B3LYP

Sm	0.00000000	-0.00000000	-0.03000797
C	-1.84153210	-1.65395175	-0.90784596
C	-1.84153210	1.65395175	-0.90784596
C	1.84153210	1.65395175	-0.90784596
C	-1.86938410	0.00000000	1.83887500
C	1.84153210	-1.65395175	-0.90784596
C	1.86938410	0.00000000	1.83887500
O	-2.69310611	-2.32900474	-1.24527996
O	-2.69310611	2.32900474	-1.24527996
O	-2.73208411	0.00000000	2.57956298
O	2.69310611	-2.32900474	-1.24527996
O	2.69310611	2.32900474	-1.24527996
O	2.73208411	0.00000000	2.57956298

$^{9}Sm(CO)_{6}$ B3LYP

Sm	0.00000000	0.00000000	-0.46360381
C	-1.57101200	-2.13500598	-0.58862682
C	-1.57101200	2.13500598	-0.58862682
C	1.57101200	2.13500598	-0.58862682
C	-1.48038300	0.00000000	1.66492719
C	1.57101200	-2.13500598	-0.58862682
C	1.48038300	0.00000000	1.66492719
O	-2.22484200	-3.06559298	-0.58129282
O	-2.22484200	3.06559298	-0.58129282
O	-2.13986900	0.00000000	2.59428119
O	2.22484200	-3.06559298	-0.58129282
O	2.22484200	3.06559298	-0.58129282
O	2.13986900	0.00000000	2.59428119

$^{10}Eu(CO)_8$ BP86

Eu	0.00000000	0.00000000	0.00000000
C	1.51435000	1.51435000	1.51435000
C	-1.51435000	1.51435000	-1.51435000
C	-1.51435000	1.51435000	1.51435000
C	1.51435000	1.51435000	-1.51435000
C	-1.51435000	-1.51435000	-1.51435000
C	1.51435000	-1.51435000	1.51435000
C	1.51435000	-1.51435000	-1.51435000
C	-1.51435000	-1.51435000	1.51435000
O	-2.17753100	2.17753100	-2.17753100
O	2.17753100	2.17753100	2.17753100
O	2.17753100	2.17753100	-2.17753100
O	-2.17753100	2.17753100	2.17753100
O	2.17753100	-2.17753100	2.17753100
O	-2.17753100	-2.17753100	-2.17753100
O	-2.17753100	-2.17753100	2.17753100
O	2.17753100	-2.17753100	-2.17753100

$^{8}Eu(CO)_8$ BP86

Eu	0.00000000	0.00000000	0.00000000
C	0.00000000	2.05026400	1.54974500
C	1.44975600	1.44975600	-1.54974500
C	-1.44975600	1.44975600	-1.54974500
C	2.05026400	0.00000000	1.54974500
C	1.44975600	-1.44975600	-1.54974500
C	-2.05026400	0.00000000	1.54974500
C	0.00000000	-2.05026400	1.54974500
C	-1.44975600	-1.44975600	-1.54974500
O	2.07644200	2.07644200	-2.28060400
O	0.00000000	2.93653300	2.28060400
O	2.93653300	0.00000000	2.28060400
O	-2.07644200	2.07644200	-2.28060400
O	-2.93653300	0.00000000	2.28060400
O	2.07644200	-2.07644200	-2.28060400
O	-2.07644200	-2.07644200	-2.28060400
O	0.00000000	-2.93653300	2.28060400

$^{10}Eu(CO)_8$ B3LYP

Eu	0.00000000	0.00000000	0.00000000
C	1.56129400	1.56129400	1.56129400
C	-1.56129400	1.56129400	-1.56129400
C	-1.56129400	1.56129400	1.56129400
C	1.56129400	1.56129400	-1.56129400
C	-1.56129400	-1.56129400	-1.56129400
C	1.56129400	-1.56129400	1.56129400
C	1.56129400	-1.56129400	-1.56129400
C	-1.56129400	-1.56129400	1.56129400
O	-2.21648900	2.21648900	-2.21648900
O	2.21648900	2.21648900	2.21648900
O	2.21648900	2.21648900	-2.21648900
O	-2.21648900	2.21648900	2.21648900
O	2.21648900	-2.21648900	2.21648900
O	-2.21648900	-2.21648900	-2.21648900
O	-2.21648900	-2.21648900	2.21648900
O	2.21648900	-2.21648900	-2.21648900

$^{8}Eu(CO)_8$ B3LYP

Eu	0.00000000	0.00000000	0.00000000
C	0.00000000	2.13668700	1.60610900
C	1.51086600	1.51086600	-1.60610900
C	-1.51086600	1.51086600	-1.60610900
C	2.13668700	0.00000000	1.60610900
C	1.51086600	-1.51086600	-1.60610900
C	-2.13668700	0.00000000	1.60610900
C	0.00000000	-2.13668700	1.60610900
C	-1.51086600	-1.51086600	-1.60610900
O	2.13497000	2.13497000	-2.31924000
O	0.00000000	3.01930300	2.31924000
O	3.01930300	0.00000000	2.31924000
O	-2.13497000	2.13497000	-2.31924000
O	-3.01930300	0.00000000	2.31924000
O	2.13497000	-2.13497000	-2.31924000
O	-2.13497000	-2.13497000	-2.31924000
O	0.00000000	-3.01930300	2.31924000

$^{10}Eu(CO)_7$ BP86

Eu	0.00000000	0.00000000	-0.09981200
O	0.00000000	0.00000000	3.59720700
O	3.09493000	-1.78685900	0.96138600
O	0.00000000	-3.27391300	-1.93548300
O	-2.83529200	1.63695700	-1.93548300
O	0.00000000	3.57371700	0.96138600
O	2.83529200	1.63695700	-1.93548300
O	-3.09493000	-1.78685900	0.96138600
C	1.94851600	1.12497600	-1.41536600
C	-1.94851600	1.12497600	-1.41536600
C	0.00000000	2.46641000	0.64926100
C	0.00000000	0.00000000	2.44645000
C	0.00000000	-2.24995200	-1.41536600
C	2.13597300	-1.23320500	0.64926100
C	-2.13597300	-1.23320500	0.64926100

$^{8}Eu(CO)_7$ BP86

Eu	-0.35051690	0.02978705	0.00000000
C	1.17648871	2.07548034	0.00000000
C	1.59317260	-0.86614023	1.35215680
C	1.59317260	-0.86614023	-1.35215680
C	-0.96746294	-1.86106949	-1.62649131
C	-0.91777374	1.66195044	1.90026076
C	-0.91777374	1.66195044	-1.90026076
C	-0.96746294	-1.86106949	1.62649131
O	-1.12908996	-2.73591271	-2.35557004
O	-1.09684103	2.42027319	-2.74673039
O	-1.09684103	2.42027319	2.74673039
O	2.47732383	-1.29777091	1.95088470
O	2.47732383	-1.29777091	-1.95088470
O	1.81383153	3.03273146	0.00000000
O	-1.12908996	-2.73591271	2.35557004

$^{10}Eu(CO)_7$ B3LYP

Eu	0.00000000	0.00000000	-0.09957000
C	2.00822800	1.15945100	-1.44881900
C	-2.00822800	1.15945100	-1.44881900
C	0.00000000	2.54006600	0.67271500
C	0.00000000	0.00000000	2.53394400
C	0.00000000	-2.31890200	-1.44881900
C	2.19976200	-1.27003300	0.67271500
C	-2.19976200	-1.27003300	0.67271500
O	0.00000000	0.00000000	3.67078600
O	3.14911400	-1.81814200	0.97364600
O	0.00000000	-3.31764800	-1.98727900
O	-2.87316700	1.65882400	-1.98727900
O	0.00000000	3.63628400	0.97364600
O	2.87316700	1.65882400	-1.98727900
O	-3.14911400	-1.81814200	0.97364600

$^{8}Eu(CO)_7$ B3LYP

Eu	-0.03492600	0.03320200	-0.04394300
C	-1.60473100	-1.67683100	-1.38535300
C	2.00859500	0.00124900	-1.79371400
C	1.23413300	-2.28451000	0.18938000
C	0.67239700	-0.25265100	2.48195400
C	-1.42784500	2.03563500	-1.16635500
C	-2.35267300	0.02008500	1.27006400
C	1.55749300	2.10579300	0.51619800
O	0.97439000	-0.38412700	3.57041700
O	-3.36125800	0.01131200	1.79431500
O	-2.03930300	2.87474800	-1.62358200
O	2.88731700	-0.02869800	-2.51162900
O	1.78050800	-3.27980700	0.25689800
O	-2.27677300	-2.40504100	-1.93944200
O	2.24463400	2.98857300	0.71494400

$^{10}Eu(CO)_6$ BP86

Eu	0.00000000	0.00000000	0.30712100
C	0.00000000	2.49840800	0.96000500
C	2.16368500	-1.24920400	0.96000500
C	1.83979900	1.06220800	-1.13962800
C	-2.16368500	-1.24920400	0.96000500
C	-1.83979900	1.06220800	-1.13962800
C	0.00000000	-2.12441600	-1.13962800
O	0.00000000	3.64466100	1.07873500
O	3.15636900	-1.82233000	1.07873500
O	-3.15636900	-1.82233000	1.07873500
O	-2.68469600	1.55001000	-1.75020900
O	2.68469600	1.55001000	-1.75020900
O	0.00000000	-3.10002000	-1.75020900

$^{8}Eu(CO)_6$ BP86

Eu	0.52604000	-0.05777000	0.00000000
C	0.79394800	-1.16204000	2.32169200
C	0.79394800	-1.16204000	-2.32169200
C	0.20970400	1.76066900	-1.77933700
C	-1.17073000	-1.89602800	0.00000000
C	0.20970400	1.76066900	1.77933700
C	-1.81441400	0.76362100	0.00000000
O	0.79394800	-1.59874400	3.38749500
O	0.79394800	-1.59874400	-3.38749500
O	-1.98509200	-2.71433100	0.00000000
O	-0.05705500	2.57575800	2.54857000
O	-0.05705500	2.57575800	-2.54857000
O	-2.89788400	1.16660000	0.00000000

$^{10}Eu(CO)_6$ B3LYP

Eu	-0.00000000	0.00000000	0.00000000
C	0.00000000	2.41414392	1.09561870
C	2.09070996	-1.20707196	1.09561870
C	2.09070996	1.20707196	-1.09561870
C	-2.09070996	-1.20707196	1.09561870
C	-2.09070996	1.20707196	-1.09561870
C	-0.00000000	-2.41414392	-1.09561870
O	0.00000000	3.48536588	1.47805856
O	3.01841539	-1.74268294	1.47805856
O	-3.01841539	-1.74268294	1.47805856
O	-3.01841539	1.74268294	-1.47805856
O	3.01841539	1.74268294	-1.47805856
O	-0.00000000	-3.48536588	-1.47805856

$^{8}Eu(CO)_6$ B3LYP

Eu	0.00000000	0.00000000	0.43961600
C	2.13143300	1.59360000	0.61888800
C	-2.13143300	1.59360000	0.61888800
C	-2.13143300	-1.59360000	0.61888800
C	0.00000000	1.47278000	-1.69587600
C	2.13143300	-1.59360000	0.61888800
C	0.00000000	-1.47278000	-1.69587600
O	3.05507200	2.25692800	0.62099400
O	-3.05507200	2.25692800	0.62099400
O	0.00000000	2.12770500	-2.62940100
O	3.05507200	-2.25692800	0.62099400
O	-3.05507200	-2.25692800	0.62099400
O	0.00000000	-2.12770500	-2.62940100

$^{9}Gd(CO)_8$ BP86

Gd	0.00000000	0.00000000	0.00000000
C	0.00000000	2.00087200	1.61468400
C	-2.00087200	0.00000000	-1.61468400
C	-2.00087200	0.00000000	1.61468400
C	0.00000000	2.00087200	-1.61468400
C	0.00000000	-2.00087200	-1.61468400
C	2.00087200	0.00000000	1.61468400
C	2.00087200	0.00000000	-1.61468400
C	0.00000000	-2.00087200	1.61468400
O	-2.96459500	0.00000000	-2.24106600
O	0.00000000	2.96459500	2.24106600
O	0.00000000	2.96459500	-2.24106600
O	-2.96459500	0.00000000	2.24106600
O	2.96459500	0.00000000	2.24106600
O	0.00000000	-2.96459500	-2.24106600
O	0.00000000	-2.96459500	2.24106600
O	2.96459500	0.00000000	-2.24106600

$^{11}Gd(CO)_8$ BP86

Gd	0.00000600	-0.03206900	0.00045800
C	-1.85205300	-0.78542400	1.54249500
C	-0.81991700	-1.88118800	-1.40471400
C	0.91054000	-1.82809400	1.42200300
C	-2.04065300	0.76086900	-1.40765800
C	1.88943600	-0.71582600	-1.53684600
C	-0.78916100	1.96684100	1.53205300
C	0.69677500	1.98664500	-1.55130200
C	2.00488200	0.86849900	1.40154100
O	-1.18977400	-2.81075100	-1.98983300
O	-2.70685300	-1.24529000	2.16740400
O	-3.03169000	1.00529700	-1.93879300
O	1.32158500	-2.73502800	2.01476400
O	-1.21630100	2.85448700	2.12279800
O	2.76342200	-1.14506000	-2.15644600
O	2.98337700	1.16413900	1.92954900
O	1.07629800	2.88951700	-2.15128600

$^{9}Gd(CO)_8$ B3LYP

Gd	0.00000000	0.00000000	0.00000000
C	0.00000000	2.04921800	1.61071300
C	-2.04921800	0.00000000	-1.61071300
C	-2.04921800	0.00000000	1.61071300
C	0.00000000	2.04921800	-1.61071300
C	0.00000000	-2.04921800	-1.61071300
C	2.04921800	0.00000000	1.61071300
C	2.04921800	0.00000000	-1.61071300
C	0.00000000	-2.04921800	1.61071300
O	-3.01771900	0.00000000	-2.20418100
O	0.00000000	3.01771900	2.20418100
O	0.00000000	3.01771900	-2.20418100
O	-3.01771900	0.00000000	2.20418100
O	3.01771900	0.00000000	2.20418100
O	0.00000000	-3.01771900	-2.20418100
O	0.00000000	-3.01771900	2.20418100
O	3.01771900	0.00000000	-2.20418100

$^{11}Gd(CO)_8$ B3LYP

Gd	-0.00011100	-0.05708800	-0.00023300
C	-1.93715400	-0.80010700	1.45361500
C	-0.73253700	-1.87734700	-1.45963000
C	0.82414500	-1.84844200	1.45141200
C	-2.00312100	0.79824100	-1.52254400
C	1.97755900	-0.70210200	-1.45939000
C	-0.90368000	2.03863600	1.52607800
C	0.80721900	2.08890700	-1.51669400
C	1.96856400	0.88501100	1.52869000
O	-1.04648000	-2.78321000	-2.08861300
O	-2.78620100	-1.28713700	2.04011400
O	-2.96950900	0.98676700	-2.08926800
O	1.17705000	-2.74336900	2.07493500
O	-1.40074400	2.90066300	2.06689300
O	2.84715200	-1.15083300	-2.04559700
O	2.92570100	1.11559700	2.09501900
O	1.25317100	2.98112800	-2.05277000

$^{9}Gd(CO)_7$ BP86

Gd	-0.12786700	-0.05446600	0.00000000
C	-0.99343500	-1.82593500	-1.66621800
C	-1.70673400	1.94127900	0.00000000
C	0.23593200	1.49090400	-1.95177100
C	2.10087200	1.03151300	0.00000000
C	-0.99343500	-1.82593500	1.66621800
C	1.32483900	-2.14107300	0.00000000
C	0.23593200	1.49090400	1.95177100
O	3.18554900	1.42363300	0.00000000
O	2.07210000	-3.01665300	0.00000000
O	-1.32390100	-2.56065000	2.48356200
O	-2.46961900	2.80337100	0.00000000
O	0.36486500	2.11271700	-2.91339400
O	-1.32390100	-2.56065000	-2.48356200
O	0.36486500	2.11271700	2.91339400

$^{11}Gd(CO)_7$ BP86

Gd	0.00050993	0.04098909	0.00000000
C	1.78570776	-0.37749906	1.69682229
C	-0.00438717	-2.32525991	0.00000000
C	1.78570776	-0.37749906	-1.69682229
C	0.00278516	2.17307416	-1.64980175
C	-1.78990724	-0.36976892	1.69282597
C	0.00278516	2.17307416	1.64980175
C	-1.78990724	-0.36976892	-1.69282597
O	0.00206327	2.85836120	-2.56864272
O	0.00206327	2.85836120	2.56864272
O	-2.55459032	-0.73107392	2.47742089
O	-0.00723021	-3.49217491	0.00000000
O	2.55233612	-0.73861290	-2.47867866
O	2.55233612	-0.73861290	2.47867866
O	-2.55459032	-0.73107392	-2.47742089

$^{9}Gd(CO)_7$ B3LYP

Gd	-0.08368700	-0.04842200	0.00000000
C	-1.03276800	-1.81773700	-1.66847400
C	-1.79364200	1.87775400	0.00000000
C	0.21245500	1.48518300	-2.01983600
C	2.17307200	1.08864600	0.00000000
C	-1.03276800	-1.81773700	1.66847400
C	1.44255600	-2.12118500	0.00000000
C	0.21245500	1.48518300	2.01983600
O	3.24611300	1.47106700	0.00000000
O	2.20723900	-2.96276600	0.00000000
O	-1.43979000	-2.51658700	2.46355400
O	-2.62670100	2.65231200	0.00000000
O	0.29320100	2.06242700	-2.99780200
O	-1.43979000	-2.51658700	-2.46355400
O	0.29320100	2.06242700	2.99780200

$^{11}Gd(CO)_7$ B3LYP

Gd	0.00000000	0.00000000	-0.00535700
C	1.60747500	0.92807600	-1.58723700
C	-1.60747500	0.92807600	-1.58723700
C	0.00000000	2.47164300	0.82186600
C	0.00000000	0.00000000	2.81674400
C	0.00000000	-1.85615300	-1.58723700
C	2.14050600	-1.23582200	0.82186600
C	-2.14050600	-1.23582200	0.82186600
O	0.00000000	0.00000000	3.94720100
O	3.11165100	-1.79651300	0.99690900
O	0.00000000	-2.63434000	-2.42851600
O	-2.28140500	1.31717000	-2.42851600
O	0.00000000	3.59302500	0.99690900
O	2.28140500	1.31717000	-2.42851600
O	-3.11165100	-1.79651300	0.99690900

$^{9}Gd(CO)_6$ BP86

Gd	-0.48309000	0.11287200	0.00000000
C	-0.65460200	-1.99053200	1.36061300
C	-0.37094200	2.25772200	1.41910000
C	-0.37094200	2.25772200	-1.41910000
C	1.53179100	-0.40569800	1.27869100
C	-0.65460200	-1.99053200	-1.36061300
C	1.53179100	-0.40569800	-1.27869100
O	-0.75082700	-2.92330200	2.03268100
O	-0.15118300	3.13997700	2.12344500
O	2.45468700	-0.56428000	1.95749800
O	-0.75082700	-2.92330200	-2.03268100
O	-0.15118300	3.13997700	-2.12344500
O	2.45468700	-0.56428000	-1.95749800

$^{11}Gd(CO)_6$ BP86

Gd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.48091000
C	0.00000000	2.48091000	0.00000000
C	2.48091000	0.00000000	0.00000000
C	-2.48091000	0.00000000	0.00000000
C	0.00000000	-2.48091000	0.00000000
C	0.00000000	0.00000000	-2.48091000
O	0.00000000	0.00000000	3.63469200
O	0.00000000	3.63469200	0.00000000
O	-3.63469200	0.00000000	0.00000000
O	0.00000000	-3.63469200	0.00000000
O	3.63469200	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.63469200

$^{9}Gd(CO)_6$ B3LYP

Gd	-0.41434800	0.11024500	0.00000000
C	-0.71864200	-1.98713500	1.40782500
C	-0.40709600	2.25259700	1.47968500
C	-0.40709600	2.25259700	-1.47968500
C	1.61440400	-0.41932600	1.34376500
C	-0.71864200	-1.98713500	-1.40782500
C	1.61440400	-0.41932600	-1.34376500
O	-0.91672500	-2.87350200	2.09588900
O	-0.29627500	3.10936800	2.21721000
O	2.50389300	-0.56144700	2.04550100
O	-0.91672500	-2.87350200	-2.09588900
O	-0.29627500	3.10936800	-2.21721000
O	2.50389300	-0.56144700	-2.04550100

$^{11}Gd(CO)_6$ B3LYP

Gd	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.49796600
C	0.00000000	2.49796600	0.00000000
C	2.49796600	0.00000000	0.00000000
C	-2.49796600	0.00000000	0.00000000
C	0.00000000	-2.49796600	0.00000000
C	0.00000000	0.00000000	-2.49796600
O	0.00000000	0.00000000	3.63732300
O	0.00000000	3.63732300	0.00000000
O	-3.63732300	0.00000000	0.00000000
O	0.00000000	-3.63732300	0.00000000
O	3.63732300	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.63732300

$^{8}Tb(CO)_8$ B3LYP

Tb	-0.00000000	0.00000000	0.00000000
C	-1.48795569	1.48827719	1.42659489
C	1.48827719	1.48795569	-1.42659489
C	-1.48827719	1.48795569	-1.42659489
C	1.48795569	1.48827719	1.42659489
C	1.48827719	-1.48795569	-1.42659489
C	-1.48795569	-1.48827719	1.42659489
C	1.48795569	-1.48827719	1.42659489
C	-1.48827719	-1.48795569	-1.42659489
O	2.15443036	2.16291168	-2.05320536
O	-2.16291168	2.15443036	2.05320536
O	2.16291168	2.15443036	2.05320536
O	-2.15443036	2.16291168	-2.05320536
O	-2.16291168	-2.15443036	2.05320536
O	2.15443036	-2.16291168	-2.05320536
O	-2.15443036	-2.16291168	-2.05320536
O	2.16291168	-2.15443036	2.05320536

$^{10}Tb(CO)_8$ B3LYP

Tb	0.00000000	-0.00000000	0.00000000
C	-1.43205512	1.39751730	-1.52815948
C	1.39751730	1.43205512	1.52815948
C	1.43205512	1.39751730	-1.52815948
C	-1.39751730	1.43205512	1.52815948
C	1.39751730	-1.43205512	1.52815948
C	-1.43205512	-1.39751730	-1.52815948
C	-1.39751730	-1.43205512	1.52815948
C	1.43205512	-1.39751730	-1.52815948
O	2.13102826	1.94126896	2.23206060
O	-1.94126896	2.13102826	-2.23206060
O	-2.13102826	1.94126896	2.23206060
O	1.94126896	2.13102826	-2.23206060
O	-1.94126896	-2.13102826	-2.23206060
O	2.13102826	-1.94126896	2.23206060
O	1.94126896	-2.13102826	-2.23206060
O	-2.13102826	-1.94126896	2.23206060

$^{7}Dy(CO)_{8}$ B3LYP

Dy	0.00000000	-0.00242900	0.00912000
C	1.48931700	-1.46079300	-1.41088900
C	-1.46203400	1.46547200	-1.43484200
C	1.46198900	1.46550300	-1.43485600
C	-1.48929800	-1.46082400	-1.41087700
C	-1.46852900	1.46323300	1.43072300
C	1.49149100	-1.46573800	1.40065200
C	-1.49144800	-1.46577000	1.40066600
C	1.46851200	1.46326200	1.43071000
O	-2.13065300	2.12943000	-2.07009800
O	2.16535300	-2.12052900	-2.04286900
O	-2.16532500	-2.12057400	-2.04285400
O	2.13058900	2.12947600	-2.07011700
O	2.17172600	-2.12923400	2.02466700
O	-2.14030400	2.12872600	2.06145100
O	2.14027900	2.12876700	2.06143400
O	-2.17166500	-2.12928100	2.02468400

$^{9}Dy(CO)_{8}$ B3LYP

Dy	0.02209600	0.00163100	-0.00438000
C	-0.34784600	1.88770500	-1.65715800
C	-0.35432500	-2.20949200	-1.20639600
C	-2.37308400	-0.10861600	-0.94306600
C	1.62759300	-0.22497900	-1.91997900
C	1.70724600	-1.34860200	1.30305800
C	-1.03093200	1.72380900	1.56201500
C	1.81093500	1.49016000	0.97581900
C	-1.15188700	-1.21359100	1.90925900
O	-0.47053200	-3.24020300	-1.67590100
O	-0.46416300	2.78514800	-2.34842600
O	2.40671200	-0.31840800	-2.74677100
O	-3.46446200	-0.14594300	-1.26099400
O	-1.53405900	2.53455300	2.18203600
O	2.49498600	-1.98595400	1.82391300
O	-1.71395800	-1.80959500	2.69896200
O	2.64741200	2.16964900	1.34565300

$^{6}Ho(CO)_{8}$ B3LYP

Ho	0.00000000	0.00000000	0.00000000
C	0.00000000	2.00970000	1.47685800
C	-2.00970000	0.00000000	-1.47685800
C	-2.00970000	0.00000000	1.47685800
C	0.00000000	2.00970000	-1.47685800
C	0.00000000	-2.00970000	-1.47685800
C	2.00970000	0.00000000	1.47685800
C	2.00970000	0.00000000	-1.47685800
C	0.00000000	-2.00970000	1.47685800
O	-2.91685400	0.00000000	-2.16253100
O	0.00000000	2.91685400	2.16253100
O	0.00000000	2.91685400	-2.16253100
O	-2.91685400	0.00000000	2.16253100
O	2.91685400	0.00000000	2.16253100
O	0.00000000	-2.91685400	-2.16253100
O	0.00000000	-2.91685400	2.16253100
O	2.91685400	0.00000000	-2.16253100

$^{8}Ho(CO)_{8}$ B3LYP

Ho	-0.00110500	-0.00000200	-0.00000800
C	0.85636400	-1.86149900	-1.46274100
C	-0.85216700	-1.82372600	1.51164900
C	-1.86186900	-0.87835000	-1.44581900
C	1.86574900	-0.83748600	1.46518900
C	-1.84823100	0.87502300	1.46533400
C	1.84839500	0.84125600	-1.48444600
C	0.86839600	1.86303000	1.45368500
C	-0.87204300	1.82156200	-1.50251500
O	-1.25812100	-2.68388900	2.13851700
O	1.26352800	-2.73763500	-2.06619300
O	2.74526300	-1.23914900	2.06742000
O	-2.73928800	-1.29642300	-2.04003400
O	2.72049700	1.24491200	-2.09606300
O	-2.71998700	1.29170500	2.06875600
O	-1.28660900	2.68067200	-2.12519100
O	1.28052900	2.73996600	2.05259900

$^{6}Ho(CO)_{7}$ B3LYP

Ho	0.00509300	0.05844800	-0.01063600
C	-0.04816400	2.53652700	-0.10665000
C	-1.99172800	0.16418300	-1.45201400
C	-2.00098900	0.35141800	1.38504100
C	0.01899600	-1.80510900	1.54298500
C	1.99467700	0.21177700	-1.45660600
C	2.00109900	0.39918200	1.38690200
C	0.01948100	-2.01692100	-1.27494800
O	0.02305200	-2.66990600	2.28549300
O	2.94170400	0.57457100	2.00334300
O	2.93284700	0.30141400	-2.09421500
O	-2.93411300	0.23030800	-2.08613700
O	-2.94767600	0.50208400	1.99853900
O	-0.07747900	3.67119400	-0.15201500
O	0.02398100	-2.97995900	-1.88446800

$^{8}Ho(CO)_{7}$ B3LYP

Ho	0.00000000	-0.00000000	0.04167596
O	0.00000000	-0.00000000	3.79723096
O	-3.14834706	-1.56688090	0.98455823
O	-2.17966816	1.35262744	-2.44137421
O	2.26124380	1.21133427	-2.44137421
O	2.93113219	-1.94310808	0.98455823
O	-0.08157565	-2.56396171	-2.44137421
O	0.21721487	3.50998898	0.98455823
C	-0.06228479	-1.81924341	-1.57194698
C	1.60665341	0.85568150	-1.57194698
C	2.00288584	-1.32037636	0.78485021
C	0.00000000	-0.00000000	2.66340896
C	-1.54436862	0.96356192	-1.57194698
C	-2.14492239	-1.07436184	0.78485021
C	0.14203655	2.39473820	0.78485021

^{6}Ho(CO)$_{6}$ B3LYP

Ho	0.00009600	0.00129600	0.30728200
C	1.56828400	-1.84175000	0.62343700
C	1.57792700	1.83264300	0.63205700
C	-1.57802500	1.83243900	0.63165700
C	1.41472900	0.00677500	-1.60843700
C	-1.56899400	-1.84100900	0.62316200
C	-1.41400500	0.00696800	-1.60880000
O	2.30739500	-2.70084700	0.74168300
O	2.32098100	2.68803000	0.75276800
O	2.11009100	0.00832600	-2.51533100
O	-2.30868000	-2.69962900	0.74128400
O	-2.32137500	2.68760000	0.75216500
O	-2.10915000	0.00862000	-2.51586300

^{8}Ho(CO)$_{6}$ B3LYP

Ho	0.00000000	0.00000000	0.00000000
C	0.00000000	2.02888663	1.37054815
C	1.75706736	1.01444331	-1.37054815
C	-0.00000000	-2.02888663	-1.37054815
C	1.75706736	-1.01444331	1.37054815
C	-1.75706736	1.01444331	-1.37054815
C	-1.75706736	-1.01444331	1.37054815
O	0.00000000	2.97282971	2.00773604
O	2.57454605	1.48641486	-2.00773604
O	2.57454605	-1.48641486	2.00773604
O	-2.57454605	1.48641486	-2.00773604
O	-0.00000000	-2.97282971	-2.00773604
O	-2.57454605	-1.48641486	2.00773604

^{5}Er(CO)$_{8}$ B3LYP

Er	-0.00000000	0.00000000	-0.00000000
C	0.00000000	1.99614666	1.46962650
C	0.00000000	-1.99614666	1.46962650
C	1.99614666	0.00000000	1.46962650
C	-1.99614666	-0.00000000	1.46962650
C	-0.00000000	-1.99614666	-1.46962650
C	-0.00000000	1.99614666	-1.46962650
C	-1.99614666	0.00000000	-1.46962650
C	1.99614666	-0.00000000	-1.46962650
O	0.00000000	-2.90000417	2.16039178
O	-0.00000000	2.90000417	2.16039178
O	-2.90000417	-0.00000000	2.16039178
O	2.90000417	0.00000000	2.16039178
O	0.00000000	2.90000417	-2.16039178
O	-0.00000000	-2.90000417	-2.16039178
O	2.90000417	-0.00000000	-2.16039178
O	-2.90000417	0.00000000	-2.16039178

^{7}Er(CO)$_{8}$ B3LYP

Er	0.00886400	-0.01598000	-0.00054300
C	-0.29892000	2.01104700	1.43594900
C	0.48007000	-1.98078800	1.46776600
C	2.08372400	0.41889900	1.32863400
C	-1.90276000	-0.35870300	1.57520500
C	1.59635800	-1.15422900	-1.55393700
C	-1.76395700	1.12528400	-1.35261100
C	-1.23863300	-1.70482600	-1.36410900
C	1.03774600	1.66062400	-1.53886300
O	0.70882200	-2.90986100	2.08628600
O	-0.47066700	2.96555700	2.03466100
O	-2.81253900	-0.52563000	2.24085000
O	3.06016200	0.64246100	1.87189800
O	-2.59524200	1.66837300	-1.91190800
O	2.35436100	-1.70350700	-2.20355600
O	1.52751900	2.46871200	-2.17562600
O	-1.84298200	-2.48325500	-1.93651900

^{4}Tm(CO)$_{8}$ B3LYP

Tm	0.00000000	0.00000000	0.00000000
C	0.00000000	1.98934876	-1.45457400
C	-1.98934876	0.00000000	1.45457400
C	0.00000000	1.98934876	1.45457400
C	-1.98934876	-0.00000000	-1.45457400
C	-0.00000000	-1.98934876	1.45457400
C	1.98934876	0.00000000	-1.45457400
C	0.00000000	-1.98934876	-1.45457400
C	1.98934876	-0.00000000	1.45457400
O	-2.90100385	0.00000000	2.13470500
O	0.00000000	2.90100385	-2.13470500
O	-2.90100385	-0.00000000	-2.13470500
O	0.00000000	2.90100385	2.13470500
O	2.90100385	0.00000000	-2.13470500
O	0.00000000	-2.90100385	2.13470500
O	2.90100385	0.00000000	2.13470500
O	-0.00000000	-2.90100385	-2.13470500

^{6}Tm(CO)$_{8}$ B3LYP

Tm	0.00111200	-0.00206600	0.00048200
C	-1.23371200	1.60296600	1.44087400
C	1.19713200	-1.61356900	1.45803700
C	1.59750100	1.20411200	1.47556500
C	-1.62084400	-1.21907500	1.43244200
C	2.02196700	-0.11266000	-1.43519900
C	-1.99792200	0.12541900	-1.47069600
C	-0.10634700	-1.99812100	-1.46693100
C	0.13774400	2.02210600	-1.43344700
O	1.76449800	-2.38616700	2.07451100
O	-1.82162300	2.37047000	2.04398700
O	-2.39339700	-1.79830500	2.03778800
O	2.36403500	1.77395500	2.09683600
O	-2.95256300	0.17856100	-2.09049500
O	2.98449100	-0.16532200	-2.04317700
O	0.20065900	2.98798700	-2.03476100
O	-0.15232900	-2.95174400	-2.08933300

$^{4}Tm(CO)_{7}$ B3LYP

Tm	-0.00003800	0.04041600	-0.00034100
C	-0.00076500	2.48108700	-0.00492700
C	-1.95414800	0.29305800	-1.42070700
C	-1.96988700	0.29736200	1.40227900
C	-0.00672500	-1.89333200	1.42757200
C	1.96911500	0.28988000	-1.40557800
C	1.95462600	0.30273400	1.41723200
C	0.00785500	-1.90321500	-1.41499300
O	-0.01058200	-2.79733200	2.12179100
O	2.88799400	0.44839200	2.05268200
O	2.90935400	0.42437000	-2.03276600
O	-2.88724700	0.43422100	-2.05753600
O	-2.91047300	0.43529500	2.02822700
O	-0.00108600	3.61767500	-0.00704200
O	0.01231300	-2.81189300	-2.10306900

$^{6}Tm(CO)_{7}$ B3LYP

Tm	0.04869798	-0.00019409	0.00000000
C	-1.54402659	1.79523140	0.00000000
C	-1.55422972	-0.85939316	1.58062668
C	0.81376063	1.20143798	2.01954376
C	2.60411501	-0.11173228	0.00000000
C	-1.55422972	-0.85939316	-1.58062668
C	0.81376063	1.20143798	-2.01954376
C	0.66618274	-2.40561190	0.00000000
O	3.73849002	-0.15119092	0.00000000
O	1.05079236	1.78555953	-2.96457077
O	-2.42898468	-1.20620290	-2.23116899
O	-2.42898468	-1.20620290	2.23116899
O	1.05079236	1.78555953	2.96457077
O	-2.40401083	2.55192813	0.00000000
O	0.81643209	-3.53126285	0.00000000

$^{4}Tm(CO)_{6}$ B3LYP

Tm	-0.26358793	0.01247094	0.00000000
C	-0.67267527	1.53412901	1.82257540
C	-0.67267527	1.53412901	-1.82257540
C	-0.63428659	-1.57437596	-1.76531718
C	1.61300327	1.45252267	0.00000000
C	-0.63428659	-1.57437596	1.76531718
C	1.63761987	-1.38738233	0.00000000
O	-0.84144195	2.25122600	2.69209165
O	-0.84144195	2.25122600	-2.69209165
O	2.50987937	2.16038955	0.00000000
O	-0.78954163	-2.33782411	2.59669671
O	-0.78954163	-2.33782411	-2.59669671
O	2.54149877	-2.08643646	0.00000000

$^{6}Tm(CO)_{6}$ B3LYP

Tm	0.00000000	0.00000000	0.00000000
C	0.00000000	2.41193500	0.00000000
C	0.00000000	0.00000000	2.41091200
C	2.41674400	-0.05376000	0.00000000
C	-2.41674400	0.05376000	0.00000000
C	0.00000000	0.00000000	-2.41091200
C	0.00000000	-2.41193500	0.00000000
O	-0.00304600	3.55136400	0.00000000
O	0.00000000	0.00000000	3.55033000
O	-3.55570500	0.07881700	0.00000000
O	0.00000000	0.00000000	-3.55033000
O	3.55570500	-0.07881700	0.00000000
O	0.00304600	-3.55136400	0.00000000

$^{1}Yb(CO)_{8}$ BP86

Yb	0.00000000	0.00000000	0.00000000
C	0.00000000	1.97349000	1.40960000
C	0.00000000	-1.97349000	1.40960000
C	1.97349000	0.00000000	1.40960000
C	-1.97349000	0.00000000	1.40960000
C	1.39546800	-1.39546800	-1.40960000
C	-1.39546800	1.39546800	-1.40960000
C	-1.39546800	-1.39546800	-1.40960000
C	1.39546800	1.39546800	-1.40960000
O	0.00000000	-2.89128900	2.10250200
O	0.00000000	2.89128900	2.10250200
O	-2.89128900	0.00000000	2.10250200
O	2.89128900	0.00000000	2.10250200
O	-2.04445000	2.04445000	-2.10250200
O	2.04445000	-2.04445000	-2.10250200
O	2.04445000	2.04445000	-2.10250200
O	-2.04445000	-2.04445000	-2.10250200

$^{3}Yb(CO)_{8}$ BP86

Yb	0.00000000	0.00000000	0.00000000
C	-0.40344600	2.00525500	1.39879500
C	0.40344600	-2.00525500	1.39879500
C	2.00525500	0.40344600	1.39879500
C	-2.00525500	-0.40344600	1.39879500
C	2.00525500	-0.40344600	-1.39879500
C	-2.00525500	0.40344600	-1.39879500
C	-0.40344600	-2.00525500	-1.39879500
C	0.40344600	2.00525500	-1.39879500
O	0.64670600	-2.93125400	2.03611900
O	-0.64670600	2.93125400	2.03611900
O	-2.93125400	-0.64670600	2.03611900
O	2.93125400	0.64670600	2.03611900
O	-2.93125400	0.64670600	-2.03611900
O	2.93125400	-0.64670600	-2.03611900
O	0.64670600	2.93125400	-2.03611900
O	-0.64670600	-2.93125400	-2.03611900

$^{1}Yb(CO)_{8}$ B3LYP

Yb	0.00000000	0.00000000	0.00000000
C	0.00000000	2.04778600	1.48289800
C	0.00000000	-2.04778600	1.48289800
C	2.04778600	0.00000000	1.48289800
C	-2.04778600	0.00000000	1.48289800
C	1.44800300	-1.44800300	-1.48289800
C	-1.44800300	1.44800300	-1.48289800
C	-1.44800300	-1.44800300	-1.48289800
C	1.44800300	1.44800300	-1.48289800
O	0.00000000	-2.94958200	2.17325200
O	0.00000000	2.94958200	2.17325200
O	-2.94958200	0.00000000	2.17325200
O	2.94958200	0.00000000	2.17325200
O	-2.08567000	2.08567000	-2.17325200
O	2.08567000	-2.08567000	-2.17325200
O	2.08567000	2.08567000	-2.17325200
O	-2.08567000	-2.08567000	-2.17325200

$^3Yb(CO)_8$ B3LYP

Yb	0.00000000	0.00000000	0.00000000
C	-1.49163059	1.49163059	1.49163059
C	1.49163059	-1.49163059	1.49163059
C	1.49163059	1.49163059	1.49163059
C	-1.49163059	-1.49163059	1.49163059
C	1.49163059	1.49163059	-1.49163059
C	-1.49163059	-1.49163059	-1.49163059
C	1.49163059	-1.49163059	-1.49163059
C	-1.49163059	1.49163059	-1.49163059
O	2.14744811	-2.14744811	2.14744811
O	-2.14744811	2.14744811	2.14744811
O	-2.14744811	-2.14744811	2.14744811
O	2.14744811	2.14744811	2.14744811
O	-2.14744811	-2.14744811	-2.14744811
O	2.14744811	2.14744811	-2.14744811
O	-2.14744811	2.14744811	-2.14744811
O	2.14744811	-2.14744811	-2.14744811

$^1Yb(CO)_7$ BP86

Yb	0.05545800	0.02998200	0.00000000
C	-2.38797600	-0.08045700	0.00000000
C	-0.68892400	1.13415800	-2.03267900
C	0.02840900	-1.83380000	-1.57589600
C	2.37821400	-0.72048200	0.00000000
C	-0.68892400	1.13415800	2.03267900
C	0.02840900	-1.83380000	1.57589600
C	1.21416900	2.15801700	0.00000000
O	3.45777000	-1.12071300	0.00000000
O	0.02840900	-2.71486800	2.31451300
O	-1.06973200	1.63865500	2.99569900
O	-1.06973200	1.63865500	-2.99569900
O	0.02840900	-2.71486800	-2.31451300
O	-3.53719100	-0.12753300	0.00000000
O	1.76427300	3.16998000	0.00000000

$^3Yb(CO)_7$ BP86

Yb	0.00000000	0.00000000	-0.05061300
C	-1.65572000	0.95593000	1.47159100
C	1.65572000	0.95593000	1.47159100
C	0.00000000	2.36593400	-0.61562000
C	0.00000000	0.00000000	-2.47314900
C	0.00000000	-1.91186100	1.47159100
C	-2.04895900	-1.18296700	-0.61562000
C	2.04895900	-1.18296700	-0.61562000
O	0.00000000	0.00000000	-3.62486500
O	-3.02594400	-1.74703000	-0.84764000
O	0.00000000	-2.81736800	2.17985800
O	2.43991200	1.40868400	2.17985800
O	0.00000000	3.49405900	-0.84764000
O	-2.43991200	1.40868400	2.17985800
O	3.02594400	-1.74703000	-0.84764000

$^1Yb(CO)_7$ B3LYP

Yb	0.01896700	0.00280300	0.00000000
C	-2.51177800	0.05846000	0.00000000
C	-0.63514900	1.18668100	-2.12051500
C	-0.00022900	-1.88105400	-1.68753000
C	2.40451000	-0.78875100	0.00000000
C	-0.63514900	1.18668100	2.12051500
C	-0.00022900	-1.88105400	1.68753000
C	1.33740800	2.13183700	0.00000000
O	3.47438900	-1.17609800	0.00000000
O	-0.00022900	-2.72357800	2.44891700
O	-0.95326200	1.70541900	3.08180500
O	-0.95326200	1.70541900	-3.08180500
O	-0.00022900	-2.72357800	-2.44891700
O	-3.64745700	0.08404500	0.00000000
O	1.94455200	3.09424800	0.00000000

$^3Yb(CO)_7$ B3LYP

Yb	0.00000000	0.00000000	-0.01382400
C	-1.75983400	1.01604100	1.49304100
C	1.75983400	1.01604100	1.49304100
C	0.00000000	2.43056400	-0.64952000
C	0.00000000	0.00000000	-2.51685400
C	0.00000000	-2.03208100	1.49304100
C	-2.10493100	-1.21528200	-0.64952000
C	2.10493100	-1.21528200	-0.64952000
O	0.00000000	0.00000000	-3.65473600
O	-3.06456200	-1.76932600	-0.90790300
O	0.00000000	-2.94901600	2.16304200
O	2.55392300	1.47450800	2.16304200
O	0.00000000	3.53865200	-0.90790300
O	-2.55392300	1.47450800	2.16304200
O	3.06456200	-1.76932600	-0.90790300

$^1Yb(CO)_6$ BP86

Yb	0.00000000	0.00000000	0.00000000
C	0.00000000	1.74399500	1.67271200
C	-1.51034400	-0.87199700	1.67271200
C	-1.51034400	-0.87199700	-1.67271200
C	1.51034400	-0.87199700	1.67271200
C	0.00000000	1.74399500	-1.67271200
C	1.51034400	-0.87199700	-1.67271200
O	0.00000000	2.52744100	2.51831200
O	-2.18882800	-1.26372100	2.51831200
O	2.18882800	-1.26372100	2.51831200
O	0.00000000	2.52744100	-2.51831200
O	-2.18882800	-1.26372100	-2.51831200
O	2.18882800	-1.26372100	-2.51831200

$^3Yb(CO)_6$ BP86

Yb	0.00000000	0.00000000	0.30109900
C	0.00000000	2.34904800	0.94960700
C	2.03433600	-1.17452400	0.94960700
C	1.67055400	0.96449500	-1.16683900
C	-2.03433600	-1.17452400	0.94960700
C	-1.67055400	0.96449500	-1.16683900
C	0.00000000	-1.92898900	-1.16683900
O	0.00000000	3.48912700	1.12570100
O	3.02167200	-1.74456300	1.12570100
O	-3.02167200	-1.74456300	1.12570100
O	-2.47978800	1.43170600	-1.84098200
O	2.47978800	1.43170600	-1.84098200
O	0.00000000	-2.86341200	-1.84098200

^{1}Yb(CO)$_{6}$ B3LYP

Yb	0.00000000	0.00000000	0.00000000
C	0.00000000	1.79761200	1.72044700
C	-1.55677800	-0.89880600	1.72044700
C	-1.55677800	-0.89880600	-1.72044700
C	1.55677800	-0.89880600	1.72044700
C	0.00000000	1.79761200	-1.72044700
C	1.55677800	-0.89880600	-1.72044700
O	0.00000000	2.58548400	2.54189900
O	-2.23909500	-1.29274200	2.54189900
O	2.23909500	-1.29274200	2.54189900
O	0.00000000	2.58548400	-2.54189900
O	-2.23909500	-1.29274200	-2.54189900
O	2.23909500	-1.29274200	-2.54189900

^{3}Yb(CO)$_{6}$ B3LYP

Yb	0.00000000	0.00000000	0.00000000
C	0.00000000	2.23211900	1.14394100
C	1.93307200	-1.11606000	1.14394100
C	1.93307200	1.11606000	-1.14394100
C	-1.93307200	-1.11606000	1.14394100
C	-1.93307200	1.11606000	-1.14394100
C	0.00000000	-2.23211900	-1.14394100
O	0.00000000	3.27523600	1.59981300
O	2.83643800	-1.63761800	1.59981300
O	-2.83643800	-1.63761800	1.59981300
O	-2.83643800	1.63761800	-1.59981300
O	2.83643800	1.63761800	-1.59981300
O	0.00000000	-3.27523600	-1.59981300

^{2}Lu(CO)$_{8}$ B3LYP

Lu	0.00000000	0.00000000	0.00000000
C	-1.44454000	1.39967400	-1.39335400
C	1.44454000	-1.39967400	-1.39335400
C	-1.44454000	-1.39967400	-1.39335400
C	1.44454000	1.39967400	-1.39335400
C	1.44454000	-1.39967400	1.39335400
C	-1.44454000	1.39967400	1.39335400
C	1.44454000	1.39967400	1.39335400
C	-1.44454000	-1.39967400	1.39335400
O	2.12497900	-2.04658000	-2.03559300
O	-2.12497900	2.04658000	-2.03559300
O	2.12497900	2.04658000	-2.03559300
O	-2.12497900	-2.04658000	-2.03559300
O	-2.12497900	2.04658000	2.03559300
O	2.12497900	-2.04658000	2.03559300
O	-2.12497900	-2.04658000	2.03559300
O	2.12497900	2.04658000	2.03559300

^{4}Lu(CO)$_{8}$ B3LYP

Lu	0.00000000	0.00000000	0.00000000
C	0.00000000	1.99409300	1.43104000
C	0.00000000	-1.99409300	1.43104000
C	1.99409300	0.00000000	1.43104000
C	-1.99409300	0.00000000	1.43104000
C	1.41003600	-1.41003600	-1.43104000
C	-1.41003600	1.41003600	-1.43104000
C	-1.41003600	-1.41003600	-1.43104000
C	1.41003600	1.41003600	-1.43104000
O	0.00000000	-2.95525400	2.04375400
O	0.00000000	2.95525400	2.04375400
O	-2.95525400	0.00000000	2.04375400
O	2.95525400	0.00000000	2.04375400
O	-2.08968000	2.08968000	-2.04375400
O	2.08968000	-2.08968000	-2.04375400
O	2.08968000	2.08968000	-2.04375400
O	-2.08968000	-2.08968000	-2.04375400

^{2}Lu(CO)$_{7}$ B3LYP

Lu	0.00000000	0.00000000	0.03153495
C	0.00000000	0.00000000	2.43831137
C	1.92421800	-1.41053899	0.30499700
C	1.92421800	1.41053899	0.30499700
C	0.00000000	1.39741834	-1.88588551
C	-1.92421800	-1.41053899	0.30499700
C	-1.92421800	1.41053899	0.30499700
C	0.00000000	-1.39741834	-1.88588551
O	0.00000000	2.08332943	-2.79667779
O	-2.85273900	2.05223808	0.45512581
O	-2.85273900	-2.05223808	0.45512581
O	2.85273900	-2.05223808	0.45512581
O	2.85273900	2.05223808	0.45512581
O	0.00000000	0.00000000	3.57474817
O	0.00000000	-2.08332943	-2.79667779

^{4}Lu(CO)$_{7}$ B3LYP

Lu	0.00000000	0.00000000	0.06180700
C	1.51789200	0.87635500	-1.54195200
C	-1.51789200	0.87635500	-1.54195200
C	0.00000000	2.34833400	0.74868300
C	0.00000000	0.00000000	2.58691300
C	0.00000000	-1.75271100	-1.54195200
C	2.03371700	-1.17416700	0.74868300
C	-2.03371700	-1.17416700	0.74868300
O	0.00000000	0.00000000	3.72217600
O	3.00238400	-1.73342700	0.94697900
O	0.00000000	-2.48467600	-2.42232500
O	-2.15179200	1.24233800	-2.42232500
O	0.00000000	3.46685500	0.94697900
O	2.15179200	1.24233800	-2.42232500
O	-3.00238400	-1.73342700	0.94697900

^{2}Lu(CO)$_{6}$ B3LYP

Lu	0.00000000	0.00000000	0.21426800
C	1.72557800	1.56293400	0.68602200
C	-1.72557800	1.56293400	0.68602200
C	-1.72557800	-1.56293400	0.68602200
C	0.00000000	1.42030500	-1.63823100
C	1.72557800	-1.56293400	0.68602200
C	0.00000000	-1.42030500	-1.63823100
O	2.55391900	2.31812100	0.89229800
O	-2.55391900	2.31812100	0.89229800
O	0.00000000	2.12801800	-2.53577100
O	2.55391900	-2.31812100	0.89229800
O	-2.55391900	-2.31812100	0.89229800
O	0.00000000	-2.12801800	-2.53577100

^{4}Lu(CO)$_{6}$ B3LYP

Lu	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.38184300
C	0.00000000	2.38184300	0.00000000
C	-2.38184300	0.00000000	0.00000000
C	2.38184300	0.00000000	0.00000000
C	0.00000000	-2.38184300	0.00000000
C	0.00000000	0.00000000	-2.38184300
O	0.00000000	0.00000000	3.52131600
O	0.00000000	3.52131600	0.00000000
O	3.52131600	0.00000000	0.00000000
O	0.00000000	-3.52131600	0.00000000
O	-3.52131600	0.00000000	0.00000000
O	0.00000000	0.00000000	-3.52131600