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Table S1. Vibrational frequencies (cm^{-1}) for $[M(CO)_6]$ (M = Cr, Mo, W)

			Exp.[a] (vapor)	Exp.[a,b] (solution)	$\Delta\nu_S$[c]	BP86 ECP1	$\Delta\nu$[d]	BP86 ECP2	$\Delta\nu$[d]
$[Cr(CO)_6]$									
A_{1g}	ν_1	[CO]	2119	2112	- 7	2100	-19	2091	-28
A_{1g}	ν_2	[MC]	379	381	+ 2	401	22	397	18
E_g	ν_3	[CO]	2027	2018	- 9	2017	-10	2003	-24
E_g	ν_4	[MC]	391	394	+ 3	407	16	404	13
T_{1g}	ν_5	[δMCO]	364			358	- 6	365	1
T_{1u}	ν_6	[CO]	2000	1984	-16	1999	- 1	1983	-17
T_{1u}	ν_7	[δMCO]	668	665	- 3	691	23	688	20
T_{1u}	ν_8	[MC]	441	444	+ 3	458	17	458	17
T_{1u}	ν_9	[δCMC]	97	103	+ 6	103	6	98	1
T_{2g}	ν_{10}	[δMCO]	532			533	1	535	3
T_{2g}	ν_{11}	[δCMC]	90	101	+11	91	1	89	- 1
T_{2u}	ν_{12}	[δMCO]	511			521	10	520	9
T_{2u}	ν_{13}	[δCMC]	68			62	- 6	61	7
$[Mo(CO)_6]$									
A_{1g}	ν_1	[CO]	2121	2117	- 4	2102	- 9	2095	-26
A_{1g}	ν_2	[MC]	391	402	+11	416	25	412	21
E_g	ν_3	[CO]	2025	2019	- 6	2013	-12	2002	-23
E_g	ν_4	[MC]	381	392	+11	402	21	398	17
T_{1g}	ν_5	[δMCO]	342			341	- 1	340	- 2
T_{1u}	ν_6	[CO]	2003	1986	-17	1993	-10	1981	-22
T_{1u}	ν_7	[δMCO]	596	593	- 3	611	15	602	6
T_{1u}	ν_8	[MC]	367	367	0	396	29	389	22
T_{1u}	ν_9	[δCMC]	82	91	+ 9	88	6	81	- 1
T_{2g}	ν_{10}	[δMCO]	477			478	1	474	- 3
T_{2g}	ν_{11}	[δCMC]	79	91	+12	84	5	79	0
T_{2u}	ν_{12}	[δMCO]	507			516	9	513	6
T_{2u}	ν_{13}	[δCMC]	60			61	1	56	- 4
$[W(CO)_6]$									
A_{1g}	ν_1	[CO]	2126	2117	- 9	2102	-24	2095	-31
A_{1g}	ν_2	[MC]	426	427	+ 1	434	8	430	4
E_g	ν_3	[CO]	2021	2010	-11	2010	-11	1999	-22
E_g	ν_4	[MC]	410	412	+ 2	419	9	415	5
T_{1g}	ν_5	[δMCO]	362			349	-13	350	-12
T_{1u}	ν_6	[CO]	1998	1977	-21	1990	- 8	1977	-21
T_{1u}	ν_7	[δMCO]	587	583	- 4	588	1	581	- 6
T_{1u}	ν_8	[MC]	374	374	0	388	14	382	8
T_{1u}	ν_9	[δCMC]	82	92	+10	84	2	78	- 4
T_{2g}	ν_{10}	[δMCO]	482			472	-10	468	-14
T_{2g}	ν_{11}	[δCMC]	81	92	+11	86	5	81	0
T_{2u}	ν_{12}	[δMCO]	521			523	2	520	- 1
T_{2u}	ν_{13}	[δCMC]	61			62	1	56	- 5

a Reference 47.

b CCl_4 solution for M = Cr, Mo; CS_2 solution for M = W.

c $\Delta\nu_S$ = difference between the experimental gas phase and solution values.

d $\Delta\nu$ = difference between the calculated and the experimental gas phase values.

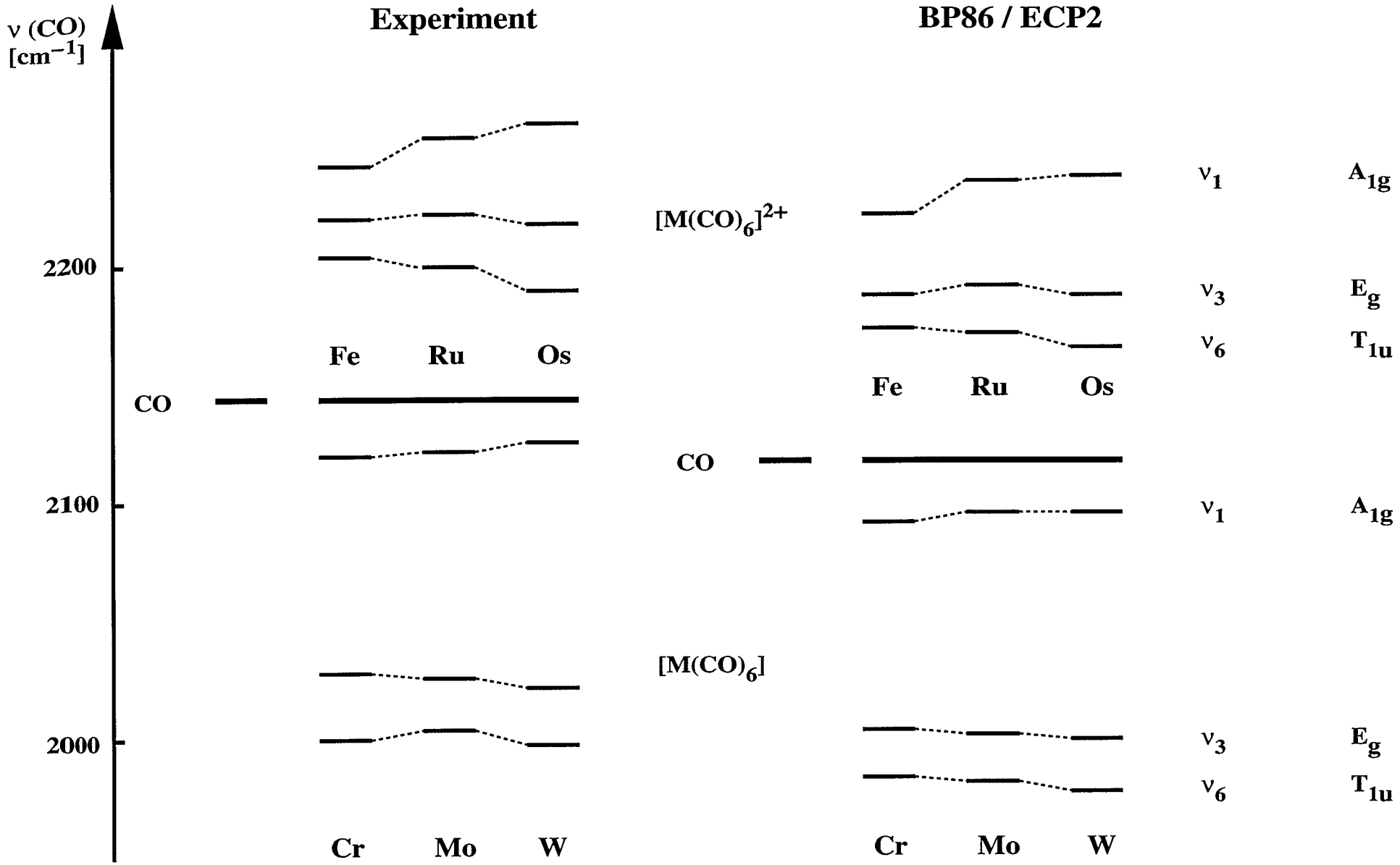

Figure S1. Experimental versus calculated CO stretching frequencies for $[M(CO)_6]$ (M = Cr, Mo, W) and $[M(CO)_6]^{2+}$ (M = Fe, Ru, Os). See Tables S1 and 5.