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

^a Reference 47.

^b CCl₄ solution for M = Cr, Mo; CS₂ solution for M = W.

^c Δv_s = difference between the experimental gas phase and solution values.

^d Δv = difference between the calculated and the experimental gas phase values.

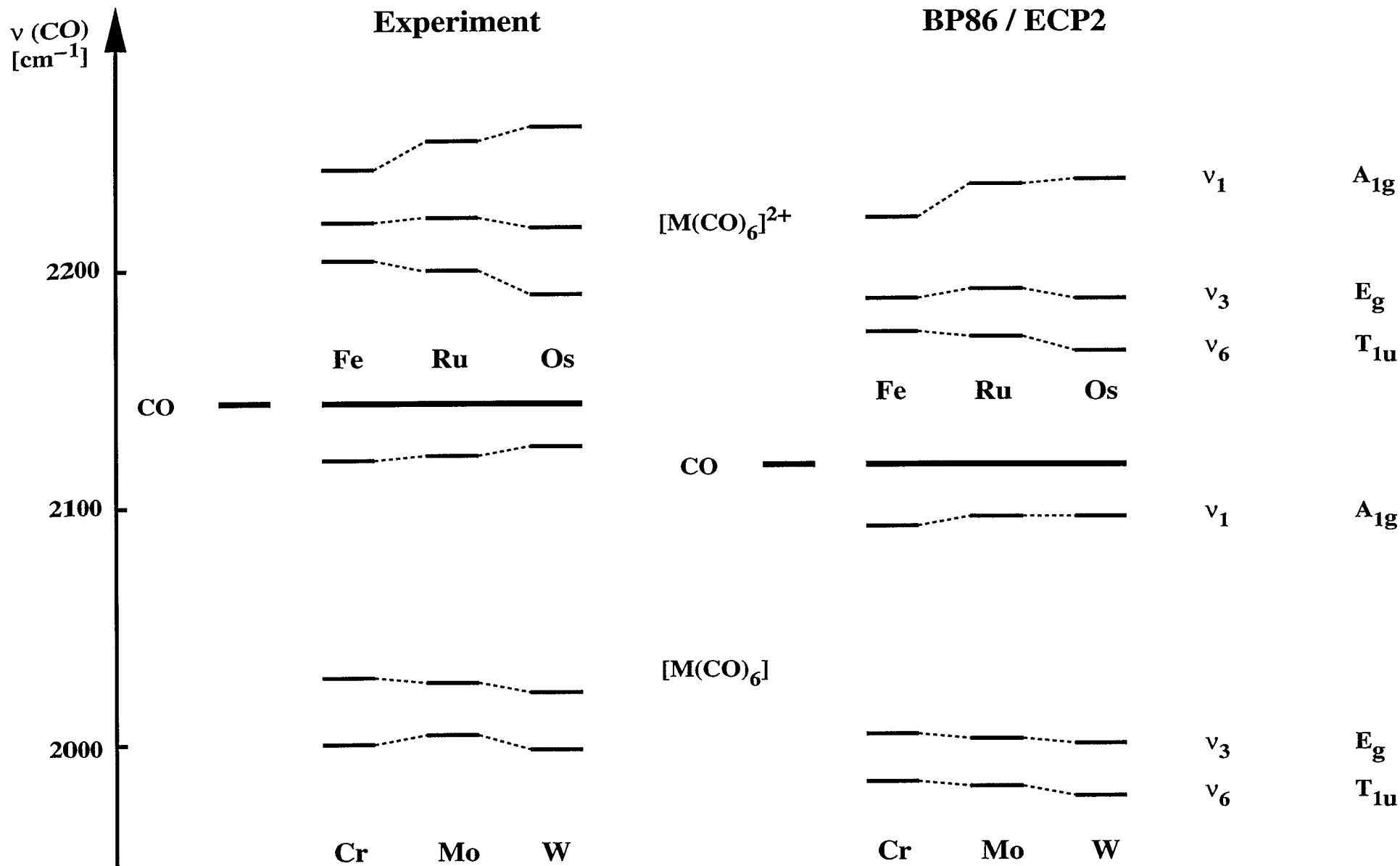


Figure S1. Experimental versus calculated CO stretching frequencies for $[\text{M}(\text{CO})_6]$ ($M = \text{Cr}, \text{Mo}, \text{W}$) and $[\text{M}(\text{CO})_6]^{2+}$ ($M = \text{Fe}, \text{Ru}, \text{Os}$). See Tables S1 and 5.