Supporting Information

Benchmarking the Fluxional Processes of Organometallic Piano Stool Complexes

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Table S1. Computed bond lengths from Cr to COT C atoms (in Å).

I (minimum)	Level of Theory	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
	PBE0/BS1	2.211	2.211	2.176	2.305	–	–	2.305	2.176
	PBE0/BS3	2.208	2.208	2.177	2.309	–	–	2.309	2.177
	PBEPBE/BS1	2.234	2.234	2.197	2.342	–	–	2.342	2.197
	PBEPBE/BS2	2.231	2.231	2.198	2.343	–	–	2.343	2.198
	PBEPBE/BS3	2.230	2.230	2.196	2.339	–	–	2.339	2.196
	B3LYP/BS1	2.260	2.260	2.235	2.410	–	–	2.410	2.235
	B3LYP/BS3	2.254	2.254	2.235	2.416	–	–	2.416	2.235
	B3LYP/BS4	2.260	2.260	2.235	2.408	–	–	2.408	2.235
	B3LYP/BS5	2.259	2.259	2.234	2.407	–	–	2.407	2.234
	B97-1/BS2	2.249	2.249	2.224	2.384	–	–	2.384	2.224
	B97-1/BS3	2.242	2.242	2.215	2.369	–	–	2.369	2.215
TS-1 (CO Rot.)	**Level of Theory**	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
	PBE0/BS1	2.213	2.213	2.187	2.265	–	–	2.265	2.187
	PBE0/BS3	2.209	2.209	2.186	2.264	–	–	2.264	2.186
	PBEPBE/BS1	2.237	2.237	2.211	2.303	–	–	2.303	2.211
	PBEPBE/BS2	2.232	2.232	2.208	2.301	–	–	2.301	2.208
	PBEPBE/BS3	2.230	2.230	2.196	2.339	–	–	2.339	2.196
	B3LYP/BS1	2.268	2.268	2.244	2.342	–	–	2.342	2.244
	B3LYP/BS3	2.262	2.262	2.240	2.338	–	–	2.338	2.240
	B3LYP/BS4	2.269	2.269	2.242	2.337	–	–	2.337	2.242
	B3LYP/BS5	2.267	2.267	2.242	2.336	–	–	2.336	2.242
	B97-1/BS2	2.253	2.253	2.229	2.312	–	–	2.312	2.229
	B97-1/BS3	2.244	2.244	2.220	2.301	–	–	2.301	2.220
TS-2 (1,3)	**Level of Theory**	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
	PBE0/BS1	2.145	2.145	2.219	–	–	–	–	2.219
	PBE0/BS3	2.147	2.147	2.228	–	–	–	–	2.228
	PBEPBE/BS1	2.167	2.167	2.263	–	–	–	–	2.263
	PBEPBE/BS2	2.167	2.167	2.265	–	–	–	–	2.265
	PBEPBE/BS3	2.168	2.168	2.268	–	–	–	–	2.268
	B3LYP/BS1	2.185	2.185	2.285	–	–	–	–	2.285
	B3LYP/BS3	2.184	2.184	2.290	–	–	–	–	2.290
	B3LYP/BS4	2.186	2.186	2.279	–	–	–	–	2.279

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	Level of Theory	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
	B3LYP/BS5	2.183	2.183	2.278	–	–	–	–	2.278
	B97-1/BS2	2.179	2.179	2.269	–	–	–	–	2.269
	B97-1/BS3	2.174	2.174	2.265	–	–	–	–	2.265
TS-3 (1,2)	**Level of Theory**	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
	PBE0/BS1	2.173	2.128	2.367	–	–	–	2.367	2.128
	PBE0/BS3	2.173	2.140	2.380	–	–	–	2.380	2.140
	PBEPBE/BS1	2.192	2.158	2.409	–	–	–	2.409	2.158
	PBEPBE/BS2	2.193	2.166	2.411	–	–	–	2.411	2.166
	PBEPBE/BS3	2.193	2.167	2.413	–	–	–	2.413	2.167
	B3LYP/BS1	2.206	2.176	2.442	–	–	–	2.442	2.176
	B3LYP/BS3	2.204	2.185	2.453	–	–	–	2.453	2.185
	B3LYP/BS4	2.207	2.180	2.440	–	–	–	2.440	2.180
	B3LYP/BS5	2.207	2.179	2.438	–	–	–	2.438	2.179
	B97-1/BS2	2.203	2.174	2.429	–	–	–	2.429	2.174
	B97-1/BS3	2.197	2.169	2.427	–	–	–	2.427	2.169
TS-4 (1,5)	**Level of Theory**	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
	PBE0/BS1	2.228	2.228	–	–	2.620	2.620	–	–
	PBE0/BS3	2.236	2.236	–	–	2.609	2.609	–	–
	PBEPBE/BS1	2.254	2.254	–	–	2.630	2.630	–	–
	PBEPBE/BS2	2.263	2.263	–	–	2.611	2.611	–	–
	PBEPBE/BS3	2.264	2.264	–	–	2.606	2.606	–	–
	B3LYP/BS1	2.288	2.288	–	–	2.706	2.706	–	–
	B3LYP/BS3	2.297	2.297	–	–	2.707	2.707	–	–
	B3LYP/BS4	2.295	2.295	–	–	2.697	2.697	–	–
	B3LYP/BS5	2.294	2.294	–	–	2.695	2.695	–	–
	B97-1/BS2	2.272	2.272	–	–	2.681	2.681	–	–
	B97-1/BS3	2.270	2.270	–	–	2.677	2.677	–	–
TS-5 (1,4)	**Level of Theory**	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8
	PBE0/BS1	2.167	2.259	–	–	2.164	–	–	2.259
	PBE0/BS3	2.175	2.272	–	–	2.175	–	–	2.272
	PBEPBE/BS1	2.193	2.291	–	–	2.212	–	–	2.292
	PBEPBE/BS2	2.198	2.300	–	–	2.231	–	–	2.300
	PBEPBE/BS3	2.199	2.302	–	–	2.233	–	–	2.302
	B3LYP/BS1	2.216	2.321	–	–	2.215	–	–	2.321
	B3LYP/BS3	2.221	2.331	–	–	2.228	–	–	2.331
	B3LYP/BS4	2.218	2.326	–	–	2.217	–	–	2.326
	B3LYP/BS5	2.215	2.326	–	–	2.220	–	–	2.325
	B97-1/BS2	2.214	2.319	–	–	2.210	–	–	2.319
	B97-1/BS3	2.207	2.310	–	–	2.204	–	–	2.310

Table S2. $\Delta G/\Delta G^{\ddagger}$ values for fluxional transition states of $(COT)Cr(CO)_3$ (in kcal mol^{-1}).

	PBE0/ BS1	PBE0/ BS3	PBEPBE/ BS1	PBEPBE/ BS2	PBEPBE/ BS3	B3LYP/ BS1	B3LYP/ BS3	B3LYP/ BS4	B3LYP/ BS5	B97-1/ BS2	B97-1/ BS3
I (minimum)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS-1 (CO-rot)	12.9	12.3	11.8	11.5	11.3	13.7	13.4	13.4	13.2	13.0	12.7
TS-2 (1,3)	13.5	13.1	12.3	12.3	12.4	9.1	8.5	9.1	8.8	9.7	10.3
TS-3 (1,2)	14.8	14.3	11.1	11.2	11.1	10.7	10.0	10.4	10.0	11.4	11.6
TS-4 (1,5)	23.3	24.2	22.2	22.6	23.5	16.9	17.7	17.0	17.1	18.6	20.5
TS-5 (1,4)	47.4	46.5	40.8	40.7	40.6	44.5	43.6	43.7	43.0	44.3	44.2

Table S3. $\Delta E_e/\Delta E_e^{\ddagger}$ values for fluxional transition states of $(COT)Cr(CO)_3$ (in kcal mol^{-1}).

	PBE0/ BS1	PBE0/ BS3	PBEPBE/ BS1	PBEPBE/ BS2	PBEPBE/ BS3	B3LYP/ BS1	B3LYP/ BS3	B3LYP/ BS4	B3LYP/ BS5	B97-1/ BS2	B97-1/ BS3	ccCA-TM
I (minimum)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS-1 (CO-rot)	12.6	12.0	11.6	11.0	11.2	13.3	12.9	13.0	12.7	12.5	12.2	11.0
TS-2 (1,3)	14.2	13.9	12.8	13.1	13.0	9.4	8.9	9.4	9.2	10.1	10.8	17.0
TS-3 (1,2)	16.8	16.3	12.7	12.9	12.9	12.3	11.6	12.0	11.7	13.2	13.5	18.8
TS-4 (1,5)	25.6	26.7	24.3	25.7	24.8	18.6	19.4	18.9	19.0	20.6	21.5	29.2
TS-5 (1,4)	48.9	47.9	42.7	42.6	42.8	46.5	45.5	45.6	44.9	46.1	45.9	47.4

Table S4. Raw Energies Utilized in Assessment of ccCA-TM Energies Using P Extrapolation (in a.u.).

	I (minimum)	TS-1 (CO-rot)	TS-2 (1,3)	TS-3 (1,2)	TS-4 (1,5)	TS-5 (1,4)
HF/aug-cc-pVTZ-DK	-1695.768876	-1695.746516	-1695.766307	-1695.752945	-1695.747831	-1695.704804
HF/aug-cc-pVQZ-DK	-1695.808584	-1695.786219	-1695.806079	-1695.792743	-1695.787631	-1695.744553
HF/CBS-DK	-1695.81826	-1695.795893	-1695.81577	-1695.80244	-1695.797329	-1695.754239
MP2/aug-cc-pVDZ-DK	-1698.109075	-1698.076155	-1698.056546	-1698.049605	-1698.071521	-1697.963276
MP2/aug-cc-pVTZ-DK	-1698.672971	-1698.64005	-1698.621527	-1698.613677	-1698.635623	-1698.527119
MP2/aug-cc-pVQZ-DK	-1698.859862	-1698.826771	-1698.808645	-1698.800487	-1698.823193	-1698.713826
MP2/CBS-DK + HF/CBS-DK (P)	-3.136330259	-3.125477818	-3.087719343	-3.092691233	-3.121012074	-3.05416263
MP2/cc-pVTZ-DK	-1698.61531	-1698.582505	-1698.565085	-1698.557464	-1698.577866	-1698.471052
CCSD(T)/cc-pVTZ-DK	-1698.722693	-1698.7046	-1698.698031	-1698.693904	-1698.675409	-1698.647357
CCSD(T)/aug-cc-pCVDZ-DK	-1698.259687	-1698.242006	-1698.232798	-1698.229627	-1698.211603	-1698.184003
CCSD(T,FC1)/aug-cc-pCVDZ-DK	-1699.123923	-1699.106407	-1699.095199	-1699.092212	-1699.073703	-1699.047402
D(CC)	-0.1073827	-0.1220958	-0.1329461	-0.1364394	-0.0975427	-0.1763049
D(CV)	-0.8642364	-0.8644015	-0.8624008	-0.8625851	-0.8620994	-0.8633987
ccCA-TM E_e (P)	-1699.926209	-1699.907868	-1699.898837	-1699.894156	-1699.877983	-1699.848105
scaled ZPE	0.159248635	0.158487913	0.15893827	0.157185185	0.157532442	0.156622985
ccCA-TM E_{ZPE} (P)	-1699.766961	-1699.74938	-1699.739898	-1699.736971	-1699.72045	-1699.691482

Table S5. $\Delta\Delta E_e/\Delta\Delta E_e^{\ddagger}$ values for fluxional transition states of $(COT)Cr(CO)_3$ and statistical parameters (R^2 = least squared regression, m = slope, b = y-intercept) in kcal mol^{-1} (relative to ccCA-TM).

	PBE0/ BS1	PBE0/ BS3	PBEPBE/ BS1	PBEPBE/ BS2	PBEPBE/ BS3	B3LYP/ BS1	B3LYP/ BS3	B3LYP/ BS4	B3LYP/ BS5	B97-1/ BS2	B97-1/ BS3
R^2	0.982	0.988	0.979	0.984	0.983	0.904	0.913	0.911	0.915	0.937	0.950
m	1.006 ± 0.069	0.998 ± 0.055	0.888 ± 0.065	0.898 ± 0.057	0.895 ± 0.059	0.925 ± 0.151	0.915 ± 0.142	0.912 ± 0.142	0.901 ± 0.137	0.933 ± 0.121	0.935 ± 0.107
b	−0.998 ± 1.739	−1.065 ± 1.398	−0.913 ± 1.657	−0.926 ± 1.438	−0.965 ± 1.502	−2.345 ± 3.827	−2.442 ± 3.592	−2.263 ± 3.604	−2.282 ± 3.480	−2.102 ± 3.080	−1.904 ± 2.710
I (minimum)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS-1 (CO-rot)	1.6	0.9	0.5	−0.1	0.2	2.3	1.9	2.0	1.7	1.4	1.1
TS-2 (1,3)	−2.8	−3.1	−4.2	−3.9	−4.0	−7.6	−8.1	−7.6	−7.8	−6.8	−6.2
TS-3 (1,2)	−2.0	−2.5	−6.1	−5.9	−5.9	−6.5	−7.2	−6.8	−7.1	−5.6	−5.3
TS-4 (1,5)	−3.6	−2.6	−5.0	−3.6	−4.4	−10.7	−9.8	−10.3	−10.3	−8.6	−7.7
TS-5 (1,4)	1.6	0.6	−4.6	−4.7	−4.6	−0.9	−1.9	−1.8	−2.4	−1.3	−1.5
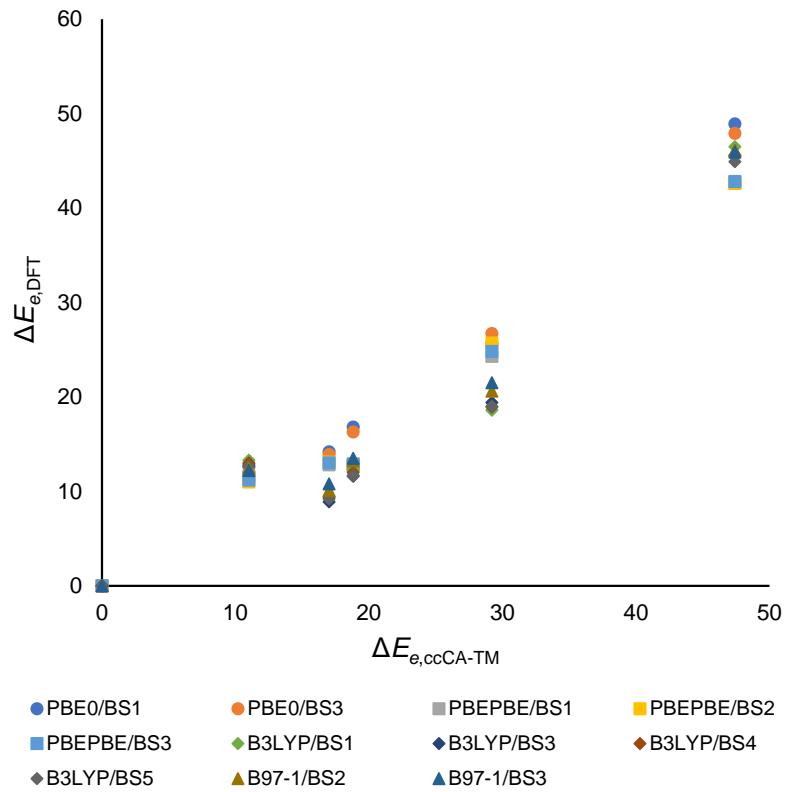
Figure S1. Plot of $\Delta E_{e,\text{DFT}}$ vs. $\Delta E_{e,\text{ccCA-TM}}$ (in kcal mol^{-1}) for (COT)Cr(CO)$_3$ computed at each level of theory.

Table S4. Experimental and computed bond lengths and angles for (TMCOT)Cr(CO)$_3$; computed bond lengths and angles for (TMCOT)Mo(CO)$_3$ and (TMCOT)W(CO)$_3$ (PBE0/BS1 level of theory). (M = Cr, Mo, W)

	(TMCOT)Cr(CO)$_3$		(TMCOT)Mo(CO)$_3$	(TMCOT)W(CO)$_3$
Bond length (Å)	Expt	Comp	Comp	Comp
M–C2	2.20	2.18	2.31	2.29
M–C3	2.29	2.25	2.39	2.36
M–C12	2.41	2.39	2.50	2.45
M–C13	2.21	2.18	2.31	2.29
M–C14	2.25	2.23	2.37	2.35
M–C15	2.23	2.22	2.35	2.33
M–C1	1.85	1.84	1.99	1.99
M–C8	1.86	1.83	1.99	1.99
M–C9	1.84	1.83	1.99	1.99
Bond angle (°)	Expt	Comp	Comp	Comp
C10–C11–C12	124.4	123.2	124.9	123.7
C11–C10–C3	121.0	120.0	121.4	120.1
C10–C3–C2	124.2	123.2	123.8	122.7
C3–C2–C15	125.1	125.0	125.6	124.9
C2–C15–C14	134.2	133.1	133.9	133.9
C1–M1–C8	94.2	93.0	91.5	92.1
C1–M1–C9	81.5	81.8	82.5	82.1
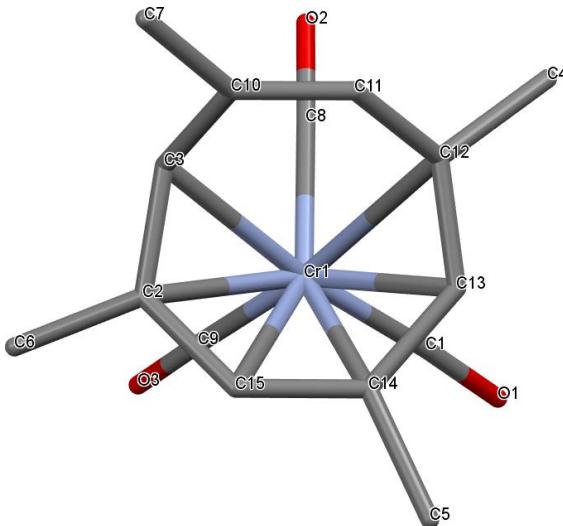
Figure S2. Top-down view of the reported crystal structure of (TMCOT)Cr(CO)$_3$ with atom labels. Hydrogens omitted for clarity.[2]
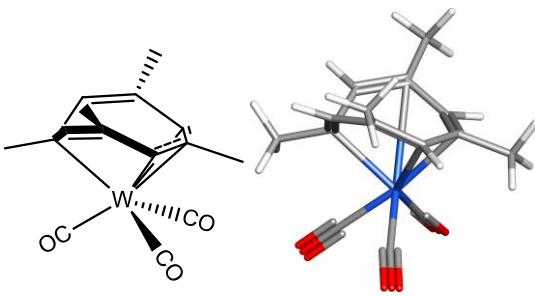
Figure S3. 2D and 3D representation of **TS-G**
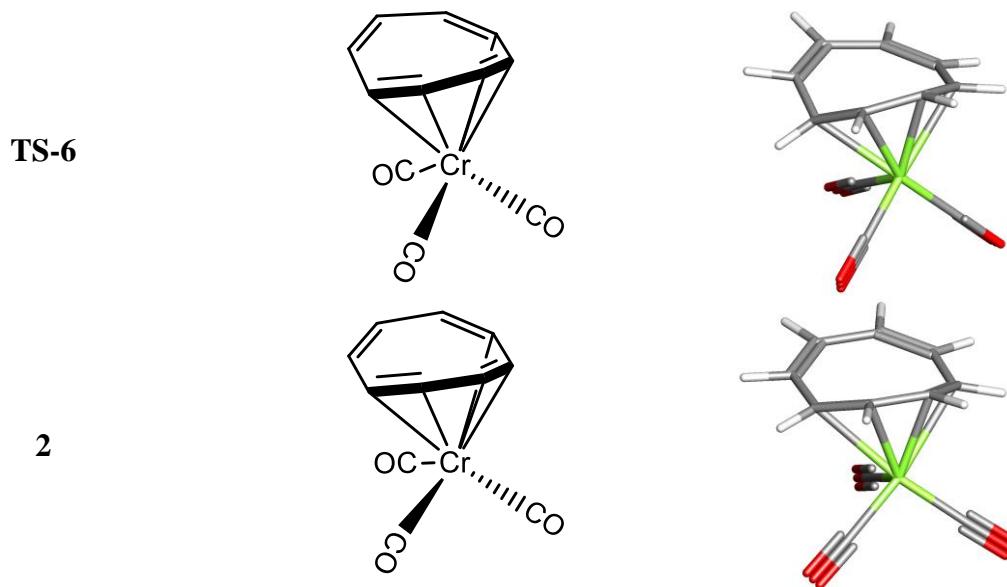
Figure S4. 2D and 3D representation of **TS-6** and **2**.

Table S7. $\Delta G^{\ddagger}_{\text{solution}}$ of (TMCOT)M(CO)$_3$ complexes with implicit chloroform solvation model at the SMD-PBE0//PBE0/BS1 level of theory (gas phase $\Delta G^{\ddagger}$ in parentheses). All relative free energies reported in kcal mol^{-1}.

Transition State	(TMCOT)Cr(CO)₃	(TMCOT)Mo(CO)₃	(TMCOT)W(CO)₃
TS-A (CO-rot)	12.8 (12.6)	13.6 (13.8)	11.7 (11.6)
TS-B (1,2-a)	14.0 (13.4)	13.9 (12.8)	14.5 (13.2)
TS-C (1,3)	18.3 (18.0)	21.1 (18.0)	27.0 (22.3)
TS-D (1,5)	23.2 (21.3)	25.7 (20.3)	33.2 (26.9)
TS-E (1,2-b)	20.9 (21.9)	22.0 (22.5)	24.0 (23.8)
TS-F (1,4)	47.4 (47.9)	47.9 (46.3)	48.5 (45.1)
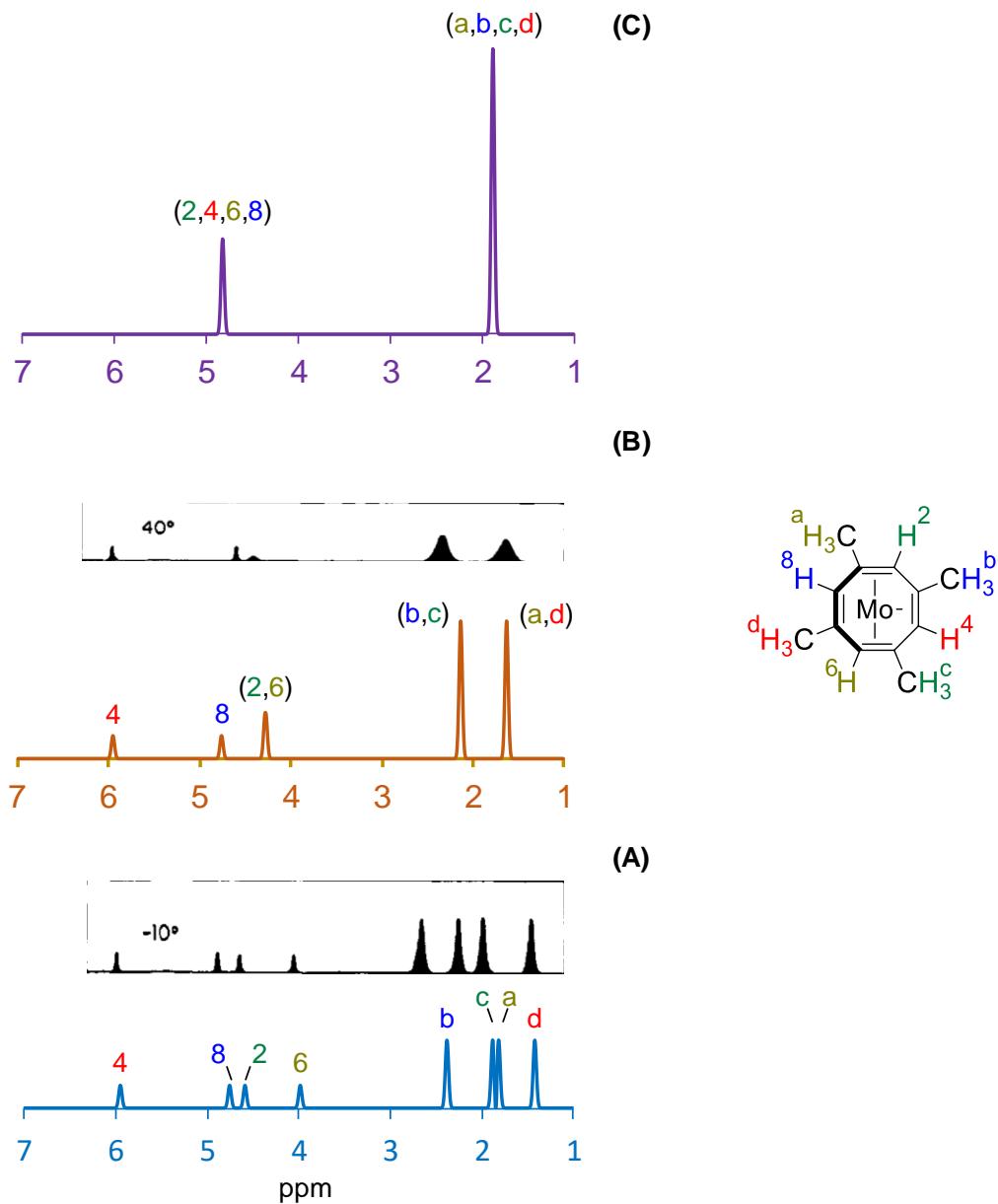
Figure S5. Simulated (colored) gas-phase and experimental (black) ^{1}H-NMR for the lowest energy structure of (TMCOT)Mo(CO)$_3$ at the GIAO-PBEPBE/BS6//PBEPBE/BS1 level of theory. Results given for low-temperature limit (**A**, −10° C), low temperature (**B**, 40° C), and high-temperature limit (**C**, >80° C). Experimental ^{1}H-NMR for high temperature limit not reported due to thermal decomposition of (TMCOT)Mo(CO)$_3$ above 80° C. Experimental spectra adapted in part with permission from Cotton, F. A.; Faller, J. W.; Musco, A. Stereochemically Nonrigid Organometallic Compounds. II. 1,3,5,7-Tetramethylcyclo-Octatetraenemolybdenum Tricarbonyl. *J. Am. Chem. Soc.* **1966**, *88* (19), 4506–4507. Copyright (1966) American Chemical Society.
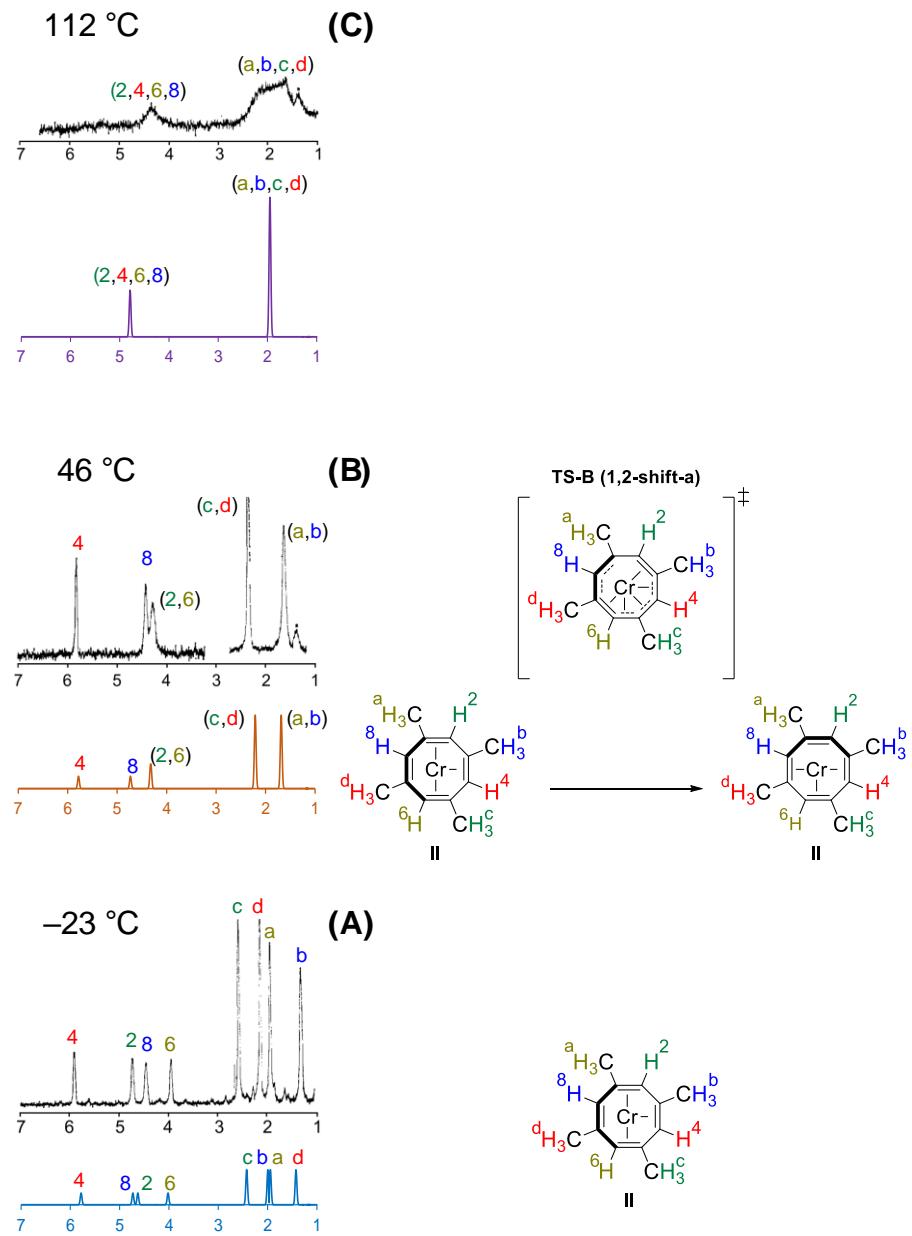
Figure S6. Simulated gas-phase (colored, GIAO-PBEPBE/BS6//PBEPBE/BS1) and experimental ^{1}H-NMR for (TMCOT)Cr(CO)$_3$ in three temperature regimes (A, B, C) with corresponding fluxional processes. (CO)$_3$ omitted for clarity. All chemical shifts are relative to tetramethylsilane (TMS). Experimental spectra adapted in part with permission from Cotton, F. A.; Faller, J. W.; Musco, A., Stereochemically nonrigid organometallic molecules. XII. Temperature dependence of the proton nuclear magnetic resonance spectra of the 1,3,5,7-tetramethylcyclooctatetraene tricarbonyl compounds of chromium, molybdenum, and tungsten *J. Am. Chem. Soc.*, **1968**, *90* (6), 1438-1444. Copyright (1968) American Chemical Society.

Table S8. Experimental and computed ^{1}H-NMR chemical shifts in (TMCOT)Cr(CO)$_3$ and (TMCOT)Mo(CO)$_3$ at the GIAO-PBEPBE/BS6//PBEPBE/auto/BS1 level of theory (measured in ppm; relative to TMS).

	(TMCOT)Cr(CO)$_3$		(TMCOT)Mo(CO)$_3$	
Low-temperature limit	**Expt (–23 °C)**	**Comp**	**Expt (–10 °C)**	**Comp**
H(2)	4.7	4.6	4.9	4.8
H(8)	4.3	4.7	4.6	4.6
H(4)	5.9	5.8	6.0	5.9
H(6)	3.9	4.0	4.0	4.0
CH$_3$(a)	2.6	2.4	1.4	1.4
CH$_3$(b)	1.9	1.9	1.9	1.8
CH$_3$(c)	1.3	1.4	2.6	2.3
CH$_3$(d)	2.1	2.0	2.2	1.9
Low temperature	**Exp (46 °C)**	**Comp**	**Exp (40 °C)**	**Comp**
Average of H(2, 6)	4.2	4.3	4.4	4.3
H(8)	4.4	4.7	4.6	4.8
H(4)	5.6	5.8	6.0	5.9
Average of CH$_3$(a, b)	2.3	2.2	1.7	1.6
Average of CH$_3$(c, d)	1.6	1.7	2.4	2.1
High-temperature limit	**Exp (112 °C)**	**Comp**	**Exp (> 80 °C)**	**Comp**
Average of H(2, 4, 6, 8)	4.3	4.8	–	4.8
Average of CH$_3$(a, b, c, d)	1.9	2.0	–	1.9
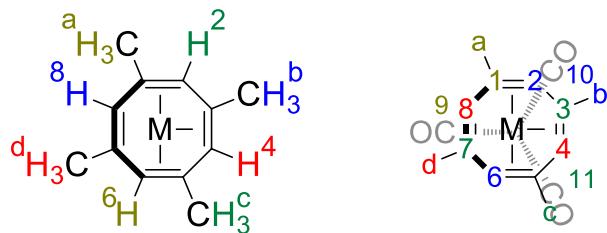
Figure S7. 2D-representation of (TMCOT)M(CO)$_3$ (M = Cr, Mo) with hydrogens labelled. (CO)$_3$ omitted for clarity.

Table S9. Computed chemical shifts for ^{13}C-NMR in (TMCOT)Cr(CO)$_3$ at the GIAO-PBEPBE/BS6//PBEPBE/auto/BS1 (relative to TMS). See Figure S for appropriate atom labelling.

Chemical Shift (ppm)	C(1)	C(2)	C(3)	C(4)	C(5)	C(6)	C(7)	C(8)	C(9)	C(10)	C(11)	C(a)	C(b)	C(c)	C(d)
Expt.	114.2	104.7	112.0	106.7	112.9	89.5	139.8	126.3	–	–	–	26.7	29.5	31.6	23.2
Comp.	123.7	111.6	120.3	113.4	121.8	98.4	150.6	134.7	245.3	226.6	245.3	29.5	33.9	35.0	25.8

*Experimental ^{13}C chemical shifts reported at –24 °C. No experimental ^{13}C chemical shift for CO groups were reported.

Table S10. Basis Sets Used in Study

Basis Set	
BS1	6-31G(d') for H, C, O mod-LANL2DZ(f) with ECP for transition metals
BS2	6-311++G(2df,2p) for H, C, O mod-LANL2TZ uncontracted to [4s4p3d] for Cr
BS3	cc-pVTZ for all atoms
BS4	aug-cc-pVDZ for H, C, O LANL2DZ with LANL2DZ ECP for Cr
BS5	aug-cc-pVDZ for H, C, O SDD with ECP for Cr
BS6	IGLO-II for H, C, O LANL08 with ECP for Cr, Mo LANl2DZ with ECP for Si

Molecular Coordinates for (COT)Cr(CO)₃ (Å)

PBE0/BS1

```
I
Cr    -0.047386  -0.350179   0.000000
C      1.792849  -0.230768   0.000000
O      2.936391  -0.104733   0.000000
C     -0.033948  -1.738162   1.212834
O     -0.011026  -2.634624   1.935405
C     -0.033948  -1.738162  -1.212834
O     -0.011026  -2.634624  -1.935405
C      0.388442   2.672437  -0.662865
C      0.251721   1.424132  -1.441166
C     -0.951791   0.746798  -1.646664
C     -1.985007   0.450346  -0.703748
C     -1.985007   0.450346   0.703748
C     -0.951791   0.746798   1.646664
C      0.251721   1.424132   1.441166
C      0.388442   2.672437   0.662865
H      0.465661   3.601360  -1.231928
H      0.961541   1.313251  -2.263119
H     -1.078535   0.227227  -2.597455
H     -2.832431  -0.084766  -1.131544
H     -2.832431  -0.084766   1.131544
H     -1.078535   0.227227   2.597455
H      0.961541   1.313251   2.263119
H      0.465661   3.601360   1.231928
       el energy= -735.149798374
             zpe= -734.986335
       th energy= -734.972586
     th enthalpy= -734.971641
     free energy= -735.026599


TS-1
Cr     0.310131   0.000000   0.018983
C      1.095356   1.232989  -1.097863
O      1.579159   2.013491  -1.793251
C      1.867616   0.000023   1.021824
O      2.830923   0.000037   1.649063
C      1.095361  -1.233030  -1.097816
O      1.579165  -2.013555  -1.793176
C     -2.706384  -0.661238  -0.645047
C     -1.420389  -1.375048  -0.475073
C     -0.885885  -1.651973   0.807857
C     -0.706449  -0.715281   1.849466
C     -0.706448   0.715333   1.849446
C     -0.885884   1.651996   0.807811
C     -1.420389   1.375036  -0.475111
C     -2.706384   0.661222  -0.645065
H     -3.618362  -1.257784  -0.723130
H     -1.251502  -2.176911  -1.197722
H     -0.417549  -2.619525   0.993061
H     -0.251507  -1.131364   2.748264
H     -0.251505   1.131441   2.748232
H     -0.417546   2.619553   0.992988
H     -1.251501   2.176878  -1.197783
H     -3.618362   1.257767  -0.723164
       el energy= -735.129678719
             zpe= -734.967003
       th energy= -734.954009
     th enthalpy= -734.953065
     free energy= -735.006011


TS-2
Cr     0.034057  -0.437936   0.000000
C     -1.170854  -0.998304   1.314095
O     -1.908003  -1.368251   2.111953
C     -1.170854  -0.998304  -1.314095
```

```
O     -1.908003  -1.368251  -2.111953
C      0.755537  -2.086267   0.000000
O      1.240084  -3.134776   0.000000
C     -0.040607   1.940984   1.663419
C      0.892715   0.810886   1.620733
C      1.877254   0.396858   0.713294
C      1.877254   0.396858  -0.713294
C      0.892715   0.810886  -1.620733
C     -0.040607   1.940984  -1.663419
C     -0.628680   2.720011  -0.729171
C     -0.628680   2.720011   0.729171
H     -0.353890   2.155900   2.685102
H      1.062675   0.403114   2.616229
H      2.633728  -0.261324   1.139553
H      2.633728  -0.261324  -1.139553
H      1.062675   0.403114  -2.616229
H     -0.353890   2.155900  -2.685102
H     -1.293090   3.478852  -1.141779
H     -1.293090   3.478852   1.141779
       el energy= -735.127176234
             zpe= -734.964222
       th energy= -734.950597
     th enthalpy= -734.949653
     free energy= -735.005093


TS-3
Cr    -0.010092  -0.469499   0.000000
C      1.869771  -0.409652   0.000000
O      3.013836  -0.349533   0.000000
C     -0.075570  -1.842036   1.217733
O     -0.114803  -2.726831   1.955049
C     -0.075570  -1.842036  -1.217733
O     -0.114803  -2.726831  -1.955049
C     -2.047149   0.285865   0.000000
C     -1.438474   0.489015   1.253561
C     -0.271033   1.222752   1.633620
C      0.246108   2.472932   1.228887
C      0.315174   3.120576   0.000000
C      0.246108   2.472932  -1.228887
C     -0.271033   1.222752  -1.633620
C     -1.438474   0.489015  -1.253561
H     -2.941106  -0.334294   0.000000
H     -1.926046  -0.033705   2.076872
H      0.050886   0.947388   2.637906
H      0.769443   2.998010   2.032970
H      0.761750   4.111780   0.000000
H      0.769443   2.998010  -2.032970
H      0.050886   0.947388  -2.637906
H     -1.926046  -0.033705  -2.076872
       el energy= -735.122989876
             zpe= -734.961852
       th energy= -734.947906
     th enthalpy= -734.946962
     free energy= -735.003058


TS-4
Cr    -0.059206   0.442055   0.000000
C     -1.592175   1.483257   0.000000
O     -2.513954   2.173374   0.000000
C      0.622660   1.559141   1.241339
O      1.065784   2.265894   2.043411
C      0.622660   1.559141  -1.241339
O      1.065784   2.265894  -2.043411
C     -1.494592  -1.642534  -0.677706
C     -0.462542  -2.152853  -1.587956
C      0.844500  -1.831234  -1.594021
C      1.561781  -0.919414  -0.694092
```

```
C      1.561781 -0.919414  0.694092
C      0.844500 -1.831234  1.594021
C     -0.462542 -2.152853  1.587956
C     -1.494592 -1.642534  0.677706
H     -2.403613 -1.285322 -1.165611
H     -0.836591 -2.771133 -2.405419
H      1.442166 -2.212310 -2.424329
H      2.383741 -0.384948 -1.169089
H      2.383741 -0.384948  1.169089
H      1.442166 -2.212310  2.424329
H     -0.836591 -2.771133  2.405419
H     -2.403613 -1.285322  1.165611
      el energy= -735.108933361
            zpe= -734.947626
       th energy= -734.933504
     th enthalpy= -734.932560
      free energy= -734.989541

TS-5
Cr     0.382049 -0.000318 -0.332554
C      1.366445 -1.528776 -0.546299
O      2.013263 -2.459863 -0.745464
C      1.423902 -0.000347  1.149780
O      2.111739 -0.000431  2.080484
C      1.368345  1.526906 -0.547007
O      2.016342  2.457104 -0.746435
C     -1.292121  1.290430 -1.128948
C     -1.295978  0.000872 -1.703259
C     -1.293409 -1.288798 -1.129173
C     -1.907995 -1.770460  0.121396
C     -1.636945 -1.237009  1.316672
C     -0.807391  0.000139  1.475153
C     -1.634994  1.238582  1.317114
C     -1.905475  1.772686  0.121957
H     -1.077127  2.078884 -1.851388
H     -0.890172  0.000822 -2.721611
H     -1.079138 -2.077354 -1.851718
H     -2.538245 -2.657651  0.046002
H     -2.060099 -1.680718  2.220206
H     -0.370478 -0.000409  2.479004
H     -2.056943  1.683104  2.220809
H     -2.534016  2.661121  0.046997
      el energy= -735.071838896
            zpe= -734.910833
       th energy= -734.897253
     th enthalpy= -734.896309
      free energy= -734.951098

TS-6
Cr    -0.766299  0.012947 -0.319934
C     -0.232826  0.011821  1.424946
O      0.080115  0.082902  2.530281
C     -1.605469  1.622479  0.122030
O     -2.079781  2.613259  0.456454


PBE0/BS3
I
Cr    -0.045253 -0.347029  0.000000
C      1.809447 -0.235706  0.000000
O      2.948540 -0.120341  0.000000
C     -0.040733 -1.746705  1.213008
O     -0.023974 -2.647616  1.922416
C     -0.040733 -1.746705 -1.213008
O     -0.023974 -2.647616 -1.922416
C      0.394486  2.669977 -0.658862
C      0.244461  1.432614 -1.441695
C     -0.953293  0.756568 -1.641569
C     -1.978682  0.457504 -0.701031
C     -1.978682  0.457504  0.701031
```

```
C     -2.192608 -1.054599  0.071969
O     -3.082539 -1.764261  0.259676
C      1.997524 -1.599727  0.477649
C      0.694821 -1.743794 -0.204947
C      0.337352 -1.313294 -1.493495
C      0.510007  0.005816 -2.023413
C      0.923385  1.202759 -1.430154
C      1.881882  1.564768 -0.391712
C      2.708394  0.854510  0.410969
C      2.841311 -0.567681  0.673283
H      2.328369 -2.549991  0.900303
H      0.200407 -2.673267  0.077919
H     -0.311768 -1.963662 -2.079582
H     -0.072897  0.166812 -2.935160
H      0.615176  2.070242 -2.012844
H      1.967870  2.646558 -0.289809
H      3.385575  1.463271  1.010365
H      3.753458 -0.822403  1.213194
      el energy= -735.109479356
            zpe= -734.947345
       th energy= -734.933640
     th enthalpy= -734.932696
      free energy= -734.988047

2
Cr    -0.875553  0.000033 -0.304650
C     -0.184098 -0.000025  1.409215
O      0.232186  0.000032  2.484271
C     -2.009346  1.425034  0.142342
O     -2.676839  2.326929  0.409551
C     -2.009994 -1.424474  0.142151
O     -2.677856 -2.326127  0.409267
C      2.034607 -1.663496  0.043727
C      0.883018 -1.630800 -0.858883
C      0.433302 -0.722114 -1.817720
C      0.433412  0.721329 -1.817999
C      0.883440  1.630420 -0.859707
C      2.034831  1.663298  0.043087
C      2.877753  0.726626  0.547517
C      2.877693 -0.726773  0.547749
H      2.266229 -2.684222  0.349721
H      0.476162 -2.628785 -1.018201
H     -0.200522 -1.155691 -2.595440
H     -0.200430  1.154615 -2.595877
H      0.476726  2.628378 -1.019513
H      2.266478  2.684105  0.348803
H      3.690494  1.140884  1.144132
H      3.690502 -1.140900  1.144364
      el energy= -735.896316253
            zpe= -735.735743
       th energy= -735.720950
     th enthalpy= -735.720006
      free energy= -735.778222


C     -0.953293  0.756568  1.641569
C      0.244461  1.432614  1.441695
C      0.394486  2.669977  0.658862
H      0.485774  3.596241 -1.221298
H      0.944533  1.330614 -2.266691
H     -1.087278  0.252302 -2.593810
H     -2.828136 -0.065143 -1.127794
H     -2.828136 -0.065143  1.127794
H     -1.087278  0.252302  2.593810
H      0.944533  1.330614  2.266691
H      0.485774  3.596241  1.221298
      el energy= -1693.41122721
            zpe= -1693.248461
```

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```
      th energy= -1693.234711
   th enthalpy= -1693.233767
    free energy= -1693.288845

TS-1
Cr   -0.022176 -0.307633  0.000000
C     1.098150 -1.101654  1.240198
O     1.789672 -1.589054  2.014344
C    -1.032211 -1.874149  0.000000
O    -1.648874 -2.837940  0.000000
C     1.098150 -1.101654 -1.240198
O     1.789672 -1.589054 -2.014344
C     0.659856  2.697981 -0.657193
C     0.471657  1.421958 -1.374191
C    -0.809403  0.896086 -1.645781
C    -1.845105  0.716888 -0.712255
C    -1.845105  0.716888  0.712255
C    -0.809403  0.896086  1.645781
C     0.471657  1.421958  1.374191
C     0.659856  2.697981  0.657193
H     0.754212  3.606867 -1.247713
H     1.185965  1.254784 -2.177149
H    -1.003388  0.449226 -2.616188
H    -2.746845  0.279796 -1.128177
H    -2.746845  0.279796  1.128177
H    -1.003388  0.449226  2.616188
H     1.185965  1.254784  2.177149
H     0.754212  3.606867  1.247713
       el energy= -1693.39215710
              zpe= -1693.230127
       th energy= -1693.217163
    th enthalpy= -1693.216219
     free energy= -1693.269197

TS-2
Cr    0.040766 -0.434714  0.000000
C    -1.163135 -1.022661  1.319652
O    -1.886009 -1.416544  2.111424
C    -1.163135 -1.022661 -1.319652
O    -1.886009 -1.416544 -2.111424
C     0.778068 -2.083933  0.000000
O     1.261671 -3.127869  0.000000
C    -0.064241  1.945093  1.654793
C     0.890589  0.842028  1.615448
C     1.871545  0.434609  0.709825
C     1.871545  0.434609 -0.709825
C     0.890589  0.842028 -1.615448
C    -0.064241  1.945093 -1.654793
C    -0.664046  2.709675 -0.725799
C    -0.664046  2.709675  0.725799
H    -0.383148  2.152262  2.671597
H     1.072535  0.449911  2.609737
H     2.645860 -0.192914  1.137438
H     2.645860 -0.192914 -1.137438
H     1.072535  0.449911 -2.609737
H    -0.383148  2.152262 -2.671597
H    -1.341534  3.450472 -1.138037
H    -1.341534  3.450472  1.138037
       el energy= -1693.38908154
              zpe= -1693.226883
       th energy= -1693.213236
    th enthalpy= -1693.212292
     free energy= -1693.267947

TS-3
Cr   -0.007357 -0.457183  0.000000
C     1.891484 -0.424342  0.000000
O     3.031051 -0.400048  0.000000
C    -0.083945 -1.841810  1.215821
O    -0.133269 -2.734442  1.935118
```

```
C    -0.083945 -1.841810 -1.215821
O    -0.133269 -2.734442 -1.935118
C    -2.046099  0.294569  0.000000
C    -1.450199  0.507815  1.250921
C    -0.295146  1.242843  1.640601
C     0.261938  2.463792  1.226644
C     0.362381  3.097465  0.000000
C     0.261938  2.463792 -1.226644
C    -0.295146  1.242843 -1.640601
C    -1.450199  0.507815 -1.250921
H    -2.941166 -0.315361  0.000000
H    -1.943490 -0.005085  2.069920
H     0.008071  0.977109  2.648366
H     0.795292  2.974992  2.026653
H     0.843517  4.067334  0.000000
H     0.795292  2.974992 -2.026653
H     0.008071  0.977109 -2.648366
H    -1.943490 -0.005085 -2.069920
       el energy= -1693.38518754
              zpe= -1693.224728
       th energy= -1693.210764
    th enthalpy= -1693.209820
     free energy= -1693.266117

TS-4
Cr   -0.059766  0.432854  0.000000
C    -1.590165  1.490371  0.000000
O    -2.493972  2.196050  0.000000
C     0.625629  1.561029  1.237165
O     1.068321  2.278677  2.023189
C     0.625629  1.561029 -1.237165
O     1.068321  2.278677 -2.023189
C    -1.492124 -1.641567 -0.674166
C    -0.468583 -2.142594 -1.588334
C     0.834182 -1.834722 -1.593424
C     1.561109 -0.944293 -0.690853
C     1.561109 -0.944293  0.690853
C     0.834182 -1.834722  1.593424
C    -0.468583 -2.142594  1.588334
C    -1.492124 -1.641567  0.674166
H    -2.403672 -1.297706 -1.156197
H    -0.847202 -2.740625 -2.412519
H     1.421085 -2.206499 -2.429524
H     2.385519 -0.421255 -1.162725
H     2.385519 -0.421255  1.162725
H     1.421085 -2.206499  2.429524
H    -0.847202 -2.740625  2.412519
H    -2.403672 -1.297706  1.156197
       el energy= -1693.36874019
              zpe= -1693.208124
       th energy= -1693.193999
    th enthalpy= -1693.193055
     free energy= -1693.250206

TS-5
Cr    0.339404  0.383199  0.000000
C     0.554602  1.394439  1.522448
O     0.735601  2.045680  2.447702
C    -1.154829  1.420179  0.000000
O    -2.086286  2.098804  0.000000
C     0.554602  1.394439 -1.522448
O     0.735601  2.045680 -2.447702
C     1.128399 -1.316018 -1.286005
C     1.693993 -1.317967  0.000000
C     1.128399 -1.316018  1.286005
C    -0.125317 -1.908234  1.771444
C    -1.312381 -1.642561  1.237100
C    -1.470701 -0.822788  0.000000
C    -1.312381 -1.642561 -1.237100
C    -0.125317 -1.908234 -1.771444
```

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```
H     1.853203 -1.116452 -2.069044
H     2.720663 -0.947563  0.000000
H     1.853203 -1.116452  2.069044
H    -0.056678 -2.526552  2.661990
H    -2.212670 -2.053992  1.686678
H    -2.467830 -0.384583  0.000000
H    -2.212670 -2.053992 -1.686678
```
PBEPBE/auto/BS1
```
I
Cr   -0.053397 -0.352388  0.000000
C     1.791775 -0.274455  0.000000
O     2.956245 -0.192955  0.000000
C    -0.060357 -1.753806  1.195051
O    -0.044046 -2.681154  1.908587
C    -0.060357 -1.753806 -1.195051
O    -0.044046 -2.681154 -1.908587
C     0.429587  2.700629 -0.668771
C     0.272816  1.453148 -1.455678
C    -0.946660  0.777454 -1.659266
C    -1.992670  0.501223 -0.709596
C    -1.992670  0.501223  0.709596
C    -0.946660  0.777454  1.659266
C     0.272816  1.453148  1.455678
C     0.429587  2.700629  0.668771
H     0.528432  3.636203 -1.240363
H     0.987986  1.329244 -2.282275
H    -1.083831  0.258859 -2.618499
H    -2.856074 -0.023130 -1.140303
H    -2.856074 -0.023130  1.140303
H    -1.083831  0.258859  2.618499
H     0.987986  1.329244  2.282275
H     0.528432  3.636203  1.240363
     el energy= -735.218624797
           zpe= -735.061293
     th energy= -735.047063
   th enthalpy= -735.046119
   free energy= -735.102078
```
TS-1
```
Cr   -0.311404  0.000036 -0.028314
C    -1.133581  1.222759  1.072975
O    -1.666240  1.997377  1.769280
C    -1.861648 -0.001347 -1.039936
O    -2.847917 -0.002109 -1.665224
C    -1.132487 -1.221230  1.075343
O    -1.664406 -1.995115  1.773037
C     2.730094 -0.666608  0.699252
C     1.447012 -1.390853  0.498937
C     0.922657 -1.663826 -0.801345
C     0.759318 -0.721048 -1.854705
C     0.759421  0.719775 -1.855200
C     0.922776  1.663248 -0.802473
C     1.447045  1.391505  0.498090
C     2.730071  0.667365  0.699049
H     3.648452 -1.265788  0.802213
H     1.255953 -2.195547  1.225164
H     0.455038 -2.639620 -0.994742
H     0.319494 -1.141625 -2.768830
H     0.319664  1.139691 -2.769656
H     0.455182  2.638885 -0.996738
H     1.255928  2.196895  1.223521
```

```
H    -0.056678 -2.526552 -2.661990
     el energy= -1693.33486428
           zpe= -1693.174562
     th energy= -1693.160999
   th enthalpy= -1693.160055
   free energy= -1693.214782
```

```
H     3.648411  1.266589  0.801927
     el energy= -735.200181685
           zpe= -735.043660
     th energy= -735.030153
   th enthalpy= -735.029208
   free energy= -735.083254
```

TS-2
```
Cr    0.027808 -0.444925  0.000000
C    -1.129959 -1.074035  1.320346
O    -1.849495 -1.509754  2.127971
C    -1.129959 -1.074035 -1.320346
O    -1.849495 -1.509754 -2.127971
C     0.786000 -2.068672  0.000000
O     1.293757 -3.127992  0.000000
C    -0.084169  1.990242  1.675048
C     0.870729  0.874502  1.634465
C     1.862184  0.457328  0.718644
C     1.862184  0.457328 -0.718644
C     0.870729  0.874502 -1.634465
C    -0.084169  1.990242 -1.675048
C    -0.682087  2.774580 -0.730871
C    -0.682087  2.774580  0.730871
H    -0.411247  2.196544  2.703100
H     1.043012  0.461023  2.636244
H     2.635654 -0.190912  1.150443
H     2.635654 -0.190912 -1.150443
H     1.043012  0.461023 -2.636244
H    -0.411247  2.196544 -2.703100
H    -1.358380  3.532760 -1.147741
H    -1.358380  3.532760  1.147741
     el energy= -735.198189551
           zpe= -735.041114
     th energy= -735.027043
   th enthalpy= -735.026098
   free energy= -735.082544
```

TS-3
```
Cr   -0.006078 -0.478057  0.000000
C     1.872407 -0.466279  0.000000
O     3.036203 -0.455748  0.000000
C    -0.104528 -1.864087  1.192002
O    -0.163964 -2.783061  1.916844
C    -0.104528 -1.864087 -1.192002
O    -0.163964 -2.783061 -1.916844
C    -2.043439  0.332011  0.000000
C    -1.431605  0.533175  1.265595
C    -0.253195  1.262637  1.646892
C     0.268075  2.523650  1.240292
C     0.342025  3.169324  0.000000
C     0.268075  2.523650 -1.240292
C    -0.253195  1.262637 -1.646892
C    -1.431605  0.533175 -1.265595
```

```
H    -2.951089 -0.282873  0.000000
H    -1.925359  0.005676  2.092893
H     0.076606  0.979144  2.655379
H     0.786911  3.057250  2.053103
H     0.783523  4.172218  0.000000
H     0.786911  3.057250 -2.053103
H     0.076606  0.979144 -2.655379
H    -1.925359  0.005676 -2.092893
     el energy= -735.198327495
           zpe= -735.042699
     th energy= -735.028343
   th enthalpy= -735.027399
    free energy= -735.084461


TS-4
Cr   -0.053243  0.421556  0.000000
C    -1.608039  1.426423  0.000000
O    -2.557207  2.109518  0.000000
C     0.600236  1.574062  1.216495
O     1.034495  2.324644  2.010459
C     0.600236  1.574062 -1.216495
O     1.034495  2.324644 -2.010459
C    -1.490423 -1.672075 -0.685667
C    -0.453363 -2.130123 -1.622680
C     0.868401 -1.805700 -1.627242
C     1.606311 -0.933036 -0.700348
C     1.606311 -0.933036  0.700348
C     0.868401 -1.805700  1.627242
C    -0.453363 -2.130123  1.622680
C    -1.490423 -1.672075  0.685667
H    -2.426209 -1.350456 -1.165759
H    -0.834018 -2.696614 -2.484698
H     1.451429 -2.133570 -2.500691
H     2.437717 -0.391287 -1.169815
H     2.437717 -0.391287  1.169815
H     1.451429 -2.133570  2.500691
H    -0.834018 -2.696614  2.484698
```

PBEPBE/BS2

```
I
Cr   -0.055821 -0.347342  0.000000
C     1.801726 -0.304964  0.000000
O     2.961053 -0.253093  0.000000
C    -0.079778 -1.757488  1.197275
O    -0.071014 -2.685655  1.899302
C    -0.079778 -1.757488 -1.197275
O    -0.071014 -2.685655 -1.899302
C     0.456955  2.693087 -0.664576
C     0.276968  1.458572 -1.455814
C    -0.942132  0.796059 -1.654122
C    -1.983271  0.526768 -0.706489
C    -1.983271  0.526768  0.706489
C    -0.942132  0.796059  1.654122
C     0.276968  1.458572  1.455814
C     0.456955  2.693087  0.664576
H     0.576829  3.623773 -1.229246
H     0.983830  1.334307 -2.281639
H    -1.090864  0.294313 -2.613765
H    -2.853675  0.026229 -1.136237
H    -2.853675  0.026229  1.136237
H    -1.090864  0.294313  2.613765
H     0.983830  1.334307  2.281639
```

```
H    -2.426209 -1.350456  1.165759
     el energy= -735.179977018
           zpe= -735.024338
     th energy= -735.009827
   th enthalpy= -735.008883
    free energy= -735.066692

TS-5
Cr    0.351482 -0.000448 -0.288416
C     1.369976 -1.496266 -0.552929
O     2.062771 -2.407907 -0.799886
C     1.461479  0.000604  1.157993
O     2.181570  0.001065  2.086392
C     1.370596  1.494632 -0.554604
O     2.063652  2.405842 -0.802411
C    -1.324353  1.302057 -1.153218
C    -1.302506  0.001096 -1.727667
C    -1.324905 -1.300447 -1.154556
C    -1.901952 -1.802336  0.105374
C    -1.650274 -1.269159  1.323804
C    -0.895562 -0.000542  1.538402
C    -1.649155  1.269069  1.325284
C    -1.900326  1.803559  0.107313
H    -1.103374  2.094123 -1.881338
H    -0.906809  0.001621 -2.756107
H    -1.104032 -2.091842 -1.883487
H    -2.447218 -2.754664  0.040286
H    -1.984617 -1.805042  2.224503
H    -0.445676 -0.001100  2.544670
H    -1.981899  1.805188  2.226359
H    -2.444003  2.756862  0.043184
     el energy= -735.150526632
           zpe= -734.995828
     th energy= -734.981618
   th enthalpy= -734.980673
    free energy= -735.036989



H     0.576829  3.623773  1.229246
     el energy= -735.459353623
           zpe= -735.302462
     th energy= -735.288282
   th enthalpy= -735.287337
    free energy= -735.343273

TS-1
Cr   -0.032115 -0.306246  0.000000
C     1.069437 -1.143235  1.225867
O     1.757254 -1.686785  1.990529
C    -1.049983 -1.863741  0.000000
O    -1.664310 -2.848837  0.000000
C     1.069437 -1.143235 -1.225867
O     1.757254 -1.686785 -1.990529
C     0.719191  2.720285 -0.662745
C     0.498731  1.448736 -1.390566
C    -0.799648  0.934608 -1.657513
C    -1.847251  0.776276 -0.717368
C    -1.847251  0.776276  0.717368
C    -0.799648  0.934608  1.657513
C     0.498731  1.448736  1.390566
C     0.719191  2.720285  0.662745
```

```
H       0.840744   3.633628  -1.255761
H       1.217730   1.257307  -2.193551
H      -1.001940   0.487115  -2.634270
H      -2.764766   0.357737  -1.136781
H      -2.764766   0.357737   1.136781
H      -1.001940   0.487115   2.634270
H       1.217730   1.257307   2.193551
H       0.840744   3.633628   1.255761
       el energy= -735.441512750
               zpe= -735.285408
         th energy= -735.271974
       th enthalpy= -735.271030
       free energy= -735.324976

TS-2
Cr      0.031650  -0.435678   0.000000
C      -1.118756  -1.095334   1.325567
O      -1.815586  -1.559961   2.126999
C      -1.118756  -1.095334  -1.325567
O      -1.815586  -1.559961  -2.126999
C       0.802321  -2.062637   0.000000
O       1.300996  -3.119155   0.000000
C      -0.107239   1.991301   1.666084
C       0.866182   0.900231   1.628280
C       1.855015   0.492562   0.715368
C       1.855015   0.492562  -0.715368
C       0.866182   0.900231  -1.628280
C      -0.107239   1.991301  -1.666084
C      -0.715823   2.761250  -0.727734
C      -0.715823   2.761250   0.727734
H      -0.434934   2.193238   2.688852
H       1.048785   0.500463   2.627305
H       2.644903  -0.124980   1.147296
H       2.644903  -0.124980  -1.147296
H       1.048785   0.500463  -2.627305
H      -0.434934   2.193238  -2.688852
H      -1.401083   3.503578  -1.143780
H      -1.401083   3.503578   1.143780
       el energy= -735.438707789
               zpe= -735.282152
         th energy= -735.268112
       th enthalpy= -735.267168
       free energy= -735.323658

TS-3
Cr     -0.006947  -0.465411   0.000000
C       1.885096  -0.495541   0.000000
O       3.041372  -0.529742   0.000000
C      -0.120627  -1.861292   1.192153
O      -0.188594  -2.784312   1.900392
C      -0.120627  -1.861292  -1.192153
O      -0.188594  -2.784312  -1.900392
C      -2.040747   0.355514   0.000000
C      -1.437737   0.559712   1.261923
C      -0.260880   1.276190   1.647386
C       0.292575   2.513038   1.236147
C       0.389624   3.148765   0.000000
C       0.292575   2.513038  -1.236147
C      -0.260880   1.276190  -1.647386
C      -1.437737   0.559712  -1.261923
H      -2.956120  -0.236902   0.000000
```

```
H      -1.941619   0.048994   2.085397
H       0.055037   0.996192   2.655231
H       0.820775   3.032785   2.043943
H       0.857169   4.133536   0.000000
H       0.820775   3.032785  -2.043943
H       0.055037   0.996192  -2.655231
H      -1.941619   0.048994  -2.085397
       el energy= -735.438733464
               zpe= -735.283578
         th energy= -735.269258
       th enthalpy= -735.268314
       free energy= -735.325448

TS-4
Cr     -0.049483   0.407359   0.000000
C      -1.604876   1.423283   0.000000
O      -2.540292   2.113917   0.000000
C       0.604067   1.576370   1.211574
O       1.031591   2.343685   1.983437
C       0.604067   1.576370  -1.211574
O       1.031591   2.343685  -1.983437
C      -1.489780  -1.660406  -0.682170
C      -0.462133  -2.110619  -1.622537
C       0.857007  -1.807290  -1.626242
C       1.610869  -0.963779  -0.696150
C       1.610869  -0.963779   0.696150
C       0.857007  -1.807290   1.626242
C      -0.462133  -2.110619   1.622537
C      -1.489780  -1.660406   0.682170
H      -2.426258  -1.352054  -1.156421
H      -0.848708  -2.654074  -2.489474
H       1.427266  -2.128402  -2.503310
H       2.444397  -0.434428  -1.162110
H       2.444397  -0.434428   1.162110
H       1.427266  -2.128402   2.503310
H      -0.848708  -2.654074   2.489474
H      -2.426258  -1.352054   1.156421
       el energy= -735.419810391
               zpe= -735.264726
         th energy= -735.250231
       th enthalpy= -735.249287
       free energy= -735.307221

TS-5
Cr      0.286614   0.340723   0.000000
C       0.567717   1.385630   1.484991
O       0.806441   2.083453   2.386040
C      -1.164475   1.455441   0.000000
O      -2.084257   2.176053   0.000000
C       0.567717   1.385630  -1.484991
O       0.806441   2.083453  -2.386040
C       1.155307  -1.348053  -1.297366
C       1.720624  -1.325167   0.000000
C       1.155307  -1.348053   1.297366
C      -0.111426  -1.881253   1.807480
C      -1.324712  -1.639200   1.274614
C      -1.553739  -0.919864   0.000000
C      -1.324712  -1.639200  -1.274614
C      -0.111426  -1.881253  -1.807480
H       1.887712  -1.147621  -2.082262
H       2.760364  -0.980051   0.000000
```

```
H      1.887712  -1.147621   2.082262
H     -0.056825  -2.388187   2.775053
H     -2.216772  -1.932104   1.836354
H     -2.553408  -0.473084   0.000000
H     -2.216772  -1.932104  -1.836354
H     -0.056825  -2.388187  -2.775053
      el energy= -735.391210914
```

PBEPBE/BS3

```
I
Cr    -0.053200  -0.346894   0.000000
C      1.805829  -0.285340   0.000000
O      2.965223  -0.220184   0.000000
C     -0.071181  -1.760130   1.195545
O     -0.060724  -2.691312   1.895220
C     -0.071181  -1.760130  -1.195545
O     -0.060724  -2.691312  -1.895220
C      0.441188   2.694941  -0.664416
C      0.270660   1.457270  -1.452985
C     -0.945732   0.788674  -1.653741
C     -1.984904   0.514299  -0.706563
C     -1.984904   0.514299   0.706563
C     -0.945732   0.788674   1.653741
C      0.270660   1.457270   1.452985
C      0.441188   2.694941   0.664416
H      0.551915   3.626210  -1.230226
H      0.977625   1.338947  -2.279819
H     -1.092194   0.287650  -2.614189
H     -2.851721   0.006855  -1.136080
H     -2.851721   0.006855   1.136080
H     -1.092194   0.287650   2.614189
H      0.977625   1.338947   2.279819
H      0.551915   3.626210   1.230226
      el energy= -1693.44464560
            zpe= -1693.287782
      th energy= -1693.273601
   th enthalpy= -1693.272656
   free energy= -1693.328616

TS-1
Cr    -0.032046  -0.307188   0.000000
C      1.073459  -1.137281   1.229431
O      1.765461  -1.671917   1.997760
C     -1.047473  -1.869240   0.000000
O     -1.658179  -2.857554   0.000000
C      1.073459  -1.137281  -1.229431
O      1.765461  -1.671917  -1.997760
C      0.711407   2.720574  -0.662632
C      0.495145   1.446759  -1.387631
C     -0.802843   0.930888  -1.656798
C     -1.849844   0.768305  -0.717276
C     -1.849844   0.768305   0.717276
C     -0.802843   0.930888   1.656798
C      0.495145   1.446759   1.387631
C      0.711407   2.720574   0.662632
H      0.828572   3.634289  -1.256215
H      1.213651   1.258100  -2.192015
H     -1.004444   0.486021  -2.635028
H     -2.765728   0.345646  -1.136704
H     -2.765728   0.345646   1.136704
H     -1.004444   0.486021   2.635028
H      1.213651   1.258100   2.192015
```

```
             zpe= -735.237078
       th energy= -735.222832
    th enthalpy= -735.221888
    free energy= -735.278438
```

```
H      0.828572   3.634289   1.256215
      el energy= -1693.42716645
            zpe= -1693.271070
      th energy= -1693.257640
   th enthalpy= -1693.256695
   free energy= -1693.310651

TS-2
Cr     0.030806  -0.440811   0.000000
C     -1.120408  -1.097175   1.328552
O     -1.820041  -1.555456   2.132630
C     -1.120408  -1.097175  -1.328552
O     -1.820041  -1.555456  -2.132630
C      0.801887  -2.066924   0.000000
O      1.305411  -3.122468   0.000000
C     -0.104260   1.995557   1.665297
C      0.865018   0.901211   1.627115
C      1.853518   0.489628   0.715032
C      1.853518   0.489628  -0.715032
C      0.865018   0.901211  -1.627115
C     -0.104260   1.995557  -1.665297
C     -0.710238   2.767989  -0.727430
C     -0.710238   2.767989   0.727430
H     -0.433153   2.195923   2.688135
H      1.046404   0.502162   2.626914
H      2.641887  -0.129581   1.147794
H      2.641887  -0.129581  -1.147794
H      1.046404   0.502162  -2.626914
H     -0.433153   2.195923  -2.688135
H     -1.393571   3.512261  -1.143662
H     -1.393571   3.512261   1.143662
      el energy= -1693.42374242
            zpe= -1693.267227
      th energy= -1693.253172
   th enthalpy= -1693.252227
   free energy= -1693.308778

TS-3
Cr    -0.005235  -0.465827   0.000000
C      1.890158  -0.486714   0.000000
O      3.047395  -0.513176   0.000000
C     -0.116850  -1.864179   1.189832
O     -0.185139  -2.789756   1.896462
C     -0.116850  -1.864179  -1.189832
O     -0.185139  -2.789756  -1.896462
C     -2.041040   0.348462   0.000000
C     -1.439756   0.556011   1.262016
C     -0.266334   1.277741   1.647330
C      0.286538   2.514796   1.235937
C      0.384290   3.149905   0.000000
C      0.286538   2.514796  -1.235937
C     -0.266334   1.277741  -1.647330
C     -1.439756   0.556011  -1.262016
```

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```
H   -2.952303  -0.250744   0.000000
H   -1.940752   0.042452   2.085633
H    0.048759   1.000509   2.656407
H    0.814049   3.034806   2.044158
H    0.853280   4.134219   0.000000
H    0.814049   3.034806  -2.044158
H    0.048759   1.000509  -2.656407
H   -1.940752   0.042452  -2.085633
       el energy= -1693.42403373
             zpe= -1693.268917
        th energy= -1693.254572
     th enthalpy= -1693.253628
      free energy= -1693.310894


TS-4
Cr  -0.047008   0.402558   0.000000
C   -1.612808   1.405349   0.000000
O   -2.557935   2.083911   0.000000
C    0.600526   1.575298   1.210908
O    1.026621   2.342092   1.985652
C    0.600526   1.575298  -1.210908
O    1.026621   2.342092  -1.985652
C   -1.485582  -1.660661  -0.682533
C   -0.459068  -2.094038  -1.630019
C    0.860803  -1.792443  -1.632876
C    1.619248  -0.962174  -0.696216
C    1.619248  -0.962174   0.696216
C    0.860803  -1.792443   1.632876
C   -0.459068  -2.094038   1.630019
C   -1.485582  -1.660661   0.682533
H   -2.427169  -1.362404  -1.153098
H   -0.847774  -2.621078  -2.506194
H    1.426316  -2.098301  -2.518527
H    2.454366  -0.433228  -1.160250
H    2.454366  -0.433228   1.160250
H    1.426316  -2.098301   2.518527
H   -0.847774  -2.621078   2.506194
```

B3LYP/BS1
```
I
Cr  -0.035449  -0.382273   0.000000
C    1.832639  -0.319327   0.000000
O    2.982417  -0.232082   0.000000
C   -0.065785  -1.769675   1.242922
O   -0.078972  -2.654839   1.984478
C   -0.065785  -1.769675  -1.242922
O   -0.078972  -2.654839  -1.984478
C    0.449469   2.704125  -0.664897
C    0.240104   1.492522  -1.488779
C   -0.957322   0.804268  -1.654088
C   -1.992225   0.503654  -0.702763
C   -1.992225   0.503654   0.702763
C   -0.957322   0.804268   1.654088
C    0.240104   1.492522   1.488779
C    0.449469   2.704125   0.664897
H    0.601263   3.634446  -1.217038
H    0.926800   1.391698  -2.330651
H   -1.091674   0.282646  -2.601922
H   -2.852253  -0.005862  -1.135668
H   -2.852253  -0.005862   1.135668
H   -1.091674   0.282646   2.601922
H    0.926800   1.391698   2.330651
```

```
H   -2.427169  -1.362404   1.153098
       el energy= -1693.40372685
             zpe= -1693.248588
        th energy= -1693.234081
     th enthalpy= -1693.233136
      free energy= -1693.291160

TS-5
Cr   0.287456   0.344507   0.000000
C    0.567250   1.388676   1.487105
O    0.805147   2.084136   2.391674
C   -1.167191   1.456020   0.000000
O   -2.092688   2.170995   0.000000
C    0.567250   1.388676  -1.487105
O    0.805147   2.084136  -2.391674
C    1.155661  -1.347216  -1.297602
C    1.720189  -1.323798   0.000000
C    1.155661  -1.347216   1.297602
C   -0.109395  -1.882700   1.808768
C   -1.322368  -1.644393   1.274489
C   -1.550382  -0.924564   0.000000
C   -1.322368  -1.644393  -1.274489
C   -0.109395  -1.882700  -1.808768
H    1.888581  -1.145401  -2.081880
H    2.759261  -0.975820   0.000000
H    1.888581  -1.145401   2.081880
H   -0.053330  -2.388493   2.776957
H   -2.214510  -1.940115   1.834803
H   -2.550013  -0.476839   0.000000
H   -2.214510  -1.940115  -1.834803
H   -0.053330  -2.388493  -2.776957
       el energy= -1693.37670695
             zpe= -1693.222555
        th energy= -1693.208321
     th enthalpy= -1693.207376
      free energy= -1693.263862



H    0.601263   3.634446   1.217038
       el energy= -735.924800456
             zpe= -735.763519
        th energy= -735.749249
     th enthalpy= -735.748305
      free energy= -735.804530

TS-1
Cr   0.341122  -0.000005  -0.006211
C    1.131231  -1.261507   1.112532
O    1.607233  -2.057546   1.800677
C    1.901723   0.000226  -1.042564
O    2.852010   0.000335  -1.695059
C    1.131330   1.260829   1.113173
O    1.607434   2.056539   1.801622
C   -2.723069   0.662594   0.682656
C   -1.463656   1.417833   0.461387
C   -0.927607   1.659633  -0.824552
C   -0.743194   0.715972  -1.865330
C   -0.743246  -0.715054  -1.865643
C   -0.927835  -1.659164  -0.825310
C   -1.463951  -1.418014   0.460687
C   -2.723194  -0.662656   0.682376
```

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```
   H    -3.640489  1.244758  0.802449
   H    -1.298383  2.235334  1.165472
   H    -0.458756  2.625188 -1.017295
   H    -0.307644  1.135064 -2.771661
   H    -0.307746 -1.133750 -2.772180
   H    -0.459050 -2.624666 -1.018472
   H    -1.298774 -2.235903  1.164341
   H    -3.640708 -1.244699  0.802004
        el energy= -735.903610497
               zpe= -735.743141
         th energy= -735.729690
       th enthalpy= -735.728746
       free energy= -735.782650

TS-2
   Cr   -0.025772  0.470278  0.000000
   C     1.181707  1.044266  1.338225
   O     1.920429  1.407140  2.142091
   C     1.181707  1.044266 -1.338225
   O     1.920429  1.407140 -2.142091
   C    -0.799430  2.122385  0.000000
   O    -1.311520  3.160367  0.000000
   C     0.053350 -1.978102  1.668835
   C    -0.905449 -0.865136  1.631605
   C    -1.877479 -0.441307  0.716322
   C    -1.877479 -0.441307 -0.716322
   C    -0.905449 -0.865136 -1.631605
   C     0.053350 -1.978102 -1.668835
   C     0.652325 -2.751122 -0.730938
   C     0.652325 -2.751122  0.730938
   H     0.369110 -2.189996  2.690421
   H    -1.086016 -0.470028  2.630013
   H    -2.645989  0.201911  1.142481
   H    -2.645989  0.201911 -1.142481
   H    -1.086016 -0.470028 -2.630013
   H     0.369110 -2.189996 -2.690421
   H     1.326381 -3.502558 -1.141791
   H     1.326381 -3.502558  1.141791
        el energy= -735.909824703
               zpe= -735.748805
         th energy= -735.734868
       th enthalpy= -735.733924
       free energy= -735.790018

TS-3
   Cr   -0.001775 -0.492233  0.000000
   C     1.902869 -0.455781  0.000000
   O     3.050207 -0.403907  0.000000
   C    -0.094506 -1.869757  1.247442
   O    -0.148853 -2.742660  2.001289
   C    -0.094506 -1.869757 -1.247442
   O    -0.148853 -2.742660 -2.001289
   C    -2.052299  0.321442  0.000000
   C    -1.451614  0.530001  1.260883
   C    -0.295906  1.268778  1.666631
   C     0.267675  2.495541  1.240222
   C     0.372565  3.124963  0.000000
   C     0.267675  2.495541 -1.240222
   C    -0.295906  1.268778 -1.666631
   C    -1.451614  0.530001 -1.260883
   H    -2.953733 -0.287221  0.000000
```

```
   H    -1.948908  0.006921  2.077570
   H    -0.001970  1.009183  2.683288
   H     0.791306  3.020636  2.043697
   H     0.848878  4.102648  0.000000
   H     0.791306  3.020636 -2.043697
   H    -0.001970  1.009183 -2.683288
   H    -1.948908  0.006921 -2.077570
        el energy= -735.905142409
               zpe= -735.745941
         th energy= -735.731683
       th enthalpy= -735.730739
       free energy= -735.787480

TS-4
   Cr   -0.048095  0.485602  0.000000
   C    -1.624576  1.496059  0.000000
   O    -2.581303  2.142538  0.000000
   C     0.631175  1.605856  1.273791
   O     1.064493  2.302625  2.093391
   C     0.631175  1.605856 -1.273791
   O     1.064493  2.302625 -2.093391
   C    -1.498344 -1.695306 -0.678574
   C    -0.457789 -2.180671 -1.600996
   C     0.850909 -1.854802 -1.607239
   C     1.583630 -0.960843 -0.693606
   C     1.583630 -0.960843  0.693606
   C     0.850909 -1.854802  1.607239
   C    -0.457789 -2.180671  1.600996
   C    -1.498344 -1.695306  0.678574
   H    -2.417018 -1.361196 -1.164387
   H    -0.830506 -2.785332 -2.429317
   H     1.444720 -2.219361 -2.447643
   H     2.405445 -0.426073 -1.167082
   H     2.405445 -0.426073  1.167082
   H     1.444720 -2.219361  2.447643
   H    -0.830506 -2.785332  2.429317
   H    -2.417018 -1.361196  1.164387
        el energy= -735.895186163
               zpe= -735.735587
         th energy= -735.721229
       th enthalpy= -735.720285
       free energy= -735.777570

TS-5
   Cr    0.407284  0.000281 -0.283105
   C     1.408959 -1.543744 -0.553286
   O     2.067980 -2.455405 -0.807352
   C     1.435640  0.000869  1.245006
   O     2.085939  0.001333  2.203274
   C     1.405875  1.546019 -0.552970
   O     2.062961  2.459089 -0.807108
   C    -1.304727  1.293382 -1.167309
   C    -1.269130 -0.001208 -1.733014
   C    -1.303501 -1.295775 -1.167416
   C    -1.924049 -1.790642  0.076975
   C    -1.698881 -1.257905  1.287107
   C    -0.912060 -0.000272  1.496544
   C    -1.701710  1.255669  1.286677
   C    -1.927348  1.787622  0.076410
   H    -1.082105  2.079890 -1.888600
   H    -0.857651 -0.001067 -2.747373
```

23

```
H    -1.079995 -2.082191 -1.888548
H    -2.507490 -2.708625 -0.009598
H    -2.106822 -1.745889  2.174831
H    -0.505444  0.000392  2.511786
H    -2.111672  1.742465  2.174129
H    -2.513093  2.704061 -0.010981
     el energy= -735.850711911
           zpe= -735.692071
     th energy= -735.677972
   th enthalpy= -735.677028
   free energy= -735.733629

TS-6
Cr    0.770221 -0.039960 -0.271463
C     0.334336  0.149373  1.520382
O     0.089121  0.189063  2.646979
C     1.626305 -1.650657  0.222483
O     2.121593 -2.628095  0.575895
C     2.255779  1.030721 -0.090786
O     3.176480  1.730454 -0.052516
C    -2.008754  1.633406  0.441961
C    -0.763170  1.767395 -0.339997
C    -0.385107  1.201158 -1.563663
C    -0.533652 -0.161358 -2.006025
C    -1.020795 -1.312062 -1.385244
C    -2.023482 -1.588907 -0.362741
C    -2.814631 -0.811784  0.422505
C    -2.865155  0.616739  0.695179
H    -2.283376  2.581522  0.906724
H    -0.286153  2.730224 -0.161690
H     0.265314  1.805459 -2.194522
H     0.076396 -0.378338 -2.887186
H    -0.709358 -2.219208 -1.901046
H    -2.191453 -2.660179 -0.251174
H    -3.539823 -1.373058  1.012362
H    -3.724438  0.897126  1.304440
     el energy= -735.893854093


2
Cr   -0.875553  0.000033 -0.304650
C    -0.184098 -0.000025  1.409215
O     0.232186  0.000032  2.484271
C    -2.009346  1.425034  0.142342
O    -2.676839  2.326929  0.409551
C    -2.009994 -1.424474  0.142151
O    -2.677856 -2.326127  0.409267
C     2.034607 -1.663496  0.043727
C     0.883018 -1.630800 -0.858883
C     0.433302 -0.722114 -1.817720
C     0.433412  0.721329 -1.817999
C     0.883440  1.630420 -0.859707
C     2.034831  1.663298  0.043087
C     2.877753  0.726626  0.547517
C     2.877693 -0.726773  0.547749
H     2.266229 -2.684222  0.349721
H     0.476162 -2.628785 -1.018201
H    -0.200522 -1.155691 -2.595440
H    -0.200430  1.154615 -2.595877
H     0.476726  2.628378 -1.019513
H     2.266478  2.684105  0.348803
H     3.690494  1.140884  1.144132
```

```
H     3.690502 -1.140900  1.144364
     el energy= -735.896316253
           zpe= -735.735743
     th energy= -735.720950
   th enthalpy= -735.720006
   free energy= -735.778222

TS-7
Cr    0.318661  0.012708 -0.021700
C     1.849663 -1.078847  0.129143
O     2.823619 -1.687016  0.207458
C     1.643609  1.319164 -0.154432
O     2.507891  2.083500 -0.231089
C     0.142255 -0.026245  1.847405
O    -0.027948 -0.085227  2.985157
C    -2.607066  0.574073  0.480494
C    -1.486483  1.530499  0.241620
C    -0.800639  1.645639 -0.996660
C    -0.927165  0.451001 -1.777487
C    -0.027340 -0.631596 -2.029848
C    -0.448639 -1.721019 -1.162125
C    -1.326390 -1.575774 -0.049334
C    -2.551945 -0.754597  0.264182
H    -3.551777  1.017987  0.800396
H    -1.409106  2.368861  0.933400
H    -0.181966  2.508404 -1.222255
H    -1.911944  0.038156 -1.597793
H     0.847821 -0.685478 -2.667711
H     0.125531 -2.646770 -1.191882
H    -1.288041 -2.456338  0.596325
H    -3.466041 -1.333666  0.420364
     el energy= -735.855943756
           zpe= -735.695164
     th energy= -735.681422
   th enthalpy= -735.680477
   free energy= -735.735298


3
Cr   -0.363077 -0.038963  0.008833
C    -0.112107  1.792578  0.389106
O     0.042413  2.907343  0.627057
C    -1.507364  0.337620 -1.413220
O    -2.227794  0.557320 -2.288030
C    -1.879418 -0.020881  1.084190
O    -2.823251 -0.029887  1.749166
C     0.560955 -1.476845  1.368364
C    -0.111287 -2.187772  0.290614
C     0.052310 -1.845979 -1.067442
C     1.290342 -1.087685 -1.199598
C     1.559833  0.251059 -1.451941
C     2.630783  0.727765 -0.553136
C     2.562629  0.328500  0.741468
C     1.414310 -0.332422  1.451301
H     0.106474 -1.711466  2.331378
H    -0.905092 -2.864334  0.600858
H    -0.589009 -2.232155 -1.853636
H     2.059569 -1.538673 -0.578366
H     1.142634  0.860212 -2.248379
H     3.456825  1.343829 -0.905338
H     3.357654  0.642205  1.420208
H     1.387937  0.041646  2.477490
```

el energy= -735.890534470
        zpe= -735.728992
   th energy= -735.715338
  th enthalpy= -735.714394
   free energy= -735.769016

TS-8
```
Cr    1.235836   0.000514  -0.418289
C     3.037536   0.001662  -0.923446
O     4.148938   0.002545  -1.236316
C     1.592976   1.286686   0.834359
O     1.800183   2.100756   1.631464
C     1.593908  -1.288665   0.831032
O     1.802123  -2.104938   1.625613
C    -3.917275   0.673657  -0.212391
C    -2.891909   1.603792   0.276842
C    -1.568636   1.618254   0.030825
C    -0.808819   0.689278  -0.825494
C    -0.808551  -0.689265  -0.825043
C    -1.568377  -1.617915   0.031628
C    -2.891713  -1.603598   0.277353
C    -3.917216  -0.673823  -0.212224
H    -4.838459   1.161127  -0.539240
H    -3.285923   2.439921   0.859216
H    -0.992308   2.455181   0.426252
H    -0.274793   1.187028  -1.661785
H    -0.274122  -1.187278  -1.660900
H    -0.991997  -2.454534   0.427616
H    -3.285606  -2.439607   0.859996
H    -4.838350  -1.161452  -0.538945
```
    el energy= -735.879188426
        zpe= -735.720927
   th energy= -735.705606

B3LYP/BS3
I
```
Cr   -0.034015  -0.378288   0.000000
C     1.848810  -0.338516   0.000000
O     2.994030  -0.277392   0.000000
C    -0.079040  -1.774986   1.243457
O    -0.102912  -2.662949   1.972985
C    -0.079040  -1.774986  -1.243457
O    -0.102912  -2.662949  -1.972985
C     0.463123   2.701962  -0.660579
C     0.235515   1.505227  -1.489244
C    -0.954914   0.818954  -1.647573
C    -1.981159   0.515159  -0.699479
C    -1.981159   0.515159   0.699479
C    -0.954914   0.818954   1.647573
C     0.235515   1.505227   1.489244
C     0.463123   2.701962   0.660579
H     0.634567   3.625625  -1.205487
H     0.911115   1.412145  -2.332814
H    -1.097027   0.314886  -2.596407
H    -2.840870   0.017612  -1.130865
H    -2.840870   0.017612   1.130865
H    -1.097027   0.314886   2.596407
H     0.911115   1.412145   2.332814
H     0.634567   3.625625   1.205487
```
    el energy= -1694.40027290
        zpe= -1694.239252
   th energy= -1694.225023

th enthalpy= -735.704662
   free energy= -735.764971

4
```
Cr   -1.046925  -0.207990  -0.316170
C    -2.583519  -1.207389   0.019484
O    -3.541265  -1.831999   0.191552
C    -0.781065   0.035990   1.476656
O    -0.593937   0.201510   2.606807
C    -2.023417   1.344409  -0.410547
O    -2.622719   2.335000  -0.452931
C     3.393973  -1.093910  -0.037783
C     2.102386  -1.786513  -0.048043
C     0.980295  -1.412613  -0.697564
C     0.708307  -0.212194  -1.502490
C     0.838959   1.106135  -1.116961
C     1.537113   1.660927   0.048839
C     2.711370   1.284010   0.599852
C     3.636792   0.205428   0.232110
H     4.261023  -1.743679  -0.170747
H     2.081792  -2.747840   0.469711
H     0.142446  -2.140567  -0.680301
H     0.246267  -0.395209  -2.482879
H     0.475841   1.851000  -1.825844
H     1.077906   2.565240   0.449254
H     3.088371   1.926008   1.398454
H     4.688739   0.495039   0.285700
```
    el energy= -735.885236129
        zpe= -735.726604
   th energy= -735.711320
  th enthalpy= -735.710376
   free energy= -735.770560

th enthalpy= -1694.224079
   free energy= -1694.280321

TS-1
```
Cr   -0.010765  -0.336861   0.000000
C     1.111656  -1.138693   1.265502
O     1.796176  -1.622768   2.051621
C    -1.056502  -1.905543   0.000000
O    -1.698322  -2.855859   0.000000
C     1.111656  -1.138693  -1.265502
O     1.796176  -1.622768  -2.051621
C     0.699371   2.713250  -0.658101
C     0.459314   1.464471  -1.413867
C    -0.824398   0.939174  -1.651384
C    -1.858826   0.756486  -0.712153
C    -1.858826   0.756486   0.712153
C    -0.824398   0.939174   1.651384
C     0.459314   1.464471   1.413867
C     0.699371   2.713250   0.658101
H     0.836456   3.624074  -1.234854
H     1.155158   1.300575  -2.230245
H    -1.025377   0.492765  -2.618764
H    -2.766373   0.339007  -1.130388
H    -2.766373   0.339007   1.130388
H    -1.025377   0.492765   2.618764
H     1.155158   1.300575   2.230245
H     0.836456   3.624074   1.234854
```

el energy= -1694.37967640
zpe= -1694.219424
th energy= -1694.206054
th enthalpy= -1694.205110
free energy= -1694.258914

zpe= -1694.222806
th energy= -1694.208581
th enthalpy= -1694.207637
free energy= -1694.264403

TS-2
```
Cr    0.033393  -0.473542   0.000000
C    -1.175890  -1.068746   1.343592
O    -1.904333  -1.448124   2.140536
C    -1.175890  -1.068746  -1.343592
O    -1.904333  -1.448124  -2.140536
C     0.823065  -2.125339   0.000000
O     1.336768  -3.156805   0.000000
C    -0.073686   1.985608   1.658650
C     0.895900   0.891819   1.622998
C     1.866696   0.476067   0.712125
C     1.866696   0.476067  -0.712125
C     0.895900   0.891819  -1.622998
C    -0.073686   1.985608  -1.658650
C    -0.675350   2.750799  -0.727054
C    -0.675350   2.750799   0.727054
H    -0.392055   2.191625   2.674065
H     1.085451   0.510745   2.618384
H     2.651019  -0.135576   1.139720
H     2.651019  -0.135576  -1.139720
H     1.085451   0.510745  -2.618384
H    -0.392055   2.191625  -2.674065
H    -1.352761   3.490664  -1.137102
H    -1.352761   3.490664   1.137102
```
el energy= -1694.38615001
zpe= -1694.225443
th energy= -1694.211541
th enthalpy= -1694.210597
free energy= -1694.266726

TS-3
```
Cr   -0.000802  -0.483822   0.000000
C     1.921263  -0.469347   0.000000
O     3.063093  -0.447516   0.000000
C    -0.104416  -1.872293   1.245942
O    -0.168085  -2.751537   1.983148
C    -0.104416  -1.872293  -1.245942
O    -0.168085  -2.751537  -1.983148
C    -2.047343   0.335571   0.000000
C    -1.457962   0.550816   1.257022
C    -0.311760   1.286981   1.668379
C     0.282235   2.487653   1.236508
C     0.411143   3.103621   0.000000
C     0.282235   2.487653  -1.236508
C    -0.311760   1.286981  -1.668379
C    -1.457962   0.550816  -1.257022
H    -2.950820  -0.258736   0.000000
H    -1.962567   0.042184   2.069438
H    -0.032696   1.035387   2.684781
H     0.812238   3.000785   2.034703
H     0.913203   4.061506   0.000000
H     0.812238   3.000785  -2.034703
H    -0.032696   1.035387  -2.684781
H    -1.962567   0.042184  -2.069438
```
el energy= -1694.38174046

TS-4
```
Cr   -0.047402   0.486276   0.000000
C    -1.628844   1.500719   0.000000
O    -2.577757   2.149034   0.000000
C     0.633581   1.616721   1.271819
O     1.065177   2.321841   2.077800
C     0.633581   1.616721  -1.271819
O     1.065177   2.321841  -2.077800
C    -1.490859  -1.702756  -0.674308
C    -0.457275  -2.182065  -1.596569
C     0.844319  -1.862963  -1.602642
C     1.578875  -0.981296  -0.689989
C     1.578875  -0.981296   0.689989
C     0.844319  -1.862963   1.602642
C    -0.457275  -2.182065   1.596569
C    -1.490859  -1.702756   0.674308
H    -2.408403  -1.380100  -1.155836
H    -0.830877  -2.775549  -2.424185
H     1.431234  -2.221206  -2.442314
H     2.401161  -0.457328  -1.160062
H     2.401161  -0.457328   1.160062
H     1.431234  -2.221206   2.442314
H    -0.830877  -2.775549   2.424185
H    -2.408403  -1.380100   1.155836
```
el energy= -1694.36933926
zpe= -1694.210053
th energy= -1694.195726
th enthalpy= -1694.194782
free energy= -1694.252119

TS-5
```
Cr    0.291505   0.407711   0.000000
C     0.562595   1.429376   1.541391
O     0.797388   2.085923   2.452658
C    -1.243284   1.438605   0.000000
O    -2.197460   2.085203   0.000000
C     0.562595   1.429376  -1.541391
O     0.797388   2.085923  -2.452658
C     1.162852  -1.327895  -1.289829
C     1.720142  -1.293120   0.000000
C     1.162852  -1.327895   1.289829
C    -0.084310  -1.925359   1.787277
C    -1.285489  -1.702019   1.255483
C    -1.494593  -0.924385   0.000000
C    -1.285489  -1.702019  -1.255483
C    -0.084310  -1.925359  -1.787277
H     1.885554  -1.120936  -2.070031
H     2.741399  -0.916700   0.000000
H     1.885554  -1.120936   2.070031
H    -0.004828  -2.497716   2.705308
H    -2.169488  -2.095219   1.747711
H    -2.499885  -0.512870   0.000000
H    -2.169488  -2.095219  -1.747711
H    -0.004828  -2.497716  -2.705308
```
el energy= -1694.32779678
zpe= -1694.169431
```

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```
        th energy= -1694.155391   free energy= -1694.210816
      th enthalpy= -1694.154447
```
## B3LYP/BS4
```
I   free energy= -735.893538
Cr   -0.036354 -0.374770 0.000000
C   1.838430 -0.339988 0.000000   TS-2
O   2.992106 -0.282039 0.000000   Cr   0.031299 -0.467937 0.000000
C   -0.078574 -1.768834 1.240402   C   -1.178536 -1.056240 1.337171
O   -0.098502 -2.662069 1.975804   O   -1.916271 -1.435046 2.137196
C   -0.078574 -1.768834 -1.240402   C   -1.178536 -1.056240 -1.337171
O   -0.098502 -2.662069 -1.975804   O   -1.916271 -1.435046 -2.137196
C   0.465987 2.706175 -0.665259   C   0.811767 -2.120634 0.000000
C   0.246162 1.497008 -1.489011   O   1.324816 -3.160965 0.000000
C   -0.954929 0.814447 -1.655044   C   -0.064806 1.982354 1.667714
C   -1.990049 0.516449 -0.703167   C   0.896190 0.870917 1.629042
C   -1.990049 0.516449 0.703167   C   1.877206 0.457996 0.716000
C   -0.954929 0.814447 1.655044   C   1.877206 0.457996 -0.716000
C   0.246162 1.497008 1.489011   C   0.896190 0.870917 -1.629042
C   0.465987 2.706175 0.665259   C   -0.064806 1.982354 -1.667714
H   0.628940 3.637754 -1.215773   C   -0.664711 2.757702 -0.730845
H   0.933303 1.394145 -2.332687   C   -0.664711 2.757702 0.730845
H   -1.096165 0.302256 -2.608970   H   -0.380036 2.196627 2.691250
H   -2.857110 0.016284 -1.137136   H   1.082783 0.482365 2.630969
H   -2.857110 0.016284 1.137136   H   2.661533 -0.166575 1.145881
H   -1.096165 0.302256 2.608970   H   2.661533 -0.166575 -1.145881
H   0.933303 1.394145 2.332687   H   1.082783 0.482365 -2.630969
H   0.628940 3.637754 1.215773   H   -0.380036 2.196627 -2.691250
      el energy= -736.034420863   H   -1.336323 3.512583 -1.144904
              zpe= -735.873915   H   -1.336323 3.512583 1.144904
        th energy= -735.859657   el energy= -736.019470285
      th enthalpy= -735.858713   zpe= -735.859178
      free energy= -735.914916   th energy= -735.845259
                                               th enthalpy= -735.844315
                                               free energy= -735.900362
TS-1
Cr   0.335402 0.000000 0.010538
C   1.136467 1.259857 -1.108913   TS-3
O   1.626560 2.048746 -1.799301   Cr   -0.003146 -0.486280 0.000000
C   1.898818 0.000046 1.052904   C   1.908042 -0.483942 0.000000
O   2.855410 0.000088 1.699756   O   3.058122 -0.466038 0.000000
C   1.136457 -1.259964 -1.108796   C   -0.109126 -1.868860 1.245963
O   1.626561 -2.048921 -1.799098   O   -0.171382 -2.748224 1.995315
C   -2.720064 -0.663030 -0.698444   C   -0.109126 -1.868860 -1.245963
C   -1.461914 -1.416360 -0.465358   O   -0.171382 -2.748224 -1.995315
C   -0.933746 -1.659549 0.824563   C   -2.051096 0.337419 0.000000
C   -0.756241 -0.715766 1.866087   C   -1.450680 0.546652 1.261003
C   -0.756232 0.715912 1.866037   C   -0.286827 1.276326 1.663825
C   -0.933731 1.659619 0.824440   C   0.282060 2.501318 1.241115
C   -1.461904 1.416330 -0.465459   C   0.393227 3.130170 0.000000
C   -2.720060 0.662991 -0.698485   C   0.282060 2.501318 -1.241115
H   -3.638524 -1.244467 -0.831008   C   -0.286827 1.276326 -1.663825
H   -1.294083 -2.235276 -1.170113   C   -1.450680 0.546652 -1.261003
H   -0.476616 -2.631260 1.023997   H   -2.963723 -0.257503 0.000000
H   -0.333296 -1.136441 2.779782   H   -1.956911 0.035321 2.081723
H   -0.333281 1.136646 2.779701   H   0.003638 1.017997 2.683962
H   -0.476589 2.631341 1.023797   H   0.809682 3.024008 2.046109
H   -1.294072 2.235191 -1.170279   H   0.877389 4.106341 0.000000
H   -3.638517 1.244424 -0.831086   H   0.809682 3.024008 -2.046109
      el energy= -736.013725065   H   0.003638 1.017997 -2.683962
              zpe= -735.854048   H   -1.956911 0.035321 -2.081723
        th energy= -735.840616   el energy= -736.015295215
      th enthalpy= -735.839672   zpe= -735.856839
```

```
      th energy= -735.842594                          free energy= -735.887810
    th enthalpy= -735.841650
    free energy= -735.898334                  TS-5
                                              Cr    0.403858  0.000108 -0.289282
                                              C     1.420441 -1.538102 -0.557339
  TS-4                                         O     2.085699 -2.451279 -0.797935
  Cr   -0.049301  0.486301  0.000000          C     1.432551  0.000023  1.241322
  C    -1.619351  1.509616  0.000000          O     2.090446  0.000037  2.197188
  O    -2.571983  2.166545  0.000000          C     1.419619  1.538853 -0.556939
  C     0.638783  1.607598  1.272548          O     2.084350  2.452456 -0.797388
  O     1.076489  2.310390  2.088392          C    -1.317249  1.295200 -1.166956
  C     0.638783  1.607598 -1.272548          C    -1.281219 -0.000494 -1.730755
  O     1.076489  2.310390 -2.088392          C    -1.317083 -1.296052 -1.166664
  C    -1.501885 -1.681768 -0.678857          C    -1.930508 -1.791233  0.080955
  C    -0.467767 -2.187659 -1.596680          C    -1.702337 -1.256195  1.290156
  C     0.844313 -1.873912 -1.602435          C    -0.912052  0.000073  1.495076
  C     1.577777 -0.976107 -0.693901          C    -1.703040  1.255883  1.289709
  C     1.577777 -0.976107  0.693901          C    -1.931270  1.790481  0.080359
  C     0.844313 -1.873912  1.602435          H    -1.100710  2.082962 -1.891232
  C    -0.467767 -2.187659  1.596680          H    -0.887325 -0.000618 -2.754100
  C    -1.501885 -1.681768  0.678857          H    -1.100474 -2.083948 -1.890774
  H    -2.419258 -1.340364 -1.166427          H    -2.517260 -2.710056  0.000225
  H    -0.844463 -2.800709 -2.419782          H    -2.106660 -1.746862  2.180278
  H     1.437899 -2.254506 -2.438646          H    -0.504585  0.000379  2.511052
  H     2.404180 -0.447097 -1.170038          H    -2.107974  1.746370  2.179655
  H     2.404180 -0.447097  1.170038          H    -2.518685  2.708844 -0.000800
  H     1.437899 -2.254506  2.438646            el energy= -735.961736393
  H    -0.844463 -2.800709  2.419782                  zpe= -735.803886
  H    -2.419258 -1.340364  1.166427             th energy= -735.789802
    el energy= -736.004312890              th enthalpy= -735.788858
          zpe= -735.845717              free energy= -735.845289
    th energy= -735.831323
  th enthalpy= -735.830379
```

B3LYP/BS5

```
  I                                           free energy= -736.599390
  Cr   -0.036286 -0.377801  0.000000
  C     1.836001 -0.324725  0.000000          TS-1
  O     2.989074 -0.253195  0.000000          Cr    0.336736  0.000002  0.009221
  C    -0.071009 -1.768168  1.240984          C     1.131758  1.259754 -1.111388
  O    -0.085214 -2.659920  1.978716          O     1.616904  2.049823 -1.804115
  C    -0.071009 -1.768168 -1.240984          C     1.898888  0.000014  1.049669
  O    -0.085214 -2.659920 -1.978716          O     2.855326  0.000030  1.696941
  C     0.456922  2.704834 -0.665270          C     1.131744 -1.259802 -1.111337
  C     0.241325  1.493964 -1.487574          O     1.616889 -2.049906 -1.804024
  C    -0.958145  0.807966 -1.654410          C    -2.720683 -0.663030 -0.692014
  C    -1.991929  0.506354 -0.703310          C    -1.460848 -1.414787 -0.462240
  C    -1.991929  0.506354  0.703310          C    -0.930027 -1.658807  0.826759
  C    -0.958145  0.807966  1.654410          C    -0.747735 -0.715734  1.867460
  C     0.241325  1.493964  1.487574          C    -0.747728  0.715803  1.867439
  C     0.456922  2.704834  0.665270          C    -0.930013  1.658843  0.826705
  H     0.616798  3.636456 -1.216446          C    -1.460837  1.414776 -0.462283
  H     0.928302  1.393623 -2.331771          C    -2.720679  0.663019 -0.692028
  H    -1.098550  0.297765 -2.609554          H    -3.638817 -1.244912 -0.823525
  H    -2.856688  0.002376 -1.137542          H    -1.294243 -2.233773 -1.167045
  H    -2.856688  0.002376  1.137542          H    -0.474346 -2.631443  1.025131
  H    -1.098550  0.297765  2.609554          H    -0.321446 -1.136535  2.779460
  H     0.928302  1.393623  2.331771          H    -0.321434  1.136625  2.779427
  H     0.616798  3.636456  1.216446          H    -0.474323  2.631482  1.025042
    el energy= -736.718929497                 H    -1.294232  2.233736 -1.167118
          zpe= -736.558388                    H    -3.638810  1.244904 -0.823551
    th energy= -736.544131                      el energy= -736.698685959
  th enthalpy= -736.543187                            zpe= -736.538928
```

th energy= -736.525512
th enthalpy= -736.524568
free energy= -736.578398

TS-2
Cr   0.034120 -0.475107 0.000000
C   -1.180884 -1.049919 1.334400
O   -1.923931 -1.418362 2.134541
C   -1.180884 -1.049919 -1.334400
O   -1.923931 -1.418362 -2.134541
C   0.805998 -2.131095 0.000000
O   1.313852 -3.174000 0.000000
C   -0.059847 1.984421 1.666971
C   0.894873 0.867073 1.627495
C   1.876696 0.451229 0.715574
C   1.876696 0.451229 -0.715574
C   0.894873 0.867073 -1.627495
C   -0.059847 1.984421 -1.666971
C   -0.653598 2.765375 -0.730622
C   -0.653598 2.765375 0.730622
H   -0.374385 2.198809 2.690618
H   1.079780 0.478810 2.629856
H   2.660436 -0.173143 1.146689
H   2.660436 -0.173143 -1.146689
H   1.079780 0.478810 -2.629856
H   -0.374385 2.198809 -2.690618
H   -1.320654 3.523919 -1.145260
H   -1.320654 3.523919 1.145260
el energy= -736.704324308
zpe= -736.544072
th energy= -736.530137
th enthalpy= -736.529193
free energy= -736.585308

TS-3
Cr   -0.002355 -0.488756 0.000000
C   1.906119 -0.471710 0.000000
O   3.056070 -0.443191 0.000000
C   -0.102871 -1.868005 1.246821
O   -0.163190 -2.746517 1.997524
C   -0.102871 -1.868005 -1.246821
O   -0.163190 -2.746517 -1.997524
C   -2.052117 0.329244 0.000000
C   -1.451718 0.539329 1.260557
C   -0.289008 1.272378 1.661536
C   0.275793 2.500114 1.240604
C   0.384150 3.130175 0.000000
C   0.275793 2.500114 -1.240604
C   -0.289008 1.272378 -1.661536
C   -1.451718 0.539329 -1.260557
H   -2.963413 -0.267648 0.000000
H   -1.956509 0.028431 2.082358
H   0.004855 1.012568 2.680439
H   0.802539 3.022880 2.046021
H   0.865377 4.107775 0.000000
H   0.802539 3.022880 -2.046021
H   0.004855 1.012568 -2.680439
H   -1.956509 0.028431 -2.082358
el energy= -736.700295450
zpe= -736.541839
th energy= -736.527580

th enthalpy= -736.526636
free energy= -736.583390

TS-4
Cr   -0.048050 0.490680 0.000000
C   -1.617899 1.509494 0.000000
O   -2.572781 2.163626 0.000000
C   0.640321 1.606120 1.275147
O   1.079020 2.303646 2.095229
C   0.640321 1.606120 -1.275147
O   1.079020 2.303646 -2.095229
C   -1.500832 -1.675690 -0.679092
C   -0.469900 -2.188249 -1.596449
C   0.842570 -1.876366 -1.602369
C   1.573730 -0.976139 -0.694468
C   1.573730 -0.976139 0.694468
C   0.842570 -1.876366 1.602369
C   -0.469900 -2.188249 1.596449
C   -1.500832 -1.675690 0.679092
H   -2.416306 -1.328973 -1.166479
H   -0.848831 -2.801373 -2.418349
H   1.437264 -2.258569 -2.436852
H   2.401804 -0.449451 -1.170422
H   2.401804 -0.449451 1.170422
H   1.437264 -2.258569 2.436852
H   -0.848831 -2.801373 2.418349
H   -2.416306 -1.328973 1.166479
el energy= -736.688676857
zpe= -736.530048
th energy= -736.515656
th enthalpy= -736.514711
free energy= -736.572125

TS-5
Cr   0.409457 0.000217 -0.289458
C   1.425675 -1.535964 -0.552887
O   2.088867 -2.451363 -0.791104
C   1.424454 -0.000005 1.248430
O   2.072569 -0.000063 2.211111
C   1.424584 1.537084 -0.552215
O   2.087101 2.453048 -0.790215
C   -1.309098 1.295786 -1.169860
C   -1.271034 -0.000686 -1.732451
C   -1.308903 -1.296965 -1.169521
C   -1.931384 -1.793377 0.073488
C   -1.712495 -1.256410 1.283252
C   -0.921159 0.000116 1.488141
C   -1.713663 1.255890 1.282629
C   -1.932658 1.792244 0.072670
H   -1.089354 2.082701 -1.894047
H   -0.877024 -0.000843 -2.756015
H   -1.089008 -2.084039 -1.893483
H   -2.518037 -2.711643 -0.012333
H   -2.124023 -1.743596 2.171856
H   -0.517055 0.000571 2.505440
H   -2.126244 1.742656 2.170978
H   -2.520439 2.709731 -0.013801
el energy= -736.647320934
zpe= -736.489463
th energy= -736.475376
th enthalpy= -736.474432

```
     free energy= -736.530891
```
B97-1/BS2
```
I
Cr   -0.038992 -0.369002  0.000000        TS-2
C     1.839242 -0.311717  0.000000        Cr    0.034257 -0.451314  0.000000
O     2.983930 -0.231529  0.000000        C    -1.181779 -1.042223  1.334958
C    -0.068125 -1.768103  1.241783        O    -1.910646 -1.428018  2.128728
O    -0.076850 -2.656716  1.970363        C    -1.181779 -1.042223 -1.334958
C    -0.068125 -1.768103 -1.241783        O    -1.910646 -1.428018 -2.128728
O    -0.076850 -2.656716 -1.970363        C     0.808568 -2.116820  0.000000
C     0.449549  2.694287 -0.661995        O     1.307959 -3.154110  0.000000
C     0.242305  1.479747 -1.478665        C    -0.065875  1.965750  1.663648
C    -0.958557  0.802036 -1.651419        C     0.905641  0.867922  1.627450
C    -1.990093  0.501094 -0.702380        C     1.882784  0.455737  0.714260
C    -1.990093  0.501094  0.702380        C     1.882784  0.455737 -0.714260
C    -0.958557  0.802036  1.651419        C     0.905641  0.867922 -1.627450
C     0.242305  1.479747  1.478665        C    -0.065875  1.965750 -1.663648
C     0.449549  2.694287  0.661995        C    -0.674015  2.727973 -0.729150
H     0.598902  3.620220 -1.213613        C    -0.674015  2.727973  0.729150
H     0.926728  1.378580 -2.317213        H    -0.384326  2.173533  2.681101
H    -1.097593  0.292502 -2.600744        H     1.094058  0.482497  2.623736
H    -2.849255 -0.002658 -1.133178        H     2.662668 -0.166074  1.141242
H    -2.849255 -0.002658  1.133178        H     2.662668 -0.166074 -1.141242
H    -1.097593  0.292502  2.600744        H     1.094058  0.482497 -2.623736
H     0.926728  1.378580  2.317213        H    -0.384326  2.173533 -2.681101
H     0.598902  3.620220  1.213613        H    -1.356398  3.465902 -1.140137
       el energy= -735.952274029         H    -1.356398  3.465902  1.140137
               zpe= -735.791612                el energy= -735.936108899
           th energy= -735.777451                    zpe= -735.775819
        th enthalpy= -735.776506              th energy= -735.761924
        free energy= -735.832561           th enthalpy= -735.760980
                                            free energy= -735.817108

TS-1
Cr   -0.012677 -0.326144  0.000000        TS-3
C     1.112355 -1.127188  1.262536        Cr   -0.004281 -0.471909  0.000000
O     1.800469 -1.610597  2.045678        C     1.913936 -0.464229  0.000000
C    -1.051983 -1.896204  0.000000        O     3.056188 -0.449525  0.000000
O    -1.689569 -2.849489  0.000000        C    -0.099774 -1.860493  1.247136
C     1.112355 -1.127188 -1.262536        O    -0.157730 -2.738846  1.985175
O     1.800469 -1.610597 -2.045678        C    -0.099774 -1.860493 -1.247136
C     0.688429  2.710429 -0.659833        O    -0.157730 -2.738846 -1.985175
C     0.465446  1.446778 -1.404795        C    -2.058415  0.325131  0.000000
C    -0.824638  0.925004 -1.656599        C    -1.461654  0.536356  1.258588
C    -1.862146  0.743123 -0.715378        C    -0.305328  1.270924  1.665367
C    -1.862146  0.743123  0.715378        C     0.283118  2.479320  1.237402
C    -0.824638  0.925004  1.656599        C     0.405198  3.103240  0.000000
C     0.465446  1.446778  1.404795        C     0.283118  2.479320 -1.237402
C     0.688429  2.710429  0.659833        C    -0.305328  1.270924 -1.665367
H     0.812092  3.621667 -1.242543        C    -1.461654  0.536356 -1.258588
H     1.166707  1.282792 -2.219980        H    -2.962059 -0.272633  0.000000
H    -1.023805  0.474569 -2.625050        H    -1.964207  0.026143  2.074465
H    -2.769069  0.317165 -1.132448        H    -0.018716  1.011449  2.680170
H    -2.769069  0.317165  1.132448        H     0.819382  2.989303  2.036805
H    -1.023805  0.474569  2.625050        H     0.905402  4.064260  0.000000
H     1.166707  1.282792  2.219980        H     0.819382  2.989303 -2.036805
H     0.812092  3.621667  1.242543        H    -0.018716  1.011449 -2.680170
       el energy= -735.932422381         H    -1.964207  0.026143 -2.074465
               zpe= -735.772405                el energy= -735.931273438
           th energy= -735.759124                    zpe= -735.772810
        th enthalpy= -735.758180              th energy= -735.758573
        free energy= -735.811790           th enthalpy= -735.757629
```

```
   free energy= -735.814455                      TS-5
                                              Cr    0.314527  0.404906  0.000000
TS-4                                          C     0.566566  1.419701  1.549758
Cr   -0.052467  0.463225  0.000000            O     0.774584  2.071981  2.469633
C    -1.616556  1.505425  0.000000            C    -1.218898  1.429405  0.000000
O    -2.540862  2.188293  0.000000            O    -2.168586  2.083046  0.000000
C     0.632218  1.597024  1.271753            C     0.566566  1.419701 -1.549758
O     1.063512  2.309327  2.070854            O     0.774584  2.071981 -2.469633
C     0.632218  1.597024 -1.271753            C     1.152800 -1.327652 -1.293372
O     1.063512  2.309327 -2.070854            C     1.715731 -1.309360  0.000000
C    -1.498012 -1.691091 -0.676293            C     1.152800 -1.327652  1.293372
C    -0.461312 -2.175921 -1.598316            C    -0.102917 -1.923768  1.787689
C     0.843318 -1.853119 -1.604724            C    -1.301453 -1.679430  1.253096
C     1.575560 -0.962299 -0.693062            C    -1.486298 -0.876672  0.000000
C     1.575560 -0.962299  0.693062            C    -1.301453 -1.679430 -1.253096
C     0.843318 -1.853119  1.604724            C    -0.102917 -1.923768 -1.787689
C    -0.461312 -2.175921  1.598316            H     1.879401 -1.127421 -2.075344
C    -1.498012 -1.691091  0.676293            H     2.741805 -0.937380  0.000000
H    -2.415484 -1.362477 -1.159292            H     1.879401 -1.127421  2.075344
H    -0.834128 -2.773998 -2.425775            H    -0.027631 -2.519254  2.693967
H     1.431869 -2.214020 -2.444998            H    -2.194173 -2.084076  1.724888
H     2.401738 -0.439842 -1.163462            H    -2.493470 -0.461377  0.000000
H     2.401738 -0.439842  1.163462            H    -2.194173 -2.084076 -1.724888
H     1.431869 -2.214020  2.444998            H    -0.027631 -2.519254 -2.693967
H    -0.834128 -2.773998  2.425775               el energy= -735.878795739
H    -2.415484 -1.362477  1.159292                     zpe= -735.720729
   el energy= -735.919438863                     th energy= -735.706713
         zpe= -735.760586                      th enthalpy= -735.705769
    th energy= -735.746238                     free energy= -735.761911
   th enthalpy= -735.745294
    free energy= -735.802882
B97-1/BS3
I
Cr    0.039971  0.364415  0.000000            TS-1
C    -1.832378  0.295517  0.000000            Cr   -0.016701 -0.321932  0.000000
O    -2.978120  0.211929  0.000000            C     1.104750 -1.124931  1.253956
C     0.063260  1.764261  1.230069            O     1.793949 -1.615879  2.034042
O     0.067905  2.661702  1.950982            C    -1.048323 -1.890433  0.000000
C     0.063260  1.764261 -1.230069            O    -1.678449 -2.850527  0.000000
O     0.067905  2.661702 -1.950982            C     1.104750 -1.124931 -1.253956
C    -0.436903 -2.695320 -0.661614            O     1.793949 -1.615879 -2.034042
C    -0.245475 -1.471322 -1.469427            C     0.686141  2.714199 -0.659569
C     0.956488 -0.793244 -1.650581            C     0.471594  1.442451 -1.394392
C     1.987722 -0.493980 -0.702916            C    -0.819246  0.922150 -1.654697
C     1.987722 -0.493980  0.702916            C    -1.858037  0.742064 -0.715436
C     0.956488 -0.793244  1.650581            C    -1.858037  0.742064  0.715436
C    -0.245475 -1.471322  1.469427            C    -0.819246  0.922150  1.654697
C    -0.436903 -2.695320  0.661614            C     0.471594  1.442451  1.394392
H    -0.569045 -3.621482 -1.217280            C     0.686141  2.714199  0.659569
H    -0.934717 -1.370077 -2.304176            H     0.800739  3.623996 -1.246310
H     1.095291 -0.286522 -2.601416            H     1.177842  1.273944 -2.204605
H     2.844643  0.014858 -1.132707            H    -1.017805  0.475832 -2.625186
H     2.844643  0.014858  1.132707            H    -2.764406  0.314248 -1.132249
H     1.095291 -0.286522  2.601416            H    -2.764406  0.314248  1.132249
H    -0.934717 -1.370077  2.304176            H    -1.017805  0.475832  2.625186
H    -0.569045 -3.621482  1.217280            H     1.177842  1.273944  2.204605
   el energy= -1694.10660525                   H     0.800739  3.623996  1.246310
         zpe= -1693.945839                        el energy= -1694.08719667
    th energy= -1693.931761                           zpe= -1693.927120
   th enthalpy= -1693.930817                     th energy= -1693.913894
    free energy= -1693.986681                   th enthalpy= -1693.912950
```

free energy= -1693.966451

TS-2
Cr   0.036832 -0.455918   0.000000
C   -1.170502 -1.050324   1.331244
O   -1.898097 -1.441046   2.126273
C   -1.170502 -1.050324 -1.331244
O   -1.898097 -1.441046 -2.126273
C   0.803392 -2.110995   0.000000
O   1.302418 -3.151589   0.000000
C   -0.071023   1.973593   1.662494
C   0.893830   0.869309   1.624466
C   1.875524   0.458860   0.713669
C   1.875524   0.458860 -0.713669
C   0.893830   0.869309 -1.624466
C   -0.071023   1.973593 -1.662494
C   -0.673131   2.741106 -0.729167
C   -0.673131   2.741106   0.729167
H   -0.389524   2.179814   2.680250
H   1.079401   0.482444   2.620870
H   2.655552 -0.162249   1.141635
H   2.655552 -0.162249 -1.141635
H   1.079401   0.482444 -2.620870
H   -0.389524   2.179814 -2.680250
H   -1.350677   3.483459 -1.140316
H   -1.350677   3.483459   1.140316
      el energy= -1694.08940965
            zpe= -1693.929066
       th energy= -1693.915209
     th enthalpy= -1693.914265
      free energy= -1693.970322

TS-3
Cr   -0.002889 -0.471521   0.000000
C   1.910513 -0.461363   0.000000
O   3.054369 -0.449975   0.000000
C   -0.099484 -1.859286   1.232500
O   -0.160045 -2.747577   1.962348
C   -0.099484 -1.859286 -1.232500
O   -0.160045 -2.747577 -1.962348
C   -2.052293   0.320791   0.000000
C   -1.456177   0.533775   1.258500
C   -0.300985   1.271725   1.661644
C   0.277736   2.486315   1.236323
C   0.394583   3.112029   0.000000
C   0.277736   2.486315 -1.236323
C   -0.300985   1.271725 -1.661644
C   -1.456177   0.533775 -1.258500
H   -2.952367 -0.282713   0.000000
H   -1.955524   0.021185   2.074830
H   -0.010116   1.012276   2.675322
H   0.810345   2.998848   2.036560
H   0.888149   4.076531   0.000000
H   0.810345   2.998848 -2.036560
H   -0.010116   1.012276 -2.675322
H   -1.955524   0.021185 -2.074830
      el energy= -1694.08508337
            zpe= -1693.926505
       th energy= -1693.912320
     th enthalpy= -1693.911376
      free energy= -1693.968123

TS-4
Cr   0.054040 -0.461316   0.000000
C   1.616258 -1.491710   0.000000
O   2.547053 -2.168688   0.000000
C   -0.624765 -1.597806   1.257742
O   -1.058980 -2.315302   2.053847
C   -0.624765 -1.597806 -1.257742
O   -1.058980 -2.315302 -2.053847
C   1.492181   1.692637 -0.676397
C   0.455654   2.173221 -1.600241
C   -0.848207   1.848405 -1.606105
C   -1.577354   0.956533 -0.693227
C   -1.577354   0.956533   0.693227
C   -0.848207   1.848405   1.606105
C   0.455654   2.173221   1.600241
C   1.492181   1.692637   0.676397
H   2.410980   1.366455 -1.158426
H   0.828440   2.768803 -2.429536
H   -1.437391   2.204951 -2.447841
H   -2.400710   0.429937 -1.164174
H   -2.400710   0.429937   1.164174
H   -1.437391   2.204951   2.447841
H   0.828440   2.768803   2.429536
H   2.410980   1.366455   1.158426
      el energy= -1694.07114528
            zpe= -1693.912207
       th energy= -1693.897902
     th enthalpy= -1693.896957
      free energy= -1693.954437

TS-5
Cr   0.316115   0.400117   0.000000
C   0.561382   1.412549   1.540620
O   0.769225   2.064400   2.464304
C   -1.198907   1.441945   0.000000
O   -2.142870   2.107532   0.000000
C   0.561382   1.412549 -1.540620
O   0.769225   2.064400 -2.464304
C   1.146494 -1.325013 -1.292809
C   1.711020 -1.310281   0.000000
C   1.146494 -1.325013   1.292809
C   -0.107603 -1.925827   1.786471
C   -1.304642 -1.679507   1.250976
C   -1.483910 -0.872007   0.000000
C   -1.304642 -1.679507 -1.250976
C   -0.107603 -1.925827 -1.786471
H   1.871740 -1.121277 -2.075164
H   2.735819 -0.934285   0.000000
H   1.871740 -1.121277   2.075164
H   -0.031266 -2.523664   2.690967
H   -2.199451 -2.084606   1.718314
H   -2.486039 -0.444458   0.000000
H   -2.199451 -2.084606 -1.718314
H   -0.031266 -2.523664 -2.690967
      el energy= -1694.03350669
            zpe= -1693.875316
       th energy= -1693.861397
     th enthalpy= -1693.860453
      free energy= -1693.916280

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Molecular Coordinates for (TMCOT)Cr(CO)$_3$ (Å)

PBE0/BS1

II

C	2.536410	0.095897	-0.033772
C	1.436369	1.005236	-0.447383
C	0.629885	1.704174	0.467701
C	-0.016077	1.121367	1.607909
C	-0.347127	-0.205973	1.954110
C	-0.050450	-1.429564	1.255388
C	0.902653	-1.727650	0.285608
C	2.266687	-1.159078	0.306592
Cr	-0.596720	0.055258	-0.249506
C	-0.138524	-0.514084	-1.929636
C	-2.182585	-0.877961	-0.257590
C	-1.670453	1.373412	-0.934524
O	0.208143	-0.886999	-2.964154
O	-3.192919	-1.433478	-0.283883
O	-2.390130	2.151490	-1.390379
C	3.910982	0.697922	-0.002866
C	0.343599	3.169642	0.230233
C	-1.315618	-0.371507	3.105563
C	0.797510	-3.065007	-0.408864
H	3.954835	1.540872	0.701309
H	4.185730	1.097747	-0.989454
H	4.668722	-0.036800	0.291370
H	1.478553	-3.792371	0.058414
H	1.091381	-2.982947	-1.462329
H	-0.220326	-3.468928	-0.370689
H	-2.118636	-1.073166	2.850421
H	-1.775719	0.577697	3.397490
H	-0.792089	-0.778644	3.981428
H	-0.639279	3.477900	0.603277
H	0.394932	3.410082	-0.837247
H	1.106968	3.775033	0.739838
H	3.058645	-1.839810	0.630812
H	-0.782970	-2.212697	1.461554
H	-0.567888	1.851675	2.199983
H	1.658102	1.579116	-1.351535

    el energy= -892.224976056
          zpe= -891.949782
    th energy= -891.929554
  th enthalpy= -891.928610
  free energy= -891.996913

TS-A

C	-2.592326	0.043452	-0.254779
C	-1.451513	-0.833917	-0.634508
C	-0.803093	-1.624133	0.359589
C	-0.258544	-1.054911	1.536996
C	0.106865	0.283473	1.905299
C	-0.060219	1.498650	1.183685
C	-0.916646	1.782515	0.102530
C	-2.312289	1.291620	0.089931
Cr	0.597783	-0.035409	-0.235078
C	0.878146	-1.027079	-1.747466
C	1.477417	1.263038	-1.181496
C	2.244342	-0.579484	0.375305

O	1.036444	-1.665537	-2.695391
O	2.055109	2.058312	-1.786623
O	3.266432	-0.933831	0.772435
C	-3.959515	-0.573380	-0.245807
C	-0.592778	-3.102891	0.142639
C	0.959700	0.377142	3.152946
C	-0.742614	3.115219	-0.587445
H	-4.008467	-1.409699	0.466221
H	-4.211882	-0.985655	-1.233107
H	-4.731220	0.154906	0.027828
H	-1.485838	3.830138	-0.201318
H	-0.917016	3.025379	-1.665983
H	0.252930	3.544431	-0.437157
H	0.311760	0.434796	4.038462
H	1.615582	-0.491713	3.275236
H	1.584821	1.276054	3.144454
H	-1.484739	-3.657984	0.467026
H	-0.446834	-3.320229	-0.921385
H	0.273190	-3.489721	0.691405
H	-3.081998	2.002275	0.405062
H	0.659418	2.270659	1.462711
H	0.213627	-1.790813	2.188841
H	-1.615608	-1.370440	-1.574313

    el energy= -892.204187881
          zpe= -891.929758
    th energy= -891.910224
  th enthalpy= -891.909280
  free energy= -891.975636

TS-B

C	-0.026757	2.201392	1.231760
C	-0.184448	2.834822	0.000000
C	-0.026757	2.201392	-1.231760
C	-0.157248	0.818047	-1.546812
C	-1.274475	-0.054202	-1.262036
C	-1.858438	-0.296024	0.000000
C	-1.274475	-0.054202	1.262036
C	-0.157248	0.818047	1.546812
Cr	0.268776	-0.797800	0.000000
C	2.086315	-0.426321	0.000000
C	0.450651	-2.155562	1.209893
C	0.450651	-2.155562	-1.209893
O	3.201200	-0.145433	0.000000
O	0.578948	-3.034516	1.949411
O	0.578948	-3.034516	-1.949411
C	0.418398	3.065448	2.380878
C	0.418398	3.065448	-2.380878
C	-1.914107	-0.725748	-2.453388
C	-1.914107	-0.725748	2.453388
H	0.620566	4.098510	2.081956
H	1.329639	2.646106	2.829028
H	-0.343647	3.069320	3.172745
H	-2.612134	-0.032586	2.944456
H	-1.161771	-1.014207	3.195858
H	-2.469641	-1.625037	2.164051

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H    -2.469641 -1.625037 -2.164051          C    -0.432155 -1.611168  0.651830
H    -2.612134 -0.032586 -2.944456          C    -1.165495 -0.880133  1.690327
H    -1.161771 -1.014207 -3.195858          C    -1.436206  0.443924  1.777572
H    -0.343647  3.069320 -3.172745          C    -1.086370  1.471193  0.777429
H     0.620566  4.098510 -2.081956          C    -1.422083  1.517277 -0.539840
H     1.329639  2.646106 -2.829028          C    -2.182134  0.465605 -1.236780
H     0.263653  0.590069  2.528631          Cr    0.811929  0.141105 -0.156152
H    -2.699161 -0.988110  0.000000          C     1.893923 -0.600616 -1.381883
H     0.263653  0.590069 -2.528631          C     1.823724  1.671743 -0.294077
H    -0.095658  3.919312  0.000000          C     1.986625 -0.402519  1.094104
      el energy= -892.203247978            O     2.573424 -1.092789 -2.182426
             zpe= -891.929558              O     2.497804  2.603707 -0.391301
       th energy= -891.909679              O     2.735973 -0.739682  1.911293
     th enthalpy= -891.908734              C    -2.619080 -1.775038 -2.200357
      free energy= -891.976785             C     0.303204 -2.836468  1.142010
                                           C    -2.041101  1.014013  3.032264
                                           C    -1.142233  2.751310 -1.357299
TS-C                                       H    -2.967020 -2.630592 -1.605235
C     1.580892  1.686035  0.258653          H    -1.993674 -2.185772 -3.005648
C     0.215079  1.628120  0.816565          H    -3.489023 -1.288853 -2.654855
C    -0.477713  0.770357  1.691344          H    -2.090913  3.206264 -1.678215
C    -0.457368 -0.660234  1.722405          H    -0.585704  2.505286 -2.270275
C     0.223644 -1.620610  0.957524          H    -0.574677  3.498463 -0.793089
C     1.607155 -1.648583  0.455806          H    -2.985157  1.531744  2.813185
C     2.543839 -0.737496  0.103386          H    -2.236636  0.236183  3.777890
C     2.500455  0.726408  0.009399          H    -1.369888  1.759549  3.482611
Cr   -0.688690 -0.003353 -0.315531          H    -0.424345 -3.625723  1.387035
C    -0.826508  1.233049 -1.695366          H     0.975595 -3.225781  0.370491
C    -0.838282 -1.387385 -1.543710          H     0.894998 -2.639524  2.042642
C    -2.477367  0.006395 -0.165402          H    -3.060765  0.814725 -1.784129
O    -0.934402  2.003416 -2.542176          H    -0.624527  2.367310  1.199183
O    -0.944821 -2.250022 -2.296641          H    -1.398682 -1.475924  2.576426
O    -3.628317  0.010050 -0.049067          H    -0.162547 -2.199930 -1.345868
C     1.932003  3.100770 -0.138251               el energy= -892.188172977
C    -1.567717  1.404718  2.528647                      zpe= -891.914867
C    -0.339966 -3.027517  1.069597                th energy= -891.894566
C     3.880288 -1.272684 -0.354733              th enthalpy= -891.893621
H     1.874520  3.777702  0.725981               free energy= -891.963048
H     1.216303  3.477252 -0.883885
H     2.936568  3.172176 -0.566460
H     4.691072 -0.863692  0.265439          TS-E
H     4.091923 -0.964871 -1.388981          C     0.884883 -1.629468  0.192299
H     3.930879 -2.364775 -0.305785          C     2.224749 -1.218249 -0.009715
H     0.196343 -3.592878  1.845624          C     2.895376 -0.000126  0.080720
H    -1.405266 -3.019083  1.320622          C     2.224670  1.218067 -0.008403
H    -0.222749 -3.575635  0.127134          C     0.884887  1.629115  0.194239
H    -1.176518  1.630160  3.530726          C     0.026338  1.245624  1.281259
H    -1.914885  2.345867  2.089295          C    -0.247018 -0.001217  1.890877
H    -2.435151  0.746212  2.649423          C     0.026484 -1.247340  1.279967
H     3.425133  1.117133 -0.416595          Cr   -0.769222 -0.000045 -0.226553
H     1.930142 -2.679879  0.307893          C    -2.151218 -1.196182 -0.317052
H    -1.312949 -1.065151  2.263232          C    -2.151030  1.196384 -0.315529
H    -0.227096  2.624312  0.816956          C    -0.479573  0.001803 -2.078724
      el energy= -892.196067018            O    -3.050250 -1.918310 -0.376557
             zpe= -891.921207              O    -3.049922  1.918760 -0.374164
       th energy= -891.901404              O    -0.273920  0.003124 -3.207078
     th enthalpy= -891.900460              C     0.585567 -3.019946 -0.356012
      free energy= -891.968284             C     4.399673  0.000016 -0.037075
                                           C     0.585528  3.020190 -0.352507
                                           C    -1.135792 -0.002020  3.110266
TS-D                                       H     1.068841 -3.803135  0.248693
C    -1.824772 -0.822530 -1.349770          H     0.942841 -3.127335 -1.386481
C    -0.631007 -1.440567 -0.716371
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H     -0.489179 -3.227673 -0.366670          C      0.487754 -0.004194  2.039654
H     -0.531970 -0.003796  4.028042          C      1.601734 -1.544320  0.793131
H     -1.779843 -0.888648  3.134973          O      2.205406  2.467875  1.110960
H     -1.778204  0.885713  3.137353          O      0.313782 -0.004652  3.184463
H      1.068893  3.802684  0.253012          O      2.182840 -2.489282  1.107403
H      0.942688  3.128732 -1.382893          C      1.033240  2.442579 -2.064396
H     -0.489213  3.227953 -0.362811          C      1.011989 -2.446587 -2.069599
H      4.881471  0.000252  0.950751          C     -3.089841 -1.848358  0.483847
H      4.764013 -0.887826 -0.569795          C     -3.074940  1.872930  0.485980
H      4.763841  0.887726 -0.570137          H      2.059733  2.131668 -2.290137
H     -0.537773 -2.079606  1.708507          H      1.080182  3.281836 -1.360874
H     -0.537929  2.077355  1.710795          H      0.587233  2.823761 -2.995586
H      2.862147  2.029831 -0.379683          H     -3.351143  2.759152 -0.096931
H      2.862307 -2.029651 -0.381658          H     -2.957384  2.177870  1.536043
      el energy= -892.185219784             H     -3.918624  1.169407  0.457198
            zpe= -891.913395                H     -3.928318 -1.138590  0.456089
      th energy= -891.892696                H     -3.372812 -2.731948 -0.099802
   th enthalpy= -891.891752                H     -2.974165 -2.155169  1.533575
   free energy= -891.962076                H      0.562775 -2.822003 -3.001587
                                            H      2.041141 -2.144077 -2.294648
                                            H      1.051623 -3.287647 -1.367778
TS-F                                        H     -1.527852  2.640831 -1.574073
C      0.195152  1.303588 -1.516431          H     -1.720217  0.006234  1.690786
C      0.589509 -0.000295 -1.902516          H     -1.550111 -2.624660 -1.578523
C      0.183712 -1.301525 -1.519302          H      1.597041 -0.004299 -2.336577
C     -1.155107 -1.739575 -1.073947                el energy= -892.146807420
C     -1.819852 -1.231960 -0.026630                      zpe= -891.873611
C     -1.319747  0.005179  0.669695                th energy= -891.853765
C     -1.809407  1.247603 -0.024718             th enthalpy= -891.852821
C     -1.140090  1.751846 -1.070726             free energy= -891.920639
Cr     0.785286 -0.003662  0.254282
C      1.615529  1.528754  0.795533
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PBEPBE/auto/BS1

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II
C      2.558381  0.131923 -0.079889
C      1.431314  1.025845 -0.483668
C      0.623703  1.730889  0.446958
C      0.008837  1.140956  1.612852
C     -0.295740 -0.201070  1.978810
C     -0.000650 -1.432027  1.271973
C      0.957477 -1.736742  0.289486
C      2.314373 -1.136960  0.276743
Cr    -0.610811  0.048842 -0.241843
C     -0.184405 -0.529210 -1.931142
C     -2.193244 -0.891681 -0.224401
C     -1.734349  1.333777 -0.909564
O      0.132619 -0.914654 -2.989539          H     -0.663974  3.505384  0.606783
O     -3.222096 -1.451896 -0.247988          H      0.334499  3.432803 -0.873296
O     -2.501404  2.096765 -1.361355          H      1.095841  3.823298  0.689335
C      3.931510  0.758520 -0.079917          H      3.134480 -1.806733  0.582719
C      0.317717  3.200471  0.205321          H     -0.720807 -2.230951  1.503363
C     -1.236736 -0.373981  3.163168          H     -0.544035  1.871783  2.219172
C      0.858218 -3.087294 -0.397231          H      1.625363  1.594814 -1.407262
H      3.978799  1.615669  0.620259                el energy= -892.262116341
H      4.184474  1.159144 -1.081489                      zpe= -891.996490
H      4.712665  0.033671  0.207745                th energy= -891.975575
H      1.584370 -3.799084  0.045217             th enthalpy= -891.974630
H      1.106946 -3.002200 -1.470660             free energy= -892.044549
H     -0.152804 -3.521985 -0.314398
H     -2.044599 -1.090696  2.930329          TS-A
H     -1.701714  0.577966  3.468689          C     -2.613263  0.004616 -0.321206
H     -0.681422 -0.777303  4.031790          C     -1.444914 -0.866674 -0.664273
                                            C     -0.804708 -1.650319  0.356778
                                            C     -0.295804 -1.058850  1.552196
                                            C      0.036457  0.300190  1.919963
                                            C     -0.127020  1.513717  1.173299
                                            C     -0.975214  1.799346  0.069339
                                            C     -2.363350  1.276323  0.008856
                                            Cr     0.614787 -0.036388 -0.220210
                                            C      0.984893 -1.048985 -1.700807
                                            C      1.489501  1.257445 -1.179224
                                            C      2.267772 -0.514899  0.429509
                                            O      1.222885 -1.702167 -2.644057
                                            O      2.080338  2.057260 -1.800802
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O     3.317197 -0.832866  0.839304
C    -3.977480 -0.638724 -0.333437
C    -0.574199 -3.137091  0.156516
C     0.850529  0.423747  3.201003
C    -0.788767  3.138066 -0.621747
H    -4.030260 -1.471772  0.395177
H    -4.203532 -1.076613 -1.325572
H    -4.774583  0.084015 -0.086791
H    -1.554280  3.854608 -0.258449
H    -0.932225  3.045340 -1.712768
H     0.206998  3.575698 -0.442231
H     0.167534  0.477060  4.070865
H     1.523318 -0.437388  3.354724
H     1.461982  1.341754  3.204716
H    -1.478533 -3.703099  0.455660
H    -0.388454 -3.361270 -0.908379
H     0.281922 -3.516531  0.741004
H    -3.165145  1.983866  0.278139
H     0.578162  2.304489  1.469417
H     0.169540 -1.786412  2.231720
H    -1.567300 -1.405692 -1.618352
        el energy= -892.243386222
               zpe= -891.978555
        th energy= -891.958304
      th enthalpy= -891.957360
      free energy= -892.025422


TS-B
C    -0.013843  2.233859  1.243549
C    -0.155261  2.869280  0.000000
C    -0.013843  2.233859 -1.243549
C    -0.163900  0.841985 -1.560995
C    -1.287799 -0.035073 -1.274302
C    -1.871821 -0.281064  0.000000
C    -1.287799 -0.035073  1.274302
C    -0.163900  0.841985  1.560995
Cr    0.270961 -0.807375  0.000000
C     2.093925 -0.457344  0.000000
C     0.438856 -2.183192  1.190692
C     0.438856 -2.183192 -1.190692
O     3.233039 -0.201151  0.000000
O     0.561997 -3.093507  1.922840
O     0.561997 -3.093507 -1.922840
C     0.436443  3.099313  2.401175
C     0.436443  3.099313 -2.401175
C    -1.931337 -0.712004 -2.471708
C    -1.931337 -0.712004  2.471708
H     0.667007  4.133906  2.098016
H     1.337936  2.661693  2.871807
H    -0.339878  3.127931  3.190844
H    -2.629597 -0.013537  2.973853
H    -1.172115 -1.010751  3.215161
H    -2.496780 -1.613575  2.178195
H    -2.496780 -1.613575 -2.178195
H    -2.629597 -0.013537 -2.973853
H    -1.172115 -1.010751 -3.215161
H    -0.339878  3.127931 -3.190844
H     0.667007  4.133906 -2.098016
H     1.337936  2.661693 -2.871807
H     0.269132  0.602131  2.544274
H    -2.718991 -0.978649  0.000000
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H     0.269132  0.602131 -2.544274
H    -0.053827  3.961478  0.000000
        el energy= -892.245859145
               zpe= -891.981232
        th energy= -891.960778
      th enthalpy= -891.959834
      free energy= -892.029126


TS-C
C     1.576459  1.722250  0.243140
C     0.231684  1.622375  0.855217
C    -0.429294  0.720540  1.729926
C    -0.380300 -0.720339  1.718723
C     0.328082 -1.659685  0.931776
C     1.696635 -1.638188  0.387834
C     2.612185 -0.685414  0.030559
C     2.524666  0.781311 -0.045358
Cr   -0.708904 -0.004143 -0.310506
C    -0.957424  1.267638 -1.637254
C    -0.913132 -1.374823 -1.542820
C    -2.486406 -0.033993 -0.107937
O    -1.150551  2.069840 -2.464971
O    -1.066152 -2.241771 -2.311383
O    -3.654103 -0.053462  0.034376
C     1.871521  3.153483 -0.173634
C    -1.504639  1.315519  2.627940
C    -0.205928 -3.089337  1.019850
C     3.958017 -1.185273 -0.466334
H     1.822182  3.841296  0.693217
H     1.112258  3.505448 -0.900462
H     2.864401  3.255451 -0.641670
H     4.779089 -0.765792  0.148405
H     4.146016 -0.849841 -1.505557
H     4.035918 -2.284564 -0.439835
H     0.381840 -3.672827  1.755851
H    -1.266160 -3.116220  1.320401
H    -0.117317 -3.605758  0.047342
H    -2.364451  0.635442  2.757632
H    -1.080361  1.516816  3.631128
H    -1.882438  2.271912  2.228281
H     3.429461  1.206815 -0.501552
H     2.043544 -2.664104  0.199394
H    -1.217918 -1.162137  2.275255
H    -0.238683  2.614250  0.890380
        el energy= -892.235458690
               zpe= -891.970046
        th energy= -891.949575
      th enthalpy= -891.948631
      free energy= -892.018088


TS-D
C    -1.859301 -0.786930 -1.373056
C    -0.655835 -1.431964 -0.767088
C    -0.449583 -1.661794  0.607114
C    -1.145988 -0.949922  1.687270
C    -1.398785  0.389661  1.828786
C    -1.081105  1.451150  0.848140
C    -1.440284  1.539238 -0.477452
C    -2.211819  0.509957 -1.207105
Cr    0.798621  0.145433 -0.173969
C     1.918013 -0.577116 -1.373598
```

```
C      1.799662   1.679155  -0.317564        H      0.991019   3.160233  -1.386486
C      1.979784  -0.393207   1.065960        H     -0.483393   3.229184  -0.399722
O      2.642257  -1.056093  -2.170294        H      1.057771   3.837933   0.265329
O      2.480827   2.627603  -0.428260        H      4.809035  -0.893350  -0.611684
O      2.747936  -0.749008   1.884321        H      4.809289   0.895997  -0.607641
C     -2.663450  -1.705502  -2.264908        H      4.935226  -0.002148   0.920766
C      0.302523  -2.907400   1.044611        H     -0.520529  -2.094960   1.718110
C     -1.930526   0.921057   3.142682        H     -0.520607   2.092920   1.720693
C     -1.187086   2.817832  -1.251161        H      2.904555   2.051520  -0.387272
H     -3.021089  -2.589002  -1.701459        H      2.904721  -2.050701  -0.389898
H     -2.035089  -2.095404  -3.089773          el energy= -892.230238929
H     -3.535470  -1.193748  -2.706657                zpe= -891.967386
H     -2.152995   3.280937  -1.536570          th energy= -891.946100
H     -0.643646   2.616938  -2.192474        th enthalpy= -891.945156
H     -0.609886   3.551392  -0.663894        free energy= -892.016913
H     -2.890963   1.452570   2.997816
H     -2.084935   0.114736   3.879374
H     -1.227912   1.657892   3.579967        TS-F
H     -0.421937  -3.706496   1.304184        C      0.154148   1.315713  -1.553447
H      0.948091  -3.285729   0.234434        C      0.565700   0.000440  -1.925259
H      0.934916  -2.729759   1.931822        C      0.155950  -1.315391  -1.553376
H     -3.095502   0.885530  -1.746406        C     -1.170576  -1.763686  -1.073389
H     -0.625273   2.349591   1.292275        C     -1.836647  -1.257794  -0.006527
H     -1.338831  -1.566513   2.579509        C     -1.372206  -0.000939   0.679910
H     -0.191856  -2.178645  -1.428821        C     -1.838157   1.255453  -0.006266
      el energy= -892.226613058              C     -1.172830   1.762275  -1.073182
            zpe= -891.962625                 Cr     0.753959   0.000424   0.252914
      th energy= -891.941714                 C      1.622375   1.519596   0.773155
    th enthalpy= -891.940770                 C      0.555430   0.000208   2.063074
    free energy= -892.011671                 C      1.624126  -1.517678   0.773166
                                             O      2.258183   2.456632   1.080277
                                             O      0.428214  -0.000006   3.231710
TS-E                                         O      2.260970  -2.454010   1.080320
C      0.914012  -1.649231   0.194455        C      0.987974   2.462206  -2.115975
C      2.261758  -1.230613  -0.021612        C      0.991281  -2.460767  -2.115933
C      2.932241   0.000134   0.055340        C     -3.067413  -1.927486   0.555148
C      2.261668   1.230836  -0.020190        C     -3.069317   1.923998   0.555906
C      0.913724   1.648955   0.196235        H      2.011293   2.142598  -2.378104
C      0.051909   1.257771   1.287519        H      1.065484   3.298406  -1.399202
C     -0.223533  -0.001132   1.899929        H      0.512972   2.861064  -3.035288
C      0.051968  -1.259248   1.285989        H     -3.345213   2.823588  -0.021874
Cr    -0.784344   0.000158  -0.229907        H     -2.900652   2.230116   1.607655
C     -2.182187  -1.173775  -0.297052        H     -3.940108   1.239533   0.565737
C     -2.182300   1.174003  -0.296247        H     -3.939298  -1.244364   0.562885
C     -0.521679   0.001265  -2.086215        H     -3.341231  -2.828334  -0.021659
O     -3.112600  -1.888444  -0.344750        H     -2.899576  -2.231784   1.607545
O     -3.112639   1.888750  -0.343748        H      0.516929  -2.860074  -3.035385
O     -0.347129   0.002074  -3.238124        H      2.014263  -2.139872  -2.377819
C      0.603036  -3.042362  -0.363315        H      1.069688  -3.296964  -1.399258
C      4.444517   0.000169  -0.072039        H     -1.554086   2.683356  -1.541187
C      0.602618   3.042715  -0.360029        H     -1.742698  -0.001240   1.720398
C     -1.104601  -0.002181   3.135257        H     -1.550664  -2.685142  -1.541598
H      1.057665  -3.838249   0.261567        H      1.569917   0.001122  -2.383286
H      0.992051  -3.158951  -1.389646          el energy= -892.193987396
H     -0.482983  -3.228621  -0.403824                zpe= -891.930296
H     -0.485817  -0.005739   4.053257          th energy= -891.909788
H     -1.753803  -0.894775   3.167361        th enthalpy= -891.908844
H     -1.749905   0.893044   3.171690        free energy= -891.978007
```

B3LYP/BS1

II
```
C      0.578212   1.719731   0.549062
C     -0.023827   1.051563   1.674651
C     -0.285753  -0.302932   1.959354
C      0.069163  -1.490628   1.205908
C      1.053771  -1.749549   0.267091
C      2.366203  -1.067144   0.223970
C      2.548882   0.214878  -0.087376
C      1.405992   1.117557  -0.411765
Cr    -0.646792   0.055748  -0.272289
C     -1.786560   1.383109  -0.875369
C     -0.219520  -0.450244  -2.004864
C     -2.202199  -0.968429  -0.256784
O     -2.537686   2.170128  -1.269703
O      0.108108  -0.788320  -3.060674
O     -3.184516  -1.578366  -0.256175
C      0.229054   3.192412   0.399264
C     -1.203542  -0.578721   3.141597
C      1.022981  -3.081159  -0.457951
C      3.910834   0.866905  -0.118768
H      0.960866   3.796520   0.956038
H     -0.768814   3.435729   0.779924
H      0.280237   3.503402  -0.649737
H      3.970298   1.692383   0.605536
H      4.113999   1.302666  -1.108090
H      4.708642   0.150799   0.109417
H      1.817384  -3.741525  -0.077623
H      0.061739  -3.593712  -0.341213
H      1.209770  -2.945282  -1.530764
H     -0.629404  -1.011859   3.973065
H     -1.691302   0.331354   3.505380
H     -1.985500  -1.300878   2.876956
H      1.593372   1.751101  -1.281876
H      3.223154  -1.703448   0.460657
H     -0.633940  -2.306419   1.377922
H     -0.576890   1.729582   2.323644
      el energy= -893.191300325
            zpe= -892.918704
      th energy= -892.898013
    th enthalpy= -892.897069
    free energy= -892.966648
```

TS-A
```
C     -2.599949  -0.057461  -0.294655
C     -1.433771  -0.940488  -0.609190
C     -0.767697  -1.661902   0.422409
C     -0.246854  -1.032610   1.584664
C      0.066373   0.329561   1.907410
C     -0.149757   1.526378   1.152789
C     -1.030637   1.805890   0.097449
C     -2.387282   1.216434   0.015791
Cr     0.645845  -0.035891  -0.259180
C      1.461162   1.309705  -1.236129
C      2.321255  -0.493434   0.401376
C      0.977852  -1.087719  -1.746829
O      1.977136   2.147332  -1.846323
O      3.348908  -0.794548   0.836398
O      1.158813  -1.762281  -2.668977
C     -3.960886  -0.709352  -0.318505
C     -0.510188  -3.149618   0.261962
```

C   0.887227   0.506644   3.177742
C   -0.902098   3.150643 -0.591808
H   -4.019891 -1.525236   0.416895
H   -4.166317 -1.157745 -1.301487
H   -4.759006   0.008769 -0.097105
H   -1.689181   3.830539 -0.228732
H   -1.042050   3.053166 -1.675106
H   0.068040   3.625099 -0.414791
H   0.216341   0.602031   4.043622
H   1.552763 -0.343284   3.364103
H   1.498816   1.414324   3.136879
H   -1.391547 -3.719024   0.592570
H   -0.339661 -3.402047 -0.790553
H   0.356017 -3.492165   0.839181
H   -3.212589   1.892836   0.256676
H   0.548838   2.322199   1.413844
H   0.226290 -1.730041   2.275215
H   -1.574511 -1.518080 -1.526507
      el energy= -893.169934552
            zpe= -892.898189
      th energy= -892.878188
    th enthalpy= -892.877244
    free energy= -892.944715
```

TS-B
```
C     -0.023863   2.217057   1.242410
C     -0.147530   2.846140   0.000000
C     -0.023863   2.217057  -1.242410
C     -0.204835   0.842264  -1.581016
C     -1.306158  -0.040552  -1.268716
C     -1.877345  -0.293543   0.000000
C     -1.306158  -0.040552   1.268716
C     -0.204835   0.842264   1.581016
Cr     0.286899  -0.819614   0.000000
C      2.126944  -0.438820   0.000000
C      0.465143  -2.183955   1.238903
C      0.465143  -2.183955  -1.238903
O      3.242822  -0.150501   0.000000
O      0.590438  -3.052885   1.994031
O      0.590438  -3.052885  -1.994031
C      0.440082   3.086978   2.392969
C      0.440082   3.086978  -2.392969
C     -1.961943  -0.721585  -2.457910
C     -1.961943  -0.721585   2.457910
H      0.691103   4.104647   2.078150
H      1.325662   2.641339   2.866859
H     -0.335102   3.141851   3.170793
H     -2.665713  -0.029612   2.943795
H     -1.219101  -1.011857   3.209123
H     -2.515476  -1.619599   2.160920
H     -2.515476  -1.619599  -2.160920
H     -2.665713  -0.029612  -2.943795
H     -1.219101  -1.011857  -3.209123
H     -0.335102   3.141851  -3.170793
H      0.691103   4.104647  -2.078150
H      1.325662   2.641339  -2.866859
H      0.195339   0.618504   2.571268
H     -2.720558  -0.981270   0.000000
H      0.195339   0.618504  -2.571268
H     -0.021577   3.926505   0.000000
```

```
    el energy= -893.174501287
          zpe= -892.903215
     th energy= -892.882966
   th enthalpy= -892.882022
   free energy= -892.950901

TS-C
C     -1.566071   1.716923  -0.268948
C     -0.215012   1.626545  -0.868021
C      0.454393   0.731158  -1.721701
C      0.404181  -0.705970  -1.725442
C     -0.306926  -1.648792  -0.970260
C     -1.676548  -1.631028  -0.423529
C     -2.583349  -0.689384  -0.058507
C     -2.502349   0.778129   0.015390
Cr     0.729878  -0.005937   0.334160
C      0.912117   1.272198   1.698066
C      0.859053  -1.397789   1.589378
C      2.538331  -0.033860   0.135242
O      1.032821   2.061083   2.530328
O      0.936054  -2.258268   2.352995
O      3.688256  -0.052175  -0.010113
C     -1.886253   3.152554   0.114423
C      1.535018   1.327299  -2.612982
C      0.210784  -3.081879  -1.086177
C     -3.928894  -1.190516   0.439259
H     -1.842289   3.814180  -0.762888
H     -1.147017   3.532635   0.834860
H     -2.878609   3.246553   0.566316
H     -4.745094  -0.772735  -0.168533
H     -4.111811  -0.864590   1.473821
H     -4.004294  -2.281902   0.406742
H     -0.391546  -3.645929  -1.813865
H      1.256665  -3.115081  -1.406615
H      0.135605  -3.608149  -0.126947
H      1.124888   1.508575  -3.617253
H      1.893763   2.286409  -2.224472
H      2.397846   0.660686  -2.722704
H     -3.408096   1.194141   0.455925
H     -2.022514  -2.650845  -0.255633
H      1.239887  -1.136084  -2.275281
H      0.237641   2.615984  -0.906152
    el energy= -893.169530211
          zpe= -892.897022
     th energy= -892.876881
   th enthalpy= -892.875937
   free energy= -892.944553

TS-D
C     -1.697599  -0.719456  -1.540725
C     -0.584084  -1.423523  -0.844601
C     -0.488826  -1.699573   0.513385
C     -1.317698  -1.070480   1.556094
C     -1.627143   0.234234   1.739898
C     -1.207306   1.363218   0.874239
C     -1.443261   1.549191  -0.453420
C     -2.084153   0.554376  -1.337420
Cr     0.878438   0.157869  -0.071210
C      1.990139  -0.400734  -1.398605
C      1.830253   1.751028   0.004333
C      2.049811  -0.526222   1.143405

O      2.677814  -0.763479  -2.262365
O      2.444445   2.731594   0.043215
O      2.782462  -0.952054   1.938327
C     -2.373533  -1.566212  -2.596955
C      0.240810  -2.953746   0.963225
C     -2.381077   0.674200   2.976187
C     -1.162564   2.889106  -1.102908
H     -2.791103  -2.482499  -2.156225
H     -1.647689  -1.886507  -3.358451
H     -3.181131  -1.023345  -3.100252
H     -2.107609   3.343256  -1.436987
H     -0.532416   2.778207  -1.994194
H     -0.672576   3.584301  -0.413697
H     -3.315226   1.187263   2.706423
H     -2.627351  -0.174258   3.623687
H     -1.786825   1.391189   3.561820
H     -0.488128  -3.765216   1.117475
H      0.960712  -3.286228   0.208451
H      0.777515  -2.810130   1.907201
H     -2.886089   0.951557  -1.963469
H     -0.806113   2.217905   1.423575
H     -1.626807  -1.756501   2.348293
H     -0.052080  -2.118783  -1.494822
    el energy= -893.165191791
          zpe= -892.894111
     th energy= -892.873513
   th enthalpy= -892.872569
   free energy= -892.942677

TS-E
C     -0.233088   0.910408   1.665850
C      0.015259   2.238076   1.229690
C     -0.041977   2.900650   0.000000
C      0.015259   2.238076  -1.229690
C     -0.233088   0.910408  -1.665850
C     -1.299621   0.039934  -1.253282
C     -1.901532  -0.239587   0.000000
C     -1.299621   0.039934   1.253282
Cr     0.245613  -0.797803   0.000000
C      0.329997  -2.185485   1.228215
C      0.329997  -2.185485  -1.228215
C      2.121620  -0.502778   0.000000
O      0.389189  -3.071713   1.969200
O      0.389189  -3.071713  -1.969200
O      3.251930  -0.292034   0.000000
C      0.276505   0.621764   3.082719
C      0.121487   4.410406   0.000000
C      0.276505   0.621764  -3.082719
C     -3.141768  -1.114353   0.000000
H     -0.376320   1.077143   3.844429
H      1.286888   1.019346   3.232028
H      0.319925  -0.452602   3.287758
H     -4.050980  -0.496407   0.000000
H     -3.179996  -1.756879   0.887594
H     -3.179996  -1.756879  -0.887594
H     -0.376320   1.077143  -3.844429
H      1.286888   1.019346  -3.232028
H      0.319925  -0.452602  -3.287758
H      0.665242   4.759135   0.887764
H      0.665242   4.759135  -0.887764
H     -0.851445   4.923236   0.000000
```

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```
H    -1.734537 -0.531207  2.076242        C    -0.939336 -2.452075 -2.144203
H    -1.734537 -0.531207 -2.076242        C    -0.948930  2.450069 -2.138449
H     0.393621  2.875942 -2.036346        C     3.092885  1.894958  0.552940
H     0.393621  2.875942  2.036346        C     3.087847 -1.895328  0.565322
     el energy= -893.158036811            H    -1.955566 -2.142543 -2.413838
            zpe= -892.888629              H    -1.015125 -3.299446 -1.452869
      th energy= -892.867584              H    -0.451072 -2.823702 -3.058703
    th enthalpy= -892.866640              H     3.366313 -2.789906 -0.004414
    free energy= -892.937776              H     2.937596 -2.192159  1.614096
                                          H     3.943810 -1.205289  0.556066
TS-F                                      H     3.946470  1.202000  0.539831
C    -0.126400 -1.308173 -1.547917        H     3.371285  2.787726 -0.019675
C    -0.533387 -0.000642 -1.914027        H     2.949509  2.193864  1.602075
C    -0.131805  1.307932 -1.544406        H    -0.464334  2.822907 -3.054439
C     1.191702  1.756078 -1.055132        H    -1.965342  2.138309 -2.404965
C     1.840857  1.251768  0.007663        H    -1.024564  3.297206 -1.446818
C     1.348444  0.002558  0.696386        H     1.588472 -2.654508 -1.529567
C     1.841025 -1.248480  0.012518        H     1.721093  0.004724  1.726112
C     1.194644 -1.754570 -1.051666        H     1.585632  2.652949 -1.538783
Cr   -0.797081  0.001824  0.283343        H    -1.520633 -0.002367 -2.388131
C    -1.675386 -1.564814  0.747473             el energy= -893.116737517
C    -0.553346 -0.005798  2.106304                    zpe= -892.846219
C    -1.669343  1.568277  0.756664              th energy= -892.825942
O    -2.307613 -2.497433  1.002335            th enthalpy= -892.824998
O    -0.393384 -0.009572  3.253938            free energy= -892.895198
O    -2.299055  2.501494  1.015847
```

Molecular Coordinates for (TMCOT)Mo(CO)$_3$ (Å)

PBE0/BS1

II

C	2.649382	0.131574	-0.268016
C	1.526790	1.066024	-0.545696
C	0.803913	1.740549	0.455026
C	0.289374	1.145081	1.668052
C	0.020426	-0.184350	2.070104
C	0.252580	-1.428175	1.362758
C	1.092251	-1.730556	0.290992
C	2.428959	-1.121141	0.119594
Mo	-0.605908	0.038026	-0.206581
C	-0.370064	-0.630275	-2.062628
C	-2.307861	-0.980591	0.001626
C	-1.837491	1.462237	-0.836504
O	-0.140036	-1.048705	-3.110600
O	-3.315113	-1.532149	0.108170
O	-2.601884	2.245284	-1.202361
C	4.024235	0.716908	-0.421222
C	0.467461	3.201889	0.261062
C	-0.766626	-0.343635	3.353256
C	0.951397	-3.096399	-0.341467
H	4.166384	1.569717	0.257696
H	4.174771	1.099145	-1.441074
H	4.805663	-0.022842	-0.214572
H	1.705429	-3.787629	0.065301
H	1.115200	-3.044829	-1.424437
H	-0.042089	-3.524612	-0.168133
H	-0.103412	-0.692235	4.157137
H	-1.224907	0.596407	3.675843
H	-1.562294	-1.088918	3.240559
H	1.246293	3.821857	0.728662
H	0.441421	3.454992	-0.804148
H	-0.497278	3.477051	0.701569
H	3.269484	-1.784588	0.342803
H	-0.428326	-2.220437	1.679605
H	-0.178527	1.876852	2.326927
H	1.668239	1.662684	-1.450646

el energy= -873.521605073
zpe= -873.248247
th energy= -873.227411
th enthalpy= -873.226467
free energy= -873.296868

TS-A

C	-2.667131	0.104261	-0.466839
C	-1.518651	-0.808129	-0.742278
C	-1.012580	-1.640017	0.312968
C	-0.557516	-1.091934	1.538686
C	-0.226705	0.242424	1.998750
C	-0.311989	1.489439	1.321385
C	-0.991351	1.799640	0.108014
C	-2.391238	1.339490	-0.072482
Mo	0.597421	-0.022068	-0.196067
C	0.998218	-0.956014	-1.899193
C	1.734481	1.414746	-0.977389
C	2.270188	-0.813549	0.575031
O	1.195303	-1.534026	-2.877959

O	2.401703	2.236764	-1.434164
O	3.200891	-1.283704	1.061794
C	-4.044780	-0.474572	-0.602502
C	-0.857534	-3.126474	0.104319
C	0.470912	0.264724	3.343316
C	-0.731771	3.169851	-0.478191
H	-4.186729	-1.321090	0.084726
H	-4.210777	-0.862382	-1.617725
H	-4.819630	0.270734	-0.390915
H	-1.472279	3.891097	-0.095896
H	-0.832747	3.152174	-1.569177
H	0.266186	3.549688	-0.234822
H	-0.274210	0.203956	4.148722
H	1.160699	-0.577965	3.464365
H	1.036604	1.190843	3.485904
H	-0.593440	-3.340640	-0.937331
H	-0.086775	-3.564089	0.748617
H	-1.809991	-3.636419	0.309999
H	-3.176432	2.058075	0.182702
H	0.327110	2.263724	1.750932
H	-0.169471	-1.848855	2.221991
H	-1.608294	-1.337578	-1.696206

el energy= -873.500378975
zpe= -873.227731
th energy= -873.207662
th enthalpy= -873.206718
free energy= -873.274824

TS-B

C	0.036655	2.373919	1.242803
C	-0.040157	3.003574	0.000000
C	0.036655	2.373919	-1.242803
C	-0.251134	1.028558	-1.605098
C	-1.379025	0.189008	-1.275601
C	-1.954158	-0.040506	0.000000
C	-1.379025	0.189008	1.275601
C	-0.251134	1.028558	1.605098
Mo	0.263842	-0.741689	0.000000
C	2.274794	-0.606359	0.000000
C	0.301634	-2.227538	1.289929
C	0.301634	-2.227538	-1.289929
O	3.417713	-0.485463	0.000000
O	0.305400	-3.124944	2.019476
O	0.305400	-3.124944	-2.019476
C	0.574549	3.209280	2.376549
C	0.574549	3.209280	-2.376549
C	-2.064999	-0.469687	-2.449663
C	-2.064999	-0.469687	2.449663
H	0.926885	4.191658	2.048151
H	1.407578	2.686698	2.865394
H	-0.198329	3.352222	3.144975
H	-2.755975	0.241391	2.924935
H	-1.336562	-0.777092	3.208007
H	-2.635111	-1.354549	2.145747
H	-2.635111	-1.354549	-2.145747
H	-2.755975	0.241391	-2.924935

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H     -1.336562  -0.777092  -3.208007
H     -0.198329   3.352222  -3.144975
H      0.926885   4.191658  -2.048151
H      1.407578   2.686698  -2.865394
H      0.110597   0.798243   2.609166
H     -2.824246  -0.694817   0.000000
H      0.110597   0.798243  -2.609166
H      0.181593   4.068697   0.000000
        el energy= -873.500002766
              zpe= -873.227718
        th energy= -873.207234
      th enthalpy= -873.206290
      free energy= -873.276518


TS-C
C     -1.750179  -1.684788   0.247242
C     -0.475115  -1.636784   0.980690
C      0.179648  -0.738722   1.840949
C      0.163612   0.704345   1.839289
C     -0.473891   1.664862   1.042656
C     -1.775627   1.669633   0.362878
C     -2.654285   0.746508  -0.101376
C     -2.609915  -0.718160  -0.157226
Mo     0.636775  -0.006826  -0.299198
C      0.984755  -1.387751  -1.713054
C      1.067095   1.507210  -1.538707
C      2.513260  -0.067059   0.057245
O      1.210003  -2.202121  -2.493668
O      1.330580   2.405181  -2.208508
O      3.650183  -0.103967   0.287870
C     -2.068626  -3.102911  -0.167759
C      1.195123  -1.340929   2.788817
C      0.053971   3.080366   1.209458
C     -3.911492   1.274526  -0.752775
H     -2.151561  -3.759123   0.710109
H     -1.260383  -3.509082  -0.793108
H     -3.001734  -3.167676  -0.735490
H     -4.801679   0.881143  -0.240884
H     -3.980292   0.943532  -1.798966
H     -3.963103   2.367428  -0.735674
H     -0.599655   3.651051   1.885286
H      1.069013   3.093734   1.618103
H      0.072160   3.609702   0.249448
H      0.739405  -1.470872   3.780761
H      1.532135  -2.324013   2.444590
H      2.077254  -0.701929   2.907309
H     -3.464981  -1.110598  -0.707892
H     -2.075998   2.694731   0.143903
H      0.970736   1.114386   2.445630
H     -0.062003  -2.640534   1.077672
        el energy= -873.493675568
              zpe= -873.219863
        th energy= -873.199620
      th enthalpy= -873.198675
      free energy= -873.268243


TS-D
C     -1.790483  -0.672096  -1.603979
C     -0.733340  -1.426487  -0.885317
C     -0.685410  -1.700455   0.480212
C     -1.566009  -1.078475   1.483578
```

```
C     -1.867085   0.222367   1.684912
C     -1.380062   1.363269   0.878667
C     -1.539644   1.573401  -0.456611
C     -2.150406   0.607509  -1.386481
Mo     0.798014   0.152837  -0.027410
C      2.028103  -0.459992  -1.364147
C      1.916438   1.781679   0.141301
C      2.011780  -0.695826   1.184217
O      2.751412  -0.837516  -2.191398
O      2.589743   2.715466   0.226754
O      2.727809  -1.218310   1.935323
C     -2.435730  -1.460873  -2.711025
C     -0.007102  -2.966705   0.950088
C     -2.695054   0.643237   2.869053
C     -1.203057   2.911597  -1.063763
H     -2.893144  -2.378866  -2.317325
H     -1.682547  -1.775344  -3.447190
H     -3.205692  -0.882473  -3.232533
H     -2.124294   3.394767  -1.421852
H     -0.543717   2.804574  -1.933745
H     -0.723522   3.578925  -0.340446
H     -3.600541   1.175372   2.545790
H     -2.996847  -0.215652   3.477679
H     -2.133652   1.337881   3.510420
H     -0.756421  -3.765933   1.063466
H      0.743120  -3.304229   0.227558
H      0.488377  -2.838115   1.918590
H     -2.907636   1.037861  -2.045898
H     -0.999664   2.203419   1.465498
H     -1.942482  -1.780234   2.232634
H     -0.207294  -2.141139  -1.521067
        el energy= -873.488028007
              zpe= -873.215518
        th energy= -873.194981
      th enthalpy= -873.194037
      free energy= -873.264532


TS-E
C     -0.276816   1.073282   1.685384
C      0.077190   2.365380   1.230078
C      0.069321   3.024518   0.000000
C      0.077190   2.365380  -1.230078
C     -0.276816   1.073282  -1.685384
C     -1.374862   0.250517  -1.259008
C     -1.982129  -0.004734   0.000000
C     -1.374862   0.250517   1.259008
Mo     0.236795  -0.712153   0.000000
C      0.202242  -2.207898   1.276084
C      0.202242  -2.207898  -1.276084
C      2.271882  -0.642514   0.000000
O      0.161534  -3.113982   1.992201
O      0.161534  -3.113982  -1.992201
O      3.416960  -0.583013   0.000000
C      0.178579   0.763045   3.107486
C      0.360567   4.507080   0.000000
C      0.178579   0.763045  -3.107486
C     -3.253912  -0.819236   0.000000
H     -0.499579   1.207720   3.852501
H      1.185094   1.151218   3.297815
H      0.211397  -0.316381   3.292766
H     -4.131301  -0.157575   0.000000
```

```
H    -3.321293 -1.458916  0.887293
H    -3.321293 -1.458916 -0.887293
H    -0.499579  1.207720 -3.852501
H     1.185094  1.151218 -3.297815
H     0.211397 -0.316381 -3.292766
H     0.932363  4.808362  0.887301
H     0.932363  4.808362 -0.887301
H    -0.564465  5.100860  0.000000
H    -1.844024 -0.301068  2.077351
H    -1.844024 -0.301068 -2.077351
H     0.515937  2.975236 -2.028146
H     0.515937  2.975236  2.028146
        el energy= -873.482256329
               zpe= -873.211284
         th energy= -873.190240
       th enthalpy= -873.189296
       free energy= -873.261034


TS-F
C     0.321311  1.298890  1.622812
C     0.032783 -0.002055  2.106298
C     0.318303 -1.302675  1.619791
C     1.505834 -1.744960  0.850737
C     1.921112 -1.244763 -0.322790
C     1.298188 -0.000869 -0.896375
C     1.921609  1.242399 -0.322388
C     1.507849  1.741255  0.852388
Mo   -0.775017  0.000093 -0.094194
C    -1.791373  1.646888 -0.501590
C    -0.911915  0.003218 -2.054414
```

PBEPBE/auto/BS1
```
II
C    -2.670790  0.155114  0.304182
C    -1.531041  1.086675  0.562385
C    -0.807379  1.758896 -0.455615
C    -0.313272  1.148710 -1.681835
C    -0.060822 -0.194870 -2.084560
C    -0.292375 -1.440765 -1.359817
C    -1.142574 -1.748307 -0.283187
C    -2.469548 -1.113629 -0.084412
Mo    0.622541  0.037469  0.206101
C     0.426060 -0.615133  2.072606
C     2.312381 -0.999620 -0.018182
C     1.881605  1.451144  0.800430
O     0.219026 -1.035634  3.143915
O     3.329703 -1.567325 -0.135607
O     2.674983  2.241149  1.145865
C    -4.045648  0.755437  0.481725
C    -0.460978  3.228536 -0.272264
C     0.705874 -0.369857 -3.388376
C    -1.006485 -3.123212  0.350297
H    -4.196900  1.615032 -0.200530
H    -4.177157  1.146661  1.510010
H    -4.843260  0.016845  0.290150
H    -1.811842 -3.795636 -0.009378
H    -1.106422 -3.063464  1.448969
H    -0.033243 -3.589462  0.119117
H     0.023671 -0.733913 -4.180989
H     1.158875  0.573423 -3.735758
H     1.510679 -1.118440 -3.281475
H    -1.243493  3.855002 -0.745027
```

```
C    -1.793437 -1.643902 -0.506524
O    -2.459501  2.574764 -0.653985
O    -0.945425  0.004829 -3.209763
O    -2.463104 -2.570234 -0.661773
C    -0.348329  2.447722  2.353652
C    -0.353832 -2.451701  2.348016
C     3.027045 -1.883693 -1.111035
C     3.024984  1.883770 -1.112219
H    -1.286771  2.142338  2.830825
H    -0.569480  3.279903  1.675539
H     0.314557  2.838421  3.141258
H     3.419560  2.771675 -0.605054
H     2.661278  2.189597 -2.103994
H     3.859369  1.189510 -1.284512
H     3.861749 -1.188688 -1.278812
H     3.420393 -2.772764 -0.604950
H     2.666588 -2.187045 -2.104745
H     0.307653 -2.844961  3.135536
H    -1.292226 -2.145633  2.824872
H    -0.575805 -3.282247  1.668170
H     1.998549  2.636821  1.242715
H     1.443681 -0.000783 -1.982772
H     1.996603 -2.640315  1.241519
H    -0.811515 -0.001754  2.806554
        el energy= -873.446752008
               zpe= -873.175165
         th energy= -873.154805
       th enthalpy= -873.153861
       free energy= -873.223139



H    -0.430449  3.491429  0.798692
H     0.510875  3.498588 -0.720376
H    -3.330899 -1.773485 -0.279353
H     0.385252 -2.244999 -1.682301
H     0.151572  1.879417 -2.358200
H    -1.653725  1.689077  1.476546
        el energy= -873.518012298
               zpe= -873.254164
         th energy= -873.232606
       th enthalpy= -873.231662
       free energy= -873.303858


TS-A
C    -2.691918 -0.080176  0.507711
C    -1.526815  0.832775  0.757230
C    -1.022362  1.655612 -0.320066
C    -0.587471  1.086410 -1.556361
C    -0.272596 -0.264863 -2.006918
C    -0.353623 -1.511218 -1.303779
C    -1.036533 -1.818449 -0.079978
C    -2.431572 -1.334887  0.124187
Mo    0.613537  0.023697  0.192905
C     1.072193  0.995773  1.861904
C     1.747839 -1.404283  0.991950
C     2.287026  0.757794 -0.619673
O     1.315003  1.602767  2.833657
O     2.425143 -2.235512  1.462877
O     3.234067  1.207167 -1.137744
C    -4.070432  0.515866  0.653621
C    -0.852926  3.151349 -0.126678
```

```
C      0.403519 -0.314241 -3.371384
C     -0.767039 -3.185115  0.528888
H     -4.215057  1.364112 -0.044492
H     -4.224207  0.920685  1.673378
H     -4.861342 -0.228553  0.456910
H     -1.526287 -3.915307  0.177346
H     -0.843704 -3.146095  1.629382
H      0.230902 -3.576094  0.268342
H     -0.362144 -0.263928 -4.169715
H      1.098822  0.529672 -3.521888
H      0.966512 -1.252142 -3.510309
H     -0.552976  3.373834  0.912285
H     -0.095449  3.584668 -0.802713
H     -1.815760  3.669792 -0.306526
H     -3.235179 -2.055542 -0.103627
H      0.284475 -2.299320 -1.731315
H     -0.203811  1.838200 -2.260879
H     -1.590779  1.371276  1.717553
      el energy= -873.498902969
              zpe= -873.235697
        th energy= -873.214940
     th enthalpy= -873.213996
      free energy= -873.283689


TS-B
C      0.054578  2.404544  1.253551
C     -0.012475  3.035259  0.000000
C      0.054578  2.404544 -1.253551
C     -0.241947  1.049032 -1.614592
C     -1.384714  0.214095 -1.286558
C     -1.963454 -0.015327  0.000000
C     -1.384714  0.214095  1.286558
C     -0.241947  1.049032  1.614592
Mo     0.267728 -0.761090  0.000000
C      2.277479 -0.655614  0.000000
C      0.283271 -2.251293  1.288161
C      0.283271 -2.251293 -1.288161
O      3.440135 -0.549027  0.000000
O      0.271215 -3.162902  2.028135
O      0.271215 -3.162902 -2.028135
C      0.591538  3.243781  2.396636
C      0.591538  3.243781 -2.396636
C     -2.081347 -0.440586 -2.468188
C     -2.081347 -0.440586  2.468188
H      0.958403  4.229526  2.066665
H      1.421201  2.713557  2.901933
H     -0.190252  3.399857  3.165958
H     -2.773035  0.281215  2.945788
H     -1.351153 -0.753518  3.234258
H     -2.662527 -1.328310  2.164275
H     -2.662527 -1.328310 -2.164275
H     -2.773035  0.281215 -2.945788
H     -1.351153 -0.753518 -3.234258
H     -0.190252  3.399857 -3.165958
H      0.958403  4.229526 -2.066665
H      1.421201  2.713557 -2.901933
H      0.129594  0.808028  2.621941
H     -2.846649 -0.666053  0.000000
H      0.129594  0.808028 -2.621941
H      0.211229  4.109002  0.000000
      el energy= -873.501856739
```

```
           zpe= -873.238728
     th energy= -873.217603
   th enthalpy= -873.216659
    free energy= -873.288396

TS-C
C      1.752627 -1.721366 -0.228757
C      0.486074 -1.640187 -0.985838
C     -0.144860 -0.715530 -1.854827
C     -0.105792  0.737890 -1.830753
C      0.557136  1.686725 -1.020736
C      1.847967  1.654696 -0.315554
C      2.718344  0.699095  0.143590
C      2.643745 -0.768059  0.186167
Mo    -0.663638 -0.002247  0.304282
C     -1.094621 -1.402515  1.669877
C     -1.107921  1.510073  1.539401
C     -2.533577 -0.021228 -0.109220
O     -1.376512 -2.243751  2.430854
O     -1.378548  2.423453  2.216898
O     -3.680055 -0.034716 -0.379070
C      2.030832 -3.153892  0.198114
C     -1.144747 -1.293120 -2.847230
C      0.052088  3.121838 -1.176305
C      3.988478  1.204480  0.808597
H      2.104201 -3.825048 -0.679948
H      1.199047 -3.537891  0.821693
H      2.962454 -3.242343  0.780655
H      4.881833  0.801131  0.291636
H      4.053661  0.856350  1.858370
H      4.057976  2.304605  0.805702
H      0.737353  3.698299 -1.828800
H     -0.959018  3.160668 -1.613521
H      0.018618  3.638029 -0.200310
H     -0.665283 -1.389985 -3.841224
H     -1.487078 -2.296050 -2.541731
H     -2.032846 -0.648038 -2.965749
H      3.493133 -1.188510  0.742108
H      2.164840  2.677430 -0.067889
H     -0.899988  1.174366 -2.450360
H      0.050167 -2.641942 -1.099078
      el energy= -873.493614740
              zpe= -873.229197
        th energy= -873.208295
     th enthalpy= -873.207351
      free energy= -873.278505


TS-D
C     -1.788207 -0.668946 -1.634433
C     -0.730556 -1.439623 -0.919904
C     -0.680707 -1.748267  0.453129
C     -1.540656 -1.138877  1.486878
C     -1.846320  0.171535  1.718659
C     -1.393283  1.334915  0.916025
C     -1.568567  1.572481 -0.428572
C     -2.159638  0.616853 -1.388867
Mo     0.793490  0.151206 -0.033370
C      2.058319 -0.423205 -1.363759
C      1.854802  1.818657  0.138138
C      2.022367 -0.672348  1.188811
O      2.810679 -0.778852 -2.198906
```

```
O      2.490622  2.799836  0.221659          H      0.254457 -0.306918 -3.297592
O      2.749005 -1.193019  1.957527          H      0.943999  4.875594  0.894316
C     -2.410909 -1.428646 -2.785328          H      0.943999  4.875594 -0.894316
C      0.014301 -3.028362  0.889868          H     -0.566267  5.152501  0.000000
C     -2.630649  0.563853  2.952479          H     -1.841641 -0.260446  2.093580
C     -1.272825  2.946010 -1.000833          H     -1.841641 -0.260446 -2.093580
H     -2.883419 -2.364388 -2.429153          H      0.533893  3.028424 -2.048482
H     -1.634828 -1.729659 -3.516156          H      0.533893  3.028424  2.048482
H     -3.171323 -0.830329 -3.315346              el energy= -873.486221470
H     -2.217322  3.421661 -1.333826                   zpe= -873.224261
H     -0.619556  2.884357 -1.889865              th energy= -873.202654
H     -0.795224  3.607910 -0.259410            th enthalpy= -873.201710
H     -3.563701  1.094219  2.679529            free energy= -873.274699
H     -2.896062 -0.314481  3.564835
H     -2.047398  1.262197  3.584845          TS-F
H     -0.734263 -3.838627  1.010725          C     -0.329249  1.315456 -1.642078
H      0.753074 -3.355239  0.139081          C     -0.023074  0.002164 -2.115392
H      0.537425 -2.913428  1.854966          C     -0.327316 -1.312421 -1.644243
H     -2.906360  1.061957 -2.064719          C     -1.510433 -1.762222 -0.866164
H     -1.033662  2.184933  1.516962          C     -1.941442 -1.261349  0.318144
H     -1.881478 -1.852187  2.254516          C     -1.351563 -0.001664  0.900333
H     -0.199769 -2.149446 -1.571425          C     -1.943086  1.258315  0.320397
       el energy= -873.487677852              C     -1.512823  1.762076 -0.862928
            zpe= -873.224584                  Mo     0.758383  0.000368  0.113088
       th energy= -873.203374                 C      1.803483  1.634128  0.498585
     th enthalpy= -873.202430                 C      0.924462 -0.001780  2.080860
     free energy= -873.274605                 C      1.805702 -1.632630  0.495688
                                              O      2.514220  2.557556  0.630844
TS-E                                          O      0.970283 -0.003207  3.252861
C     -0.247039  1.103834  1.694400          O      2.517646 -2.555291  0.626571
C      0.103913  2.409998  1.240357          C      0.349816  2.468193 -2.376873
C      0.095652  3.070945  0.000000          C      0.353372 -2.462833 -2.381249
C      0.103913  2.409998 -1.240357          C     -3.023116 -1.940575  1.122046
C     -0.247039  1.103834 -1.694400          C     -3.025913  1.934325  1.125472
C     -1.363403  0.290912 -1.268689          H      1.288248  2.152694 -2.865126
C     -1.981989  0.044454  0.000000          H      0.586388  3.302117 -1.693259
C     -1.363403  0.290912  1.268689          H     -0.320365  2.870836 -3.163982
Mo     0.238860 -0.739858  0.000000          H     -3.405302  2.838439  0.617842
C      0.152694 -2.235828  1.274510          H     -2.642590  2.234400  2.121106
C      0.152694 -2.235828 -1.274510          H     -3.882958  1.257372  1.311125
C      2.270108 -0.734962  0.000000          H     -3.880883 -1.265134  1.309820
O      0.075712 -3.152511  2.003312          H     -3.401632 -2.843886  0.612332
O      0.075712 -3.152511 -2.003312          H     -2.638923 -2.242692  2.116732
O      3.435055 -0.710988  0.000000          H     -0.315573 -2.863900 -3.170218
C      0.226765  0.781574  3.117363          H      1.292183 -2.145449 -2.867554
C      0.372645  4.564952  0.000000          H      0.589690 -3.298327 -1.699483
C      0.226765  0.781574 -3.117363          H     -1.982891  2.687173 -1.233505
C     -3.279840 -0.744136  0.000000          H     -1.496063 -0.002678  1.994712
H     -0.443959  1.230408  3.878674          H     -1.979137 -2.687291 -1.238556
H      1.245072  1.166361  3.297448          H      0.827602  0.003318 -2.819483
H      0.254457 -0.306918  3.297592              el energy= -873.452042126
H     -4.148683 -0.057606  0.000000                   zpe= -873.189973
H     -3.363620 -1.386515  0.894104              th energy= -873.168890
H     -3.363620 -1.386515 -0.894104            th enthalpy= -873.167945
H     -0.443959  1.230408 -3.878674            free energy= -873.238889
H      1.245072  1.166361 -3.297448
```

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B3LYP/BS1

II
```
C     2.660489   0.216908  -0.326334
C     1.514236   1.154621  -0.508769
C     0.785395   1.745318   0.537367
C     0.313917   1.074526   1.734773
C     0.092982  -0.278065   2.074297
C     0.352128  -1.486880   1.301891
C     1.209560  -1.752982   0.241630
C     2.501051  -1.061428   0.017470
Mo   -0.647976   0.038678  -0.216029
C    -0.461397  -0.525909  -2.124798
C    -2.312498  -1.061398  -0.004207
C    -1.929300   1.472327  -0.733435
O    -0.264599  -0.881715  -3.206648
O    -3.292461  -1.664297   0.117391
O    -2.714700   2.271785  -1.025737
C     4.022826   0.835567  -0.538179
C     0.412643   3.216096   0.433054
C    -0.639369  -0.532174   3.384082
C     1.117588  -3.114759  -0.424553
H     4.193591   1.665758   0.162643
H     4.108158   1.257571  -1.550395
H     4.826318   0.102090  -0.405315
H     1.950997  -3.756168  -0.098038
H     1.194234  -3.024623  -1.515015
H     0.177386  -3.625692  -0.189419
H     0.064152  -0.908855   4.140560
H    -1.105755   0.376149   3.778754
H    -1.421086  -1.291103   3.261988
H     1.177024   3.823870   0.940380
H     0.380261   3.536192  -0.613661
H    -0.557108   3.441513   0.890051
H     3.380076  -1.698940   0.146414
H    -0.307811  -2.305881   1.589525
H    -0.139442   1.762011   2.448093
H     1.626584   1.804821  -1.379099
    el energy= -874.457243362
          zpe= -874.186011
    th energy= -874.164869
  th enthalpy= -874.163925
  free energy= -874.235147
```

TS-A
```
C    -2.676022   0.074974  -0.513618
C    -1.525966  -0.861921  -0.733515
C    -1.030774  -1.656484   0.355945
C    -0.587526  -1.080083   1.575184
C    -0.268271   0.266288   2.009469
C    -0.361738   1.506608   1.312167
C    -1.039942   1.823091   0.103585
C    -2.421774   1.322125  -0.134461
Mo    0.630169  -0.029458  -0.209115
C     1.068506  -1.027920  -1.881173
C     1.735424   1.422443  -1.029892
C     2.323412  -0.746537   0.619137
O     1.283695  -1.640371  -2.839387
O     2.373540   2.264644  -1.502288
O     3.258348  -1.177487   1.142036
C    -4.059879  -0.500342  -0.691042
C    -0.877767  -3.157509   0.189505
```

C   0.399855   0.326349   3.377330
C   -0.787757   3.202798 -0.481343
H   -4.234836 -1.334510   0.004465
H   -4.191856 -0.904794 -1.705292
H   -4.836907   0.253914 -0.521178
H   -1.546593   3.913390 -0.114059
H   -0.867571   3.185279 -1.574293
H   0.199462   3.596446 -0.218376
H   -0.364987   0.291307   4.166531
H   1.082889 -0.514676   3.540810
H   0.965098   1.254748   3.508034
H   -0.600007 -3.403942 -0.841228
H   -0.120354 -3.581653   0.858348
H   -1.836281 -3.657100   0.395362
H   -3.227347   2.035071   0.067336
H   0.272184   2.287445   1.735175
H   -0.219158 -1.820770   2.284867
H   -1.604168 -1.420491 -1.670230
```
    el energy= -874.434871656
          zpe= -874.164517
    th energy= -874.144120
  th enthalpy= -874.143176
  free energy= -874.212041
```

TS-B
```
C     0.060556   2.389042   1.251635
C     0.013399   3.012758   0.000000
C     0.060556   2.389042  -1.251635
C    -0.269789   1.053230  -1.627741
C    -1.399609   0.221532  -1.281100
C    -1.969212  -0.008103   0.000000
C    -1.399609   0.221532   1.281100
C    -0.269789   1.053230   1.627741
Mo    0.270540  -0.767288   0.000000
C     2.296797  -0.649232   0.000000
C     0.291673  -2.254448   1.312826
C     0.291673  -2.254448  -1.312826
O     3.444019  -0.533458   0.000000
O     0.287670  -3.142963   2.058011
O     0.287670  -3.142963  -2.058011
C     0.609353   3.227285   2.390801
C     0.609353   3.227285  -2.390801
C    -2.111889  -0.428334  -2.456312
C    -2.111889  -0.428334   2.456312
H     0.999325   4.192403   2.053352
H     1.417095   2.687336   2.903134
H    -0.171088   3.410305   3.143668
H    -2.798643   0.294601   2.921095
H    -1.398320  -0.742733   3.225682
H    -2.692749  -1.305324   2.149972
H    -2.692749  -1.305324  -2.149972
H    -2.798643   0.294601  -2.921095
H    -1.398320  -0.742733  -3.225682
H    -0.171088   3.410305  -3.143668
H     0.999325   4.192403  -2.053352
H     1.417095   2.687336  -2.903134
H     0.074449   0.825071   2.637213
H    -2.850768  -0.645449   0.000000
H     0.074449   0.825071  -2.637213
H     0.263651   4.071090   0.000000
```

```
     el energy= -874.440306836
            zpe= -874.170197
      th energy= -874.149419
   th enthalpy= -874.148475
    free energy= -874.219432

TS-C
C    -1.766297 -1.708290  0.212161
C    -0.506545 -1.638341  0.981476
C     0.111208 -0.724122  1.853154
C     0.078012  0.724346  1.838790
C    -0.563669  1.676522  1.035942
C    -1.847068  1.655028  0.313686
C    -2.705291  0.713708 -0.162074
C    -2.637272 -0.754835 -0.208953
Mo    0.688780 -0.003276 -0.304248
C     1.108138 -1.402096 -1.697461
C     1.128170  1.516165 -1.558457
C     2.564156 -0.031098  0.143935
O     1.360318 -2.223372 -2.468262
O     1.377172  2.412790 -2.241598
O     3.691729 -0.049630  0.430914
C    -2.064478 -3.142220 -0.196408
C     1.085067 -1.308487  2.867259
C    -0.068499  3.110598  1.222146
C    -3.967101  1.223449 -0.839308
H    -2.163981 -3.790298  0.686387
H    -1.239715 -3.551097 -0.798139
H    -2.984017 -3.220265 -0.784567
H    -4.860512  0.823142 -0.337604
H    -4.018111  0.885033 -1.884542
H    -4.032570  2.315825 -0.830446
H    -0.756793  3.667173  1.875707
H     0.931178  3.145393  1.665879
H    -0.030014  3.642409  0.264091
H     0.586202 -1.399827  3.843406
H     1.423193 -2.307252  2.572616
H     1.968820 -0.675334  3.004267
H    -3.479771 -1.162095 -0.766900
H    -2.159668  2.673633  0.085566
H     0.853866  1.148253  2.473895
H    -0.091805 -2.637379  1.105018
     el energy= -874.435363396
            zpe= -874.163648
      th energy= -874.143171
   th enthalpy= -874.142226
    free energy= -874.212335

TS-D
C    -1.794308 -0.614418 -1.651709
C    -0.764862 -1.412668 -0.927769
C    -0.744623 -1.732353  0.426940
C    -1.631576 -1.129618  1.444061
C    -1.929072  0.167969  1.679544
C    -1.425954  1.336762  0.912603
C    -1.569615  1.598690 -0.416867
C    -2.153093  0.662193 -1.400438
Mo    0.849947  0.147340 -0.009496
C     2.074508 -0.416053 -1.396396
C     1.955438  1.788646  0.219143
C     2.057492 -0.753315  1.197577

O     2.786228 -0.757833 -2.253148
O     2.601858  2.742279  0.341609
O     2.757655 -1.306500  1.946833
C    -2.414644 -1.358994 -2.814274
C    -0.079226 -3.024571  0.871243
C    -2.779969  0.556930  2.869275
C    -1.245815  2.974141 -0.966452
H    -2.899150 -2.284214 -2.471920
H    -1.642048 -1.657750 -3.537401
H    -3.158724 -0.750461 -3.339514
H    -2.171670  3.460373 -1.309450
H    -0.579085  2.915729 -1.835565
H    -0.780841  3.616702 -0.211838
H    -3.679752  1.101654  2.549245
H    -3.094232 -0.319770  3.445811
H    -2.228138  1.229731  3.542178
H    -0.844236 -3.808463  0.991665
H     0.648014 -3.372977  0.130955
H     0.436478 -2.918852  1.831873
H    -2.884781  1.118808 -2.070374
H    -1.060022  2.156760  1.534894
H    -2.023479 -1.852351  2.163839
H    -0.230103 -2.106835 -1.576821
     el energy= -874.432515279
            zpe= -874.161998
      th energy= -874.141262
   th enthalpy= -874.140318
    free energy= -874.211174

TS-E
C    -0.282003  1.104591  1.705818
C     0.102266  2.388332  1.238344
C     0.117840  3.040424  0.000000
C     0.102266  2.388332 -1.238344
C    -0.282003  1.104591 -1.705818
C    -1.379013  0.286515 -1.263872
C    -1.986409  0.036453  0.000000
C    -1.379013  0.286515  1.263872
Mo    0.244294 -0.745124  0.000000
C     0.177970 -2.240002  1.301282
C     0.177970 -2.240002 -1.301282
C     2.295411 -0.712607  0.000000
O     0.120721 -3.133923  2.036178
O     0.120721 -3.133923 -2.036178
O     3.444938 -0.668265  0.000000
C     0.147352  0.806021  3.147851
C     0.438432  4.526516  0.000000
C     0.147352  0.806021 -3.147851
C    -3.286860 -0.748603  0.000000
H    -0.542788  1.263077  3.874930
H     1.151244  1.193493  3.353654
H     0.170254 -0.270655  3.348060
H    -4.147902 -0.064690  0.000000
H    -3.372520 -1.386330  0.887513
H    -3.372520 -1.386330 -0.887513
H    -0.542788  1.263077 -3.874930
H     1.151244  1.193493 -3.353654
H     0.170254 -0.270655 -3.348060
H     1.015995  4.817256  0.887320
H     1.015995  4.817256 -0.887320
H    -0.475344  5.138719  0.000000
```

```
H    -1.860648 -0.259249  2.077671          C    -0.282670  2.456055  2.390891
H    -1.860648 -0.259249 -2.077671          C    -0.283385 -2.458064  2.389144
H     0.539727  2.998137 -2.035847          C     3.031686 -1.906248 -1.161610
H     0.539727  2.998137  2.035847          C     3.032187  1.906299 -1.160291
     el energy= -874.423497037             H    -1.208648  2.149820  2.891307
           zpe= -874.154881                H    -0.518645  3.296755  1.728431
     th energy= -874.133497                H     0.403227  2.837004  3.164277
   th enthalpy= -874.132553                H     3.425107  2.799337 -0.660120
   free energy= -874.205149                H     2.652925  2.207408 -2.148236
                                           H     3.871944  1.220487 -1.343208
TS-F                                       H     3.871408 -1.220313 -1.344223
C     0.366678  1.305038  1.628255         H     3.424665 -2.799527 -0.661914
C     0.075424 -0.000933  2.103917         H     2.652377 -2.206863 -2.149689
C     0.366207 -1.306649  1.627338         H     0.402844 -2.840321  3.161590
C     1.540609 -1.752238  0.832182         H    -1.208771 -2.151741  2.890597
C     1.940361 -1.252220 -0.349978         H    -0.520411 -3.297884  1.725936
C     1.316211  0.000144 -0.918226         H     2.031484  2.651317  1.212200
C     1.940807  1.251871 -0.349067         H     1.442315  0.000481 -2.005500
C     1.541287  1.750964  0.833551         H     2.030566 -2.653049  1.210059
Mo   -0.794633  0.000160 -0.112442         H    -0.748414 -0.001018  2.825723
C    -1.827924  1.676363 -0.456878              el energy= -874.386357438
C    -0.970179  0.001097 -2.091859                    zpe= -874.117063
C    -1.828740 -1.675362 -0.458201              th energy= -874.096420
O    -2.514464  2.601844 -0.557658            th enthalpy= -874.095475
O    -1.017377  0.001667 -3.248960            free energy= -874.165576
O    -2.515753 -2.600425 -0.559590
```

Molecular Coordinates for (TMCOT)W(CO)₃ (Å)

PBE0/BS1

```
II
C     0.903707  1.734886  0.435617        O     3.036325 -1.393994  1.097722
C     0.380669  1.171798  1.657244        C    -4.127688 -0.444329 -0.611761
C     0.096704 -0.152948  2.089802        C    -0.979439 -3.118894  0.082151
C     0.325141 -1.410981  1.413434        C     0.365388  0.222273  3.371657
C     1.152577 -1.716497  0.320360        C    -0.785878  3.169205 -0.441719
C     2.510225 -1.140462  0.180581        H    -4.275606 -1.300141  0.062609
C     2.745108  0.101171 -0.231361        H    -4.288443 -0.817568 -1.633341
C     1.608861  1.007142 -0.554720        H    -4.902924  0.298919 -0.394445
W    -0.499193  0.027035 -0.171608        H    -1.507775  3.895742 -0.034773
C    -1.721209  1.452238 -0.823359        H    -0.903825  3.170476 -1.531090
C    -0.270867 -0.696502 -2.009014        H     0.221626  3.530731 -0.209564
C    -2.217779 -0.951327  0.080384        H    -0.382013  0.138821  4.172654
O    -2.475456  2.243008 -1.199543        H     1.059979 -0.618892  3.474191
O    -0.042156 -1.147591 -3.044847        H     0.925807  1.147829  3.536214
O    -3.233998 -1.484039  0.217315        H    -1.942654 -3.612983  0.276257
C     0.601792  3.198463  0.210318        H    -0.710646 -3.327978 -0.959239
C    -0.715417 -0.270191  3.362400        H    -0.221670 -3.575713  0.728740
C     1.000708 -3.093189 -0.289188        H    -3.243731  2.080326  0.224558
C     4.117622  0.695193 -0.359331        H     0.229176  2.254238  1.814385
H     1.406685  3.809236  0.644341        H    -0.275290 -1.866463  2.213355
H    -0.346754  3.509641  0.662106        H    -1.677600 -1.286370 -1.706527
H     0.559027  3.422903 -0.860809          el energy= -873.802256715
H     4.235823  1.560525  0.308364                zpe= -873.529467
H     4.291441  1.061329 -1.381364           th energy= -873.509501
H     4.899753 -0.033927 -0.119924         th enthalpy= -873.508557
H     1.725849 -3.792658  0.154246         free energy= -873.576771
H    -0.007342 -3.495570 -0.138025
H     1.196578 -3.067518 -1.367679
H    -0.062760 -0.570873  4.193641        TS-B
H    -1.196420  0.674879  3.632879        C     0.039764  2.496184  1.236992
H    -1.496323 -1.032729  3.265500        C    -0.047133  3.133842  0.000000
H     1.753414  1.579791 -1.474904        C     0.039764  2.496184 -1.236992
H     3.333953 -1.806719  0.452181        C    -0.229136  1.136880 -1.571489
H    -0.345228 -2.200752  1.757691        C    -1.395409  0.323638 -1.272639
H    -0.101546  1.918103  2.288365        C    -1.986525  0.115114  0.000000
      el energy= -873.819967054        C    -1.395409  0.323638  1.272639
              zpe= -873.546548        C    -0.229136  1.136880  1.571489
         th energy= -873.525835        W     0.208513 -0.631433  0.000000
       th enthalpy= -873.524891        C     2.213073 -0.540618  0.000000
       free energy= -873.595265        C     0.212427 -2.119327  1.288584
                                       C     0.212427 -2.119327 -1.288584
                                       O     3.360247 -0.437454  0.000000
TS-A                                    O     0.190409 -3.012788  2.027149
C    -2.751085  0.130965 -0.460722        O     0.190409 -3.012788 -2.027149
C    -1.593652 -0.768998 -0.745046        C     0.575138  3.319889  2.378364
C    -1.109115 -1.632576  0.302839        C     0.575138  3.319889 -2.378364
C    -0.663756 -1.100136  1.540911        C    -2.091736 -0.297777 -2.459879
C    -0.328968  0.227700  2.024956        C    -2.091736 -0.297777  2.459879
C    -0.396112  1.482941  1.360081        H     0.906884  4.314227  2.064620
C    -1.055907  1.791187  0.126056        H     1.422048  2.802132  2.848454
C    -2.467434  1.357982 -0.045380        H    -0.191383  3.434286  3.157881
W     0.494411 -0.013695 -0.158502        H    -2.756513  0.438783  2.933685
C     0.913658 -0.902504 -1.883053        H    -1.365791 -0.621644  3.213757
C     1.683694  1.422623 -0.865832        H    -2.690572 -1.168350  2.169568
C     2.125478 -0.882295  0.610415        H    -2.690572 -1.168350 -2.169568
O     1.122977 -1.451385 -2.877855        H    -2.756513  0.438783 -2.933685
O     2.382462  2.241827 -1.282138        H    -1.365791 -0.621644 -3.213757
                                       H    -0.191383  3.434286 -3.157881
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H     0.906884   4.314227  -2.064620          C    -0.820200   1.682393  -0.484837
H     1.422048   2.802132  -2.848454          C    -1.567561   1.013052  -1.554248
H     0.144903   0.893319   2.568443          W     0.653277  -0.102266   0.091134
H    -2.870645  -0.520348   0.000000          C     1.832187  -1.698463   0.011983
H     0.144903   0.893319  -2.568443          C     1.782314   0.729229  -1.222263
H     0.163948   4.201248   0.000000          C     1.906973   0.649244   1.341752
       el energy= -873.797612222              O     2.529431  -2.620923  -0.015401
               zpe= -873.525220               O     2.427370   1.246097  -2.041149
        th energy= -873.504828                O     2.635110   1.107121   2.127076
      th enthalpy= -873.503884                C    -2.397016  -0.774764  -3.066483
      free energy= -873.574237                C    -1.233630  -2.907025   1.087921
                                              C    -2.887617   1.437322   2.457578
TS-C                                          C    -0.209840   3.007684  -0.877554
C    -1.871134  -1.676311   0.227647          H    -3.319462  -1.340962  -2.876439
C    -0.595221  -1.620821   0.965064          H    -1.718028  -1.449219  -3.607602
C     0.023627  -0.736590   1.880538          H    -2.637213   0.066916  -3.724243
C     0.012484   0.700994   1.878657          H    -1.004761   3.758901  -1.006827
C    -0.583717   1.648932   1.020671          H     0.349391   2.947155  -1.817870
C    -1.899246   1.664398   0.359667          H     0.473279   3.367301  -0.101108
C    -2.792822   0.748816  -0.088001          H    -3.297152   2.329305   1.963885
C    -2.742870  -0.714457  -0.160107          H    -3.715626   0.862669   2.886470
W     0.562168  -0.007421  -0.225332          H    -2.253706   1.797658   3.280094
C     0.918404  -1.360020  -1.659461          H    -2.156327  -3.447727   1.346727
C     1.007680   1.494735  -1.465503          H    -0.628178  -3.546875   0.437787
C     2.433108  -0.065912   0.173516          H    -0.689638  -2.745973   2.026543
O     1.132316  -2.161042  -2.459698          H    -1.864004   1.677736  -2.369823
O     1.265553   2.391591  -2.142778          H    -0.499713   2.098093   1.558833
O     3.563487  -0.105119   0.446085          H    -3.206131  -1.121978   1.789558
C    -2.162816  -3.090499  -0.217977          H    -0.884583  -2.260901  -1.440468
C     0.997649  -1.356570   2.859155                 el energy= -873.775013738
C    -0.048760   3.064040   1.184349                         zpe= -873.502858
C    -4.062710   1.282530  -0.708640                  th energy= -873.482294
H    -2.237170  -3.766530   0.645470                th enthalpy= -873.481350
H    -1.345371  -3.468395  -0.849019                free energy= -873.552459
H    -3.092272  -3.159035  -0.791268
H    -4.942340   0.886496  -0.180882          TS-E
H    -4.154267   0.960012  -1.755769          C    -0.262420   1.176704   1.656849
H    -4.112485   2.375358  -0.681716          C     0.076754   2.482802   1.224542
H    -0.694325   3.637076   1.865719          C     0.063520   3.149365   0.000000
H     0.969955   3.071346   1.584191          C     0.076754   2.482802  -1.224542
H    -0.033725   3.592290   0.223884          C    -0.262420   1.176704  -1.656849
H     0.490457  -1.536034   3.817657          C    -1.397949   0.379720  -1.256070
H     1.373080  -2.318277   2.494440          C    -2.019537   0.144252   0.000000
H     1.858847  -0.706748   3.049632          C    -1.397949   0.379720   1.256070
H    -3.595586  -1.106811  -0.714568          W     0.183503  -0.605599   0.000000
H    -2.193325   2.692633   0.146136          C     0.132073  -2.100014   1.275055
H     0.794770   1.116431   2.513342          C     0.132073  -2.100014  -1.275055
H    -0.179432  -2.623674   1.060963          C     2.202406  -0.564394   0.000000
       el energy= -873.784791038              O     0.077095  -3.001206   2.001205
               zpe= -873.511046               O     0.077095  -3.001206  -2.001205
        th energy= -873.490847                O     3.350428  -0.506262   0.000000
      th enthalpy= -873.489903                C     0.207747   0.854759   3.072938
      free energy= -873.559773                C     0.347993   4.632417   0.000000
                                              C     0.207747   0.854759  -3.072938
TS-D                                          C    -3.306674  -0.644702   0.000000
C    -1.772949  -0.311127  -1.777747          H    -0.435575   1.335651   3.826233
C    -1.334114  -1.418840  -0.908376          H     1.234306   1.198749   3.239874
C    -1.589429  -1.601074   0.423071          H     0.195123  -0.223563   3.265256
C    -2.370087  -0.666738   1.253780          H    -4.168776   0.036534   0.000000
C    -2.077822   0.622390   1.489369          H    -3.385986  -1.282562   0.887397
C    -0.932205   1.356258   0.883785          H    -3.385986  -1.282562  -0.887397
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H    -0.435575   1.335651  -3.826233        H    -2.151758   2.642817   1.225189
H     1.234306   1.198749  -3.239874        H     0.646550  -0.000548   2.802849
H     0.195123  -0.223563  -3.265256            el energy= -873.746999809
H     0.918149   4.935783   0.887482                   zpe= -873.475227
H     0.918149   4.935783  -0.887482            th energy= -873.454966
H    -0.580331   5.220662   0.000000          th enthalpy= -873.454021
H    -1.876058  -0.150243   2.082981          free energy= -873.523376
H    -1.876058  -0.150243  -2.082981
H     0.516166   3.084819  -2.028243    TS-G
H     0.516166   3.084819   2.028243    C     1.332133  -1.272614  -0.923936
     el energy= -873.778974693          C     1.413934  -0.000004  -1.545468
            zpe= -873.507541            C     1.332141   1.272607  -0.923935
     th energy= -873.486716             C     1.825664   1.759848   0.390409
   th enthalpy= -873.485772             C     1.422983   1.230776   1.555167
    free energy= -873.557290            C     0.575034   0.000001   1.703745
                                        C     1.422968  -1.230783   1.555168
TS-F                                    C     1.825644  -1.759861   0.390410
C    -0.470570  -1.305851   1.610850    W    -0.556934   0.000002  -0.250707
C    -0.198439  -0.000761   2.101198    C    -1.649738  -1.580389  -0.650533
C    -0.471834   1.304366   1.611734    C    -2.004203   0.000010   1.094250
C    -1.656343   1.749006   0.837455    C    -1.649726   1.580399  -0.650537
C    -2.054913   1.243644  -0.339399    O    -2.281205  -2.486346  -0.996356
C    -1.408162  -0.000373  -0.894509    O    -2.870754   0.000015   1.862907
C    -2.054398  -1.244793  -0.339554    O    -2.281188   2.486359  -0.996363
C    -1.655257  -1.750642   0.836872    H     1.210065  -2.085710  -1.642394
W     0.649728   0.000005  -0.063298    H     1.210072   2.085705  -1.642391
C     1.708995  -1.610804  -0.454969    H     1.749765   1.699936   2.487592
C     0.838726   0.001434  -2.029198    H     1.749739  -1.699950   2.487593
C     1.707768   1.612158  -0.452754    C     2.709280  -2.972685   0.328686
O     2.378665  -2.543756  -0.595401    C    -0.080935   0.000005   3.080702
O     0.903186   0.002231  -3.185059    C     2.709322   2.972655   0.328680
O     2.376536   2.545927  -0.591888    C     1.200305  -0.000007  -3.051444
C     0.199121  -2.450685   2.347956    H     2.985412  -3.319458   1.330590
C     0.196873   2.449286   2.349619    H     2.209134  -3.801596  -0.192964
C    -3.150998   1.873294  -1.147120    H     3.631371  -2.758194  -0.230250
C    -3.151119  -1.873874  -1.146875    H     0.662686   0.889658  -3.397190
H     1.128886  -2.138866   2.838120    H     2.185612  -0.000051  -3.538353
H     0.437664  -3.276906   1.668553    H     0.662614  -0.889633  -3.397177
H    -0.470122  -2.849832   3.125475    H     2.985457   3.319430   1.330583
H    -3.558877  -2.761174  -0.649198    H     3.631411   2.758143  -0.230250
H    -2.775682  -2.178126  -2.134624    H     2.209194   3.801573  -0.192977
H    -3.977849  -1.172834  -1.327519    H    -0.704475  -0.887371   3.234285
H    -3.977739   1.172517  -1.328717    H     0.695859  -0.000004   3.861638
H    -3.558919   2.760432  -0.649294    H    -0.704456   0.887394   3.234288
H    -2.774807   2.177964  -2.134453        el energy= -873.742780949
H    -0.473238   2.848074   3.126570               zpe= -873.470843
H     1.126245   2.137648   2.840639        th energy= -873.450690
H     0.435805   3.275740   1.670645      th enthalpy= -873.449746
H    -2.150520  -2.644549   1.224604        free energy= -873.518944
H    -1.529304  -0.000380  -1.983808
```
PBEPBE/auto/BS1
```
II
C     0.916790   1.751205   0.432822    C    -1.752410   1.453794  -0.796623
C     0.409202   1.176757   1.669682    C    -0.328587  -0.688460  -2.016041
C     0.139818  -0.160247   2.105291    C    -2.222881  -0.964545   0.103813
C     0.359976  -1.423537   1.410301    O    -2.528142   2.255739  -1.159382
C     1.194819  -1.739046   0.311944    O    -0.118988  -1.148977  -3.071661
C     2.548083  -1.145533   0.145843    O    -3.247838  -1.513727   0.257206
C     2.770511   0.111642  -0.265299    C     0.609570   3.224339   0.215827
C     1.621300   1.020707  -0.571609    C    -0.651543  -0.290357   3.400594
W    -0.513545   0.029637  -0.170787    C     1.035064  -3.120394  -0.304850
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```
C     4.145971   0.715326  -0.415757              th energy=   -873.523983
H     1.420813   3.839686   0.653118           th enthalpy=   -873.523039
H    -0.344706   3.534732   0.675733           free energy=   -873.592805
H     0.562382   3.457274  -0.861539
H     4.275794   1.586008   0.257002     TS-B
H     4.302848   1.091525  -1.446091     C     0.055726   2.524995   1.248397
H     4.942035  -0.015906  -0.191908     C    -0.020363   3.163010   0.000000
H     1.795794  -3.817443   0.101977     C     0.055726   2.524995  -1.248397
H     0.033704  -3.542604  -0.111721     C    -0.223863   1.156544  -1.583810
H     1.184280  -3.082983  -1.398791     C    -1.403884   0.347929  -1.283822
H     0.020424  -0.611803   4.219834     C    -1.997822   0.137455   0.000000
H    -1.122298   0.660997   3.698774     C    -1.403884   0.347929   1.283822
H    -1.445658  -1.051866   3.309107     C    -0.223863   1.156544   1.583810
H     1.750455   1.595156  -1.503140     W     0.210507  -0.648118   0.000000
H     3.389557  -1.814038   0.391263     C     2.214003  -0.573796   0.000000
H    -0.311010  -2.221235   1.761567     C     0.200495  -2.137832   1.292758
H    -0.066418   1.925184   2.318139     C     0.200495  -2.137832  -1.292758
     el energy=   -873.824313113        O     3.379460  -0.470683   0.000000
            zpe=   -873.560388           O     0.170943  -3.041667   2.045472
       th energy=   -873.538969          O     0.170943  -3.041667  -2.045472
    th enthalpy=   -873.538025           C     0.587976   3.353886   2.399315
     free energy=   -873.610001          C     0.587976   3.353886  -2.399315
                                         C    -2.110856  -0.270940  -2.478126
                                         C    -2.110856  -0.270940   2.478126
TS-A                                     H     0.933317   4.352134   2.083859
C    -2.781697   0.123523  -0.488088     H     1.431985   2.829781   2.887330
C    -1.610425  -0.778678  -0.757360     H    -0.188718   3.480556   3.179143
C    -1.127864  -1.641946   0.307251     H    -2.784673   0.472908   2.947401
C    -0.691336  -1.093512   1.554805     H    -1.384008  -0.590236   3.244759
C    -0.366796   0.249608   2.031402     H    -2.711802  -1.150603   2.188784
C    -0.425146   1.505374   1.340726     H    -2.711802  -1.150603  -2.188784
C    -1.092745   1.814992   0.099189     H    -2.784673   0.472908  -2.947401
C    -2.505205   1.368868  -0.084810     H    -1.384008  -0.590236  -3.244759
W     0.507766  -0.018525  -0.159121     H    -0.188718   3.480556  -3.179143
C     0.964888  -0.930164  -1.865940     H     0.933317   4.352134  -2.083859
C     1.710418   1.409922  -0.863525     H     1.431985   2.829781  -2.887330
C     2.134049  -0.856247   0.646928     H     0.159571   0.902307   2.583949
O     1.204736  -1.498282  -2.863251     H    -2.894486  -0.494994   0.000000
O     2.429414   2.238289  -1.277016     H     0.159571   0.902307  -2.583949
O     3.053132  -1.360147   1.169443     H     0.192848   4.239160   0.000000
C    -4.161000  -0.466571  -0.640515         el energy=   -873.807253555
C    -0.998100  -3.139107   0.099230                zpe=   -873.544100
C     0.311318   0.267215   3.396257           th energy=   -873.523072
C    -0.806476   3.187891  -0.493173        th enthalpy=   -873.522128
H    -4.309192  -1.323615   0.046102         free energy=   -873.593888
H    -4.316672  -0.857048  -1.665656
H    -4.949690   0.277534  -0.433759
H    -1.544349   3.927854  -0.117391     TS-C
H    -0.900242   3.166554  -1.592777     C    -1.858226  -1.719941   0.233959
H     0.203203   3.555708  -0.243638     C    -0.586915  -1.628936   0.988735
H    -0.454647   0.210658   4.193698     C     0.019288  -0.715936   1.900305
H     0.998600  -0.585957   3.530167     C    -0.018953   0.734287   1.875670
H     0.884487   1.196498   3.550228     C    -0.657599   1.670117   1.018870
H    -1.971374  -3.634571   0.288241     C    -1.964980   1.643783   0.336326
H    -0.717797  -3.359715  -0.945470     C    -2.846348   0.692484  -0.107593
H    -0.242626  -3.596514   0.761766     C    -2.762657  -0.773592  -0.165804
H    -3.293146   2.098839   0.165205     W     0.578974  -0.002242  -0.233598
H     0.203185   2.287891   1.792372     C     0.995385  -1.381975  -1.620729
H    -0.308126  -1.858476   2.245324     C     0.991535   1.502783  -1.483608
H    -1.677845  -1.300702  -1.727117     C     2.451880  -0.006463   0.189682
     el energy=   -873.807982496         O     1.245943  -2.216745  -2.402689
            zpe=   -873.544639           O     1.219580   2.418487  -2.177235
```

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O      3.594765 -0.013717  0.484314          H     -1.795634 -1.404278  2.489408
C     -2.109995 -3.149254 -0.218692          H     -1.269295 -1.757440 -1.709837
C      0.997923 -1.305458  2.906534            el energy= -873.784889171
C     -0.149138  3.107114  1.166694                    zpe= -873.522580
C     -4.130984  1.199556 -0.741986            th energy= -873.501285
H     -2.169228 -3.837562  0.647056          th enthalpy= -873.500341
H     -1.272378 -3.505529 -0.850828          free energy= -873.572972
H     -3.040445 -3.243766 -0.802196
H     -5.012590  0.793317 -0.207478       TS-E
H     -4.218952  0.856540 -1.791819       C     -0.238419  1.207195  1.668463
H     -4.200910  2.299614 -0.732358       C      0.102644  2.525327  1.235505
H     -0.826879  3.684408  1.826128       C      0.093684  3.192891  0.000000
H      0.867027  3.144531  1.592281       C      0.102644  2.525327 -1.235505
H     -0.123986  3.620665  0.189191       C     -0.238419  1.207195 -1.668463
H      0.488658 -1.443716  3.880547       C     -1.391265  0.420214 -1.266035
H      1.369229 -2.291394  2.579818       C     -2.023291  0.192519  0.000000
H      1.869303 -0.648167  3.071707       C     -1.391265  0.420214  1.266035
H     -3.610328 -1.196197 -0.722771       W      0.181347 -0.627915  0.000000
H     -2.279959  2.668765  0.094970       C      0.094116 -2.121862  1.278927
H      0.759341  1.177907  2.510728       C      0.094116 -2.121862 -1.278927
H     -0.145563 -2.629143  1.095960       C      2.197217 -0.637246  0.000000
    el energy= -873.793480660               O      0.019750 -3.032546  2.019523
            zpe= -873.529099               O      0.019750 -3.032546 -2.019523
    th energy= -873.508251                 O      3.364717 -0.601548  0.000000
  th enthalpy= -873.507307                 C      0.244494  0.875269  3.087752
  free energy= -873.578629                 C      0.369029  4.686507  0.000000
                                           C      0.244494  0.875269 -3.087752
TS-D                                       C     -3.334719 -0.573259  0.000000
C     -2.413558  0.072179 -1.293600       H     -0.386604  1.371293  3.853545
C     -1.451064 -1.016369 -0.913777       H      1.285723  1.205654  3.243775
C     -1.384739 -1.557721  0.398936       H      0.215248 -0.210549  3.281481
C     -1.587115 -0.784759  1.604535       H     -4.189862  0.130219  0.000000
C     -1.291746  0.554644  1.915445       H     -3.428944 -1.213897  0.894217
C     -0.712001  1.576074  1.061973       H     -3.428944 -1.213897 -0.894217
C     -0.883862  1.812646 -0.331282       H     -0.386604  1.371293 -3.853545
C     -2.128501  1.357115 -1.022309       H      1.285723  1.205654 -3.243775
W      0.603452 -0.063599 -0.189145       H      0.215248 -0.210549 -3.281481
C      1.598863 -1.516432 -1.074954       H      0.940021  4.997238  0.894357
C      2.085137  1.052020 -0.799469       H      0.940021  4.997238 -0.894357
C      1.651020 -0.326805  1.436115       H     -0.570791  5.272258  0.000000
O      2.181325 -2.371241 -1.635518       H     -1.879535 -0.108331  2.099577
O      2.961076  1.720242 -1.220401       H     -1.879535 -0.108331 -2.099577
O      2.215576 -0.489372  2.455849       H      0.532522  3.135691 -2.049940
C     -3.681795 -0.381271 -1.973477       H      0.532522  3.135691  2.049940
C     -1.157323 -3.046910  0.584721           el energy= -873.790516382
C     -1.309467  0.928625  3.387163                   zpe= -873.528248
C     -0.294347  3.101339 -0.893773           th energy= -873.506825
H     -4.260778 -1.066182 -1.323220         th enthalpy= -873.505881
H     -3.455276 -0.947138 -2.898942         free energy= -873.578681
H     -4.328354  0.471844 -2.243043
H     -1.046758  3.915995 -0.847291       TS-F
H     -0.006610  2.983444 -1.952666       C     -0.469538 -1.318781  1.634770
H      0.598857  3.423876 -0.333059       C     -0.175870 -0.000351  2.112025
H     -1.875673  1.864008  3.551061       C     -0.469729  1.318288  1.635790
H     -1.755458  0.136066  4.010522       C     -1.654063  1.768915  0.858092
H     -0.278397  1.106279  3.750018       C     -2.072126  1.260019 -0.326809
H     -2.134441 -3.567054  0.655609       C     -1.455141 -0.000009 -0.892217
H     -0.619068 -3.471104 -0.279574       C     -2.072946 -1.259703 -0.326731
H     -0.582761 -3.275253  1.498396       C     -1.654767 -1.768880  0.857940
H     -2.836899  2.155183 -1.299446       W      0.638168 -0.000262 -0.082505
H     -0.109729  2.314820  1.611825       C      1.717417 -1.609670 -0.447960
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C      0.842856   0.000881  -2.059296
C      1.718095   1.609242  -0.446292
O      2.423956  -2.542495  -0.561435
O      0.911601   0.001592  -3.231415
O      2.424877   2.541937  -0.558811
C      0.210692  -2.466202   2.377157
C      0.210351   2.465341   2.378837
C     -3.152603   1.922851  -1.144512
C     -3.155083  -1.920870  -1.143591
H      0.457310  -3.298796   1.695510
H     -0.462063  -2.870729   3.160735
H      1.144578  -2.144909   2.870689
H     -3.548369  -2.823075  -0.643259
H     -2.765736  -2.221175  -2.136721
H     -4.003151  -1.234308  -1.334549
H     -4.000067   1.236587  -1.339026
H     -3.547131   2.823868  -0.643032
H     -2.761001   2.225519  -2.136053
H     -0.462995   2.870104   3.161776
H      1.143579   2.143570   2.873266
H      0.457981   3.297896   1.697521
H     -2.131141  -2.689373   1.231531
H     -1.582587   0.000050  -1.988916
H     -2.129793   2.689962   1.231107
H      0.677428  -0.000522   2.814869
   el energy= -873.759083233
        zpe= -873.496980
   th energy= -873.475949
 th enthalpy= -873.475005
 free energy= -873.546141

TS-G
C      1.354734  -1.284905  -0.943913
C      1.423059  -0.000056  -1.567534
C      1.354736   1.284823  -0.943950
C      1.810189   1.797300   0.377060
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B3LYP/BS1

II
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C      0.905245   1.741675   0.494467
C      0.412839   1.125812   1.708557
C      0.162346  -0.217434   2.098423
C      0.406587  -1.453837   1.374612
C      1.242419  -1.743185   0.289739
C      2.570069  -1.107988   0.094766
C      2.762085   0.153667  -0.286765
C      1.609355   1.071804  -0.535230
W     -0.529349   0.030275  -0.178119
C     -1.781820   1.470070  -0.748881
C     -0.349813  -0.628155  -2.055162
C     -2.220641  -1.008456   0.090055
O     -2.547946   2.279688  -1.070713
O     -0.151187  -1.042016  -3.117387
O     -3.216568  -1.580596   0.248174
C      0.584763   3.219044   0.334882
C     -0.602894  -0.400960   3.401800
C      1.118567  -3.120513  -0.341503
C      4.131515   0.763556  -0.465423
H      1.384562   3.818297   0.795182
H     -0.364646   3.500838   0.803422
H      0.536939   3.493346  -0.724216
H      4.279267   1.612374   0.218234
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C      1.426193   1.258780   1.562419
C      0.633291   0.000030   1.756296
C      1.426130  -1.258752   1.562478
C      1.810130  -1.797332   0.377141
W     -0.544503   0.000003  -0.229008
C     -1.645146  -1.562705  -0.685857
C     -2.007278   0.000016   1.115093
C     -1.645081   1.562744  -0.685848
O     -2.293005  -2.457283  -1.089849
O     -2.884439   0.000027   1.897561
O     -2.292906   2.457358  -1.089829
H      1.230640  -2.098303  -1.673424
H      1.230637   2.098186  -1.673499
H      1.685089   1.798731   2.487381
H      1.684988  -1.798698   2.487449
C      2.602714  -3.082250   0.322330
C     -0.023712   0.000083   3.141956
C      2.602812   3.082169   0.322176
C      1.247735  -0.000077  -3.087076
H      2.841734  -3.457227   1.332356
H      2.042658  -3.873555  -0.214211
H      3.551483  -2.938106  -0.230847
H      0.712517   0.895213  -3.446917
H      2.250747  -0.000076  -3.556920
H      0.712525  -0.895379  -3.446894
H      2.841865   3.457196   1.332177
H      3.551567   2.937979  -0.231010
H      2.042778   3.873473  -0.214391
H     -0.652714  -0.893052   3.293839
H      0.759156   0.000102   3.928064
H     -0.652690   0.893247   3.293777
   el energy= -873.755722199
        zpe= -873.493412
   th energy= -873.472448
 th enthalpy= -873.471504
 free energy= -873.542635


H      4.255315   1.157446  -1.484960
H      4.927948   0.032895  -0.282940
H      1.913371  -3.785151   0.031592
H      0.150519  -3.585639  -0.124461
H      1.232999  -3.065273  -1.430824
H      0.084170  -0.728026   4.195362
H     -1.083539   0.525647   3.731348
H     -1.378067  -1.169504   3.303680
H      1.732628   1.683478  -1.432030
H      3.424901  -1.761231   0.290440
H     -0.250458  -2.260466   1.701463
H     -0.052168   1.843408   2.382928
   el energy= -874.751367540
        zpe= -874.480216
   th energy= -874.459127
 th enthalpy= -874.458183
 free energy= -874.529633

TS-A
C     -2.762565   0.121687  -0.501754
C     -1.603407  -0.801060  -0.741425
C     -1.136820  -1.643856   0.335122
C     -0.696301  -1.095393   1.568583
C     -0.367807   0.241967   2.037827
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C    -0.438534  1.493852  1.361399
C    -1.089296  1.813597  0.126524
C    -2.491618  1.357066 -0.096046
W     0.518233 -0.020595 -0.167939
C     0.961213 -0.952856 -1.874799
C     1.690075  1.430195 -0.895397
C     2.164018 -0.843018  0.647252
O     1.180618 -1.525399 -2.858641
O     2.370818  2.267522 -1.317609
O     3.076924 -1.328939  1.165372
C    -4.147223 -0.445304 -0.689300
C    -1.025545 -3.144527  0.144536
C     0.297851  0.259799  3.408269
C    -0.818812  3.203376 -0.432032
H    -4.326971 -1.291405 -0.009551
H    -4.281016 -0.830091 -1.711035
H    -4.921356  0.308736 -0.505646
H    -1.548782  3.923738 -0.027064
H    -0.926852  3.213320 -1.522600
H     0.184259  3.568099 -0.187648
H    -0.468586  0.190918  4.193399
H     0.987808 -0.580628  3.543171
H     0.855618  1.187453  3.571220
H    -1.999341 -3.619468  0.336875
H    -0.748471 -3.381576 -0.888499
H    -0.284734 -3.600886  0.811029
H    -3.281075  2.079802  0.131356
H     0.179840  2.269053  1.816730
H    -0.328691 -1.852560  2.261099
H    -1.679145 -1.339088 -1.690897
      el energy= -874.732922814
             zpe= -874.462400
      th energy= -874.442146
    th enthalpy= -874.441202
    free energy= -874.510043


TS-B
C     0.060956  2.512547  1.245525
C     0.002167  3.144930  0.000000
C     0.060956  2.512547 -1.245525
C    -0.246846  1.160652 -1.592827
C    -1.415513  0.355224 -1.277315
C    -2.002468  0.147571  0.000000
C    -1.415513  0.355224  1.277315
C    -0.246846  1.160652  1.592827
W     0.212777 -0.652460  0.000000
C     2.227856 -0.571357  0.000000
C     0.205344 -2.138209  1.309467
C     0.205344 -2.138209 -1.309467
O     3.378877 -0.466184  0.000000
O     0.178795 -3.022474  2.063987
O     0.178795 -3.022474 -2.063987
C     0.606701  3.339003  2.392489
C     0.606701  3.339003 -2.392489
C    -2.136328 -0.256567 -2.466605
C    -2.136328 -0.256567  2.466605
H     0.971176  4.319194  2.070061
H     1.432715  2.805712  2.882516
H    -0.166666  3.488616  3.159877
H    -2.789855  0.494184  2.935123
H    -1.424382 -0.593772  3.227790
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H    -2.752520 -1.114070  2.173740
H    -2.752520 -1.114070 -2.173740
H    -2.789855  0.494184 -2.935123
H    -1.424382 -0.593772 -3.227790
H    -0.166666  3.488616 -3.159877
H     0.971176  4.319194 -2.070061
H     1.432715  2.805712 -2.882516
H     0.111876  0.918159  2.594357
H    -2.898141 -0.470089  0.000000
H     0.111876  0.918159 -2.594357
H     0.239135  4.206453  0.000000
      el energy= -874.734763768
             zpe= -874.464468
      th energy= -874.443807
    th enthalpy= -874.442863
    free energy= -874.513851


TS-C
C    -1.888327 -1.701927  0.189557
C    -0.624036 -1.623967  0.957358
C    -0.044841 -0.726169  1.887899
C    -0.072903  0.716047  1.874472
C    -0.672123  1.656119  1.009506
C    -1.975601  1.646616  0.315114
C    -2.850810  0.713051 -0.141267
C    -2.774365 -0.753740 -0.209157
W     0.603218 -0.004419 -0.227325
C     1.040191 -1.375883 -1.633644
C     1.039153  1.503495 -1.484521
C     2.469812 -0.015512  0.253753
O     1.289236 -2.185558 -2.420787
O     1.270104  2.399894 -2.178145
O     3.590395 -0.027896  0.578301
C    -2.158693 -3.131375 -0.251310
C     0.886744 -1.330629  2.928641
C    -0.167384  3.089816  1.188899
C    -4.131279  1.228133 -0.777407
H    -2.245229 -3.801237  0.616457
H    -1.326649 -3.510010 -0.862654
H    -3.076537 -3.213097 -0.841679
H    -5.010195  0.822794 -0.254662
H    -4.211863  0.900658 -1.824313
H    -4.196561  2.320390 -0.755391
H    -0.845723  3.650843  1.848827
H     0.837227  3.118470  1.621909
H    -0.133460  3.618882  0.229365
H     0.339916 -1.468414  3.872964
H     1.258211 -2.311497  2.614286
H     1.750565 -0.688155  3.132470
H    -3.616492 -1.160993 -0.767878
H    -2.284528  2.668956  0.098017
H     0.677340  1.145463  2.536522
H    -0.205227 -2.622024  1.075472
      el energy= -874.724031045
             zpe= -874.452307
      th energy= -874.431922
    th enthalpy= -874.430978
    free energy= -874.501214


TS-D
C    -1.959928 -0.174092 -1.718057
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C    -1.478126 -1.327766 -0.918823
C    -1.672170 -1.580617  0.411995
C    -2.313429 -0.646979  1.359093
C    -1.960661  0.630285  1.612659
C    -0.875083  1.391877  0.927201
C    -0.828364  1.734510 -0.438431
C    -1.681627  1.130313 -1.477755
W     0.693294 -0.113965  0.039563
C     1.780446 -1.775566 -0.143241
C     1.867146  0.750018 -1.230380
C     1.963223  0.507532  1.361853
O     2.405576 -2.749282 -0.234741
O     2.533701  1.286299 -2.024871
O     2.693508  0.883603  2.192253
C    -2.741549 -0.580455 -2.948145
C    -1.364310 -2.953250  0.977977
C    -2.632044  1.399426  2.727677
C    -0.191825  3.054224 -0.842905
H    -3.656894 -1.124397 -2.674014
H    -2.150607 -1.257840 -3.582106
H    -3.024847  0.289361 -3.550477
H    -0.972202  3.825338 -0.946560
H     0.335710  2.985465 -1.800713
H     0.522716  3.396160 -0.087325
H    -3.089289  2.321897  2.342958
H    -3.407295  0.806959  3.225769
H    -1.893859  1.706282  3.482508
H    -2.305201 -3.447694  1.263773
H    -0.848941 -3.590075  0.252015
H    -0.752396 -2.889489  1.885838
H    -2.036287  1.841996 -2.227115
H    -0.382765  2.105215  1.589464
H    -3.080152 -1.100867  1.990187
H    -1.093912 -2.156606 -1.517278
      el energy= -874.716840926
             zpe= -874.446552
      th energy= -874.425843
    th enthalpy= -874.424899
    free energy= -874.496189

TS-E
C    -0.268465  1.209032  1.678362
C     0.099769  2.507335  1.232973
C     0.108745  3.166859  0.000000
C     0.099769  2.507335 -1.232973
C    -0.268465  1.209032 -1.678362
C    -1.402000  0.415982 -1.260573
C    -2.024678  0.186874  0.000000
C    -1.402000  0.415982  1.260573
W     0.188973 -0.632015  0.000000
C     0.109837 -2.121987  1.297987
C     0.109837 -2.121987 -1.297987
C     2.219062 -0.621961  0.000000
O     0.040121 -3.010795  2.043054
O     0.040121 -3.010795 -2.043054
O     3.371645 -0.574553  0.000000
C     0.178484  0.896514  3.113371
C     0.419718  4.654111  0.000000
C     0.178484  0.896514 -3.113371
C    -3.339916 -0.571875  0.000000
H    -0.480842  1.381107  3.851018
```

```
H     1.199823  1.247498  3.297887
H     0.165453 -0.179645  3.315630
H    -4.184921  0.131517  0.000000
H    -3.437878 -1.207354  0.887647
H    -3.437878 -1.207354 -0.887647
H    -0.480842  1.381107 -3.851018
H     1.199823  1.247498 -3.297887
H     0.165453 -0.179645 -3.315630
H     0.995126  4.948076  0.887527
H     0.995126  4.948076 -0.887527
H    -0.498556  5.259192  0.000000
H    -1.892045 -0.108889  2.082697
H    -1.892045 -0.108889 -2.082697
H     0.538001  3.109688 -2.035801
H     0.538001  3.109688  2.035801
      el energy= -874.717102870
             zpe= -874.447974
      th energy= -874.426834
    th enthalpy= -874.425889
    free energy= -874.498107


TS-F
C     0.530102  1.309985  1.622744
C     0.240007  0.003098  2.101642
C     0.500410 -1.309777  1.614689
C     1.679976 -1.765205  0.828608
C     2.072333 -1.264805 -0.354645
C     1.426360 -0.013268 -0.913045
C     2.077270  1.240608 -0.370012
C     1.698655  1.750647  0.814971
W    -0.665436 -0.001586 -0.076512
C    -1.737185  1.637365 -0.398325
C    -0.883953  0.016967 -2.057176
C    -1.744999 -1.627218 -0.423525
O    -2.417414  2.573297 -0.483990
O    -0.960015  0.024560 -3.214821
O    -2.432476 -2.556965 -0.522905
C    -0.107678  2.463661  2.391059
C    -0.158305 -2.451917  2.383293
C     3.168143 -1.903335 -1.170947
C     3.154181  1.883183 -1.208012
H    -1.022169  2.157797  2.912543
H    -0.361533  3.297334  1.726352
H     0.592262  2.852704  3.147151
H     3.565533  2.774854 -0.720433
H     2.753770  2.184101 -2.187540
H     3.983692  1.190152 -1.408480
H     4.000321 -1.208192 -1.352787
H     3.571383 -2.793958 -0.674669
H     2.789995 -2.205168 -2.158943
H     0.528409 -2.845369  3.149307
H    -1.075004 -2.132769  2.893170
H    -0.415368 -3.285832  1.720156
H     2.194891  2.651960  1.182503
H     1.531464 -0.019977 -2.002537
H     2.175343 -2.658849  1.216109
H    -0.583404  0.011491  2.825805
      el energy= -874.684131689
             zpe= -874.414575
      th energy= -874.394062
    th enthalpy= -874.393118
```

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```
    free energy= -874.463380

TS-G
C      1.339820 -1.276830 -0.942752
C      1.409193  0.000064 -1.563482
C      1.339860  1.276922 -0.942712
C      1.845535  1.773706  0.368865
C      1.470503  1.242325  1.544886
C      0.637879 -0.000041  1.720998
C      1.470599 -1.242340  1.544824
C      1.845625 -1.773647  0.368771
W     -0.583402 -0.000023 -0.235001
C     -1.668217 -1.598034 -0.663602
C     -2.015538  0.000020  1.150332
C     -1.668247  1.597969 -0.663679
O     -2.289090 -2.503025 -1.041086
O     -2.862772  0.000035  1.943977
O     -2.289125  2.502934 -1.041194
H      1.218158 -2.087464 -1.662560
H      1.218201  2.087586 -1.662484
H      1.799782  1.726375  2.468290
H      1.799980 -1.726364  2.468206
C      2.711646 -3.008441  0.293473
C      0.003759 -0.000103  3.117098
C      2.711416  3.008604  0.293665
C      1.215695  0.000084 -3.080843
H      2.992682 -3.363610  1.291384
H      2.191911 -3.827633 -0.225374
H      3.632329 -2.809804 -0.274655
H      0.682816  0.889574 -3.434201
H      2.207642 -0.000051 -3.555175
H      0.682591 -0.889277 -3.434192
H      2.992338  3.363779  1.291606
H      3.632164  2.810092 -0.274400
H      2.191625  3.827749 -0.225197
H     -0.616946 -0.887050  3.282670
H      0.794183 -0.000119  3.884812
H     -0.616978  0.886806  3.282741
     el energy= -874.680149928
            zpe= -874.410540
      th energy= -874.390095
    th enthalpy= -874.389151
    free energy= -874.459206
```

References

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(2)   Bennett, M. J.; Cotton, F. A.; Takats, J. Stereochemically Nonrigid Organometallic Molecules. XI. Molecular Structure of (1,3,5,7-Tetramethylcyclooctatetraene)Chromium Tricarbonyl. *J. Am. Chem. Soc.* **1968**, *90* (4), 903–909. https://doi.org/10.1021/ja01006a011.