

Accurate Thermochemistry for Transition Metal Oxide Clusters

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Supporting Information Metal-oxygen bond lengths and bond angles calculated at various levels of theory. Total atomization energies, normalized clustering energies, heats of formations, estimated metal-oxygen bond energies calculated at the CCSD(T) level with the RECP basis sets. Differences in the extrapolated B3LYP energies and calculated total atomization energies at 0 K using the exponential and mixed Gaussian/exponential formulae. Total atomization energies and normalized and differential clustering energies calculated at the DFT level with various exchange-correlation functionals and their deviations from the CCSD(T) or CCSD(T)-DK results. Energies calculated at the various levels of theory. Cartesian coordinates in Angstroms calculated at the various levels of theory.

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Table S1. Metal-oxygen bond lengths and bond angles calculated at the B3LYP/aVDZ-PP, B3LYP/aVTZ-PP, and compared with those calculated at the CCSD(T)/aVTZ-PP levels.

Molecule	M=O			O=M=O		
	B3LYP/ aVDZ-PP	B3LYP/ aVTZ-PP	CCSD(T) aVTZ-PP	B3LYP/ aVDZ-PP	B3LYP/ aVTZ-PP	CCSD(T)/ aVTZ-PP
TiO ₂	1.645	1.642	1.666	112.1	111.7	112.4
ZrO ₂	1.786	1.775	1.802	108.8	108.5	109.7
HfO ₂	1.781	1.771	1.798	108.2	107.9	109.6
CrO ₃	1.578	1.578	1.596	115.1	114.8	115.1
MoO ₃	1.713	1.707	1.719	110.9	110.8	110.9
WO ₃	1.725	1.719	1.732	108.0	107.8	108.4

Table S2. Total atomization energies at 0 K ($\Sigma D_{0,0K}$, kcal/mol) and heats of formation at 0 and 298 K for the ground states of $(MO_2)_n$ and $(M'O_3)_n$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$; $n = 1-2$) calculated at the CCSD(T) level with the RECP basis sets.

Molecule	ΔE_{Val}^a	ΔE_{CV}^b	$\Sigma D_{0,0K}^c$	$\Delta H_{f,0K}^d$	$\Delta H_{f,298K}^e$
TiO ₂	298.99	+3.30	297.95	-67.6	-68.2
ZrO ₂	330.59	+2.25	327.42	-65.6	-66.3
HfO ₂	329.64	+0.80	319.32	-53.7	-54.5
CrO ₃	339.63	+2.90	336.09	-64.7	-65.6
MoO ₃	416.70	+0.17	410.87	-76.8	-77.8
WO ₃	475.13	-0.94	459.71	-79.7	-80.8
Ti ₂ O ₄	719.40	+9.80	718.37	-257.7	-259.5
Zr ₂ O ₄	789.51	+7.26	784.10	-260.4	-262.2
Hf ₂ O ₄	808.96	+4.15	788.99	-257.7	-259.6
Cr ₂ O ₆	771.62	+9.44	766.06	-223.2	-225.6
Mo ₂ O ₆	945.26	+3.82	935.36	-267.3	-269.5
W ₂ O ₆	1078.82	-0.44	1048.06	-288.0	-290.3

^a ΔE_{Val} (PP) from Tables 1 and 2.

^b Calculated from the CCSD(T)/awCVTZ-PP energy differences with and without correlating the metal $(n-1)s^2(n-1)p^6$ ($n = 3$ for Ti and Cr, $n = 4$ for Zr and Mo, $n = 5$ for W) and oxygen $1s^2$ electrons.

^c $\Sigma D_{0,0K} = \Delta E_{\text{Val}} + \Delta E_{\text{CV}} + \Delta E_{\text{ZPE}} + \Delta E_{\text{SO}}$, where ΔE_{ZPE} and ΔE_{SO} are taken from Table 3. For $M = W$, it is corrected by the energy difference between the 7S_3 and 5D_0 states (8.44 kcal/mol).

^d $\Delta H_{f,0K} [(MO_m)_n] = n \Delta H_{f,0K} (M) + m*n \Delta H_{f,0K} (O) - \Sigma D_{0,0K} [(MO_m)_n]$. $\Delta H_{f,0K}$ is 58.98±0.02 kcal/mol for O, 112.4±0.7 kcal/mol for Ti, 143.9±2.0 kcal/mol for Zr, 147.7±1.5 kcal/mol for Hf, 94.5±1.0 kcal/mol for Cr, 157.1±0.9 kcal/mol for Mo, and 203.1±1.5 kcal/mol for W.

^e $\Delta H_{f,298K} [(MO_m)_n] = \Delta H_{f,0K} [(MO_m)_n] + \Delta H_{0K \rightarrow 298K} [(MO_m)_n] - n \Delta H_{0K \rightarrow 298K} (Ti) - n*m \Delta H_{0K \rightarrow 298K} (O)$. $\Delta H_{0K \rightarrow 298K}$ is 1.04 kcal/mol for O, 1.15 kcal/mol for Ti, 1.31 kcal/mol for Zr, 1.40 kcal/mol for Hf, 0.97 kcal/mol for Cr, 1.10 kcal/mol for Mo, and 1.19 kcal/mol for W. The enthalpy change from 0 K to 298 K for the cluster is calculated at the BP86/aVDZ-PP level.

Table S3. Normalized clustering energies at 0 K (ΔE_{0K} , kcal/mol) for the ground states of $(MO_2)_n$ and $(M'O_3)_n$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$; $n = 2-4$) calculated at the CCSD(T) level with the RECP basis sets.

Molecule	$\Delta E_{\text{Val}}^{\text{a}}$	$\Delta E_{\text{CV}}^{\text{b}}$	ΔE_{0K}^{c}	Molecule	$\Delta E_{\text{Val}}^{\text{a}}$	$\Delta E_{\text{CV}}^{\text{b}}$	ΔE_{0K}^{c}
Ti ₂ O ₄	60.72	+1.60	61.2	Cr ₂ O ₆	46.18	+1.82	47.0
Zr ₂ O ₄	64.16	+1.37	64.6	Mo ₂ O ₆	55.93	+1.74	56.8
Hf ₂ O ₄	74.84	+1.27	75.2	W ₂ O ₆	64.28	+0.72	64.3
Ti ₃ O ₆	82.53	+2.29	83.5	Cr ₃ O ₉	56.16	+1.81	56.8
Zr ₃ O ₆	87.30	+1.84	88.0	Mo ₃ O ₉	69.68	+1.52	70.2
Hf ₃ O ₆	100.46	+1.54	100.9	W ₃ O ₉	81.87	+0.61	81.7
Ti ₄ O ₈	95.04	+2.62	96.2	Cr ₄ O ₁₂	58.91	+2.08	59.8
Zr ₄ O ₈	104.29	+1.86	104.8	Mo ₄ O ₁₂	72.88	+1.95	73.9
Hf ₄ O ₈	119.86	+1.42	120.0	W ₄ O ₁₂	85.97	+0.61	86.6

^a ΔE_{Val} (PP) from Tables 4 to 6.

^b Calculated at the CCSD(T)/awCVTZ-PP level for $n = 2$ and CCSD(T)/wCVTZ-PP level for $n = 3$ and 4 (for Cr₄O₁₂ and Mo₄O₁₂, at the CCSD(T)/wCVDZ-PP level). See Table 7.

^c $\Delta E_{0K} = \Delta E_{\text{Val}} + \Delta E_{\text{CV}} + \Delta E_{\text{ZPE}}$, where ΔE_{ZPE} was taken from Table 8.

Table S4. Heats of formation at 0 and 298 K ($\Delta H_{f,0K}$ and $\Delta H_{f,298K}$, kcal/mol) calculated at the CCSD(T) level with the RECP basis sets from the calculated normalized clustering energies and heats of formation^a for the ground states of $(MO_2)_n$ and $(M'O_3)_n$ (M = Ti, Zr, Hf; M' = Cr, Mo, W; n = 3, 4).

Molecule	$\Delta H_{f,0K}$	$\Delta H_{f,298K}$	Molecule	$\Delta H_{f,0K}$	$\Delta H_{f,298K}$
	CCSD(T) ^b	CCSD(T) ^c		CCSD(T) ^b	CCSD(T) ^c
Ti ₃ O ₆	-453.3	-456.1	Cr ₃ O ₉	-364.5	-367.9
Zr ₃ O ₆	-460.8	-463.5	Mo ₃ O ₉	-441.0	-444.0
Hf ₃ O ₆	-463.8	-466.7	W ₃ O ₉	-484.2	-487.3
Ti ₄ O ₈	-655.2	-659.3	Cr ₄ O ₁₂	-498.0	-502.8
Zr ₄ O ₈	-681.6	-685.5	Mo ₄ O ₁₂	-602.8	-606.8
Hf ₄ O ₈	-694.8	-698.8	W ₄ O ₁₂	-665.2	-668.7

^a Error bars due to errors in the experimental heats of formation of the atoms are $\pm 0.7*n$ for $(TiO_2)_n$, $\pm 2.0*n$ for $(ZrO_2)_n$, $\pm 1.5*n$ for $(HfO_2)_n$, $\pm 1.0*n$ for $(CrO_3)_n$, $\pm 0.9*n$ for $(MoO_3)_n$, and $\pm 1.5*n$ for $(WO_3)_n$.

^b $\Delta H_{f,0K} [(MO_m)_n] = n \Delta H_{f,0K} (MO_m) - n \Delta E_{norm,n} [(MO_m)_n]$, where heats of formation of the monomers are taken from Table S2, and normalized clustering energies are taken from Table S3.

^c $\Delta H_{f,298K} [(MO_m)_n] = \Delta H_{f,0K} [(MO_m)_n] + \Delta H_{0K \rightarrow 298K} [(MO_m)_n] - n \Delta H_{0K \rightarrow 298K} (Ti) - n*m \Delta H_{0K \rightarrow 298K} (O)$. $\Delta H_{0K \rightarrow 298K}$ is 1.04 kcal/mol for O, 1.15 kcal/mol for Ti, 1.31 kcal/mol for Zr, 1.40 kcal/mol for Hf, 0.97 kcal/mol for Cr, 1.10 kcal/mol for Mo, and 1.19 kcal/mol for W. The enthalpy change from 0 K to 298 K for the cluster is calculated at the BP86/aVDZ-PP level.

Table S5. Estimated M=O and M–O (M = Ti, Zr, Hf, Cr, Mo, W) bond energies at 0 K in kcal/mol from the total atomization energies of the monomers and dimers calculated at the CCSD(T) level with the RECP basis sets.^a

	M = Ti	M = Zr	M = Hf	M = Cr	M = Mo	M = W
M=O ^a	149.0	163.7	159.7	112.0	137.0	153.2
M–O ^b	105.1	114.2	117.4	79.5	96.9	108.8

^a From Table S2.

^b $\frac{1}{2} \Sigma D_{0,0K}(\text{MO}_2)$ for M = Ti, Zr, Hf, and $\frac{1}{3} \Sigma D_{0,0K}(\text{MO}_3)$ for M = Cr, Mo, W.

^c $\frac{1}{4} [\Sigma D_{0,0K}(\text{M}_2\text{O}_4) - \Sigma D_{0,0K}(\text{MO}_2)]$ for M = Ti, Zr, Hf, and $\frac{1}{4} [\Sigma D_{0,0K}(\text{M}_2\text{O}_6) - \frac{4}{3} \Sigma D_{0,0K}(\text{MO}_3)]$ for M = Cr, Mo, W.

Table S6. Differences in the extrapolated B3LYP energies ($\Delta E = E_{\text{exp}} - E_{\text{mixed}}$) and calculated total atomization energies at 0 K ($\Delta\Delta E = \Delta E_{\text{exp}} - \Delta E_{\text{mixed}}$) in kcal/mol using the exponential and mixed Gaussian/exponential formulae for the ground states of $(\text{MO}_2)_n$ and $(\text{M}'\text{O}_3)_n$ ($\text{M} = \text{Ti, Zr, Hf}$; $\text{M}' = \text{Cr, Mo, W}$; $n = 1-2$) and the atoms.^a

Atom	ΔE	Molecule	ΔE	$\Delta\Delta E$	Molecule	ΔE	$\Delta\Delta E$
Ti	0.08	TiO ₂	0.90	0.12	Ti ₂ O ₄	1.87	0.17
Zr	0.04	ZrO ₂	1.17	-0.19	Zr ₂ O ₄	2.28	-0.33
Hf	0.05	HfO ₂	1.39	-0.39	Hf ₂ O ₄	2.80	-0.81
Cr	0.13	CrO ₃	1.27	-0.28	Cr ₂ O ₆	2.66	-0.43
Mo	0.03	MoO ₃	1.72	-0.28	Mo ₂ O ₆	3.56	-0.67
W	0.02	WO ₃	2.09	-0.65	W ₂ O ₆	4.22	-1.35
O	0.47						

^a The ⁷S₃ state for the W atom.

Table S7. Total atomization energies at 0 K ($\Sigma D_{0,0K}$, kcal/mol) for the ground states of MO_2 and $M'O_3$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$) calculated with the various DFT exchange-correlation functionals with the aVTZ-PP basis sets at the B3LYP/aVDZ-PP geometries. The ZPEs and spin-orbit corrections are taken from Table 3.

Method	TiO ₂	ZrO ₂	HfO ₂	TiO ₂	ZrO ₂	HfO ₂	CrO ₃	MoO ₃	WO ₃
	M(³ F ₂) ^a			M(⁵ F ₁) ^b			M'(⁷ S ₃) ^c		
B3LYP	288.5	321.3	310.8	279.8	316.1	305.1	312.9	406.1	451.1
B3P86	304.3	335.4	323.8	288.3	323.0	310.6	321.4	414.2	456.7
B3PW91	295.0	326.7	315.2	276.7	311.5	298.8	302.9	396.5	438.7
B1B95	287.1	323.5	313.5	273.4	313.7	302.8	288.0	395.6	442.3
B1LYP	272.6	308.8	299.4	266.3	305.0	295.1	288.8	387.1	434.6
mPW1PW91	285.3	320.3	309.6	268.1	305.0	293.0	284.9	383.4	427.9
B98	288.7	324.8	314.8	286.9	326.2	315.5	321.3	417.6	461.3
B971	291.8	327.5	317.4	291.0	330.0	319.3	329.9	424.9	468.4
B972	298.1	329.1	317.4	293.7	330.7	318.9	318.1	419.0	463.7
PBE1PBE	288.3	322.7	312.1	272.2	308.7	296.9	290.9	389.5	434.1
O3LYP	302.5	331.0	318.1	286.0	319.2	304.9	318.3	409.1	448.1
TPSSh	295.8	326.8	315.8	280.6	314.4	302.0	317.1	406.0	446.1
BMK	243.8	304.8	304.8	259.0	317.2	316.2	312.3	419.5	464.0
SVWN5	392.8	406.1	390.6	372.4	395.2	379.3	462.2	536.4	572.3
BLYP	320.0	342.3	328.2	307.9	336.8	322.3	376.8	450.1	486.5
BP86	334.9	355.0	339.8	315.8	342.4	326.4	384.6	457.3	490.9

BPW91	329.9	350.8	335.3	305.8	332.8	316.1	367.5	440.9	474.0
BB95	340.7	360.6	345.5	320.4	349.0	333.0	387.6	466.1	500.4
PW91	338.1	358.7	343.5	316.8	343.7	327.4	383.6	457.0	491.0
mPWPW91	333.5	354.4	339.1	310.8	337.9	321.4	374.8	448.3	481.9
PBE	337.0	357.2	342.0	316.1	342.6	326.4	382.4	456.0	489.7
OLYP	320.8	343.2	327.6	301.4	330.1	313.1	352.1	432.2	465.5
TPSS	313.4	339.2	326.2	296.3	326.2	311.9	351.0	430.2	465.9
VSXC	312.4	334.0	321.5	305.4	331.9	318.8	360.5	428.7	465.5
HCTH93	323.8	342.1	325.9	307.7	335.8	318.9	350.3	433.6	466.5
HCTH147	328.1	345.3	329.2	316.6	344.6	328.5	361.7	445.0	478.6
HCTH407	325.6	342.1	325.7	313.6	340.8	324.2	351.1	435.4	469.8

^a The 3F_2 state of $(n-1)d^2ns^2$ configuration was used in Equation (5) for the Ti, Zr, and Hf atoms.

^b The 5F_1 state of $(n-1)d^3ns^1$ configuration was used in Equation (5) for the Ti, Zr, and Hf atoms.

^c The 7S_3 state of $(n-1)d^5ns^1$ configuration was used in Equation (5) for the Cr, Mo, and W atoms.

Table S8. Total atomization energies at 0 K ($\Sigma D_{0,0K}$, kcal/mol) for the ground states of M_2O_4 and M'_2O_6 ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$) calculated with the various DFT exchange-correlation functionals with the aVTZ-PP basis sets at the B3LYP/aVDZ-PP geometries. The ZPEs and spin-orbit corrections are taken from Table 3.

Method	Ti ₂ O ₄	Zr ₂ O ₄	Hf ₂ O ₄	Ti ₂ O ₄	Zr ₂ O ₄	Hf ₂ O ₄	Cr ₂ O ₆	Mo ₂ O ₆	W ₂ O ₆
	M(³ F ₂) ^a			M(⁵ F ₁) ^b			M'(⁷ S ₃) ^c		
B3LYP	692.6	764.8	763.0	675.2	754.5	751.7	717.7	920.4	1022.7
B3P86	726.7	796.2	793.0	694.8	771.4	766.4	739.1	940.9	1038.5
B3PW91	705.0	775.7	772.6	668.5	745.4	739.8	698.9	902.3	999.7
B1B95	691.5	772.3	772.8	664.0	752.8	751.3	670.0	903.7	1010.8
B1LYP	662.1	741.0	741.5	649.6	733.4	732.9	669.4	883.4	991.5
mPW1PW91	688.9	765.8	764.7	654.3	735.2	731.5	664.9	879.2	981.8
B98	693.5	772.8	772.6	689.7	775.5	773.9	735.1	945.1	1045.2
B971	699.9	778.0	777.6	698.2	783.1	781.4	752.7	959.5	1059.3
B972	707.9	777.6	774.5	699.2	780.9	777.4	725.0	944.4	1047.3
PBE1PBE	695.9	771.5	770.6	663.9	743.5	740.2	678.5	892.7	995.2
O3LYP	708.0	772.1	766.2	675.0	748.4	739.9	718.5	915.8	1006.2
TPSSh	709.0	778.4	776.0	678.7	753.6	748.4	729.6	923.0	1015.6
BMK	617.0	745.6	766.1	647.5	770.4	788.8	727.2	965.0	1066.6
SVWN5	912.8	946.2	934.6	871.9	924.6	911.9	1037.7	1195.8	1276.0
BLYP	747.7	798.9	788.5	723.6	787.9	776.8	841.1	999.8	1082.3
BP86	780.1	827.6	815.8	742.0	802.5	788.9	861.5	1018.8	1096.0

BPW91	767.2	816.3	804.2	719.0	780.3	765.7	824.2	983.3	1059.9
BB95	788.5	836.8	825.2	747.9	813.5	800.2	864.7	1034.2	1112.8
PW91	788.6	836.8	825.3	745.9	806.8	793.2	861.6	1020.1	1098.2
mPWPW91	776.8	825.8	813.9	731.4	792.6	778.5	841.3	1000.1	1077.6
PBE	785.3	832.6	821.0	743.4	803.4	789.8	858.2	1017.0	1094.4
OLYP	738.1	790.0	778.2	699.3	763.7	749.3	781.5	955.2	1033.2
TPSS	741.7	800.6	793.5	707.4	774.7	765.0	796.4	968.3	1051.2
VSXC	749.5	796.4	790.5	735.5	792.0	785.2	822.0	968.1	1053.7
HCTH93	743.4	788.2	775.2	711.2	775.6	761.2	777.4	958.2	1035.5
HCTH147	757.1	799.9	787.2	734.2	798.5	785.8	805.4	985.9	1064.2
HCTH407	749.3	790.2	777.1	725.4	787.6	774.1	781.3	963.9	1044.3

^a The 3F_2 state of $(n-1)d^2ns^2$ configuration was used in Equation (5) for the Ti, Zr, and Hf atoms.

^b The 5F_1 state of $(n-1)d^3ns^1$ configuration was used in Equation (5) for the Ti, Zr, and Hf atoms.

^c The 7S_3 state of $(n-1)d^5ns^1$ configuration was used in Equation (5) for the Cr, Mo, and W atoms.

Table S9. Absolute and average deviations in kcal/mol with respect to those calculated at the CCSD(T)-DK level or at the CCSD(T) level with the pseudopotential corrections^a for the total atomization energies at 0 K for the ground states of M₂O₄ and M'₂O₆ (M = Ti, Zr, Hf; M' = Cr, Mo, W) calculated with various DFT exchange-correlation functionals and the aVTZ-PP basis set at the B3LYP/aVDZ-PP geometries.

Method	Ti ₂ O ₄	Zr ₂ O ₄	Hf ₂ O ₄	Ti ₂ O ₄	Zr ₂ O ₄	Hf ₂ O ₄	Cr ₂ O ₆	Mo ₂ O ₆	W ₂ O ₆	Average		
	M(³ F ₂) ^b			M(⁵ F ₁) ^c			M'(⁷ S ₃) ^d			M(³ F ₂) ^b	M(⁵ F ₁) ^c	M'(⁷ S ₃) ^d
B3LYP	-24.1	-20.6	-16.3	-41.4	-30.9	-27.6	-41.5	-17.2	-22.8	20.3	33.3	27.2
B3P86	+10.1	+10.8	+13.6	-21.9	-14.0	-13.0	-20.1	+3.3	-7.0	11.5	16.3	10.1
B3PW91	-11.6	-9.8	-6.8	-48.1	-40.1	-39.5	-60.4	-35.4	-45.8	9.4	42.6	47.2
B1B95	-25.1	-13.2	-6.6	-52.6	-32.7	-28.1	-89.2	-34.0	-34.7	14.9	37.8	52.6
B1LYP	-54.6	-44.4	-37.9	-67.1	-52.1	-46.5	-89.8	-54.2	-54.0	45.6	55.2	66.0
mPW1PW91	-27.7	-19.7	-14.7	-62.3	-50.3	-47.9	-94.3	-58.5	-63.7	20.7	53.5	72.2
B98	-23.1	-12.7	-6.7	-26.9	-10.0	-5.5	-24.2	+7.4	-0.3	14.2	14.1	10.6
B971	-16.7	-7.4	-1.8	-18.4	-2.4	+2.1	-6.6	+21.9	+13.3	8.7	7.6	14.1
B972	-8.7	-7.8	-4.8	-17.5	-4.6	-1.9	-34.2	+6.7	+1.8	7.1	8.0	14.2
PBE1PBE	-20.7	-14.0	-8.8	-52.7	-41.9	-39.1	-80.8	-44.9	-50.3	14.5	44.6	58.7
O3LYP	-8.7	-13.4	-13.2	-41.6	-37.1	-39.4	-40.8	-21.8	-39.3	11.8	39.4	34.0
TPSSh	-7.6	-7.0	-3.4	-37.9	-31.8	-30.9	-29.7	-14.7	-29.9	6.0	33.6	24.8
BMK	-99.6	-39.8	-13.3	-69.1	-15.1	+9.5	-32.1	+27.4	+21.1	50.9	31.2	26.9
SVWN5	+196.1	+160.8	+155.2	+155.3	+139.1	+132.5	+278.5	+258.2	+230.5	170.7	142.3	255.7
BLYP	+31.1	+13.4	+9.1	+6.9	+2.4	-2.6	+81.9	+62.1	+36.8	17.9	4.0	60.3

BP86	+63.5	+42.1	+36.4	+25.4	+17.1	+9.5	+102.2	+81.2	+50.5	47.3	17.3	78.0
BPW91	+50.6	+30.8	+24.8	+2.4	-5.2	-13.7	+64.9	+45.6	+14.4	35.4	7.1	41.6
BB95	+71.9	+51.3	+45.9	+31.3	+28.0	+20.8	+105.4	+96.5	+67.3	56.3	26.7	89.7
PW91	+71.9	+51.4	+45.9	+29.3	+21.3	+13.8	+102.3	+82.4	+52.7	56.4	21.5	79.1
mPWPW91	+60.1	+40.3	+34.5	+14.7	+7.2	-0.9	+82.0	+62.5	+32.1	45.0	7.6	58.9
PBE	+68.6	+47.1	+41.7	+26.8	+17.9	+10.4	+99.0	+79.3	+48.9	52.5	18.4	75.7
OLYP	+21.5	+4.5	-1.2	-17.4	-21.8	-30.1	+22.2	+17.6	-12.3	9.1	23.1	17.4
TPSS	+25.0	+15.1	+14.1	-9.2	-10.7	-14.3	+37.1	+30.7	+5.7	18.1	11.4	24.5
VSXC	+32.8	+10.9	+11.2	+18.9	+6.6	+5.8	+62.8	+30.5	+8.2	18.3	10.4	33.8
HCTH93	+26.7	+2.7	-4.2	-5.5	-9	-18.1	+18.1	+20.5	-10.0	11.2	11.2	16.2
HCTH147	+40.5	+14.5	+7.8	+17.5	+13.1	+6.4	+46.2	+48.2	+18.7	20.9	12.3	37.7
HCTH407	+32.7	+4.8	-2.3	+8.7	+2.1	-5.3	+22.1	+26.2	-1.2	13.2	5.4	16.5

^a From Table 3.

^b The 3F_2 state of $(n-1)d^2ns^2$ configuration was used in Equation (5) for the Ti, Zr, and Hf atoms.

^c The 5F_1 state of $(n-1)d^3ns^1$ configuration was used in Equation (5) for the Ti, Zr, and Hf atoms.

^d The 7S_3 state of $(n-1)d^5ns^1$ configuration was used in Equation (5) for the Cr, Mo, and W atoms.

Table S10. Normalized clustering energies at 0 K (ΔE_{0K} , kcal/mol) for the ground states of $(MO_2)_2$ and $(M'O_3)_2$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$) calculated with the various DFT exchange-correlation functionals and the aVTZ-PP basis sets at the B3LYP/aVDZ-PP geometries. The ZPE corrections are taken from Table 8.

Method	Ti ₂ O ₄	Zr ₂ O ₄	Hf ₂ O ₄	Cr ₂ O ₆	Mo ₂ O ₆	W ₂ O ₆
B3LYP	57.8	61.1	70.7	46.0	54.1	60.3
B3P86	59.0	62.7	72.6	48.2	56.3	62.6
B3PW91	57.6	61.1	71.1	46.5	54.7	61.1
B1B95	58.6	62.7	72.9	47.0	56.3	63.1
B1LYP	58.5	61.7	71.4	45.9	54.6	61.1
mPW1PW91	59.1	62.6	72.7	47.6	56.2	63.0
B98	58.0	61.6	71.5	46.2	54.9	61.3
B971	58.1	61.5	71.4	46.4	54.9	61.2
B972	55.9	59.7	69.8	44.4	53.2	60.0
PBE1PBE	59.7	63.1	73.2	48.3	56.8	63.5
O3LYP	51.5	55.0	65.0	40.9	48.8	54.9
TPSSh	58.8	62.4	72.2	47.7	55.5	61.7
BMK	64.8	68.0	78.2	51.3	63.0	69.4
SVWN5	63.5	67.0	76.7	56.6	61.5	65.7
BLYP	53.9	57.2	66.0	43.8	49.8	54.6
BP86	55.2	58.8	68.0	46.1	52.1	57.1
BPW91	53.7	57.4	66.8	44.6	50.7	55.9
BB95	53.5	57.7	67.1	44.7	51.0	56.0
PW91	56.2	59.7	69.2	47.2	53.0	58.1
mPWPW91	54.8	58.4	67.9	45.8	51.7	56.9
PBE	55.7	59.1	68.5	46.7	52.5	57.5
OLYP	48.2	51.8	61.5	38.7	45.5	51.1
TPSS	57.4	61.1	70.6	47.2	54.0	59.7
VSXC	62.3	64.2	73.8	50.6	55.4	61.4
HCTH93	47.9	52.0	61.7	38.4	45.5	51.3
HCTH147	50.5	54.7	64.4	41.0	47.9	53.5
HCTH407	49.1	53.0	62.9	39.6	46.5	52.3

Table S11. Normalized clustering energies at 0 K (ΔE_{0K} , kcal/mol) for the ground states of $(MO_2)_n$ and $(M'O_3)_n$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$; $n = 3, 4$) calculated with the various DFT exchange-correlation functionals and the aVTZ-PP basis sets at the B3LYP/aVDZ-PP geometries. The ZPE corrections are taken from Table 8.

Method	Ti ₃ O ₆	Ti ₄ O ₈	Zr ₃ O ₆	Zr ₄ O ₈	Hf ₃ O ₆	Hf ₄ O ₈	Cr ₃ O ₉	Cr ₄ O ₁₂	Mo ₃ O ₉	Mo ₄ O ₁₂	W ₃ O ₉	W ₄ O ₁₂
B3LYP	77.3	88.3	81.7	96.8	93.1	110.0	55.0	57.8	67.6	71.2	77.6	81.9
B3P86	78.9	90.5	83.7	99.4	95.6	113.2	57.2	59.7	69.6	72.8	79.8	83.8
B3PW91	76.8	87.9	81.5	96.7	93.4	110.6	55.1	57.4	67.5	70.7	77.8	81.7
B1B95	79.0	90.7	84.3	100.3	96.5	114.2	54.9	57.1	68.6	71.6	79.2	83.0
B1LYP	78.3	89.5	82.6	97.9	94.1	111.3	54.9	57.7	68.3	71.9	78.6	83.0
mPW1PW91	79.1	90.7	83.7	99.4	95.8	113.5	56.4	58.9	69.3	72.5	80.0	83.9
B98	77.6	88.6	82.3	97.5	94.1	111.3	54.9	57.6	68.1	71.5	78.4	82.6
B971	77.8	88.8	82.3	97.5	94.1	111.2	55.2	57.9	68.1	71.4	78.2	82.4
B972	74.5	84.9	79.6	94.3	91.7	108.3	52.6	55.1	65.9	69.1	76.5	80.5
PBE1PBE	80.1	91.8	84.4	100.2	96.5	114.3	57.2	59.8	70.0	73.2	80.5	84.5
O3LYP	68.3	77.2	72.7	85.6	84.6	99.4	47.9	50.2	60.2	63.3	70.1	74.1
TPSSh	78.7	90.5	83.6	99.4	95.2	113.0	56.3	58.6	68.1	71.2	78.1	81.9
BMK	87.2	99.4	91.2	108.8	103.7	123.4	59.7	62.7	77.5	81.2	87.4	92.0
SVWN5	85.2	98.2	89.2	106.0	100.3	118.9	67.8	70.4	75.8	79.0	84.0	87.8
BLYP	71.5	81.1	75.6	89.1	86.0	101.3	52.7	55.1	62.5	65.8	71.0	75.0
BP86	73.2	83.5	77.8	92.0	88.6	104.7	54.9	57.1	64.6	67.5	73.4	77.0
BPW91	71.1	81.0	75.8	89.5	86.9	102.5	52.9	54.9	62.7	65.5	71.7	75.2

BB95	63.8	81.5	76.7	81.0	85.5	103.7	52.5	54.3	62.4	69.5	71.1	74.4
PW91	74.8	85.3	79.1	93.5	90.2	106.5	56.4	58.8	65.7	68.8	74.5	78.3
mPWPW91	17.6	83.0	77.3	91.4	88.4	104.3	54.5	56.7	64.1	67.0	73.0	76.6
PBE	74.1	84.5	78.3	92.4	89.3	105.4	55.6	57.9	64.9	68.0	73.7	77.4
OLYP	63.5	69.9	67.8	79.4	79.3	92.9	45.1	47.2	56.0	59.0	65.3	69.0
TPSS	76.7	88.1	81.5	96.8	92.8	110.0	55.8	58.0	66.3	69.2	75.7	79.3
VSXC	85.9	99.6	88.2	105.5	99.8	119.1	62.2	64.4	68.6	70.5	78.3	81.0
HCTH93	62.8	70.5	68.0	79.8	79.5	93.3	45.2	47.4	56.6	59.6	66.1	69.8
HCTH147	66.6	75.2	71.9	84.6	83.3	97.9	48.9	51.3	59.9	63.0	69.2	73.0
HCTH407	64.7	72.7	69.7	81.6	81.2	95.1	47.0	49.6	58.1	61.5	67.7	71.7

Table S12. Differential clustering energies at 0 K (ΔE_{0K} , kcal/mol) for the ground states of $(MO_2)_n$ and $(M'O_3)_n$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$; $n = 3, 4$) calculated with the various DFT exchange-correlation functionals and the aVTZ-PP basis sets at the B3LYP/aVDZ-PP geometries. The ZPE corrections are from BP86/aVDZ-PP.

Method	Ti ₃ O ₆	Ti ₄ O ₈	Zr ₃ O ₆	Zr ₄ O ₈	Hf ₃ O ₆	Hf ₄ O ₈	Cr ₃ O ₉	Cr ₄ O ₁₂	Mo ₃ O ₉	Mo ₄ O ₁₂	W ₃ O ₉	W ₄ O ₁₂
B3LYP	116.3	121.2	122.8	142.0	137.7	160.9	73.2	65.9	94.7	81.7	112.3	94.9
B3P86	118.8	125.0	125.7	146.5	141.4	166.1	75.4	67.3	96.3	82.4	114.3	95.8
B3PW91	115.4	121.2	122.3	142.4	138.1	162.1	72.1	64.6	93.3	80.0	111.3	93.4
B1B95	119.7	125.8	127.5	148.2	143.8	167.3	70.8	63.7	93.4	80.6	111.6	94.3
B1LYP	117.9	123.1	124.5	143.8	139.6	163.0	73.0	66.1	95.6	82.6	113.5	96.1
mPW1PW91	119.2	125.4	126.0	146.6	142.1	166.6	73.9	66.3	95.6	82.0	113.9	95.8
B98	116.8	121.5	123.8	143.3	139.3	162.8	72.4	65.6	94.6	81.6	112.5	95.1
B971	117.3	121.7	123.8	143.0	139.3	162.6	72.7	65.9	94.5	81.5	112.2	94.9
B972	111.7	116.2	119.3	138.3	135.3	158.4	69.1	62.6	91.4	78.7	109.7	92.5
PBE1PBE	120.9	127.0	127.2	147.6	143.2	167.6	75.0	67.4	96.4	82.9	114.5	96.5
O3LYP	101.8	103.9	108.1	124.2	123.6	143.9	61.8	57.2	82.9	72.8	100.5	86.0
TPSSh	118.6	125.9	125.9	146.9	141.2	166.3	73.5	65.4	93.2	80.4	110.9	93.4
BMK	132.1	135.9	137.7	161.6	154.6	182.5	76.7	71.4	106.3	92.2	123.5	105.8
SVWN5	128.6	137.1	133.6	156.3	147.6	174.6	90.0	78.2	104.5	88.5	120.6	99.4
BLYP	106.6	110.2	112.5	129.5	125.8	147.2	70.3	62.5	87.8	75.7	103.9	87.0
BP86	109.3	114.3	115.8	134.5	129.8	152.8	72.5	63.7	89.5	76.4	105.9	87.8
BPW91	106.0	110.6	112.6	130.7	127.0	149.5	69.4	61.1	86.6	74.0	103.2	85.6

BB95	84.2	134.8	114.7	93.8	122.3	158.4	68.0	59.8	85.0	90.8	101.3	84.5
PW91	112.0	117.0	118.1	136.6	132.3	155.3	74.8	65.9	91.0	78.0	107.5	89.5
mPWPW91	108.8	113.5	115.1	133.4	129.4	152.2	72.0	63.4	88.7	75.9	105.3	87.5
PBE	111.0	115.5	116.7	134.8	131.0	153.5	73.5	64.8	89.8	77.0	106.1	88.4
OLYP	94.0	89.2	99.9	114.2	114.8	133.8	57.9	53.7	76.9	68.0	93.7	80.0
TPSS	115.2	122.2	122.4	142.8	137.1	161.9	73.0	64.4	90.8	78.2	107.8	90.2
VSXC	133.2	140.7	136.4	157.2	151.8	176.8	85.5	70.9	94.9	76.2	112.1	89.0
HCTH93	92.6	93.6	100.1	115.1	115.1	134.7	58.8	53.9	78.7	68.6	95.9	80.9
HCTH147	98.9	100.8	106.4	122.5	121.1	141.8	64.6	58.3	83.7	72.4	100.8	84.5
HCTH407	96.1	96.7	103.0	117.4	117.8	136.9	62.0	57.4	81.3	71.5	98.4	83.8

Table S13. Absolute and average deviations in kcal/mol with respect to the CCSD(T)-DK or CCSD(T) values^a for the normalized clustering energies at 0 K for the ground states of (MO₂)_{3,4} and (M'O₃)_{3,4} (M = Ti, Zr, Hf; M' = Cr, Mo, W) calculated with additional DFT exchange-correlation functionals and the aVTZ-PP basis set at the B3LYP/aVDZ-PP geometries.

	Ti ₃ O ₆	Ti ₄ O ₈	Zr ₃ O ₆	Zr ₄ O ₈	Hf ₃ O ₆	Hf ₄ O ₈	Cr ₃ O ₉	Cr ₄ O ₁₂	Mo ₃ O ₉	Mo ₄ O ₁₂	W ₃ O ₉	W ₄ O ₁₂	Average
B972	-8.3	-10.4	-7.8	-9.4	-9.2	-11.7	-3.8	-4.9	-3.9	-4.8	-4.6	-5.3	7.0
O3LYP	-14.5	-18.1	-14.7	-18.1	-16.3	-20.6	-8.5	-9.8	-9.6	-10.6	-11.0	-11.7	13.6
BMK	+4.4	+4.1	+3.8	+5.1	+2.8	+3.4	+3.3	+2.7	+7.7	+7.3	+6.3	+6.2	4.7
SVWN5	+2.4	+2.9	+1.8	+2.3	-0.6	-1.1	+11.4	+10.4	+6.0	+5.1	+2.9	+2.0	4.1
BLYP	-11.3	-14.2	-11.8	-14.6	-14.9	-18.7	-3.7	-4.9	-7.3	-8.1	-10.1	-10.8	10.9
BP86	-9.6	-11.8	-9.6	-11.7	-12.3	-15.3	-1.5	-2.9	-5.2	-6.4	-7.7	-8.8	8.6
BPW91	-11.7	-14.3	-11.6	-14.2	-14.0	-17.5	-3.5	-5.1	-7.1	-8.4	-9.4	-10.6	10.6
BB95	-19.0	-13.8	-10.7	-22.7	-15.4	-16.3	-3.9	-5.7	-7.4	-4.4	-10.0	-11.4	11.7
PW91	-8.0	-10.0	-8.3	-10.2	-10.7	-13.5	-0.0	-1.2	-4.1	-5.1	-6.6	-7.5	7.1
mPWPW91	-10.0	-12.3	-10.1	-12.3	-12.5	-15.7	-1.9	-3.3	-5.7	-6.9	-8.1	-9.2	9.0
PBE	-8.7	-10.8	-9.1	-11.3	-11.6	-14.6	-0.8	-2.1	-4.9	-5.9	-7.4	-8.4	8.0
OLYP	-19.3	-25.4	-19.6	-24.3	-21.6	-27.1	-11.3	-12.8	-13.8	-14.9	-15.8	-16.8	18.6
HCTH93	-20.0	-24.8	-19.4	-23.9	-21.4	-26.7	-11.2	-12.6	-13.2	-14.3	-15.0	-16.0	18.2
HCTH147	-16.2	-20.1	-15.5	-19.1	-17.6	-22.1	-7.5	-8.7	-9.9	-10.9	-11.9	-12.8	14.4
HCTH407	-18.1	-22.6	-17.7	-22.1	-19.7	-24.9	-9.4	-10.4	-11.7	-12.4	-13.4	-14.1	16.4

^a From Table 8.

Table S14. Absolute and average deviations in kcal/mol with respect to the CCSD(T)-DK or CCSD(T) values^a for the differential clustering energies at 0 K for the ground states of (MO₂)_{3,4} and (M'O₃)_{3,4} (M = Ti, Zr, Hf; M' = Cr, Mo, W) calculated with various DFT exchange-correlation functionals and the aVTZ-PP basis set at the B3LYP/aVDZ-PP geometries.

Functional	Ti ₃ O ₆	Ti ₄ O ₈	Zr ₃ O ₆	Zr ₄ O ₈	Hf ₃ O ₆	Hf ₄ O ₈	Cr ₃ O ₉	Cr ₄ O ₁₂	Mo ₃ O ₉	Mo ₄ O ₁₂	W ₃ O ₉	W ₄ O ₁₂	Average
B3LYP	-10.8	-11.6	-11.1	-10.6	-15.4	-16.4	-2.4	-4.9	-1.7	-4.5	-2.5	-5.0	8.1
B3P86	-8.3	-7.8	-8.2	-6.1	-11.7	-11.2	-0.2	-3.5	-0.1	-3.8	-0.5	-4.1	5.5
B3PW91	-11.7	-11.6	-11.6	-10.2	-15.0	-15.2	-3.5	-6.2	-3.1	-6.2	-3.5	-6.5	8.7
B1B95	-7.4	-7.0	-6.4	-4.4	-9.3	-10.0	-4.8	-7.1	-3.0	-5.6	-3.2	-5.6	6.1
B1LYP	-9.2	-9.7	-9.4	-8.8	-13.5	-14.3	-2.6	-4.7	-0.8	-3.6	-1.3	-3.8	6.8
mPW1PW91	-7.9	-7.4	-7.9	-6.0	-11.0	-10.7	-1.7	-4.5	-0.8	-4.2	-0.9	-4.1	5.6
B98	-10.3	-11.3	-10.1	-9.3	-13.8	-14.5	-3.2	-5.2	-1.8	-4.6	-2.3	-4.8	7.6
B971	-9.8	-11.1	-10.1	-9.6	-13.8	-14.7	-2.9	-4.9	-1.9	-4.7	-2.6	-5.0	7.6
B972	-15.4	-16.6	-14.6	-14.3	-17.8	-18.9	-6.5	-8.2	-5.0	-7.5	-5.1	-7.4	11.5
PBE1PBE	-6.2	-5.8	-6.7	-5.0	-9.9	-9.7	-0.6	-3.4	+0.0	-3.3	-0.3	-3.4	4.5
O3LYP	-25.3	-28.9	-25.8	-28.4	-29.5	-33.4	-13.8	-13.6	-13.5	-13.4	-14.3	-13.9	21.2
TPSSh	-8.5	-6.9	-8.0	-5.7	-11.9	-11.0	-2.1	-5.4	-3.2	-5.8	-3.9	-6.5	6.6
BMK	+5.0	+3.1	+3.8	+9.0	+1.5	+5.2	+1.1	+0.6	+9.9	+6.0	+8.7	+5.9	5.0
SVWN5	+1.5	+4.3	-0.3	+3.7	-5.5	-2.7	+14.4	+7.4	+8.1	+2.3	+5.8	-0.5	4.7
BLYP	-20.5	-22.6	-21.4	-23.1	-27.3	-30.1	-5.3	-8.3	-8.6	-10.5	-10.9	-12.9	16.8
BP86	-17.8	-18.5	-18.1	-18.1	-23.3	-24.5	-3.1	-7.1	-6.9	-9.8	-8.9	-12.1	14.0
BPW91	-21.1	-22.2	-21.3	-21.9	-26.1	-27.8	-6.2	-9.7	-9.8	-12.2	-11.6	-14.3	17.0

BB95	-42.9	+2.0	-19.2	-58.8	-30.8	-18.9	-7.6	-11.0	-11.4	+4.6	-13.5	-15.4	19.7
PW91	-15.1	-15.8	-15.8	-16.0	-20.8	-22.0	-0.8	-4.9	-5.4	-8.2	-7.3	-10.4	11.9
mPWPW91	-18.3	-19.3	-18.8	-19.2	-23.7	-25.1	-3.6	-7.4	-7.7	-10.3	-9.5	-12.4	14.6
PBE	-16.1	-17.3	-17.2	-17.8	-22.1	-23.8	-2.1	-6.0	-6.6	-9.2	-8.7	-11.5	13.2
OLYP	-33.1	-43.6	-34.0	-38.4	-38.3	-43.5	-17.7	-17.1	-19.5	-18.2	-21.1	-19.9	28.7
TPSS	-11.9	-10.6	-11.5	-9.8	-16.0	-15.4	-2.6	-6.4	-5.6	-8.0	-7.0	-9.7	9.5
VSXC	+6.1	+7.9	+2.5	+4.6	-1.3	-0.5	+9.9	+0.1	-1.5	-10.0	-2.7	-10.9	4.8
HCTH93	-34.5	-39.2	-33.8	-37.5	-38.0	-42.6	-16.8	-16.9	-17.7	-17.6	-18.9	-19.0	27.7
HCTH147	-28.2	-32.0	-27.5	-30.1	-32.0	-35.5	-11.0	-12.5	-12.7	-13.8	-14.0	-15.4	22.0
HCTH407	-31.0	-36.1	-30.9	-35.2	-35.3	-40.4	-13.6	-13.4	-15.1	-14.7	-16.4	-16.1	24.9

^a From Table 11.

Table S15. Zero-point energies (ZPE) at the BP86/aVDZ-PP level, electronic energies (E_e) at the CCSD(T)/aVDZ-PP, CCSD(T)/aVTZ-PP, CCSD(T)/aVQZ-PP, and CCSD(T)/CBS levels, core-valence corrections (ΔE_{CV}) at the CCSD(T)/wCVDZ-PP, CCSD(T)/awCVDZ-PP, CCSD(T)/wCVTZ-PP, and CCSD(T)/awCVTZ-PP levels, and scalar relativistic corrections (ΔE_{CV}) at the CISD/aVTZ-PP level for the ground states of the $(MO_2)_n$ and $(M'O_3)_n$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$; $n = 1-4$) clusters. All energies are shown in Hartree.

Molecule	ZPE ^a	E_e^b	E_e^c	E_e^d	E_e^e	ΔE_{CV}^f	ΔE_{CV}^g	ΔE_{CV}^h	ΔE_{CV}^i	ΔE_{SR}^j
TiO ₂	0.00519	-207.76127	-207.89273	-207.93536	-207.95963	-0.39883	-0.40088	-0.50207	-0.50291	-0.10795
Ti ₂ O ₄	0.01382	-415.71596	-415.97941	-416.06501	-416.11376	-0.80424	-0.80986	-1.00854	-1.01092	-0.21489
Ti ₃ O ₆	0.02195	-623.67988	-624.07475	–	–	-1.21116	-1.22100	-1.51715	–	-0.32181
Ti ₄ O ₈	0.03021	-831.65251	-832.18012	–	–	-1.61954	-1.63406	-2.02498	–	-0.42839
ZrO ₂	0.00463	-196.69661	-196.83391	-196.87709	-196.90152	-0.33170	-0.33528	-0.43863	-0.44013	-0.10515
Zr ₂ O ₄	0.01220	-393.59946	-393.87212	-393.95877	-394.00791	-0.66949	-0.67943	-0.88062	-0.88464	-0.20991
Zr ₃ O ₆	0.01925	-590.51134	-590.91990	–	–	-1.00876	-1.02661	-1.32470	–	-0.31464
Zr ₄ O ₈	0.02686	-787.45745	-788.00175	–	–	-1.34788	-1.37437	-1.76642	–	-0.41925
HfO ₂	0.00451	-198.34029	-198.48117	-198.52437	-198.54870	-0.29043	-0.29312	-0.39556	-0.39681	-0.10596
Hf ₂ O ₄	0.01201	-396.91973	-397.20049	-397.28730	-397.33626	-0.58431	-0.59171	-0.79403	-0.79767	-0.21158
Hf ₃ O ₆	0.01884	-595.50427	-595.92443	–	–	-0.87947	-0.89212	-1.19401	–	-0.31719
Hf ₄ O ₈	0.02625	-794.13007	-794.68985	–	–	-1.17370	-1.19199	-1.59128	–	-0.42268
CrO ₃	0.00920	-311.23346	-311.43681	-311.50223	-311.53942	-0.45579	-0.46026	-0.59186	-0.59369	-0.16713
Cr ₂ O ₆	0.02176	-622.61237	-623.02261	-623.15327	-623.22739	-0.91773	-0.92860	-1.18872	-1.19317	-0.33289
Cr ₃ O ₉	0.03326	-933.96305	-934.58026	–	–	-1.37743	-1.39388	-1.78422	–	–

Cr ₄ O ₁₂	0.04458	-1245.30043	-1246.12467	–	–	-1.83641	-1.85894	–	–	–
MoO ₃	0.00849	-292.79837	-293.01388	-293.08140	-293.11958	-0.38140	-0.38651	-0.52463	-0.52666	-0.15827
Mo ₂ O ₆	0.01970	-585.77319	-586.20667	-586.34167	-586.41792	-0.76859	-0.78127	-1.05377	-1.05884	-0.31605
Mo ₃ O ₉	0.03017	-878.72108	-879.37527	–	–	-1.15348	-1.17353	-1.58115	–	–
Mo ₄ O ₁₂	0.03986	-1171.64620	-1172.52082	–	–	-1.53801	-1.56554	–	–	–
WO ₃	0.00857	-292.26175	-292.47949	-292.54577	-292.58303	-0.33725	-0.34162	-0.47691	-0.47870	-0.15886
W ₂ O ₆	0.01932	-584.72537	-585.16398	-585.29681	-585.37140	-0.67698	-0.68808	-0.95504	-0.95970	-0.31725
W ₃ O ₉	0.02990	-877.16857	-877.83035	–	–	-1.01605	-1.03359	-1.43366	–	–
W ₄ O ₁₂	0.03952	-1169.57986	-1170.46595	–	–	-1.35457	-1.37824	-1.91154	–	–

^a BP86/aVDZ-PP. ^b CCSD(T)/aVDZ-PP. ^c CCSD(T)/aVTZ-PP. ^d CCSD(T)/aVQZ-PP. ^e CCSD(T)/CBS using Equation (1).

^f CCSD(T)/wCVDZ-PP. ^g CCSD(T)/awCVDZ-PP. ^h CCSD(T)/wCVTZ-PP. ⁱ CCSD(T)/awCVTZ-PP. ^j CISD/aVTZ-PP.

Table S16. Electronic energies (E_e) at the CCSD(T)-DK/aVDZ-DK, CCSD(T)-DK/aVTZ-DK, CCSD(T)-DK/aVQZ-DK, and CCSD(T)-DK/CBS levels, core-valence corrections (ΔE_{CV}) at the CCSD(T)-DK/wCVTZ-DK and CCSD(T)-DK/awCVTZ-DK for the ground states of the $(MO_2)_n$ and $(M'O_3)_n$ ($M = \text{Ti, Zr, Hf}$; $M' = \text{Cr, Mo, W}$; $n = 1-4$) clusters. All energies are shown in Hartree.

Molecule	E_e^a	E_e^b	E_e^c	E_e^d	ΔE_{CV}^e	ΔE_{CV}^f
TiO ₂	-1003.18955	-1003.32372	-1003.36668	-1003.39108	-0.47389	-0.47462
Ti ₂ O ₄	-2006.57175	-2006.84121	-2006.92738	-2006.97630	-0.94972	-0.95184
Ti ₃ O ₆	-3009.96460	-3010.36733	–	–	-1.42762	–
Ti ₄ O ₈	-4013.36566	-4013.90346	–	–	-1.90365	–
ZrO ₂	–	-3746.45389	–	–	-0.41687	-0.41819
Zr ₂ O ₄	–	-7493.11180	–	–	-0.83554	-0.83901
Zr ₃ O ₆	–	-11239.77910	–	–	-1.25621	–
Zr ₄ O ₈	–	-14986.47869	–	–	-1.67392	–
HfO ₂	–	-15216.07870	–	–	–	–
Hf ₂ O ₄	–	-30432.39672	–	–	–	–
CrO ₃	-1275.16539	-1275.37354	-1275.43938	-1275.47668	-0.56275	-0.56446
Cr ₂ O ₆	-2550.48022	-2550.89593	-2551.02742	-2551.10191	-1.12888	-1.13298
Cr ₃ O ₉	-3825.76896	-3826.39013	–	–	-1.69400	–
Cr ₄ O ₁₂	-5101.04239	-5101.87115	–	–	–	–
MoO ₃	–	-4271.53855	–	–	-0.49888	-0.50060
Mo ₂ O ₆	–	-8543.25591	–	–	-1.00099	-1.00518
Mo ₃ O ₉	–	-12814.94883	–	–	-1.50177	–

Mo ₄ O ₁₂	–	-17086.61872	–	–	–	–
WO ₃	–	-16353.40350	–	–	-1.39578	-1.39761
W ₂ O ₆	–	-32707.01110	–	–	-2.79237	-2.79713
W ₃ O ₉	–	-49060.59994	–	–	-4.19004	–

^a CCSD(T)-DK/aVDZ-DK.

^b CCSD(T)-DK/aVTZ-DK. For M = Hf, CCSD(T)-DK/awCVTZ-DK by correlating Hf 4f5s5p orbitals with additional high angular momentum functions. See text.

^c CCSD(T)-DK/aVQZ-DK. ^d CCSD(T)-DK/CBS using Equation (1).

^e CCSD(T)-DK/wCVTZ-DK. For M = W, the core-valence corrections were calculated from the energy differences with and without correlating W 4f5s5porbitals by using additional high angular momentum functions. See text.

^f CCSD(T)-DK/awCVTZ-DK. For M = W, the core-valence corrections were calculated from the energy differences with and without correlating W 4f5s5p orbitals by using additional high angular momentum functions. See text.

Table S17. Cartesian coordinates in Angstroms optimized at the B3LYP/aVDZ-PP level for the ground states of the (MO₂)_n and (M'O₃)_n (M = Ti, Zr, Hf; M' = Cr, Mo, W; n = 1–4) clusters.

TiO₂ / ¹A₁ (C_{2v})

Ti	0.000000	0.000000	0.386906
O	0.000000	1.364619	-0.531996
O	0.000000	-1.364619	-0.531996

Ti₂O₄ / ¹A_g (C_{2h})

Ti	0.000000	1.358493	0.000000
O	0.000000	0.000000	1.254563
O	0.000000	0.000000	-1.254563
Ti	0.000000	-1.358493	0.000000
O	1.342483	-2.283197	0.000000
O	-1.342483	2.283197	0.000000

Ti₃O₆ / ¹A' (C_s)

Ti	-0.276993	-0.564058	1.434118
O	1.168219	-0.102305	0.000000
O	-1.198363	-1.305108	0.000000
Ti	-0.276993	-0.564058	-1.434118
O	0.083691	-1.452887	-2.748265
O	0.083691	-1.452887	2.748265
Ti	0.705530	1.643280	0.000000
O	-0.276993	1.448243	1.417026
O	-0.276993	1.448243	-1.417026

Ti₄O₈ / ¹A₁ (C_{2v})

Ti	0.000000	2.029741	-0.618921
O	1.692413	1.678279	0.289710
O	0.000000	2.765914	-2.058792
O	0.000000	0.000000	2.049982
O	0.000000	0.000000	-0.515803
Ti	1.410571	0.000000	0.877932
O	1.692413	-1.678279	0.289710
Ti	0.000000	-2.029741	-0.618921
O	0.000000	-2.765914	-2.058792
O	-1.692413	1.678279	0.289710
Ti	-1.410571	0.000000	0.877932
O	-1.692413	-1.678279	0.289710

ZrO₂ / ¹A₁ (C_{2v})

Zr	0.000000	0.000000	0.297103
O	0.000000	1.452364	-0.742757
O	0.000000	-1.452364	-0.742757

Zr₂O₄ / ¹A_g (C_{2h})

ZR	0.000000	1.505482	0.000000
ZR	0.000000	-1.505482	0.000000
O	0.000000	0.000000	1.315252
O	0.000000	0.000000	-1.315252
O	-1.565913	2.351735	0.000000
O	1.565913	-2.351735	0.000000

Zr₃O₆ / ¹A' (C_s)

ZR	-0.334253	-0.690314	1.588476
O	1.154696	-0.125647	0.000000
O	-1.257382	-1.524851	0.000000
ZR	-0.334253	-0.690314	-1.588476
O	0.224306	-1.663907	-2.975275
O	0.224306	-1.663907	2.975275
ZR	0.733023	1.782125	0.000000
O	-0.334253	1.485413	1.526091
O	-0.334253	1.485413	-1.526091

Zr₄O₈ / ¹A₁ (C_{2v})

ZR	0.000000	2.181178	-0.765408
O	1.806591	1.793307	0.239505
O	0.000000	2.795278	-2.431649
O	0.000000	0.000000	2.201388
O	0.000000	0.000000	-0.464014
ZR	1.577808	0.000000	0.982198
O	1.806591	-1.793307	0.239505
ZR	0.000000	-2.181178	-0.765408
O	0.000000	-2.795278	-2.431649
O	-1.806591	1.793307	0.239505
ZR	-1.577808	0.000000	0.982198
O	-1.806591	-1.793307	0.239505

HfO₂ / ¹A₁ (C_{2v})

HF	0.000000	0.000000	0.189979
O	0.000000	1.442175	-0.854905
O	0.000000	-1.442175	-0.854905

Hf₂O₄ / ¹A_g (C_{2h})

HF	0.000000	1.483301	0.000000
HF	0.000000	-1.483301	0.000000
O	0.000000	0.000000	1.303775
O	0.000000	0.000000	-1.303775
O	-1.584478	2.284673	0.000000
O	1.584478	-2.284673	0.000000

Hf₃O₆ / ¹A' (C_s)

HF	-0.345622	-0.726962	1.567496
O	1.123760	-0.182226	0.000000
O	-1.258894	-1.569957	0.000000
HF	-0.345622	-0.726962	-1.567496
O	0.277286	-1.680293	-2.938739
O	0.277286	-1.680293	2.938739
HF	0.721445	1.707246	0.000000
O	-0.345622	1.416441	1.509418
O	-0.345622	1.416441	-1.509418

Hf₄O₈ / ¹A₁ (C_{2v})

HF	0.000000	2.159785	-0.792679
O	1.783750	1.786460	0.203460
O	0.000000	2.733212	-2.471181
O	0.000000	0.000000	2.140874
O	0.000000	0.000000	-0.499483
HF	1.558371	0.000000	0.930853
O	1.783750	-1.786460	0.203460
HF	0.000000	-2.159785	-0.792679
O	0.000000	-2.733212	-2.471181
O	-1.783750	1.786460	0.203460
HF	-1.558371	0.000000	0.930853
O	-1.783750	-1.786460	0.203460

CrO₃ / ¹A₁ (C_{3v})

CR	0.000000	0.000000	0.176747
O	0.000000	1.537530	-0.176747
O	1.331540	-0.768765	-0.176747
O	-1.331540	-0.768765	-0.176747

Cr₂O₆ / ¹A_g (D_{2h})

CR	1.291280	0.000000	0.000000
CR	-1.291280	0.000000	0.000000
O	0.000000	0.000000	1.217165
O	0.000000	0.000000	-1.217165
O	2.173407	1.284293	0.000000
O	2.173407	-1.284293	0.000000
O	-2.173407	1.284293	0.000000
O	-2.173407	-1.284293	0.000000

Cr₃O₉ / ¹A₁ (C_{3v})

CR	0.000000	1.791635	-0.052041
CR	1.551602	-0.895818	-0.052041
CR	-1.551602	-0.895818	-0.052041
O	0.000000	3.142453	-0.821556
O	0.000000	2.049546	1.484329
O	1.387768	0.801228	-0.506650
O	-1.387768	0.801228	-0.506650
O	1.774959	-1.024773	1.484329
O	2.721444	-1.571226	-0.821556
O	-2.721444	-1.571226	-0.821556
O	0.000000	-1.602456	-0.506650
O	-1.774959	-1.024773	1.484329

Cr₄O₁₂ / ¹A₁ (C_{4v})

CR	0.000000	2.313497	-0.061950
O	0.000000	3.721731	-0.721919
O	0.000000	2.464390	1.486380
O	1.424868	1.424868	-0.578611
CR	2.313497	0.000000	-0.061950
CR	0.000000	-2.313497	-0.061950
O	2.464390	0.000000	1.486380
O	3.721731	0.000000	-0.721919
O	1.424868	-1.424868	-0.578611
O	0.000000	-3.721731	-0.721919
O	0.000000	-2.464390	1.486380
O	-1.424868	-1.424868	-0.578611
CR	-2.313497	0.000000	-0.061950
O	-1.424868	1.424868	-0.578611
O	-2.464390	0.000000	1.486380
O	-3.721731	0.000000	-0.721919

MoO₃ / ¹A₁ (C_{3v})

MO	0.000000	0.000000	0.192793
O	0.000000	1.629311	-0.337387
O	1.411025	-0.814656	-0.337387
O	-1.411025	-0.814656	-0.337387

Mo₂O₆ / ¹A_g (D_{2h})

MO	1.441086	0.000000	0.000000
MO	-1.441086	0.000000	0.000000
O	0.000000	0.000000	1.276071
O	0.000000	0.000000	-1.276071
O	2.413212	1.385316	0.000000
O	2.413212	-1.385316	0.000000
O	-2.413212	1.385316	0.000000
O	-2.413212	-1.385316	0.000000

Mo₃O₉ / ¹A₁' (D_{3h})

MO	1.766326	1.019789	0.000000
MO	-1.766326	1.019789	0.000000
MO	0.000000	-2.039577	0.000000
O	2.628780	1.517727	1.364399
O	2.628780	1.517727	-1.364399
O	0.000000	1.724934	0.000000
O	1.493836	-0.862467	0.000000
O	-2.628780	1.517727	-1.364399
O	-2.628780	1.517727	1.364399
O	0.000000	-3.035454	1.364399
O	-1.493836	-0.862467	0.000000
O	0.000000	-3.035454	-1.364399

Mo₄O₁₂ / ¹A₁ (C_{4v})

MO	0.000000	2.623463	-0.024123
O	0.000000	3.900239	-1.129844
O	0.000000	3.286546	1.529498
O	1.519648	1.519648	-0.273006
MO	2.623463	0.000000	-0.024123
MO	0.000000	-2.623463	-0.024123
O	3.286546	0.000000	1.529498
O	3.900239	0.000000	-1.129844
O	1.519648	-1.519648	-0.273006
O	0.000000	-3.900239	-1.129844
O	0.000000	-3.286546	1.529498
O	-1.519648	-1.519648	-0.273006
MO	-2.623463	0.000000	-0.024123
O	-1.519648	1.519648	-0.273006
O	-3.286546	0.000000	1.529498
O	-3.900239	0.000000	-1.129844

WO₃ / ¹A₁ (C_{3v})

W	0.000000	0.000000	0.151072
O	0.000000	1.611436	-0.465807
O	1.395544	-0.805718	-0.465807
O	-1.395544	-0.805718	-0.465807

W₂O₆ / ¹A_g (D_{2h})

W	1.448048	0.000000	0.000000
O	2.423994	1.403978	0.000000
O	2.423994	-1.403978	0.000000
O	0.000000	0.000000	1.277963
O	0.000000	0.000000	-1.277963
W	-1.448048	0.000000	0.000000
O	-2.423994	-1.403978	0.000000
O	-2.423994	1.403978	0.000000

$W_3O_9 / {}^1A_1' (D_{3h})$

W	1.769351	1.021535	0.000000
W	-1.769351	1.021535	0.000000
W	0.000000	-2.043070	0.000000
O	2.635048	1.521346	1.382087
O	2.635048	1.521346	-1.382087
O	0.000000	1.728181	0.000000
O	1.496649	-0.864090	0.000000
O	-2.635048	1.521346	-1.382087
O	-2.635048	1.521346	1.382087
O	0.000000	-3.042692	1.382087
O	-1.496649	-0.864090	0.000000
O	0.000000	-3.042692	-1.382087

$W_4O_{12} / {}^1A_1' (D_{4h})$

W	1.875177	1.875177	0.000000
W	-1.875177	-1.875177	0.000000
W	1.875177	-1.875177	0.000000
O	2.584546	2.584546	1.378806
O	2.584546	2.584546	-1.378806
O	0.000000	2.158466	0.000000
O	2.158466	0.000000	0.000000
O	-2.584546	-2.584546	-1.378806
O	-2.584546	-2.584546	1.378806
O	2.584546	-2.584546	1.378806
O	0.000000	-2.158466	0.000000
O	2.584546	-2.584546	-1.378806
W	-1.875177	1.875177	0.000000
O	-2.584546	2.584546	1.378806
O	-2.584546	2.584546	-1.378806
O	-2.158466	0.000000	0.000000

Table S18. Cartesian coordinates in Angstroms optimized at the B3LYP/aVTZ-PP level for the ground states of the MO₂ and M'O₃ (M = Ti, Zr, Hf; M' = Cr, Mo, W) clusters.

TiO₂ / ¹A₁ (C_{2v})

Ti	0.000000	0.000000	0.387908
O	0.000000	1.359178	-0.533374
O	0.000000	-1.359178	-0.533374

ZrO₂ / ¹A₁ (C_{2v})

Zr	0.000000	0.000000	0.296247
O	0.000000	1.440235	-0.740618
O	0.000000	-1.440235	-0.740618

HfO₂ / ¹A₁ (C_{2v})

Hf	0.000000	0.000000	0.189555
O	0.000000	1.431352	-0.852999
O	0.000000	-1.431352	-0.852999

CrO₃ / ¹A₁ (C_{3v})

Cr	0.000000	0.000000	0.182090
O	0.000000	1.535222	-0.182090
O	1.329541	-0.767611	-0.182090
O	-1.329541	-0.767611	-0.182090

MoO₃ / ¹A₁ (C_{3v})

Mo	0.000000	0.000000	0.192850
O	0.000000	1.622575	-0.337488
O	1.405191	-0.811288	-0.337488
O	-1.405191	-0.811288	-0.337488

WO₃ / ¹A₁ (C_{3v})

W	0.000000	0.000000	0.151304
O	0.000000	1.604355	-0.466522
O	1.389412	-0.802178	-0.466522
O	-1.389412	-0.802178	-0.466522

Table S19. Cartesian coordinates in Angstroms optimized at the CCSD(T)/aVDZ-PP level for the ground states of the (MO₂)_n and (M'O₃)_n (M = Ti, Zr, Hf; M' = Cr, Mo, W; n = 1, 2) clusters.

TiO₂ / ¹A₁ (C_{2v})

TI	0.00000000	0.00000000	-0.36992374
O	0.00000000	1.39377441	0.55351915
O	0.00000000	-1.39377441	0.55351915

Ti₂O₄ / ¹A_g (C_{2h})

TI	-1.30600500	-0.39956416	0.00000000
TI	1.30600500	0.39956416	0.00000000
O	0.00000000	0.00000000	1.27494183
O	0.00000000	0.00000000	-1.27494183
O	-2.62642358	0.59458923	0.00000000
O	2.62642358	-0.59458923	0.00000000

ZrO₂ / ¹A₁ (C_{2v})

ZR	0.00000000	0.00000000	-0.26980609
O	0.00000000	1.49099905	0.76914483
O	0.00000000	-1.49099905	0.76914483

Zr₂O₄ / ¹A_g (C_{2h})

ZR	-1.48740678	-0.32118601	0.00000000
ZR	1.48740678	0.32118601	0.00000000
O	0.00000000	0.00000000	1.33855941
O	0.00000000	0.00000000	-1.33855941
O	-2.71956401	1.00155191	0.00000000
O	2.71956401	-1.00155191	0.00000000

HfO₂ / ¹A₁ (C_{2v})

HF	0.00000000	0.00000000	-0.15782636
O	0.00000000	1.48600374	0.88035884
O	0.00000000	-1.48600374	0.88035884

Hf₂O₄ / ¹A_g (C_{2h})

HF	-1.48728606	-0.19317990	0.00000000
HF	1.48728606	0.19317990	0.00000000
O	0.00000000	0.00000000	1.32899165
O	0.00000000	0.00000000	-1.32899165
O	-2.57845674	1.24310208	0.00000000
O	2.57845674	-1.24310208	0.00000000

CrO₃ / ¹A₁ (C_{3v})

CR	0.00000000	0.00000000	0.16118813
O	1.56403771	0.00000000	-0.17461359
O	-0.78201886	1.35449639	-0.17461359
O	-0.78201886	-1.35449639	-0.17461359

Cr₂O₆ / ¹A_g (D_{2h})

CR	0.00000000	0.00000000	-1.29255341
CR	0.00000000	0.00000000	1.29255341
O	-1.23546658	0.00000000	0.00000000
O	1.23546658	0.00000000	0.00000000
O	0.00000000	1.29900551	-2.18209306
O	0.00000000	-1.29900551	-2.18209306
O	0.00000000	1.29900551	2.18209306
O	0.00000000	-1.29900551	2.18209306

MoO₃ / ¹A₁ (C_{3v})

MO	0.00000000	0.00000000	0.17762197
O	1.64633311	0.00000000	-0.35503523
O	-0.82316656	1.42576630	-0.35503523
O	-0.82316656	-1.42576630	-0.35503523

Mo₂O₆ / ¹A_g (D_{2h})

MO	0.00000000	0.00000000	-1.44145764
MO	0.00000000	0.00000000	1.44145764
O	-1.29191465	0.00000000	0.00000000
O	1.29191465	0.00000000	0.00000000
O	0.00000000	1.39466802	-2.42171938
O	0.00000000	-1.39466802	-2.42171938
O	0.00000000	1.39466802	2.42171938
O	0.00000000	-1.39466802	2.42171938

WO₃ / ¹A₁ (C_{3v})

W	0.00000000	0.00000000	0.12563972
O	1.63319800	0.00000000	-0.48124435
O	-0.81659900	1.41439096	-0.48124435
O	-0.81659900	-1.41439096	-0.48124435

W₂O₆ / ¹A_g (D_{2h})

W	0.00000000	0.00000000	-1.44974531
W	0.00000000	0.00000000	1.44974531
O	-1.29289049	0.00000000	0.00000000
O	1.29289049	0.00000000	0.00000000
O	0.00000000	1.41388902	-2.43264554
O	0.00000000	-1.41388902	-2.43264554
O	0.00000000	1.41388902	2.43264554
O	0.00000000	-1.41388902	2.43264554

Table S20. Cartesian coordinates in Angstroms optimized at the CCSD(T)/aVTZ-PP level for the ground states of the $(\text{MO}_2)_n$ and $(\text{M}'\text{O}_3)_n$ ($\text{M} = \text{Ti, Zr, Hf}$; $\text{M}' = \text{Cr, Mo, W}$; $n = 1, 2$) clusters.

$\text{TiO}_2 / ^1\text{A}_1 (\text{C}_{2v})$

TI	0.00000000	0.00000000	-0.37131599
O	0.00000000	1.38438786	0.55560238
O	0.00000000	-1.38438786	0.55560238

$\text{Ti}_2\text{O}_4 / ^1\text{A}_g (\text{C}_{2h})$

TI	-1.30282991	-0.40318275	0.00000000
TI	1.30282991	0.40318275	0.00000000
O	0.00000000	0.00000000	1.26850644
O	0.00000000	0.00000000	-1.26850644
O	-2.60751220	0.60285623	0.00000000
O	2.60751220	-0.60285623	0.00000000

$\text{ZrO}_2 / ^1\text{A}_1 (\text{C}_{2v})$

ZR	0.00000000	0.00000000	-0.26920200
O	0.00000000	1.47338955	0.76742273
O	0.00000000	-1.47338955	0.76742273

$\text{Zr}_2\text{O}_4 / ^1\text{A}_g (\text{C}_{2h})$

ZR	-1.48330613	-0.31964131	0.00000000
ZR	1.48330613	0.31964131	0.00000000
O	0.00000000	0.00000000	1.32724565
O	0.00000000	0.00000000	-1.32724565
O	-2.69255549	1.00395768	0.00000000
O	2.69255549	-1.00395768	0.00000000

$\text{HfO}_2 / ^1\text{A}_1 (\text{C}_{2v})$

HF	0.00000000	0.00000000	-0.15752015
O	0.00000000	1.46990184	0.87865084
O	0.00000000	-1.46990184	0.87865084

$\text{Hf}_2\text{O}_4 / ^1\text{A}_g (\text{C}_{2h})$

HF	-1.48290028	-0.19201384	0.00000000
HF	1.48290028	0.19201384	0.00000000
O	0.00000000	0.00000000	1.31497017
O	0.00000000	0.00000000	-1.31497017
O	-2.55251980	1.24447322	0.00000000
O	2.55251980	-1.24447322	0.00000000

$\text{CrO}_3 / ^1\text{A}_1 (\text{C}_{3v})$

CR	0.00000000	0.00000000	0.17248980
O	1.55486578	0.00000000	-0.18685658
O	-0.77743289	1.34655326	-0.18685658
O	-0.77743289	-1.34655326	-0.18685658

Cr₂O₆ / ¹A_g (D_{2h})

CR	0.00000000	0.00000000	-1.28959757
CR	0.00000000	0.00000000	1.28959757
O	-1.23041807	0.00000000	0.00000000
O	1.23041807	0.00000000	0.00000000
O	0.00000000	1.29582270	-2.17915107
O	0.00000000	-1.29582270	-2.17915107
O	0.00000000	1.29582270	2.17915107
O	0.00000000	-1.29582270	2.17915107

MoO₃ / ¹A₁ (C_{3v})

MO	0.00000000	0.00000000	0.17744987
O	1.63411959	0.00000000	-0.35469124
O	-0.81705979	1.41518907	-0.35469124
O	-0.81705979	-1.41518907	-0.35469124

Mo₂O₆ / ¹A_g (D_{2h})

MO	0.00000000	0.00000000	-1.43569300
MO	0.00000000	0.00000000	1.43569300
O	-1.27977726	0.00000000	0.00000000
O	1.27977726	0.00000000	0.00000000
O	0.00000000	1.38503289	-2.41113349
O	0.00000000	-1.38503289	-2.41113349
O	0.00000000	1.38503289	2.41113349
O	0.00000000	-1.38503289	2.41113349

WO₃ / ¹A₁ (C_{3v})

W	0.00000000	0.00000000	0.12587631
O	1.62137080	0.00000000	-0.48215057
O	-0.81068540	1.40414830	-0.48215057
O	-0.81068540	-1.40414830	-0.48215057

W₂O₆ / ¹A_g (D_{2h})

W	0.00000000	0.00000000	-1.44439708
W	0.00000000	0.00000000	1.44439708
O	-1.27966928	0.00000000	0.00000000
O	1.27966928	0.00000000	0.00000000
O	0.00000000	1.40645556	-2.42209896
O	0.00000000	-1.40645556	-2.42209896
O	0.00000000	1.40645556	2.42209896
O	0.00000000	-1.40645556	2.42209896