**Structural and Electronic Properties of Reduced Transition Metal Oxide Clusters,
 M_3O_8 and $M_3O_8^-$ ($M = Cr, W$), from Photoelectron Spectroscopy and Quantum
Chemical Calculations**

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Figure S1. Low-lying structures of M_3O_9 ($M = \text{Cr}, \text{W}$).

Figure S2. High-lying electronic states of Cr_3O_8 calculated at the CCSD(T)/aVDZ //B3LYP/aVDZ level. Relative energies are given in kcal/mol.

Figure S3. High-lying electronic states of Cr_3O_8^- calculated at the CCSD(T)/aVDZ //B3LYP/aVDZ level. Relative energies are given in kcal/mol.

Figure S4. High-lying electronic states of W_3O_8 calculated at the CCSD(T)/aVDZ //B3LYP/aVDZ level. Relative energies are given in kcal/mol.

Figure S5. High-lying electronic states of W_3O_8^- calculated at the CCSD(T)/aVDZ //B3LYP/aVDZ level. Relative energies are given in kcal/mol.

Table S1: Relative energies at 0 K in kcal/mol calculated at the CCSD(T), B3LYP, BP86, and PW91 levels for the high-lying electronic states of Cr_3O_8 and Cr_3O_8^- . ZPE Corrections at the BP86/aVDZ Level.

state	CCSD(T) aVDZ ^a	B3LYP aVTZ ^b	BP86 aVTZ ^c	PW91 aVTZ ^d
Cr_3O_8				
$^3\text{B}_1 / \text{D}_{2d} (\text{D})$	19.6	19.1	22.9	— ^e
$^3\text{A}_2 / \text{D}_{2d} (\text{D})$	22.3	23.9	17.5	17.7
$(^1\text{A}' \text{a}) / \text{C}_s (\text{B})$	25.5	29.5	25.8	26.8
$^1\text{A}_1 / \text{D}_{2d} (\text{D})$	26.4	37.9	17.4	18.3
$^3\text{A}' / \text{C}_s (\text{B})$	30.1	30.5	29.3	29.5
$^1\text{A} / \text{C}_2 (\text{C})$	37.7	57.1	39.5	40.3
$(^1\text{A}' \text{b}) / \text{C}_s (\text{B})$	38.0	41.4	36.3	36.9
$^3\text{B} / \text{C}_2 (\text{C})$	44.9	50.6	51.6	53.3
$^5\text{A}_2 / \text{C}_{2v} (\text{A})$	45.5	36.9	45.3	45.6
$^5\text{B}_2 / \text{C}_{2v} (\text{A})$	58.4	58.5	59.8	60.0
$^5\text{A}_1 / \text{C}_{2v} (\text{A})$	59.0	50.4	56.8	57.0
$^5\text{B}_1 / \text{C}_{2v} (\text{A})$	68.0	62.0	66.8	67.0
Cr_3O_8^-				
$(^2\text{A}_2 \text{a}) / \text{C}_{2v} (\text{A})$	19.2	40.8	10.8	10.6
$^2\text{A}_1 / \text{D}_{2d} (\text{D})$	21.2	21.6	1.6	2.4
$^4\text{A}_2 / \text{C}_{2v} (\text{A})$	22.3	25.4	14.9	14.5
$(^2\text{A}_2 \text{b}) / \text{C}_{2v} (\text{A})$	22.7	51.3	22.1	22.3
$^4\text{A}'' / \text{C}_s (\text{B})$	24.0	27.8	15.4	15.3
$(^2\text{A}'' \text{a}) / \text{C}_s (\text{B})$	29.4	34.2	18.2	18.4
$^2\text{A} / \text{C}_2 (\text{C})$	31.8	49.9	31.8	32.6
$(^2\text{A}' \text{b}) / \text{C}_s (\text{B})$	38.9	42.7	28.7	29.2
$^2\text{B} / \text{C}_2 (\text{C})$	40.1	57.6	35.9	36.7
$^4\text{B} / \text{C}_2 (\text{C})$	43.5	47.9	40.7	42.3
$(^2\text{A}'' \text{b}) / \text{C}_s (\text{B})$	56.9	59.2	19.1	19.6
$^2\text{A}' / \text{C}_s (\text{B})$	−5.8	43.7	20.1	20.9

^a CCSD(T)/aVDZ//B3LYP/aVDZ. ^b B3LYP/aVTZ//B3LYP/aVDZ.

^c BP86/aVTZ//BP86/aVDZ. ^d PW91/aVTZ//PW91/aVDZ. ^e Converged to the $^3\text{A}_2$ state.

Table S2: Relative energies at 0 K (ΔE_{0K} , kcal/mol) calculated at the CCSD(T), B3LYP, BP86, and PW91 levels for the high-lying electronic states of W_3O_8 and $W_3O_8^-$. All ZPE corrections are taken from BP86/aVDZ.

State	CCSD(T) aVDZ ^a	B3LYP aVTZ ^b	BP86 aVTZ ^c	PW91 aVTZ ^d
W_3O_8				
(¹ A ₁ <i>b</i>) / C _{2v} (<i>A</i>)	20.5	30.7	28.8	28.5
³ B ₂ / D _{2d} (<i>D</i>)	32.3	30.4	24.7	25.2
³ A' / C _s (<i>B</i>)	35.7	31.7	29.4	29.5
¹ A ₁ / D _{2d} (<i>D</i>)	38.3	38.6	31.2	31.8
³ A ₂ / D _{2d} (<i>D</i>)	42.6	38.3	38.0	38.2
(³ B ₂ <i>a</i>) / C _{2v} (<i>C</i>)	49.1	40.5	47.1	48.7
(³ B ₂ <i>b</i>) / C _{2v} (<i>C</i>)	95.7	90.9	72.0	72.5
³ A ₁ / C _{2v} (<i>C</i>)	68.8	67.0	57.6	58.8
$W_3O_8^-$				
² A ₁ / C _{2v} (<i>A</i>)	25.2	30.8	29.4	28.2
⁴ A ₂ / D _{2d} (<i>D</i>)	27.8	25.7	31.0	31.2
⁴ A'' / C _s (<i>B</i>)	28.2	25.2	29.7	29.5
⁴ B ₂ / C _{2v} (<i>A</i>)	32.3	30.5	41.4	41.5
² A ₁ / D _{2d} (<i>D</i>)	32.6	33.2	30.5	31.2
⁴ B ₁ / C _{2v} (<i>A</i>)	37.0	34.7	39.8	39.4

^a CCSD(T)/aVDZ//B3LYP/aVDZ.

^b B3LYP/aVTZ//B3LYP/aVDZ.

^c BP86/aVTZ//BP86/aVDZ.

^d PW91/aVTZ//PW91/aVDZ.

Table S3: Adiabatic and Vertical Electron Detachment Energies (ADEs and VDEs in eV) for Additional Transitions Calculated at the CCSD(T), B3LYP, BP86, and PW91 Levels for the Low-lying Structures of Cr_3O_8^- . ZPE Corrections for the ADE at the BP86/aVDZ Level.

transition	orbital ^a	CCSD(T)			B3LYP	BP86	PW91
		aVDZ ^b	aVTZ ^c	aVTZ+CV ^d	aVTZ ^e	aVTZ ^f	aVTZ ^g
<i>ADEs</i>							
⁴ B ₂ → ³ A ₁ / C _{2v} (A)	15 <i>b</i> ₂	4.78	4.85	4.85	5.58	4.57	4.52
² A ₁ → (¹ A ₁ a) / C _{2v} (A)	− ^h	4.21	4.25	4.44	4.93	4.34	4.30
² A ₁ → ³ A ₁ / C _{2v} (A)	22 <i>a</i> ₁	4.60	4.70	4.66	4.47	4.29	4.24
⁴ B ₁ → ³ A ₁ / C _{2v} (A)	− ^h	4.40	4.52	4.50	5.14	4.54	4.52
² A′ → ³ A″ / C _s (B)	23 <i>a</i> ″	4.76	–	–	3.20	3.64	3.56
<i>VDEs</i>							
⁴ B ₂ → ³ A ₁ / C _{2v} (A)	15 <i>b</i> ₂	5.16	5.24	5.26	6.04	4.95	4.91
² A ₁ → (¹ A ₁ a) / C _{2v} (A)	− ^h	5.97	6.24	6.85	7.89	7.11	7.12
² A ₁ → ³ A ₁ / C _{2v} (A)	22 <i>a</i> ₁	4.98	5.08	5.02	4.92	4.65	4.62
⁴ B ₁ → ³ A ₁ / C _{2v} (A)	− ^h	6.29	6.39	6.43	6.97	5.58	5.56
² A′ → ³ A″ / C _s (B)	23 <i>a</i> ″	4.97	–	–	3.49	3.83	3.76

^a The molecular orbital where the electron is removed. The electron configuration at the BP86/aVDZ level for the $^4\text{B}_2$ state of structure **A** is $\dots(22a_1)^1(15b_2)^1(23a_1)^1$. That for $^2\text{A}_1$ state of structure **A** is $\dots(22a_1)^2(23a_1)^1$. That for $^4\text{B}_1$ state of structure **A** is $\dots(15b_2)^1(22a_1)^1(6a_2)^1$. That for $^2\text{A}'$ state of structure **B** is $\dots(23a'')^2(31a')^1$.

^b CCSD(T)/aVDZ//B3LYP/aVDZ. ^c CCSD(T)/aVTZ//B3LYP/aVDZ.

^d CCSD(T)/aVTZ//B3LYP/aVDZ with core-valence corrections calculated at the CCSD(T)/awCVDZ//B3LYP/aVDZ level.

^e B3LYP/aVTZ//B3LYP/aVDZ. ^f BP86/aVTZ//BP86/aVDZ. ^g PW91/aVTZ//PW91/aVDZ. ^h

Transitions involving orbital relaxation.

Table S4: Adiabatic and Vertical Electron Detachment Energies (ADEs and VDEs in eV) for Additional Transitions Calculated at the CCSD(T), B3LYP, BP86, and PW91 Levels for the Low-lying Structures of W_3O_8^- . ZPE Corrections for the ADE at the BP86/aVDZ Level.

transition	orbital ^a	CCSD(T) aVDZ ^b /aVTZ ^c	B3LYP aVTZ ^d	BP86 aVTZ ^e	PW91 aVTZ ^f
ADEs					
$^2\text{A}' \rightarrow ^3\text{A}_2 / \text{C}_s (\mathbf{B})$	$-\text{g}$	3.77/3.78	3.61	4.04	4.01
$^2\text{A}'' \rightarrow ^3\text{A}_2 / \text{C}_s (\mathbf{B})$	31a'	3.65/3.66	3.55	3.91	3.88
VDEs					
$^2\text{A}' \rightarrow ^3\text{A}_2 / \text{C}_s (\mathbf{B})$	$-\text{g}$	5.87	5.98	5.92	5.89
$^2\text{A}'' \rightarrow ^3\text{A}_2 / \text{C}_s (\mathbf{B})$	31a'	4.62	4.82	4.87	4.83

^a The molecular orbital where the electron is removed. The electron configuration at the B3LYP/aVDZ level for $^2\text{A}'$ state of structure $\mathbf{B}$ is $\dots(31\text{a}')^2(32\text{a}')^1$. That for $^2\text{A}''$ state of structure $\mathbf{B}$ is $\dots(31\text{a}')^2(23\text{a}'')^1$.

^b CCSD(T)/aVDZ//B3LYP/aVDZ. ^c CCSD(T)/aVTZ//B3LYP/aVDZ.

^d B3LYP/aVTZ//B3LYP/aVDZ. ^e BP86/aVTZ//BP86/aVDZ.

^f PW91/aVTZ//PW91/aVDZ. ^g Transitions involving orbital relaxation.

Table S5: Adiabatic and Vertical Electron Detachment Energies (ADEs and VDEs in eV) to Additional Excited States of the Neutral Cluster Calculated at the CCSD(T), B3LYP, BP86, and PW91 Levels for the Ground State of $M_3O_8^-$ (M = Cr, W). ZPE Corrections at the BP86/aVDZ Level.

transition ^a	CCSD(T) aVDZ ^b	B3LYP aVTZ ^c	BP86 aVTZ ^d	PW91 aVTZ ^e
<i>Cr₃O₈⁻, ADEs</i>				
$^4B_2 \rightarrow (^3A_2 \text{ } a) / C_{2v} (A)$	4.93	5.78	4.44	4.38
$^4B_2 \rightarrow (^3B_1 \text{ } a) / C_{2v} (A)$	5.11	5.75	4.59	4.54
$^4B_2 \rightarrow (^3A_2 \text{ } b) / C_{2v} (A)$	5.37	6.16	4.94	4.88
$^4B_2 \rightarrow (^3B_1 \text{ } b) / C_{2v} (A)$	5.48	6.38	5.07	5.01
$^4B_2 \rightarrow (^3A_1 \text{ } b) / C_{2v} (A)$	6.07	7.07	5.86	5.81
<i>Cr₃O₈⁻, VDEs</i>				
$^4B_2 \rightarrow (^3A_2 \text{ } a) / C_{2v} (A)$	5.96	6.88	5.24	5.19
$^4B_2 \rightarrow (^3B_1 \text{ } a) / C_{2v} (A)$	5.72	6.49	5.09	5.04
$^4B_2 \rightarrow (^3A_2 \text{ } b) / C_{2v} (A)$	5.99	6.94	5.52	5.47
$^4B_2 \rightarrow (^3B_1 \text{ } b) / C_{2v} (A)$	6.23	6.94	5.58	5.53
$^4B_2 \rightarrow (^3A_1 \text{ } b) / C_{2v} (A)$	6.40	7.14	6.15	6.10
<i>W₃O₈⁻, ADEs</i>				
$^2A_1 \rightarrow (^3B_2 \text{ } a) / C_{2v} (C)$	5.55	5.23	5.71	5.72
$^2A_1 \rightarrow (^3B_1 \text{ } b) / C_{2v} (C)$	7.68	7.52	7.37	7.33
<i>W₃O₈⁻, VDEs</i>				
$^2A_1 \rightarrow (^3B_2 \text{ } a) / C_{2v} (C)$	8.88	8.94	8.77	8.76
$^2A_1 \rightarrow (^3B_1 \text{ } b) / C_{2v} (C)$	8.53	8.52	8.19	8.15

^a All of these transitions involve orbital relaxation.

^b CCSD(T)/aVDZ//B3LYP/aVDZ. ^c B3LYP/aVTZ//B3LYP/aVDZ.

^d BP86/aVTZ//BP86/aVDZ. ^e PW91/aVTZ//PW91/aVDZ.

Table S6: Relative energies in kcal/mol between the quintet and triplet states for structure **A** of Cr₃O₈ and the triplet and open shell singlet states for structure **C** of W₃O₈ at the neutral geometries. Electronic energies of the high spin states were calculated at the ROHF/aVDZ//B3LYP/aVDZ level, and those of the low spin states were calculated at the CASSCF/aVDZ//B3LYP/aVDZ level.

Cr₃O₈ / C_{2v} (A)		W₃O₈ / C_{2v} (C)	
E(³ A ₂) – E(⁵ A ₂)	^a	E(¹ A ₁) – E(³ A ₁)	14.9
E(³ A ₁) – E(⁵ A ₁)	0.3	E(¹ A ₂) – E(³ A ₂)	1.8
E(³ B ₂) – E(⁵ B ₂)	0.5	E(¹ B ₁ <i>a</i>) – E(³ B ₁ <i>a</i>)	4.3
E(³ B ₁) – E(⁵ B ₁)	0.6	E(¹ B ₂ <i>b</i>) – E(³ B ₂ <i>b</i>)	2.7

^a It was not possible to get good convergence for the energy of this quintet state. On the basis of comparison of the values in this Table with those in Table 7 in the text for the other quintet-triplet splittings, we expect a value of 0.4 kcal/mol.

Table S7: Valence electronic energy contributions to the total atomization energies in kcal/mol for the ground states of CrO₂ (³B₁) and WO₂ (¹A₁) calculated at the CCSD(T)-DK level or at the CCSD(T) level with the pseudopotential corrections.^a

Molecule		$\Delta E_{n=D}^b$	$\Delta E_{n=T}^c$	$\Delta E_{n=Q}^c$	ΔE_{CBS}^d	$\Delta E_{\text{SR}}^{c,e}$	ΔE_{Val}^f	$\Delta E_{\text{awCVTZ-PP}}^{c,g}$	$\Delta E_{\text{awCVTZ-DK}}^{c,h}$	$\Delta E_{\text{PP,corr}}^i$	$\Delta E_{\text{Val,corr}}^j$
CrO ₂	PP	215.00	226.54	231.45	234.37	-1.33	233.04	227.15	226.52	+0.70	233.74
	DK	210.94	225.87	230.62	233.31	–	233.31	–	–	–	–
WO ₂	PP	302.13	322.05	328.14	331.57	-0.34	331.23	324.02	323.33	-0.35	330.88

^a The ground states of Cr (⁷S₃) and the first excited state of W (⁷S₃) were used.

^b Geometries from CCSD(T)/aVDZ-PP or CCSD(T)-DK/aVDZ-DK.

^c Geometries from CCSD(T)/aVTZ-PP or CCSD(T)-DK/aVTZ-DK.

^d Extrapolated CCSD(T) or CCSD(T)-DK energies with n = D, T, and Q using the mixed Gaussian/exponential formula.

^e MVD Expectation values of the CISD/aVTZ-PP wavefunction.

^f $\Delta E_{\text{Val}}(\text{PP}) = \Delta E_{\text{CBS}}(\text{PP}) + \Delta E_{\text{SR}}$ and $\Delta E_{\text{Val}}(\text{DK}) = \Delta E_{\text{CBS}}(\text{DK})$.

^g Valence electronic energy at the CCSD(T)/awCVTZ-PP level.

^h Valence electronic energy at the CCSD(T)-DK/awCVTZ-DK level.

ⁱ $\Delta E_{\text{PP,corr}} = \Delta E_{\text{awCVTZ-DK}} - (\Delta E_{\text{awCVTZ-PP}} + \Delta E_{\text{SR}})$.

^j $\Delta E_{\text{Val,corr}}(\text{PP}) = \Delta E_{\text{Val}}(\text{PP}) + \Delta E_{\text{PP,corr}} = \Delta E_{\text{CBS}}(\text{PP}) + \Delta E_{\text{awCVTZ-DK}} - \Delta E_{\text{awCVTZ-PP}}$.

Table S8: 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 CrO_2 (3B_1) and WO_2 (1A_1) calculated at the CCSD(T) level with the pseudopotential corrections, and compared with available experimental data.

	ΔE_{Val}^a	ΔE_{CV}^b	ΔE_{ZPE}^c	ΔE_{SO}^d	$\Sigma D_{0,0K}^e$	$\Delta H_{f,0K}^f$	$\Delta H_{f,298K}^g$	Expt. (298K) ^h
CrO_2	233.31	-0.27	-3.21	-0.44	229.39	-16.9	-17.3	-18.0 ± 10
WO_2	330.88	+0.14	-3.41	-0.44	318.73	-2.3	-1.7	-18.3 ± 7

^a ΔE_{Val} (DK) for CrO_2 and $\Delta E_{\text{Val,corr}}$ (PP) for WO_2 from Table S6.

^b CCSD(T)-DK/awCVTZ-DK. For WO_2 the metal $4f^{14}$ electrons were also correlated. The core-valence corrections calculated at the CCSD(T)/awCVTZ-PP level are +2.03 and +0.37 kcal/mol for CrO_2 and WO_2 respectively.

^c BP86/aVDZ-PP.

^d Experimental atomic spin-orbit corrections (-0.22 kcal/mol for O, and 0 kcal/mol for Cr and W).

^e $\Sigma D_{0,0K} = \Delta E_{\text{Val}} + \Delta E_{\text{CV}} + \Delta E_{\text{ZPE}} + \Delta E_{\text{SO}}$. For WO_2 , it was corrected by the energy difference between the 7S_3 and 5D_0 states (8.44 kcal/mol).

^f $\Delta H_{f,0K}[(\text{MO}_m)_n] = n \Delta H_{f,0K}(\text{M}) + m \cdot n \Delta H_{f,0K}(\text{O}) - \Sigma D_{0,0K}[(\text{MO}_m)_n]$. $\Delta H_{f,0K}$ is 58.98 ± 0.02 kcal/mol for O, 94.5 ± 1.0 kcal/mol for Cr, and 203.1 ± 1.5 kcal/mol for W.

^g $\Delta H_{f,298K}[(\text{MO}_m)_n] = \Delta H_{f,0K}[(\text{MO}_m)_n] + \Delta H_{0K \rightarrow 298K}[(\text{MO}_m)_n] - n \Delta H_{0K \rightarrow 298K}(\text{M}) - n \cdot m \Delta H_{0K \rightarrow 298K}(\text{O})$. $\Delta H_{0K \rightarrow 298K}$ is 1.04 kcal/mol for O, 0.97 kcal/mol for Cr, 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.

^h Ref. 56.

Table S9: Valence electronic energy contributions and core-valence corrections to the clustering energies^a at 0 K in kcal/mol for the ground states of Cr₃O₈ (³B₂) and W₃O₈ (¹A') calculated at the CCSD(T) and CCSD(T)-DK levels.

Molecule	Basis	$\Delta E_{n=D}^b$	$\Delta E_{n=T}^b$	$\Delta E_{SR,HF}^{b,c}$	ΔE_{Val}^d	$\Delta E_{PP,corr}^e$	$\Delta E_{CV,wCVDZ}$	$\Delta E_{CV,awCVDZ}$	$\Delta E_{CV,wCVTZ}$
Cr ₃ O ₈	PP	179.16	184.26	-0.82	183.44	–	+7.14	+9.35	–
W ₃ O ₈	PP	222.70	226.94	-0.25	226.69	-0.45	+2.35	+5.11	+0.92
	DK	–	226.24	–	226.24	–	–	–	–

^a Equation (1): $\Delta E(M_3O_8) = E(MO_2) + 2 E(MO_3) - E(M_3O_8)$. For the core-valence correction for M = W, the metal 4f¹⁴ electrons were correlated at the CCSD(T)-DK level.

^b Geometries from B3LYP/aVDZ-PP.

^c MVD expectation values of the HF/aVTZ-PP wavefunction.

^d $\Delta E_{Val} (PP) = \Delta E_{n=T} (PP) + \Delta E_{SR,HF}$ and $\Delta E_{Val} (DK) = \Delta E_{n=T} (DK)$.

^e $\Delta E_{PP,corr} = \Delta E_{aVTZ-DK} - [\Delta E_{aVTZ-PP} + \Delta E_{SR,HF}]$.

Table S10: Clustering energies^a at 0 K (ΔE_{0K}) and heats of formation^b at 0 and 298 K ($\Delta H_{f,0K}$ and $\Delta H_{f,298K}$) in kcal/mol for the ground states of Cr_3O_8 (3B_2) and W_3O_8 ($^1A'$) calculated at the CCSD(T) or CCSD(T)-DK level, and compared with available experimental data.

	ΔE_{val}^c	ΔE_{CV}^d	ΔE_{ZPE}^e	ΔE_{0K}^f	$\Delta H_{f,0K}^g$	$\Delta H_{f,298K}^h$	Expt. ⁱ
Cr_3O_8	183.44	+7.14	-3.62	187.0	-326.7	-329.9	–
W_3O_8	226.24	+0.92	-2.61	224.6	-383.9	-386.8	-408.7 ± 10

^a Equation (1): $\Delta E(M_3O_8) = E(MO_2) + 2 E(MO_3) - E(M_3O_8)$.

^b Error bars due to errors in the experimental heats of formation of the atoms are ± 3 kcal/mol for Cr_3O_8 and ± 4.5 kcal/mol for W_3O_8 .

^c ΔE_{val} (PP) for Cr_3O_8 and ΔE_{val} (DK) for W_3O_8 from Table S8.

^d CCSD(T)/wCVDZ-PP for Cr_3O_8 and CCSD(T)/wCVTZ-PP for W_3O_8 from Table S8.

^e BP86/aVDZ-PP.

^f $\Delta E_{0K} = \Delta E_{val} + \Delta E_{CV} + \Delta E_{ZPE}$.

^g Equation (2): $\Delta H_{f, 0K} (M_3O_8) = \Delta H_{f, 0K} (MO_2) + 2 \Delta H_{f, 0K} (MO_3) - \Delta E_{0K} (M_3O_8)$, using calculated heats of formation of the monomers from Table S7 for CrO_2 and WO_2 from Ref. 55 for CrO_3 and WO_3 (-61.4 and -78.5 kcal/mol respectively) and calculated clustering energies.

^h $\Delta H_{f,298K} [(MO_m)_n] = \Delta H_{f,0K} [(MO_m)_n] + \Delta H_{0K \rightarrow 298K} [(MO_m)_n] - n \Delta H_{0K \rightarrow 298K} (M) - n^*m \Delta H_{0K \rightarrow 298K} (O)$. $\Delta H_{0K \rightarrow 298K}$ is 1.04 kcal/mol for O, 0.97 kcal/mol for Cr, 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.

ⁱ Ref. 56.

Table S11: Zero-point energies (ZPE) at the BP86/aVDZ level, electronic energies (E_e) at the B3LYP/aVTZ, BP86/aVTZ, PW91/aVTZ, CCSD(T)/aVDZ, CCSD(T)/aVTZ levels, core-valence corrections (ΔE_{cv}) at the CCSD(T)/awCVDZ level, and T_1 diagnostics for Cr_3O_8 and its anion. All energies are shown in Hartree.

State	ZPE ^a	E_e^b	E_e^c	E_e^d	E_e^e	ΔE_e^f	ΔE_{cv}^g	T_1^h
<i>Cr₃O₈</i>								
(¹ A ₁ <i>a</i>) / C _{2v} (A)	0.02908	-861.83829	-862.23021	-862.00575	-858.89588	-859.45363	-1.35344	0.061
(¹ A ₁ <i>b</i>) / C _{2v} (A)	0.02966	-861.84556	-862.24054	-862.01636	-858.89194	-859.45005	-1.36018	0.057
³ B ₂ / C _{2v} (A)	0.02930	-861.89176	-862.25529	-862.03120	-858.90200	-859.45927	-1.36194	0.049
³ A ₁ / C _{2v} (A)	0.02742	-861.85326	-862.23047	-862.00612	-858.87977	-859.43534	-1.36166	0.048
(³ A ₂ <i>a</i>) / C _{2v} (A)	0.02760	-861.84600	-862.23544	-862.01165	-858.87432	–	–	0.046
(³ A ₂ <i>b</i>) / C _{2v} (A)	0.02746	-861.83192	-862.21690	-861.99307	-858.85786	–	–	0.046
(³ B ₁ <i>a</i>) / C _{2v} (A)	0.02930	-861.84906	-862.23141	-862.00760	-858.86931	–	–	0.045
(³ B ₁ <i>b</i>) / C _{2v} (A)	0.02802	-861.82449	-862.21265	-861.98881	-858.85432	–	–	0.050
(³ A ₁ <i>b</i>) / C _{2v} (A)	0.02567	-861.79685	-862.18140	-861.95721	-858.83049	–	–	0.048
⁵ A ₂ / C _{2v} (A)	0.02625	-861.82989	-862.17999	-861.95550	-858.82637	-859.38177	-1.36052	0.053
⁵ A ₁ / C _{2v} (A)	0.02543	-861.80755	-862.16095	-861.93647	-858.80408	-859.35898	-1.36049	0.057
⁵ B ₂ / C _{2v} (A)	0.02733	-861.79655	-862.15802	-861.93360	-858.80697	-859.36027	-1.35980	0.057
⁵ B ₁ / C _{2v} (A)	0.02821	-861.79190	-862.14778	-861.92332	-858.79247	-859.34677	-1.36127	0.061
(¹ A' <i>a</i>) / C _{2v} (B)	0.02891	-861.84439	-862.21386	-861.98818	-858.86094	-859.41907	–	0.049
(¹ A' <i>b</i>) / C _{2v} (B)	0.02791	-861.82443	-862.19599	-861.97098	-858.84001	-859.39786	–	0.049
³ A'' / C _s (B)	0.02867	-861.87225	-862.23371	-862.00952	-858.89080	–	–	0.047
³ A' / C _s (B)	0.02764	-861.84144	-862.20688	-861.98247	-858.85244	–	–	0.050

$(^3A' b) / C_s (B)$	0.02668	-861.80894	-862.18229	-861.95862	-858.82553	–	–	0.047
$^1A / C_2 (C)$	0.02898	-861.80037	-861.80037	-861.96670	-858.84166	–	–	0.053
$^3B / C_2 (C)$	0.02733	-861.80913	-861.80913	-861.94422	-858.82841	–	–	0.051
$^1A_1 / D_{2d} (D)$	0.02942	-861.83154	-862.22760	-862.00214	-858.85999	–	–	0.066
$^3B_2 / D_{2d} (D)$	0.02858	-861.86649	-862.23988	-862.01481	-858.88113	-859.43586	-1.36185	0.050
$^3A_2 / D_{2d} (D)$	0.02850	-861.85294	-862.22667	-862.00221	-858.86567	–	–	0.050
$^3B_1 / D_{2d} (D)$	0.03041	-861.86091	-862.21832	–	-858.87039	–	–	0.047
$Cr_3O_8^-$								
$^2A_1 / C_{2v} (A)$	0.02885	-862.01909	-862.38952	-862.16351	-859.05026	-859.60962	-1.36020	0.054
$(^2A_2 a) / C_{2v} (A)$	0.02856	-861.99437	-862.38232	-862.15659	-859.02581	–	–	0.051
$(^2A_2 b) / C_{2v} (A)$	0.02641	-861.97548	-862.36207	-862.13584	-859.01814	–	–	0.059
$^4B_2 / C_{2v} (A)$	0.02819	-862.05908	-862.05908	-862.17318	-859.05602	–	–	0.048
$^4B_1 / C_{2v} (A)$	0.02767	-862.04242	-862.04242	-862.17231	-859.04179	–	–	0.049
$^4A_2 / C_{2v} (A)$	0.02770	-862.01814	-862.01814	-862.14954	-859.01999	–	–	0.050
$^2A' / C_s (B)$	0.02807	-861.98931	-862.36699	-862.36699	-862.36699	–	–	0.125
$(^2A'' a) / C_s (B)$	0.02806	-862.00446	-862.36996	-862.36996	-862.36996	–	–	0.049
$(^2A' b) / C_s (B)$	0.02906	-861.99187	-862.35433	-862.35433	-862.35433	–	–	0.052
$(^2A'' b) / C_s (B)$	0.02860	-861.96512	-862.36908	-862.36908	-862.36908	–	–	0.046
$^4A' / C_s (B)$	0.02703	-862.02440	-862.37833	-862.15240	-859.02751	–	–	0.046
$^4A'' / C_s (B)$	0.02629	-862.01291	-862.37272	-862.14696	-859.01584	–	–	0.053
$^2A / C_2 (C)$	0.02703	-861.97833	-862.34733	-862.12009	-859.00415	–	–	0.049

$^2B / C_2 (C)$	0.02590	-861.96500	-862.33968	-862.11239	-858.98988	–	–	0.111
$^4B / C_2 (C)$	0.02561	-861.98022	-862.33162	-862.10316	-858.98416	–	–	0.052
$^2A_1 / D_{2d} (D)$	0.02779	-862.02423	-862.39617	-862.16889	-859.02185	–	–	0.069
$^4B_2 / D_{2d} (D)$	0.02717	-862.04109	-862.38965	-862.16276	-859.04273	-859.59885	-1.36131	0.049
$^4A_2 / D_{2d} (D)$	0.02804	-862.03729	-862.40244	-862.17646	-859.03506	-859.59298	-1.36180	0.048
<i>Cr₃O₈ over Cr₃O₈[–]</i>								
$(^1A_1 a) \text{ over } ^2A_1 (A)$	–	-861.72927	-862.12825	-861.90202	-858.83095	-859.38023	-1.33785	0.076
$(^1A_1 b) \text{ over } ^2A_1 (A)$	–	-861.82414	-862.22845	-862.00419	-858.87169	-859.42820	-1.36006	0.058
$^3B_2 \text{ over } ^4B_2 (A)$	–	-861.86929	-862.24335	-862.01919	-858.88431	-859.43993	-1.36119	0.052
$^3A_1 \text{ over } ^4B_2 (A)$	–	-861.83705	-862.21712	-861.99267	-858.86631	-859.42184	-1.36083	0.052
$(^3A_2 a) \text{ over } ^4B_2 (A)$	–	-861.80621	-862.20641	-861.98242	-858.83698	–	–	0.051
$(^3A_2 b) \text{ over } ^4B_2 (A)$	–	-861.80400	-862.19632	-861.97228	-858.83576	–	–	0.048
$(^3B_1 a) \text{ over } ^4B_2 (A)$	–	-861.82040	-862.21208	-861.98808	-858.84576	–	–	0.047
$(^3B_2 b) \text{ over } ^4B_2 (A)$	–	-861.80421	-862.19394	-861.96982	-858.82694	–	–	0.058
$(^3A_1 b) \text{ over } ^4B_2 (A)$	–	-861.79685	-862.17324	-861.94888	-858.82101	–	–	0.050
$^3B_2 \text{ over } ^4B_1 (A)$	–	-861.88011	-862.24864	-862.02442	-858.89389	-859.44986	-1.36148	0.053
$^3A_1 \text{ over } ^4B_1 (A)$	–	-861.78633	-862.19267	-861.96792	-858.81077	-859.36688	-1.35945	0.069
$^3B_2 \text{ over } ^2A_1 (A)$	–	-861.83035	-862.20903	-861.98427	-858.84527	-859.40089	-1.36240	0.053
$^3A_1 \text{ over } ^2A_1 (A)$	–	-861.83841	-862.21846	-861.99390	-858.86734	-859.42298	-1.36251	0.051
$^5A_2 \text{ over } ^4B_2 (A)$	–	-861.82105	-862.17687	-861.95234	-858.81346	-859.36709	-1.36129	0.056
$^3A_2 \text{ over } ^4B_2 (A)$	–	-861.82071	-862.17636	-861.95198	–	–	–	–

5A_1 over 4B_2 (A)	–	-861.79869	-862.15793	-861.93344	-858.79612	-859.34901	-1.36098	0.067
5B_2 over 4B_2 (A)	–	-861.79349	-862.15691	-861.93249	-858.80353	-859.35711	-1.36003	0.059
5B_1 over 4B_2 (A)	–	-861.78011	-862.14011	-861.91559	-858.78316	-859.33656	-1.36162	0.071
3B_1 over 4B_2 (A)	–	-861.78318	-862.13990	-861.91552	–	–	–	–
$^3A''$ over ($^2A' a$) (B)	–	-861.86097	-862.22608	-862.00171	-858.88232	–	–	0.052
3B_2 over 4B_2 (D)	–	-861.84046	-862.23077	-862.00564	-858.86595	-859.41920	-1.36001	0.059
3B_2 over 4A_2 (D)	–	-861.84111	-862.23079	-862.00541	-858.86549	-859.41894	-1.36012	0.058
<i>Cr₃O₈ over Cr₃O₈</i>								
3A_1 over 3B_2 (A)	–	-861.80705	-862.20155	-861.97699	-858.82926	–	–	0.057
($^3A_2 a$) over 3B_2 (A)	–	-861.82707	-862.21910	-861.99516	-858.85603	–	–	0.047
($^3A_2 b$) over 3B_2 (A)	–	-861.82534	-862.21106	-861.98712	-858.85267	–	–	0.045
($^3B_1 a$) over 3B_2 (A)	–	-861.84413	-862.22779	-862.00390	-858.86563	–	–	0.045
($^3B_2 b$) over 3B_2 (A)	–	-861.81348	-862.20344	-861.97943	-858.84402	–	–	0.054
5A_2 over 3B_2 (A)	–	-861.81982	-862.17284	-861.94831	–	–	–	–
$^3A'$ over $^3A''$ (B)	–	-861.82913	-862.19340	-861.96856	-858.83963	–	–	0.048
($^3A' b$) over $^3A''$ (B)	–	-861.78422	-862.16447	-861.93952	–	–	–	–
3A_2 over 3B_2 (D)	–	-861.85255	-862.22247	-861.99814	-858.86619	–	–	0.050
3B_1 over 3B_2 (D)	–	-861.86078	–	–	-858.87047	–	–	0.047

^a BP86/aVDZ. ^b B3LYP/aVTZ. ^c BP86/aVTZ. ^d PW91/aVTZ. ^e CCSD(T)/aVDZ. ^f CCSD(T)/aVTZ. ^g CCSD(T)/awCVDZ.

^h from CCSD(T)/aVTZ (from CCSD(T)/aVDZ when CCSD(T)/aVTZ is not available).

Table S12: Zero-point energies (ZPE) at the BP86/aVDZ level, electronic energies (E_e) at the B3LYP/aVTZ, BP86/aVTZ, PW91/aVTZ, CCSD(T)/aVDZ, CCSD(T)/aVTZ levels, core-valence corrections (ΔE_{CV}) at the CCSD(T)/awCVDZ level, and T_1 diagnostics for W_3O_8 and its anion. All energies are shown in Hartree.

State	ZPE ^a	E_e^b	E_e^c	E_e^d	E_e^e	ΔE_e^f	ΔE_{CV}^g	T_1^h
W_3O_8								
$^1A_1 / C_{2v} (A)$	0.02651	-805.02802	-805.38705	-805.11505	-801.99054	-802.58375	-1.00746	0.030
$(^1A_1 b) / C_{2v} (A)$	0.02594	-805.00117	-805.35634	-805.08353	-801.96857	-802.56289	–	0.030
$^3B_2 / C_{2v} (A)$	0.02602	-805.03020	-805.37655	-805.10352	-801.98121	-802.57395	-1.00658	0.033
$^3A_2 / C_{2v} (A)$	0.02430	-805.00388	-805.36381	-805.09092	-801.95913	–	–	0.031
$^3A_1 / C_{2v} (A)$	0.02452	-804.99384	-805.35696	-805.08476	-801.95079	–	–	0.033
$^1A' / C_s (B)$	0.02673	-805.05092	-805.40295	-805.12974	-802.00197	-802.59774	-1.00546	0.031
$^3A_2 / C_{2v} (B)$	0.02576	-805.04099	-805.38142	-805.10766	-801.98546	-802.58067	-1.00347	0.029
$^3A' / C_s (B)$	0.02554	-804.99927	-805.35491	-805.08147	-801.94382	–	–	0.035
$^1A_1 / C_{2v} (C)$	0.02576	-805.03461	-805.38780	-805.11354	-801.98822	-802.58283	-1.00438	0.030
$^3A_1 / C_{2v} (C)$	0.02545	-804.94280	-805.30982	-805.03471	-801.89100	-802.48373	-1.00457	0.033
$(^3B_2 a) / C_{2v} (C)$	0.02437	-804.98406	-805.32552	-805.04981	-801.92135	-802.51826	-1.00187	0.031
$(^3B_2 b) / C_{2v} (C)$	0.02328	-804.90269	-805.28470	-805.01075	-801.84599	-802.43590	-1.00780	0.039
$(^3B_1 a) / C_{2v} (C)$	0.02381	-804.92153	-805.29538	-805.02141	-801.87212	-802.46153	-1.00778	0.036
$(^3B_1 b) / C_{2v} (C)$	0.02690	-804.90053	-805.26510	-804.99085	-801.84358	–	–	0.036
$^3A_2 / C_{2v} (C)$	0.02245	-804.92234	-805.29955	-805.02555	-801.86830	-802.45839	-1.00805	0.033
$^1A_1 / D_{2d} (D)$	0.02569	-804.98837	-805.35218	-805.07806	-801.93983	-802.53163	-1.00580	0.042

${}^3B_2 / D_{2d} (D)$	0.02487	-805.00063	-805.36179	-805.08765	-801.94867	-802.53895	–	0.044
${}^3A_2 / D_{2d} (D)$	0.02511	-804.98830	-805.34072	-805.06720	-801.93240	–	–	0.036
$W_3O_8^-$								
${}^2A_1 / C_{2v} (A)$	0.02518	-805.12805	-805.48950	-805.21580	-802.08593	-802.67755	–	0.033
${}^4B_2 / C_{2v} (A)$	0.02413	-805.12756	-805.46918	-805.19356	-802.07363	-802.66544	–	0.034
${}^4B_1 / C_{2v} (A)$	0.02369	-805.12040	-805.47142	-805.19638	-802.06568	–	–	0.037
${}^2A' / C_s (B)$	0.02622	-805.17426	-805.53020	-805.25539	-802.12433	-802.72020	–	0.034
${}^2A'' / C_s (B)$	0.02563	-805.17135	-805.52500	-805.25019	-802.11931	-802.71516	–	0.031
${}^4A'' / C_s (B)$	0.02524	-805.13708	-805.48893	-805.21383	-802.08123	–	–	0.033
${}^2A_1 / C_{2v} (C)$	0.02567	-805.17769	-805.53676	-805.26121	-802.12662	-802.72051	-1.00829	0.030
${}^2A_1 / D_{2d} (D)$	0.02464	-805.12375	-805.12375	-805.21045	-802.07367	-802.66467	–	0.043
${}^4A_2 / D_{2d} (D)$	0.02424	-805.13529	-805.13529	-805.21014	-802.08084	-802.67102	–	0.034
$W_3O_8^{2-}$								
${}^1A_1 / C_{2v} (C)$	0.02544	-805.17515	-805.53422	-805.25710	-802.12775	-802.72168	-1.01089	0.029
W_3O_8 over $W_3O_8^-$								
${}^1A'$ over ${}^2A' (B)$	–	-805.02476	-805.38470	-805.11145	-801.98721	-802.57896	-1.00771	0.032
${}^1A'$ over ${}^2A'' (B)$	–	-805.02624	-805.38258	-805.10914	-801.98653	-802.57821	-1.00721	0.032
3A_2 over ${}^2A' (B)$	–	-804.95439	-805.31276	-805.03904	-801.90864	–	–	0.035
3A_2 over ${}^2A'' (B)$	–	-804.99420	-805.34622	-805.07251	-801.94955	–	–	0.033
1A_1 over ${}^2A_1 (C)$	–	-805.00648	-805.36570	-805.09154	-801.96811	-802.55861	-1.00672	0.032
3A_1 over ${}^2A_1 (C)$	–	-804.92929	-805.29814	-805.02414	-801.88377	-802.47421	-1.00629	0.036

$(^3B_2 a)$ over $^2A_1 (C)$	–	-804.84903	-805.21443	-804.93936	-801.80034	–	–	0.038
$(^3B_2 b)$ over $^2A_1 (C)$	–	-804.90165	-805.28356	-805.00968	-801.83819	-802.42786	-1.00768	0.044
$(^1B_2 b)$ over $^2A_1 (C)$	–	-804.89876	-805.28193	-805.00801	–	–	–	–
$(^3B_1 a)$ over $^2A_1 (C)$	–	-804.91707	-805.28593	-805.00369	-801.85895	-802.44882	-1.00799	0.042
$(^1B_1 a)$ over $^2A_1 (C)$	–	-804.91660	-805.20679	-804.92730	–	–	–	–
$(^3B_1 b)$ over $^2A_1 (C)$	–	-804.86447	-805.23591	-804.96169	-801.81330	–	–	0.040
3A_2 over $^2A_1 (C)$	–	-804.91905	-805.29825	-805.02423	-801.86503	-802.45486	-1.00794	0.033
1A_2 over $^2A_1 (C)$	–	-804.91848	-805.29768	-805.02365	–	–	–	–
W_3O_8 over W_3O_8								
3A_2 over $^1A_1 (A)$	–	-804.97361	-805.33414	-805.06104	-801.92959	–	–	0.031
3A_1 over $^1A_1 (A)$	–	-804.95877	-805.32515	-805.05194	-801.91239	–	–	0.035
3B_2 over $^1A_1 (A)$	–	-804.94126	-805.29096	-805.01728	-801.89496	–	–	0.034
3A_2 over $^1A' (B)$	–	-805.01012	-805.34705	-805.07313	-801.95671	–	–	0.032
$^3A'$ over $^2A'' (B)$	–	-804.98934	-805.34156	-805.06787	-801.93243	–	–	0.035
3A_1 over $^1A_1 (C)$	–	-804.92817	-805.29086	-805.01653	-801.87370	–	–	0.034
$(^3B_2 a)$ over $^1A_1 (C)$	–	-804.90184	-805.25774	-804.98254	-801.84816	–	–	0.036
$(^3B_2 b)$ over $^1A_1 (C)$	–	-804.88220	-805.26376	-804.98951	-801.82893	–	–	0.080
$(^3B_1 a)$ over $^1A_1 (C)$	–	-804.90255	-805.27437	-805.00607	-801.84111	–	–	0.032
$(^3B_1 b)$ over $^1A_1 (C)$	–	-804.88961	-805.25355	-804.97934	-801.83073	–	–	0.036
3A_2 over $^1A_1 (C)$	–	-804.90561	-805.28203	-805.00768	-801.84432	–	–	0.033

^a BP86/aVDZ. ^b B3LYP/aVTZ. ^c BP86/aVTZ. ^d PW91/aVTZ. ^e CCSD(T)/aVDZ. ^f CCSD(T)/aVTZ. ^g CCSD(T)/awCVDZ.

^h from CCSD(T)/aVTZ (from CCSD(T)/aVDZ when CCSD(T)/aVTZ is not available).

Table S13: Equilibrium Geometries Optimized at the B3LYP/aVDZ Level.

$\text{Cr}_3\text{O}_8, ({}^1\text{A}_1 \text{a}) / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(15\text{b}_2)^2$

CR	0.000000	1.301323	-0.986855
CR	0.000000	-1.301323	-0.986855
O	1.112920	0.000000	-1.429718
O	-1.112920	0.000000	-1.429718
O	0.000000	1.392608	0.775418
O	0.000000	2.520234	-1.937869
O	0.000000	-1.392608	0.775418
O	0.000000	-2.520234	-1.937869
CR	0.000000	0.000000	1.865794
O	1.280738	0.000000	2.754044
O	-1.280738	0.000000	2.754044

$\text{Cr}_3\text{O}_8, ({}^1\text{A}_1 \text{b}) / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(22\text{a}_1)^2$

CR	0.000000	1.170037	-0.969377
CR	0.000000	-1.170037	-0.969377
O	1.331461	0.000000	-1.046335
O	-1.331461	0.000000	-1.046335
O	0.000000	1.502271	0.757724
O	0.000000	2.243974	-2.086636
O	0.000000	-1.502271	0.757724
O	0.000000	-2.243974	-2.086636
CR	0.000000	0.000000	1.752541
O	1.264882	0.000000	2.654567
O	-1.264882	0.000000	2.654567

$\text{Cr}_3\text{O}_8, {}^3\text{B}_2 / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(15\text{b}_2)^1(22\text{a}_1)^1$

CR	0.000000	1.286632	-0.982671
CR	0.000000	-1.286632	-0.982671
O	1.193623	0.000000	-1.309770
O	-1.193623	0.000000	-1.309770
O	0.000000	1.436810	0.783025
O	0.000000	2.473147	-1.980717
O	0.000000	-1.436810	0.783025
O	0.000000	-2.473147	-1.980717
CR	0.000000	0.000000	1.823616
O	1.272497	0.000000	2.720049
O	-1.272497	0.000000	2.720049

$\text{Cr}_3\text{O}_8, {}^3\text{A}_1 / \text{C}_{2v}(\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(23a_1)^1$

CR	0.000000	1.218016	-0.984452
CR	0.000000	-1.218016	-0.984452
O	1.272790	0.000000	-1.225585
O	-1.272790	0.000000	-1.225585
O	0.000000	1.536137	0.636544
O	0.000000	2.423024	-1.966745
O	0.000000	-1.536137	0.636544
O	0.000000	-2.423024	-1.966745
CR	0.000000	0.000000	1.878623
O	1.344026	0.000000	2.691209
O	-1.344026	0.000000	2.691209

$\text{Cr}_3\text{O}_8, ({}^3\text{B}_1 \text{a}) / \text{C}_{2v}(\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(6a_2)^1$

CR	0.000000	1.292314	-1.009424
CR	0.000000	-1.292314	-1.009424
O	1.173776	0.000000	-1.375481
O	-1.173776	0.000000	-1.375481
O	0.000000	1.412833	0.770448
O	0.000000	2.613977	-1.830034
O	0.000000	-1.412833	0.770448
O	0.000000	-2.613977	-1.830034
CR	0.000000	0.000000	1.823514
O	1.272083	0.000000	2.728068
O	-1.272083	0.000000	2.728068

$\text{Cr}_3\text{O}_8, ({}^3\text{A}_2 \text{a}) / \text{C}_{2v}(\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(6a_2)^1$

CR	0.000000	1.230104	-1.004663
CR	0.000000	-1.230104	-1.004663
O	1.275434	0.000000	-1.154596
O	-1.275434	0.000000	-1.154596
O	0.000000	1.471692	0.756549
O	0.000000	2.504081	-1.896489
O	0.000000	-1.471692	0.756549
O	0.000000	-2.504081	-1.896489
CR	0.000000	0.000000	1.758955
O	1.264784	0.000000	2.670091
O	-1.264784	0.000000	2.670091

$\text{Cr}_3\text{O}_8, (^3\text{A}_2 \text{ } \mathbf{b}) / \text{C}_{2v} (\mathbf{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(13b_1)^1$

CR	0.000000	1.291957	-1.004807
CR	0.000000	-1.291957	-1.004807
O	1.165624	0.000000	-1.437933
O	-1.165624	0.000000	-1.437933
O	0.000000	1.394843	0.770307
O	0.000000	2.618327	-1.817979
O	0.000000	-1.394843	0.770307
O	0.000000	-2.618327	-1.817979
CR	0.000000	0.000000	1.842327
O	1.278117	0.000000	2.736535
O	-1.278117	0.000000	2.736535

$\text{Cr}_3\text{O}_8, (^3\text{B}_1 \text{ } \mathbf{b}) / \text{C}_{2v} (\mathbf{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(13b_1)^1$

CR	0.000000	1.253838	-1.003497
CR	0.000000	-1.253838	-1.003497
O	1.268916	0.000000	-1.234320
O	-1.268916	0.000000	-1.234320
O	0.000000	1.452729	0.757867
O	0.000000	2.554250	-1.858397
O	0.000000	-1.452729	0.757867
O	0.000000	-2.554250	-1.858397
CR	0.000000	0.000000	1.778010
O	1.271720	0.000000	2.678325
O	-1.271720	0.000000	2.678325

$\text{Cr}_3\text{O}_8, (^3\text{A}_1 \text{ } \mathbf{b}) / \text{C}_{2v} (\mathbf{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(16b_2)^1$

CR	0.000000	1.286632	-0.982671
CR	0.000000	-1.286632	-0.982671
O	1.193623	0.000000	-1.309770
O	-1.193623	0.000000	-1.309770
O	0.000000	1.436810	0.783025
O	0.000000	2.473147	-1.980717
O	0.000000	-1.436810	0.783025
O	0.000000	-2.473147	-1.980717
CR	0.000000	0.000000	1.823616
O	1.272497	0.000000	2.720049
O	-1.272497	0.000000	2.720049

$\text{Cr}_3\text{O}_8, {}^5\text{A}_2 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.282549	-0.996346
CR	0.000000	-1.282549	-0.996346
O	1.197426	0.000000	-1.331391
O	-1.197426	0.000000	-1.331391
O	0.000000	1.432555	0.767244
O	0.000000	2.476228	-1.989747
O	0.000000	-1.432555	0.767244
O	0.000000	-2.476228	-1.989747
CR	0.000000	0.000000	1.848026
O	1.338898	0.000000	2.770892
O	-1.338898	0.000000	2.770892

$\text{Cr}_3\text{O}_8, {}^5\text{A}_1 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(21a_1)^2(11b_1)^2(12b_1)^2(14b_2)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.277507	-0.999915
CR	0.000000	-1.277507	-0.999915
O	1.196974	0.000000	-1.345588
O	-1.196974	0.000000	-1.345588
O	0.000000	1.396785	0.767265
O	0.000000	2.483712	-1.978114
O	0.000000	-1.396785	0.767265
O	0.000000	-2.483712	-1.978114
CR	0.000000	0.000000	1.907929
O	1.430679	0.000000	2.694290
O	-1.430679	0.000000	2.694290

$\text{Cr}_3\text{O}_8, {}^5\text{B}_2 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(11b_1)^2(12b_1)^2(21a_1)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.293057	-0.979835
CR	0.000000	-1.293057	-0.979835
O	1.206165	0.000000	-1.286213
O	-1.206165	0.000000	-1.286213
O	0.000000	1.503266	0.673354
O	0.000000	2.481592	-2.054463
O	0.000000	-1.503266	0.673354
O	0.000000	-2.481592	-2.054463
CR	0.000000	0.000000	1.918176
O	1.347031	0.000000	2.729564
O	-1.347031	0.000000	2.729564

$\text{Cr}_3\text{O}_8, {}^5\text{B}_1 / \text{C}_{2v} (\mathbf{A}), \dots (10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(5a_2)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.283239	-0.997704
CR	0.000000	-1.283239	-0.997704
O	1.191693	0.000000	-1.335714
O	-1.191693	0.000000	-1.335714
O	0.000000	1.452330	0.791610
O	0.000000	2.453646	-2.014656
O	0.000000	-1.452330	0.791610
O	0.000000	-2.453646	-2.014656
CR	0.000000	0.000000	1.890401
O	1.386814	0.000000	2.716270
O	-1.386814	0.000000	2.716270

$\text{Cr}_3\text{O}_8, ({}^1\text{A}'\mathbf{a}) / \text{C}_s (\mathbf{B}), \dots (31a')^2$

CR	-0.779379	0.016304	1.579556
CR	1.924867	0.122661	0.000000
CR	-0.779379	0.016304	-1.579556
O	-1.346840	0.978528	2.663557
O	-1.167331	-1.452324	1.926790
O	0.972023	0.153081	1.483298
O	-1.421020	0.472835	0.000000
O	3.406994	-0.297214	0.000000
O	-1.346840	0.978528	-2.663557
O	0.972023	0.153081	-1.483298
O	-1.167331	-1.452324	-1.926790

$\text{Cr}_3\text{O}_8, ({}^1\text{A}'\mathbf{b}) / \text{C}_s (\mathbf{B}), \dots (23a'')^2$

CR	-0.787230	0.033560	1.541001
CR	1.903203	0.024137	0.000000
CR	-0.787230	0.033560	-1.541001
O	-1.482841	0.719656	2.755261
O	-0.896048	-1.526865	1.632508
O	0.901737	0.468419	1.434117
O	-1.461779	0.574676	0.000000
O	3.429855	-0.170866	0.000000
O	-1.482841	0.719656	-2.755261
O	0.901737	0.468419	-1.434117
O	-0.896048	-1.526865	-1.632508

$\text{Cr}_3\text{O}_8, {}^3\text{A}'' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (23a'')^1$

CR	-0.794014	0.028420	1.557928
CR	1.965639	0.060911	0.000000
CR	-0.794014	0.028420	-1.557928
O	-1.413965	0.872362	2.711088
O	-1.118964	-1.484642	1.768325
O	0.934422	0.260986	1.461716
O	-1.427923	0.566459	0.000000
O	3.492106	-0.217123	0.000000
O	-1.413965	0.872362	-2.711088
O	0.934422	0.260986	-1.461716
O	-1.118964	-1.484642	-1.768325

$\text{Cr}_3\text{O}_8, {}^3\text{A}' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (32a')^1$

CR	-0.769163	0.002749	1.559675
CR	1.985108	0.336661	0.000000
CR	-0.769163	0.002749	-1.559675
O	-1.438578	0.825255	2.701119
O	-0.950105	-1.524682	1.817335
O	0.936173	0.390834	1.436237
O	-1.464660	0.446588	0.000000
O	3.029333	-0.855881	0.000000
O	-1.438578	0.825255	-2.701119
O	0.936173	0.390834	-1.436237
O	-0.950105	-1.524682	-1.817335

$\text{Cr}_3\text{O}_8, ({}^3\text{A}' \mathbf{b}) / \text{C}_s (\mathbf{B}), \dots (23a'')^1 (24a'')^1$

CR	-0.829013	0.016168	1.643075
CR	1.886566	-0.034469	0.000000
CR	-0.829013	0.016168	-1.643075
O	-1.450633	0.984275	2.704737
O	-0.999426	-1.514293	1.959412
O	1.023830	0.303478	1.418384
O	-1.275230	0.444892	0.000000
O	3.442065	0.014590	0.000000
O	-1.450633	0.984275	-2.704737
O	1.023830	0.303478	-1.418384
O	-0.999426	-1.514293	-1.959412

$\text{Cr}_3\text{O}_8, {}^1\text{A} / \text{C}_2 (\text{C}), \dots (27a)^2$

CR	-0.470750	1.181807	-0.944289
CR	0.470750	-1.181807	-0.944289
CR	0.000000	0.000000	1.809857
O	-1.956439	0.815111	-1.252438
O	0.209159	2.018311	-2.068129
O	0.000000	1.401702	0.729251
O	1.956439	-0.815111	-1.252438
O	-0.209159	-2.018311	-2.068129
O	-1.267955	-0.027307	2.709398
O	0.000000	-1.401702	0.729251
O	1.267955	0.027307	2.709398

$\text{Cr}_3\text{O}_8, {}^3\text{B} / \text{C}_2 (\text{C}), \dots (27a)^1 (27b)^1$

CR	-0.631533	2.143806	-0.890426
CR	0.631533	-2.143806	-0.890426
CR	0.000000	0.000000	1.610837
O	-1.364155	1.216546	-1.929745
O	-1.047809	3.657755	-0.912047
O	0.000000	1.422799	0.591561
O	1.364155	-1.216546	-1.929745
O	1.047809	-3.657755	-0.912047
O	-1.275602	-0.015355	2.505254
O	0.000000	-1.422799	0.591561
O	1.275602	0.015355	2.505254

$\text{Cr}_3\text{O}_8, {}^1\text{A}_1 / \text{D}_{2d} (\text{D}), \dots (12b_2)^2$

O	0.000000	1.220792	1.240471
O	0.000000	-1.220792	1.240471
O	-1.220792	0.000000	-1.240471
O	1.220792	0.000000	-1.240471
O	0.000000	-1.298872	-3.422287
O	1.298872	0.000000	3.422287
O	-1.298872	0.000000	3.422287
O	0.000000	1.298872	-3.422287
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.555932
CR	0.000000	0.000000	2.555932

$\text{Cr}_3\text{O}_8, {}^3\text{B}_2 / \text{D}_{2d} (\mathbf{D}), \dots (12b_2)^1 (12a_1)^1$

O	0.000000	1.225203	1.299873
O	0.000000	-1.225203	1.299873
O	-1.225203	0.000000	-1.299873
O	1.225203	0.000000	-1.299873
O	0.000000	-1.291327	-3.459519
O	1.291327	0.000000	3.459519
O	-1.291327	0.000000	3.459519
O	0.000000	1.291327	-3.459519
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.583616
CR	0.000000	0.000000	2.583616

$\text{Cr}_3\text{O}_8, {}^3\text{A}_2 / \text{D}_{2d} (\mathbf{D}), \dots (12b_2)^1 (3b_1)^1$

O	0.000000	1.211344	1.307602
O	0.000000	-1.211344	1.307602
O	-1.211344	0.000000	-1.307602
O	1.211344	0.000000	-1.307602
O	0.000000	-1.287795	-3.478397
O	1.287795	0.000000	3.478397
O	-1.287795	0.000000	3.478397
O	0.000000	1.287795	-3.478397
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.596633
CR	0.000000	0.000000	2.596633

$\text{Cr}_3\text{O}_8, {}^3\text{B}_1 / \text{D}_{2d} (\mathbf{D}), \dots (12a_1)^1 (3b_1)^1$

O	0.000000	1.219851	1.306370
O	0.000000	-1.219851	1.306370
O	-1.219851	0.000000	-1.306370
O	1.219851	0.000000	-1.306370
O	0.000000	-1.285387	-3.478318
O	1.285387	0.000000	3.478318
O	-1.285387	0.000000	3.478318
O	0.000000	1.285387	-3.478318
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.595329
CR	0.000000	0.000000	2.595329

$\text{Cr}_3\text{O}_8^-, {}^2\text{A}_1 / \text{C}_{2v}(\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^2(23a_1)^1$

CR	0.000000	1.156646	-0.971041
CR	0.000000	-1.156646	-0.971041
O	1.351386	0.000000	-1.107281
O	-1.351386	0.000000	-1.107281
O	0.000000	1.538250	0.677437
O	0.000000	2.259768	-2.100439
O	0.000000	-1.538250	0.677437
O	0.000000	-2.259768	-2.100439
CR	0.000000	0.000000	1.847354
O	1.352336	0.000000	2.672375
O	-1.352336	0.000000	2.672375

$\text{Cr}_3\text{O}_8^-, ({}^2\text{A}_2 \text{a}) / \text{C}_{2v}(\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^2(6a_2)^1$

CR	0.000000	1.155053	-1.011207
CR	0.000000	-1.155053	-1.011207
O	1.356161	0.000000	-1.019918
O	-1.356161	0.000000	-1.019918
O	0.000000	1.462483	0.803809
O	0.000000	2.290387	-2.103733
O	0.000000	-1.462483	0.803809
O	0.000000	-2.290387	-2.103733
CR	0.000000	0.000000	1.769994
O	1.277228	0.000000	2.698472
O	-1.277228	0.000000	2.698472

$\text{Cr}_3\text{O}_8^-, ({}^2\text{A}_2 \text{b}) / \text{C}_{2v}(\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^2(6a_2)^1$

CR	0.000000	1.313759	-1.013996
CR	0.000000	-1.313759	-1.013996
O	1.128401	0.000000	-1.417817
O	-1.128401	0.000000	-1.417817
O	0.000000	1.384115	0.809040
O	0.000000	2.627371	-1.895058
O	0.000000	-1.384115	0.809040
O	0.000000	-2.627371	-1.895058
CR	0.000000	0.000000	1.852546
O	1.292442	0.000000	2.767004
O	-1.292442	0.000000	2.767004

Cr_3O_8^- , ${}^4\text{B}_2 / \text{C}_{2v}(\text{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.283344	-0.989625
CR	0.000000	-1.283344	-0.989625
O	1.207095	0.000000	-1.342597
O	-1.207095	0.000000	-1.342597
O	0.000000	1.471072	0.703227
O	0.000000	2.515611	-1.973971
O	0.000000	-1.471072	0.703227
O	0.000000	-2.515611	-1.973971
CR	0.000000	0.000000	1.905673
O	1.360804	0.000000	2.723707
O	-1.360804	0.000000	2.723707

Cr_3O_8^- , ${}^4\text{B}_1 / \text{C}_{2v}(\text{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(6a_2)^1$

CR	0.000000	1.294301	-1.019500
CR	0.000000	-1.294301	-1.019500
O	1.217768	0.000000	-1.287832
O	-1.217768	0.000000	-1.287832
O	0.000000	1.417260	0.820499
O	0.000000	2.576553	-1.947920
O	0.000000	-1.417260	0.820499
O	0.000000	-2.576553	-1.947920
CR	0.000000	0.000000	1.821131
O	1.284872	0.000000	2.742056
O	-1.284872	0.000000	2.742056

Cr_3O_8^- , ${}^4\text{A}_2 / \text{C}_{2v}(\text{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(13b_1)^1$

CR	0.000000	1.303668	-1.012387
CR	0.000000	-1.303668	-1.012387
O	1.209845	0.000000	-1.380888
O	-1.209845	0.000000	-1.380888
O	0.000000	1.400531	0.821957
O	0.000000	2.605515	-1.913114
O	0.000000	-1.400531	0.821957
O	0.000000	-2.605515	-1.913114
CR	0.000000	0.000000	1.840486
O	1.290326	0.000000	2.748477
O	-1.290326	0.000000	2.748477

$\text{Cr}_3\text{O}_8^-, {}^2\text{A}' / \text{C}_s (\mathbf{B}), \dots (23a'')^2(31a')^1$

CR	-0.789114	0.033852	1.592943
CR	1.858767	-0.052153	0.000000
CR	-0.789114	0.033852	-1.592943
O	-1.406311	0.891934	2.767727
O	-1.062918	-1.520697	1.719678
O	0.969484	0.314953	1.474758
O	-1.269570	0.612068	0.000000
O	3.427443	-0.031102	0.000000
O	-1.406311	0.891934	-2.767727
O	0.969484	0.314953	-1.474758
O	-1.062918	-1.520697	-1.719678

$\text{Cr}_3\text{O}_8^-, ({}^2\text{A}'' \mathbf{a}) / \text{C}_s (\mathbf{B}), \dots (31a')^2(23a'')^1$

CR	-0.804675	0.015976	1.649004
CR	1.894599	0.030105	0.000000
CR	-0.804675	0.015976	-1.649004
O	-1.297962	1.132377	2.654074
O	-1.246946	-1.450175	2.042167
O	1.012113	0.054583	1.486666
O	-1.249445	0.437174	0.000000
O	3.459289	-0.096915	0.000000
O	-1.297962	1.132377	-2.654074
O	1.012113	0.054583	-1.486666
O	-1.246946	-1.450175	-2.042167

$\text{Cr}_3\text{O}_8^-, ({}^2\text{A}' \mathbf{b}) / \text{C}_s (\mathbf{B}), \dots (31a')^2(32a')^1$

CR	-0.806904	-0.000006	1.608360
CR	1.928978	0.000056	0.000000
CR	-0.806904	-0.000006	-1.608360
O	-1.219638	1.314413	2.382264
O	-1.219687	-1.314416	2.382249
O	1.009491	-0.000046	1.460108
O	-1.583251	0.000053	0.000000
O	3.497412	-0.000088	0.000000
O	-1.219638	1.314413	-2.382264
O	1.009491	-0.000046	-1.460108
O	-1.219687	-1.314416	-2.382249

$\text{Cr}_3\text{O}_8^-, (^2\text{A}'' \mathbf{b}) / \text{C}_s(\mathbf{B}), \dots (23a'')^2(24a'')^1$

CR	-0.795704	-0.006294	1.623594
CR	1.868922	0.100360	0.000000
CR	-0.795704	-0.006294	-1.623594
O	-1.568732	0.845192	2.714845
O	-0.779239	-1.572680	1.888628
O	0.912038	0.531126	1.450126
O	-1.357966	0.378618	0.000000
O	3.397289	-0.249210	0.000000
O	-1.568732	0.845192	-2.714845
O	0.912038	0.531126	-1.450126
O	-0.779239	-1.572680	-1.888628

$\text{Cr}_3\text{O}_8^-, ^4\text{A}' / \text{C}_s(\mathbf{B}), \dots (23a'')^1(31a')^1(24a'')^1$

CR	-0.655125	0.079763	1.686775
CR	1.530184	-0.220642	0.000000
CR	-0.655125	0.079763	-1.686775
O	-0.582059	1.255461	2.744503
O	-1.900895	-0.874664	1.871876
O	0.853419	-0.841305	1.579612
O	-0.391528	0.710854	0.000000
O	2.990796	0.393510	0.000000
O	-0.582059	1.255461	-2.744503
O	0.853419	-0.841305	-1.579612
O	-1.900895	-0.874664	-1.871876

$\text{Cr}_3\text{O}_8^-, ^4\text{A}'' / \text{C}_s(\mathbf{B}), \dots (31a')^1(23a'')^1(32a')^1$

CR	-0.803719	0.022543	1.578329
CR	1.932700	-0.014316	0.000000
CR	-0.803719	0.022543	-1.578329
O	-1.403118	0.951726	2.708484
O	-0.980437	-1.521311	1.897350
O	0.928355	0.396751	1.401036
O	-1.580323	0.343028	0.000000
O	3.514937	-0.089667	0.000000
O	-1.403118	0.951726	-2.708484
O	0.928355	0.396751	-1.401036
O	-0.980437	-1.521311	-1.897350

$\text{Cr}_3\text{O}_8^-, {}^2\text{A} / \text{C}_2(\text{C}), \dots (27a)^2(28a)^1$

CR	-0.531815	1.148653	-0.979807
CR	0.531815	-1.148653	-0.979807
CR	0.000000	0.000000	1.926895
O	-2.042158	0.765562	-1.217967
O	0.092632	2.068245	-2.097605
O	0.000000	1.360779	0.611638
O	2.042158	-0.765562	-1.217967
O	-0.092632	-2.068245	-2.097605
O	-1.352495	-0.040236	2.753013
O	0.000000	-1.360779	0.611638
O	1.352495	0.040236	2.753013

$\text{Cr}_3\text{O}_8^-, {}^2\text{B} / \text{C}_2(\text{C}), \dots (27a)^2(27b)^1$

CR	-0.457473	1.310308	-0.963542
CR	0.457473	-1.310308	-0.963542
CR	0.000000	0.000000	1.793600
O	-1.993955	1.122607	-1.287851
O	0.388899	2.156866	-1.997969
O	0.000000	1.410282	0.783769
O	1.993955	-1.122607	-1.287851
O	-0.388899	-2.156866	-1.997969
O	-1.285739	-0.017632	2.702278
O	0.000000	-1.410282	0.783769
O	1.285739	0.017632	2.702278

$\text{Cr}_3\text{O}_8^-, {}^4\text{B} / \text{C}_2(\text{C}), \dots (27a)^1(27b)^1(28a)^1$

CR	-0.334510	2.758768	-0.741825
CR	0.334510	-2.758768	-0.741825
CR	0.000000	0.000000	1.415365
O	-1.824867	3.240933	-1.019975
O	0.850519	3.624471	-1.359044
O	0.000000	1.391819	0.221334
O	1.824867	-3.240933	-1.019975
O	-0.850519	-3.624471	-1.359044
O	-1.339988	-0.009509	2.260111
O	0.000000	-1.391819	0.221334
O	1.339988	0.009509	2.260111

$\text{Cr}_3\text{O}_8^-, {}^2\text{A}_1 / \text{D}_{2d}(\boldsymbol{D}), \dots(12b_2)^2(12a_1)^1$

O	0.000000	1.222458	1.203740
O	0.000000	-1.222458	1.203740
O	-1.222458	0.000000	-1.203740
O	1.222458	0.000000	-1.203740
O	0.000000	-1.360667	-3.457551
O	1.360667	0.000000	3.457551
O	-1.360667	0.000000	3.457551
O	0.000000	1.360667	-3.457551
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.638537
CR	0.000000	0.000000	2.638537

$\text{Cr}_3\text{O}_8^-, {}^4\text{B}_2 / \text{D}_{2d}(\boldsymbol{D}), \dots(12b_2)^1(12a_1)^1(13a_1)^1$

O	0.000000	1.241695	1.178515
O	0.000000	-1.241695	1.178515
O	-1.241695	0.000000	-1.178515
O	1.241695	0.000000	-1.178515
O	0.000000	-1.358941	-3.434751
O	1.358941	0.000000	3.434751
O	-1.358941	0.000000	3.434751
O	0.000000	1.358941	-3.434751
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.614764
CR	0.000000	0.000000	2.614764

$\text{Cr}_3\text{O}_8^-, {}^4\text{A}_2 / \text{D}_{2d}(\boldsymbol{D}), \dots(12b_2)^1(12a_1)^1(3b_1)^1$

O	0.000000	1.238457	1.180743
O	0.000000	-1.238457	1.180743
O	-1.238457	0.000000	-1.180743
O	1.238457	0.000000	-1.180743
O	0.000000	-1.351955	-3.443586
O	1.351955	0.000000	3.443586
O	-1.351955	0.000000	3.443586
O	0.000000	1.351955	-3.443586
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.613578
CR	0.000000	0.000000	2.613578

$W_3O_8, {}^1A_1 / C_{2v} (A), \dots (22a_1)^2$

W	0.000000	1.269885	-1.036105
W	0.000000	-1.269885	-1.036105
O	1.469973	0.000000	-0.988555
O	-1.469973	0.000000	-0.988555
O	0.000000	1.593342	0.864564
O	0.000000	2.291494	-2.402471
O	0.000000	-1.593342	0.864564
O	0.000000	-2.291494	-2.402471
W	0.000000	0.000000	1.974286
O	-1.376506	0.000000	2.979356
O	1.376506	0.000000	2.979356

$W_3O_8, ({}^1A_1 \mathbf{b}) / C_{2v} (A), \dots (15b_2)^2$

W	0.000000	1.475930	-1.058271
W	0.000000	-1.475930	-1.058271
O	1.123555	0.000000	-1.539359
O	-1.123555	0.000000	-1.539359
O	0.000000	1.489743	0.873804
O	0.000000	2.774726	-2.156437
O	0.000000	-1.489743	0.873804
O	0.000000	-2.774726	-2.156437
W	0.000000	0.000000	2.066261
O	-1.396177	0.000000	3.054543
O	1.396177	0.000000	3.054543

$W_3O_8, {}^3B_2 / C_{2v} (A), \dots (15b_2)^1 (22a_1)^1$

W	0.000000	1.464751	-1.048401
W	0.000000	-1.464751	-1.048401
O	1.206688	0.000000	-1.442297
O	-1.206688	0.000000	-1.442297
O	0.000000	1.528676	0.870330
O	0.000000	2.769989	-2.144445
O	0.000000	-1.528676	0.870330
O	0.000000	-2.769989	-2.144445
W	0.000000	0.000000	2.030035
O	-1.387087	0.000000	3.025211
O	1.387087	0.000000	3.025211

$W_3O_8, {}^3A_2 / C_{2v} (A), \dots (22a_1)^1(6a_2)^1$

W	0.000000	1.405727	-1.056684
W	0.000000	-1.405727	-1.056684
O	1.328478	0.000000	-1.200533
O	-1.328478	0.000000	-1.200533
O	0.000000	1.565049	0.853444
O	0.000000	2.836324	-1.991659
O	0.000000	-1.565049	0.853444
O	0.000000	-2.836324	-1.991659
W	0.000000	0.000000	1.973209
O	-1.375746	0.000000	2.986982
O	1.375746	0.000000	2.986982

$W_3O_8, {}^3A_1 / C_{2v} (A), \dots (22a_1)^1(23a_1)^1$

W	0.000000	1.365021	-0.953068
W	0.000000	-1.365021	-0.953068
O	1.341241	0.000000	-1.288919
O	-1.341241	0.000000	-1.288919
O	0.000000	1.779540	0.828165
O	0.000000	2.672016	-2.060096
O	0.000000	-1.779540	0.828165
O	0.000000	-2.672016	-2.060096
W	0.000000	0.000000	1.850779
O	-1.446170	0.000000	2.776875
O	1.446170	0.000000	2.776875

$W_3O_8, {}^1A' / C_s (B), \dots (31a')^2$

W	-0.806502	0.019854	1.711637
W	-0.806502	0.019854	-1.711637
W	1.818608	-0.155138	0.000000
O	-1.633987	-1.072077	2.731365
O	-0.910924	1.573831	2.404201
O	-1.655773	-0.026683	0.000000
O	1.047434	-0.580581	1.642342
O	-0.910924	1.573831	-2.404201
O	-1.633987	-1.072077	-2.731365
O	1.047434	-0.580581	-1.642342
O	2.748895	1.252064	0.000000

$W_3O_8, {}^3A_2 / C_{2v} (B), \dots (21a_1)^1 (8a_2)^1$

W	0.000000	1.776576	-0.948820
W	0.000000	-1.776576	-0.948820
W	0.000000	0.000000	2.094264
O	-1.386468	2.638260	-1.456023
O	1.386468	2.638260	-1.456023
O	0.000000	0.000000	-1.640554
O	0.000000	1.545161	0.928807
O	1.386468	-2.638260	-1.456023
O	-1.386468	-2.638260	-1.456023
O	0.000000	-1.545161	0.928807
O	0.000000	0.000000	3.788256

$W_3O_8, {}^3A' / C_s (B), \dots (31a')^1 (32a')^1$

W	0.820735	-0.184289	1.722541
W	0.820735	-0.184289	-1.722541
W	-1.794393	0.531588	0.000000
O	1.723870	0.730649	2.848334
O	0.820735	-1.817141	2.217177
O	1.647998	-0.019694	0.000000
O	-1.004611	0.476583	1.715264
O	0.820735	-1.817141	-2.217177
O	1.723870	0.730649	-2.848334
O	-1.004611	0.476583	-1.715264
O	-3.313459	-0.268330	0.000000

$W_3O_8, {}^1A_1 / C_{2v} (C), \dots (14b_2)^2 (11b_1)^2 (8a_2)^2 (12b_1)^2 (19a_1)^2$

W	0.000000	1.451135	-1.047733
W	0.000000	-1.451135	-1.047733
W	0.000000	0.000000	2.059219
O	-1.405802	1.949425	-1.875481
O	1.405802	1.949425	-1.875481
O	0.000000	1.490639	0.861094
O	1.405802	-1.949425	-1.875481
O	-1.405802	-1.949425	-1.875481
O	-1.382956	0.000000	3.057510
O	0.000000	-1.490639	0.861094
O	1.382956	0.000000	3.057510

$W_3O_8, {}^3A_1 / C_{2v} (C), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^1(20a_1)^1$

W	0.000000	1.482225	-1.016531
W	0.000000	-1.482225	-1.016531
W	0.000000	0.000000	1.920313
O	-1.416206	2.212857	-1.640486
O	1.416206	2.212857	-1.640486
O	0.000000	1.628842	0.881098
O	1.416206	-2.212857	-1.640486
O	-1.416206	-2.212857	-1.640486
O	-1.382410	0.000000	2.921338
O	0.000000	-1.628842	0.881098
O	1.382410	0.000000	2.921338

$W_3O_8, ({}^3B_2 a) / C_{2v} (C), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^1(15b_2)^1$

W	0.000000	3.216391	-0.656229
W	0.000000	-3.216391	-0.656229
W	0.000000	0.000000	1.376802
O	-1.405896	3.682894	-1.507625
O	1.405896	3.682894	-1.507625
O	0.000000	1.574517	0.328792
O	1.405896	-3.682894	-1.507625
O	-1.405896	-3.682894	-1.507625
O	-1.375622	0.000000	2.388868
O	0.000000	-1.574517	0.328792
O	1.375622	0.000000	2.388868

$W_3O_8, ({}^3B_2 b) / C_{2v} (C), \dots (11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(14b_2)^1(20a_1)^1$

W	0.000000	1.403525	-0.949579
W	0.000000	-1.403525	-0.949579
W	0.000000	0.000000	1.843767
O	-1.435240	1.869124	-1.767064
O	1.435240	1.869124	-1.767064
O	0.000000	1.689977	0.976623
O	1.435240	-1.869124	-1.767064
O	-1.435240	-1.869124	-1.767064
O	-1.457036	0.000000	2.813692
O	0.000000	-1.689977	0.976623
O	1.457036	0.000000	2.813692

$W_3O_8, (^3B_1 \mathbf{a}) / C_{2v} (\mathbf{C}), \dots (14b_2)^2(11b_1)^2(8a_2)^2(19a_1)^2(12b_1)^1(20a_1)^1$

W	0.000000	1.409943	-0.956432
W	0.000000	-1.409943	-0.956432
W	0.000000	0.000000	1.827273
O	-1.427367	1.892403	-1.766123
O	1.427367	1.892403	-1.766123
O	0.000000	1.679004	0.997309
O	1.427367	-1.892403	-1.766123
O	-1.427367	-1.892403	-1.766123
O	-1.389949	0.000000	2.930796
O	0.000000	-1.679004	0.997309
O	1.389949	0.000000	2.930796

$W_3O_8, (^3B_1 \mathbf{b}) / C_{2v} (\mathbf{C}), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^1(13b_1)^1$

W	0.000000	1.480830	-1.062274
W	0.000000	-1.480830	-1.062274
W	0.000000	0.000000	2.055324
O	-1.361855	2.242968	-1.785002
O	1.361855	2.242968	-1.785002
O	0.000000	1.471418	0.836443
O	1.361855	-2.242968	-1.785002
O	-1.361855	-2.242968	-1.785002
O	-1.382713	0.000000	3.053722
O	0.000000	-1.471418	0.836443
O	1.382713	0.000000	3.053722

$W_3O_8, ^3A_2 / C_{2v} (\mathbf{C}), \dots (14b_2)^2(11b_1)^2(12b_1)^2(19a_1)^2(8a_2)^1(20a_1)^1$

W	0.000000	1.379673	-0.974533
W	0.000000	-1.379673	-0.974533
W	0.000000	0.000000	1.900009
O	-1.464197	1.858193	-1.782599
O	1.464197	1.858193	-1.782599
O	0.000000	1.667368	0.897202
O	1.464197	-1.858193	-1.782599
O	-1.464197	-1.858193	-1.782599
O	-1.388040	0.000000	2.894885
O	0.000000	-1.667368	0.897202
O	1.388040	0.000000	2.894885

$W_3O_8, {}^1A_1 / D_{2d}(\mathbf{D}), \dots(12b_2)^2$

O	0.000000	1.282783	1.369533
O	0.000000	-1.282783	1.369533
O	-1.282783	0.000000	-1.369533
O	1.282783	0.000000	-1.369533
O	0.000000	-1.418887	-3.841870
O	1.418887	0.000000	3.841870
O	-1.418887	0.000000	3.841870
O	0.000000	1.418887	-3.841870
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.882432
W	0.000000	0.000000	2.882432

$W_3O_8, {}^3B_2 / D_{2d}(\mathbf{D}), \dots(12b_2)^1(12a_1)^1$

O	0.000000	1.301579	1.372559
O	0.000000	-1.301579	1.372559
O	-1.301579	0.000000	-1.372559
O	1.301579	0.000000	-1.372559
O	0.000000	-1.411723	-3.836696
O	1.411723	0.000000	3.836696
O	-1.411723	0.000000	3.836696
O	0.000000	1.411723	-3.836696
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.870183
W	0.000000	0.000000	2.870183

$W_3O_8, {}^3A_2 / D_{2d}(\mathbf{D}), \dots(12b_2)^1(3b_1)^1$

O	0.000000	1.267088	1.448718
O	0.000000	-1.267088	1.448718
O	-1.267088	0.000000	-1.448718
O	1.267088	0.000000	-1.448718
O	0.000000	-1.410338	-3.884125
O	1.410338	0.000000	3.884125
O	-1.410338	0.000000	3.884125
O	0.000000	1.410338	-3.884125
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.909586
W	0.000000	0.000000	2.909586

$W_3O_8^-, ^2A_1 / C_{2v} (A), \dots (22a_1)^2(23a_1)^1$

W	0.000000	1.252240	-0.962857
W	0.000000	-1.252240	-0.962857
O	1.511225	0.000000	-1.041675
O	-1.511225	0.000000	-1.041675
O	0.000000	1.742059	0.857962
O	0.000000	2.292879	-2.358454
O	0.000000	-1.742059	0.857962
O	0.000000	-2.292879	-2.358454
W	0.000000	0.000000	1.866041
O	-1.446505	0.000000	2.818153
O	1.446505	0.000000	2.818153

$W_3O_8^-, ^4B_2 / C_{2v} (A), \dots (22a_1)^1(15b_2)^1(23a_1)^1$

W	0.000000	1.445231	-1.117796
W	0.000000	-1.445231	-1.117796
O	1.208088	0.000000	-1.622851
O	-1.208088	0.000000	-1.622851
O	0.000000	1.454905	0.725203
O	0.000000	2.900052	-2.056548
O	0.000000	-1.454905	0.725203
O	0.000000	-2.900052	-2.056548
W	0.000000	0.000000	2.194468
O	-1.446212	0.000000	3.144391
O	1.446212	0.000000	3.144391

$W_3O_8^-, ^4B_1 / C_{2v} (A), \dots (22a_1)^1(15b_2)^1(6a_2)^1$

W	0.000000	1.487557	-1.061700
W	0.000000	-1.487557	-1.061700
O	1.224443	0.000000	-1.371563
O	-1.224443	0.000000	-1.371563
O	0.000000	1.524658	0.905502
O	0.000000	2.906208	-2.059542
O	0.000000	-1.524658	0.905502
O	0.000000	-2.906208	-2.059542
W	0.000000	0.000000	2.012458
O	-1.394243	0.000000	3.038713
O	1.394243	0.000000	3.038713

$W_3O_8^-, {}^2A' / C_s (B), \dots (31a')^2(32a')^1$

W	0.168459	-0.771549	1.562333
W	0.168459	-0.771549	-1.562333
W	-0.295288	1.742818	0.000000
O	1.650393	-1.172543	2.356066
O	-1.193707	-1.285735	2.490516
O	0.171251	-1.885449	0.000000
O	0.168459	1.196718	1.722375
O	-1.193707	-1.285735	-2.490516
O	1.650393	-1.172543	-2.356066
O	0.168459	1.196718	-1.722375
O	-1.806613	2.561153	0.000000

$W_3O_8^-, {}^2A'' / C_s (B), \dots (31a')^2(23a'')^1$

W	0.751493	0.009086	1.654063
W	0.751493	0.009086	-1.654063
W	-1.714364	-0.084933	0.000000
O	0.751493	1.451958	2.595296
O	1.690213	-1.198320	2.462180
O	1.685698	0.298469	0.000000
O	-1.008201	-0.783469	1.656910
O	1.690213	-1.198320	-2.462180
O	0.751493	1.451958	-2.595296
O	-1.008201	-0.783469	-1.656910
O	-2.597464	1.378729	0.000000

$W_3O_8^-, {}^4A'' / C_s (B), \dots (31a')^1(23a'')^1(32a')^1$

W	-0.833524	0.019380	1.672838
W	-0.833524	0.019380	-1.672838
W	1.842534	-0.088448	0.000000
O	-1.698144	-1.098814	2.671432
O	-0.888772	1.593460	2.375921
O	-1.784538	0.056999	0.000000
O	0.963927	-0.615450	1.678838
O	-0.888772	1.593460	-2.375921
O	-1.698144	-1.098814	-2.671432
O	0.963927	-0.615450	-1.678838
O	3.407271	0.644229	0.000000

$W_3O_8^-, ^2A_1 / C_{2v} (C), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(20a_1)^1$

W	0.000000	1.403510	-0.963801
W	0.000000	-1.403510	-0.963801
W	0.000000	0.000000	1.863125
O	-1.445795	1.923638	-1.749319
O	1.445795	1.923638	-1.749319
O	0.000000	1.694059	0.937580
O	1.445795	-1.923638	-1.749319
O	-1.445795	-1.923638	-1.749319
O	-1.406388	0.000000	2.859269
O	0.000000	-1.694059	0.937580
O	1.406388	0.000000	2.859269

$W_3O_8^-, ^2A_1 / D_{2d} (D), \dots (12b_2)^2(12a_1)^1$

O	0.000000	1.327040	1.374839
O	0.000000	-1.327040	1.374839
O	-1.327040	0.000000	-1.374839
O	1.327040	0.000000	-1.374839
O	0.000000	-1.441586	-3.801325
O	1.441586	0.000000	3.801325
O	-1.441586	0.000000	3.801325
O	0.000000	1.441586	-3.801325
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.842059
W	0.000000	0.000000	2.842059

$W_3O_8^-, ^4A_2 / D_{2d} (D), \dots (12b_2)^1(12a_1)^1(3b_1)^1$

O	0.000000	1.298308	1.530649
O	0.000000	-1.298308	1.530649
O	-1.298308	0.000000	-1.530649
O	1.298308	0.000000	-1.530649
O	0.000000	-1.428742	-3.891841
O	1.428742	0.000000	3.891841
O	-1.428742	0.000000	3.891841
O	0.000000	1.428742	-3.891841
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.906717
W	0.000000	0.000000	2.906717

$\text{W}_3\text{O}_8^{2-}, {}^1\text{A}_1 / \text{C}_{2v}(\mathbf{C}), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(20a_1)^2$

W	0.000000	1.359356	-0.920239
W	0.000000	-1.359356	-0.920239
W	0.000000	0.000000	1.761060
O	-1.480274	1.912074	-1.665547
O	1.480274	1.912074	-1.665547
O	0.000000	1.773017	0.970461
O	1.480274	-1.912074	-1.665547
O	-1.480274	-1.912074	-1.665547
O	-1.457050	0.000000	2.727946
O	0.000000	-1.773017	0.970461
O	1.457050	0.000000	2.727946

Table S14: Equilibrium Geometries Optimized at the BP86/aVDZ Level.

$\text{Cr}_3\text{O}_8, ({}^1\text{A}_1 \text{a}) / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(15\text{b}_2)^2$

CR	0.000000	1.310516	-0.986396
CR	0.000000	-1.310516	-0.986396
O	1.117828	0.000000	-1.438314
O	-1.117828	0.000000	-1.438314
O	0.000000	1.410451	0.778088
O	0.000000	2.545490	-1.949053
O	0.000000	-1.410451	0.778088
O	0.000000	-2.545490	-1.949053
CR	0.000000	0.000000	1.868716
O	1.300196	0.000000	2.765392
O	-1.300196	0.000000	2.765392

$\text{Cr}_3\text{O}_8, ({}^1\text{A}_1 \text{b}) / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(22\text{a}_1)^2$

CR	0.000000	1.178473	-0.961571
CR	0.000000	-1.178473	-0.961571
O	1.341401	0.000000	-1.036512
O	-1.341401	0.000000	-1.036512
O	0.000000	1.538855	0.761243
O	0.000000	2.268336	-2.090541
O	0.000000	-1.538855	0.761243
O	0.000000	-2.268336	-2.090541
CR	0.000000	0.000000	1.736420
O	1.285282	0.000000	2.645893
O	-1.285282	0.000000	2.645893

$\text{Cr}_3\text{O}_8, {}^3\text{B}_2 / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(15\text{b}_2)^1(22\text{a}_1)^1$

CR	0.000000	1.286726	-0.982368
CR	0.000000	-1.286726	-0.982368
O	1.203147	0.000000	-1.318099
O	-1.203147	0.000000	-1.318099
O	0.000000	1.454366	0.780536
O	0.000000	2.503267	-1.975798
O	0.000000	-1.454366	0.780536
O	0.000000	-2.503267	-1.975798
CR	0.000000	0.000000	1.823120
O	1.293649	0.000000	2.725786
O	-1.293649	0.000000	2.725786

$\text{Cr}_3\text{O}_8, {}^3\text{A}_1 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(23a_1)^1$

CR	0.000000	1.214501	-0.968578
CR	0.000000	-1.214501	-0.968578
O	1.290942	0.000000	-1.218320
O	-1.290942	0.000000	-1.218320
O	0.000000	1.562668	0.669592
O	0.000000	2.425892	-1.975169
O	0.000000	-1.562668	0.669592
O	0.000000	-2.425892	-1.975169
CR	0.000000	0.000000	1.837972
O	1.348498	0.000000	2.672673
O	-1.348498	0.000000	2.672673

$\text{Cr}_3\text{O}_8, ({}^3\text{B}_1 \text{a}) / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(6a_2)^1$

CR	0.000000	1.291664	-1.001641
CR	0.000000	-1.291664	-1.001641
O	1.178768	0.000000	-1.367388
O	-1.178768	0.000000	-1.367388
O	0.000000	1.440063	0.768121
O	0.000000	2.619660	-1.845972
O	0.000000	-1.440063	0.768121
O	0.000000	-2.619660	-1.845972
CR	0.000000	0.000000	1.811940
O	1.286406	0.000000	2.732254
O	-1.286406	0.000000	2.732254

$\text{Cr}_3\text{O}_8, ({}^3\text{A}_2 \text{a}) / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(6a_2)^1$

CR	0.000000	1.231436	-0.994077
CR	0.000000	-1.231436	-0.994077
O	1.287524	0.000000	-1.148687
O	-1.287524	0.000000	-1.148687
O	0.000000	1.503870	0.758955
O	0.000000	2.509601	-1.909735
O	0.000000	-1.503870	0.758955
O	0.000000	-2.509601	-1.909735
CR	0.000000	0.000000	1.741606
O	1.279247	0.000000	2.669289
O	-1.279247	0.000000	2.669289

$\text{Cr}_3\text{O}_8, (^3\text{A}_2 \text{ } \mathbf{b}) / \text{C}_{2v} (\mathbf{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(13b_1)^1$

CR	0.000000	1.294004	-1.002244
CR	0.000000	-1.294004	-1.002244
O	1.172803	0.000000	-1.449221
O	-1.172803	0.000000	-1.449221
O	0.000000	1.413648	0.772774
O	0.000000	2.633542	-1.823460
O	0.000000	-1.413648	0.772774
O	0.000000	-2.633542	-1.823460
CR	0.000000	0.000000	1.840695
O	1.294917	0.000000	2.745596
O	-1.294917	0.000000	2.745596

$\text{Cr}_3\text{O}_8, (^3\text{B}_1 \text{ } \mathbf{b}) / \text{C}_{2v} (\mathbf{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(13b_1)^1$

CR	0.000000	1.252971	-0.996524
CR	0.000000	-1.252971	-0.996524
O	1.279708	0.000000	-1.242020
O	-1.279708	0.000000	-1.242020
O	0.000000	1.480438	0.757456
O	0.000000	2.568271	-1.858382
O	0.000000	-1.480438	0.757456
O	0.000000	-2.568271	-1.858382
CR	0.000000	0.000000	1.769568
O	1.289771	0.000000	2.678166
O	-1.289771	0.000000	2.678166

$\text{Cr}_3\text{O}_8, (^3\text{A}_1 \text{ } \mathbf{b}) / \text{C}_{2v} (\mathbf{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(16b_2)^1$

CR	0.000000	1.313724	-0.984188
CR	0.000000	-1.313724	-0.984188
O	1.160597	0.000000	-1.348229
O	-1.160597	0.000000	-1.348229
O	0.000000	1.572638	0.674104
O	0.000000	2.551498	-1.957428
O	0.000000	-1.572638	0.674104
O	0.000000	-2.551498	-1.957428
CR	0.000000	0.000000	1.897274
O	1.346585	0.000000	2.738206
O	-1.346585	0.000000	2.738206

$\text{Cr}_3\text{O}_8, {}^5\text{A}_2 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.292306	-0.994460
CR	0.000000	-1.292306	-0.994460
O	1.207142	0.000000	-1.371582
O	-1.207142	0.000000	-1.371582
O	0.000000	1.448322	0.748653
O	0.000000	2.518416	-1.979002
O	0.000000	-1.448322	0.748653
O	0.000000	-2.518416	-1.979002
CR	0.000000	0.000000	1.893633
O	1.372835	0.000000	2.744863
O	-1.372835	0.000000	2.744863

$\text{Cr}_3\text{O}_8, {}^5\text{A}_1 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(21a_1)^2(11b_1)^2(12b_1)^2(14b_2)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.270123	-1.019636
CR	0.000000	-1.270123	-1.019636
O	1.210118	0.000000	-1.387620
O	-1.210118	0.000000	-1.387620
O	0.000000	1.390637	0.733370
O	0.000000	2.521250	-1.990951
O	0.000000	-1.390637	0.733370
O	0.000000	-2.521250	-1.990951
CR	0.000000	0.000000	1.958681
O	1.396479	0.000000	2.766089
O	-1.396479	0.000000	2.766089

$\text{Cr}_3\text{O}_8, {}^5\text{B}_2 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(11b_1)^2(12b_1)^2(21a_1)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.285887	-0.980771
CR	0.000000	-1.285887	-0.980771
O	1.219953	0.000000	-1.303231
O	-1.219953	0.000000	-1.303231
O	0.000000	1.489137	0.706750
O	0.000000	2.497353	-2.039899
O	0.000000	-1.489137	0.706750
O	0.000000	-2.497353	-2.039899
CR	0.000000	0.000000	1.902074
O	1.365839	0.000000	2.725582
O	-1.365839	0.000000	2.725582

$\text{Cr}_3\text{O}_8, {}^5\text{B}_1 / \text{C}_{2v}(\mathbf{A}), \dots (10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(5a_2)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.280157	-0.989910
CR	0.000000	-1.280157	-0.989910
O	1.204856	0.000000	-1.341797
O	-1.204856	0.000000	-1.341797
O	0.000000	1.474492	0.804896
O	0.000000	2.466535	-2.024366
O	0.000000	-1.474492	0.804896
O	0.000000	-2.466535	-2.024366
CR	0.000000	0.000000	1.878511
O	1.397909	0.000000	2.713231
O	-1.397909	0.000000	2.713231

$\text{Cr}_3\text{O}_8, ({}^1\text{A}'\mathbf{a}) / \text{C}_s(\mathbf{B}), \dots (31a')^2$

CR	-0.761940	-0.000614	1.576889
CR	1.847260	0.143556	0.000000
CR	-0.761940	-0.000614	-1.576889
O	-1.328799	1.084224	2.574313
O	-1.080625	-1.448930	2.116000
O	1.027674	0.187789	1.517747
O	-1.541997	0.244074	0.000000
O	3.335354	-0.317222	0.000000
O	-1.328799	1.084224	-2.574313
O	1.027674	0.187789	-1.517747
O	-1.080625	-1.448930	-2.116000

$\text{Cr}_3\text{O}_8, ({}^1\text{A}'\mathbf{b}) / \text{C}_s(\mathbf{B}), \dots (23a'')^2$

CR	-0.773833	0.031261	1.555264
CR	1.763195	-0.007291	0.000000
CR	-0.773833	0.031261	-1.555264
O	-1.519526	0.661445	2.797388
O	-0.698688	-1.560044	1.589618
O	0.944007	0.554176	1.443756
O	-1.417083	0.584605	0.000000
O	3.318914	-0.061451	0.000000
O	-1.519526	0.661445	-2.797388
O	0.944007	0.554176	-1.443756
O	-0.698688	-1.560044	-1.589618

$\text{Cr}_3\text{O}_8, {}^3\text{A}'' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (23a'')^1$

CR	-0.783211	0.030324	1.550587
CR	1.910897	0.054652	0.000000
CR	-0.783211	0.030324	-1.550587
O	-1.446040	0.814273	2.748234
O	-1.040104	-1.524250	1.694492
O	0.957820	0.348689	1.478629
O	-1.428289	0.605493	0.000000
O	3.451511	-0.228815	0.000000
O	-1.446040	0.814273	-2.748234
O	0.957820	0.348689	-1.478629
O	-1.040104	-1.524250	-1.694492

$\text{Cr}_3\text{O}_8, {}^3\text{A}' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (32a')^1$

CR	-0.779440	-0.008417	1.569174
CR	2.003765	0.354000	0.000000
CR	-0.779440	-0.008417	-1.569174
O	-1.432361	0.894743	2.689423
O	-0.873467	-1.541335	1.946834
O	0.941254	0.459700	1.367632
O	-1.555645	0.284261	0.000000
O	2.950138	-0.921977	0.000000
O	-1.432361	0.894743	-2.689423
O	0.941254	0.459700	-1.367632
O	-0.873467	-1.541335	-1.946834

$\text{Cr}_3\text{O}_8, ({}^3\text{A}' \mathbf{b}) / \text{C}_s (\mathbf{B}), \dots (23a'')^1 (24a'')^1$

CR	-0.183271	-0.705940	1.565887
CR	0.265226	1.482892	0.000000
CR	-0.183271	-0.705940	-1.565887
O	-0.688517	-1.531539	2.815412
O	1.403260	-0.411835	1.436862
O	-0.688517	1.059639	1.393220
O	-0.782462	-1.294698	0.000000
O	1.033956	2.849132	0.000000
O	-0.688517	-1.531539	-2.815412
O	-0.688517	1.059639	-1.393220
O	1.403260	-0.411835	-1.436862

Cr₃O₈, ¹A / C₂ (C), ... (27a)²

CR	-0.509597	1.170483	-0.938975
CR	0.509597	-1.170483	-0.938975
CR	0.000000	0.000000	1.789944
O	-2.008283	0.749040	-1.201959
O	0.103437	2.050946	-2.092438
O	0.000000	1.428208	0.725709
O	2.008283	-0.749040	-1.201959
O	-0.103437	-2.050946	-2.092438
O	-1.284895	-0.033939	2.700696
O	0.000000	-1.428208	0.725709
O	1.284895	0.033939	2.700696

Cr₃O₈, ³B / C₂ (C), ... (27a)¹(27b)¹

CR	-0.707752	2.003035	-0.920831
CR	0.707752	-2.003035	-0.920831
CR	0.000000	0.000000	1.612747
O	-1.457942	0.937623	-1.829969
O	-1.339156	3.455612	-0.934055
O	0.000000	1.439530	0.592889
O	1.457942	-0.937623	-1.829969
O	1.339156	-3.455612	-0.934055
O	-1.294923	-0.024128	2.514506
O	0.000000	-1.439530	0.592889
O	1.294923	0.024128	2.514506

Cr₃O₈, ¹A₁ / D_{2d} (D), ... (12b₂)²

O	0.000000	1.240230	1.189818
O	0.000000	-1.240230	1.189818
O	-1.240230	0.000000	-1.189818
O	1.240230	0.000000	-1.189818
O	0.000000	-1.324011	-3.417119
O	1.324011	0.000000	3.417119
O	-1.324011	0.000000	3.417119
O	0.000000	1.324011	-3.417119
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.553445
CR	0.000000	0.000000	2.553445

$\text{Cr}_3\text{O}_8, {}^3\text{B}_2 / \text{D}_{2d} (\mathbf{D}), \dots (12\text{b}_2)^1 (12\text{a}_1)^1$

O	0.000000	1.268953	1.199563
O	0.000000	-1.268953	1.199563
O	-1.268953	0.000000	-1.199563
O	1.268953	0.000000	-1.199563
O	0.000000	-1.313557	-3.399942
O	1.313557	0.000000	3.399942
O	-1.313557	0.000000	3.399942
O	0.000000	1.313557	-3.399942
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.522358
CR	0.000000	0.000000	2.522358

$\text{Cr}_3\text{O}_8, {}^3\text{A}_2 / \text{D}_{2d} (\mathbf{D}), \dots (12\text{b}_2)^1 (3\text{b}_1)^1$

O	0.000000	1.228206	1.256491
O	0.000000	-1.228206	1.256491
O	-1.228206	0.000000	-1.256491
O	1.228206	0.000000	-1.256491
O	0.000000	-1.307018	-3.470088
O	1.307018	0.000000	3.470088
O	-1.307018	0.000000	3.470088
O	0.000000	1.307018	-3.470088
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.581011
CR	0.000000	0.000000	2.581011

$\text{Cr}_3\text{O}_8^-, {}^2\text{A}_1 / \text{C}_{2v} (\mathbf{A}), \dots (5\text{a}_2)^2 (10\text{b}_1)^2 (14\text{b}_2)^2 (21\text{a}_1)^2 (11\text{b}_1)^2 (12\text{b}_1)^2 (22\text{a}_1)^2 (23\text{a}_1)^1$

CR	0.000000	1.156259	-0.957280
CR	0.000000	-1.156259	-0.957280
O	1.369737	0.000000	-1.090839
O	-1.369737	0.000000	-1.090839
O	0.000000	1.569730	0.704421
O	0.000000	2.254229	-2.117922
O	0.000000	-1.569730	0.704421
O	0.000000	-2.254229	-2.117922
CR	0.000000	0.000000	1.812677
O	1.359129	0.000000	2.657166
O	-1.359129	0.000000	2.657166

Cr_3O_8^- , (${}^2\text{A}_2 \mathbf{a}$) / $\text{C}_{2v}(\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^2(6a_2)^1$

CR	0.000000	1.168169	-0.994764
CR	0.000000	-1.168169	-0.994764
O	1.361911	0.000000	-1.012558
O	-1.361911	0.000000	-1.012558
O	0.000000	1.506224	0.789097
O	0.000000	2.316158	-2.098503
O	0.000000	-1.506224	0.789097
O	0.000000	-2.316158	-2.098503
CR	0.000000	0.000000	1.744059
O	1.291357	0.000000	2.690167
O	-1.291357	0.000000	2.690167

Cr_3O_8^- , (${}^2\text{A}_2 \mathbf{b}$) / $\text{C}_{2v}(\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^2(6a_2)^1$

CR	0.000000	1.321761	-1.005624
CR	0.000000	-1.321761	-1.005624
O	1.132283	0.000000	-1.422419
O	-1.132283	0.000000	-1.422419
O	0.000000	1.408741	0.793581
O	0.000000	2.636010	-1.911973
O	0.000000	-1.408741	0.793581
O	0.000000	-2.636010	-1.911973
CR	0.000000	0.000000	1.850453
O	1.307757	0.000000	2.782003
O	-1.307757	0.000000	2.782003

Cr_3O_8^- , (${}^4\text{B}_2$) / $\text{C}_{2v}(\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.278741	-0.988467
CR	0.000000	-1.278741	-0.988467
O	1.220146	0.000000	-1.355481
O	-1.220146	0.000000	-1.355481
O	0.000000	1.480387	0.717827
O	0.000000	2.534008	-1.975668
O	0.000000	-1.480387	0.717827
O	0.000000	-2.534008	-1.975668
CR	0.000000	0.000000	1.898320
O	1.370833	0.000000	2.731243
O	-1.370833	0.000000	2.731243

Cr_3O_8^- , ${}^4\text{B}_1 / \text{C}_{2v} (\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(6a_2)^1$

CR	0.000000	1.292026	-1.008967
CR	0.000000	-1.292026	-1.008967
O	1.225005	0.000000	-1.292657
O	-1.225005	0.000000	-1.292657
O	0.000000	1.442663	0.799241
O	0.000000	2.589896	-1.943752
O	0.000000	-1.442663	0.799241
O	0.000000	-2.589896	-1.943752
CR	0.000000	0.000000	1.811365
O	1.301071	0.000000	2.747022
O	-1.301071	0.000000	2.747022

Cr_3O_8^- , ${}^4\text{A}_2 / \text{C}_{2v} (\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(13b_1)^1$

CR	0.000000	1.303762	-1.011433
CR	0.000000	-1.303762	-1.011433
O	1.210909	0.000000	-1.397063
O	-1.210909	0.000000	-1.397063
O	0.000000	1.416731	0.797326
O	0.000000	2.644415	-1.882612
O	0.000000	-1.416731	0.797326
O	0.000000	-2.644415	-1.882612
CR	0.000000	0.000000	1.843937
O	1.317292	0.000000	2.750745
O	-1.317292	0.000000	2.750745

Cr_3O_8^- , ${}^2\text{A}' / \text{C}_s (\mathbf{B})$, ... $(23a'')^2(31a')^1$

CR	-0.786303	0.025851	1.608186
CR	1.824141	-0.036477	0.000000
CR	-0.786303	0.025851	-1.608186
O	-1.431081	0.905297	2.778739
O	-1.013852	-1.552670	1.760779
O	0.995370	0.361925	1.487575
O	-1.262561	0.587977	0.000000
O	3.407081	-0.062756	0.000000
O	-1.431081	0.905297	-2.778739
O	0.995370	0.361925	-1.487575
O	-1.013852	-1.552670	-1.760779

$\text{Cr}_3\text{O}_8^-, (^2A'' a) / C_s (B), \dots (31a')^2(23a'')^1$

CR	0.663646	-0.022480	1.551513
CR	-1.674995	-0.065464	0.000000
CR	0.663646	-0.022480	-1.551513
O	1.513083	-1.184023	2.257779
O	0.663646	1.312175	2.424232
O	-1.019987	-0.675300	1.512107
O	1.479603	0.323009	0.000000
O	-2.749977	1.102557	0.000000
O	1.513083	-1.184023	-2.257779
O	-1.019987	-0.675300	-1.512107
O	0.663646	1.312175	-2.424232

$\text{Cr}_3\text{O}_8^-, (^2A' b) / C_s (B), \dots (31a')^2(32a')^1$

CR	0.701437	-0.137068	1.484770
CR	-1.722332	0.223250	0.000000
CR	0.701437	-0.137068	-1.484770
O	1.106581	-1.510795	2.199630
O	1.106581	1.141072	2.351931
O	-1.136833	-0.178463	1.563462
O	1.687598	-0.071794	0.000000
O	-2.881881	1.320824	0.000000
O	1.106581	-1.510795	-2.199630
O	-1.136833	-0.178463	-1.563462
O	1.106581	1.141072	-2.351931

$\text{Cr}_3\text{O}_8^-, (^2A'' b) / C_s (B), \dots (23a'')^2(24a'')^1$

CR	0.597141	-0.053384	1.736369
CR	-1.374549	0.061320	0.000000
CR	0.597141	-0.053384	-1.736369
O	1.722451	-1.172520	1.936737
O	0.597141	1.113460	2.831816
O	-1.051294	-0.806064	1.513113
O	0.448648	0.630810	0.000000
O	-2.444442	1.235784	0.000000
O	1.722451	-1.172520	-1.936737
O	-1.051294	-0.806064	-1.513113
O	0.597141	1.113460	-2.831816

$$\text{Cr}_3\text{O}_8^-, {}^4\text{A}' / \text{C}_s (\mathbf{B}), \dots (23a'')^1 (31a')^1 (24a'')^1$$

CR	-0.649013	0.084060	1.696425
CR	1.508886	-0.233926	0.000000
CR	-0.649013	0.084060	-1.696425
O	-0.551690	1.270101	2.767155
O	-1.918328	-0.864382	1.906739
O	0.851988	-0.874197	1.577106
O	-0.366119	0.721799	0.000000
O	2.969600	0.412574	0.000000
O	-0.551690	1.270101	-2.767155
O	0.851988	-0.874197	-1.577106
O	-1.918328	-0.864382	-1.906739

$$\text{Cr}_3\text{O}_8^-, {}^4\text{A}'' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (23a'')^1 (32a')^1$$

CR	-0.775488	0.022127	1.571871
CR	1.853907	-0.014022	0.000000
CR	-0.775488	0.022127	-1.571871
O	-1.454886	0.870963	2.744386
O	-0.878567	-1.557677	1.822475
O	0.928893	0.495228	1.442636
O	-1.553435	0.389692	0.000000
O	3.453763	-0.097420	0.000000
O	-1.454886	0.870963	-2.744386
O	0.928893	0.495228	-1.442636
O	-0.878567	-1.557677	-1.822475

$$\text{Cr}_3\text{O}_8^-, {}^2\text{A} / \text{C}_2 (\mathbf{C}), \dots (27a)^2 (28a)^1$$

CR	-0.581030	1.130705	-0.988834
CR	0.581030	-1.130705	-0.988834
CR	0.000000	0.000000	1.928688
O	-2.092581	0.685444	-1.227748
O	0.014189	2.107186	-2.100058
O	0.000000	1.313957	0.620881
O	2.092581	-0.685444	-1.227748
O	-0.014189	-2.107186	-2.100058
O	-1.350577	-0.108374	2.780393
O	0.000000	-1.313957	0.620881
O	1.350577	0.108374	2.780393

$\text{Cr}_3\text{O}_8^-, {}^2\text{B} / \text{C}_2(\text{C}), \dots(27a)^2(27b)^1$

CR	-0.497873	1.243143	-0.941727
CR	0.497873	-1.243143	-0.941727
CR	0.000000	0.000000	1.771560
O	-2.061336	1.038489	-1.191720
O	0.301207	2.020576	-2.083992
O	0.000000	1.445616	0.758999
O	2.061336	-1.038489	-1.191720
O	-0.301207	-2.020576	-2.083992
O	-1.307976	-0.009189	2.684552
O	0.000000	-1.445616	0.758999
O	1.307976	0.009189	2.684552

$\text{Cr}_3\text{O}_8^-, {}^4\text{B} / \text{C}_2(\text{C}), \dots(27a)^1(27b)^1(28a)^1$

CR	-0.363044	2.890637	-0.683148
CR	0.363044	-2.890637	-0.683148
CR	0.000000	0.000000	1.250688
O	-1.875180	3.373999	-0.923541
O	0.826059	3.838686	-1.201141
O	0.000000	1.396692	0.155096
O	1.875180	-3.373999	-0.923541
O	-0.826059	-3.838686	-1.201141
O	-1.324013	-0.010916	2.142997
O	0.000000	-1.396692	0.155096
O	1.324013	0.010916	2.142997

$\text{Cr}_3\text{O}_8^-, {}^2\text{A}_1 / \text{D}_{2d}(\text{D}), \dots(12b_2)^2(12a_1)^1$

O	0.000000	1.287697	1.200355
O	0.000000	-1.287697	1.200355
O	-1.287697	0.000000	-1.200355
O	1.287697	0.000000	-1.200355
O	0.000000	-1.346750	-3.361479
O	1.346750	0.000000	3.361479
O	-1.346750	0.000000	3.361479
O	0.000000	1.346750	-3.361479
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.497172
CR	0.000000	0.000000	2.497172

$\text{Cr}_3\text{O}_8^-, {}^4\text{B}_2 / \text{D}_{2d}(\mathbf{D}), \dots(12b_2)^1(12a_1)^1(13a_1)^1$

O	0.000000	1.242358	1.225896
O	0.000000	-1.242358	1.225896
O	-1.242358	0.000000	-1.225896
O	1.242358	0.000000	-1.225896
O	0.000000	-1.362329	-3.466984
O	1.362329	0.000000	3.466984
O	-1.362329	0.000000	3.466984
O	0.000000	1.362329	-3.466984
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.622300
CR	0.000000	0.000000	2.622300

$\text{Cr}_3\text{O}_8^-, {}^4\text{A}_2 / \text{D}_{2d}(\mathbf{D}), \dots(12b_2)^1(12a_1)^1(3b_1)^1$

O	0.000000	1.268447	1.319862
O	0.000000	-1.268447	1.319862
O	-1.268447	0.000000	-1.319862
O	1.268447	0.000000	-1.319862
O	0.000000	-1.323740	-3.459179
O	1.323740	0.000000	3.459179
O	-1.323740	0.000000	3.459179
O	0.000000	1.323740	-3.459179
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.556884
CR	0.000000	0.000000	2.556884

$\text{W}_3\text{O}_8, {}^1\text{A}_1 / \text{C}_{2v}(\mathbf{A}), \dots(22a_1)^2$

W	0.000000	1.270944	-1.018575
W	0.000000	-1.270944	-1.018575
O	1.482391	0.000000	-0.965712
O	-1.482391	0.000000	-0.965712
O	0.000000	1.640587	0.877592
O	0.000000	2.287205	-2.404794
O	0.000000	-1.640587	0.877592
O	0.000000	-2.287205	-2.404794
W	0.000000	0.000000	1.936995
O	-1.381874	0.000000	2.956132
O	1.381874	0.000000	2.956132

$W_3O_8, ({}^1A_1 \text{ } b) / C_{2v} (A), \dots (15b_2)^2$

W	0.000000	1.477215	-1.052152
W	0.000000	-1.477215	-1.052152
O	1.127637	0.000000	-1.553279
O	-1.127637	0.000000	-1.553279
O	0.000000	1.514422	0.882120
O	0.000000	2.784729	-2.158145
O	0.000000	-1.514422	0.882120
O	0.000000	-2.784729	-2.158145
W	0.000000	0.000000	2.055279
O	-1.402739	0.000000	3.056041
O	1.402739	0.000000	3.056041

$W_3O_8, {}^3B_2 / C_{2v} (A), \dots (15b_2)^1 (22a_1)^1$

W	0.000000	1.461935	-1.041356
W	0.000000	-1.461935	-1.041356
O	1.212525	0.000000	-1.454592
O	-1.212525	0.000000	-1.454592
O	0.000000	1.553078	0.879022
O	0.000000	2.777005	-2.145491
O	0.000000	-1.553078	0.879022
O	0.000000	-2.777005	-2.145491
W	0.000000	0.000000	2.017098
O	-1.394069	0.000000	3.024527
O	1.394069	0.000000	3.024527

$W_3O_8, {}^3A_2 / C_{2v} (A), \dots (22a_1)^1 (6a_2)^1$

W	0.000000	1.406297	-1.043330
W	0.000000	-1.406297	-1.043330
O	1.340730	0.000000	-1.196530
O	-1.340730	0.000000	-1.196530
O	0.000000	1.602671	0.862466
O	0.000000	2.843047	-1.990695
O	0.000000	-1.602671	0.862466
O	0.000000	-2.843047	-1.990695
W	0.000000	0.000000	1.945725
O	-1.379029	0.000000	2.976583
O	1.379029	0.000000	2.976583

$W_3O_8, {}^3A_1 / C_{2v} (A), \dots (22a_1)^1(23a_1)^1$

W	0.000000	1.355742	-0.937475
W	0.000000	-1.355742	-0.937475
O	1.356466	0.000000	-1.304349
O	-1.356466	0.000000	-1.304349
O	0.000000	1.797630	0.856799
O	0.000000	2.681331	-2.046396
O	0.000000	-1.797630	0.856799
O	0.000000	-2.681331	-2.046396
W	0.000000	0.000000	1.816180
O	-1.444362	0.000000	2.765762
O	1.444362	0.000000	2.765762

$W_3O_8, {}^1A' / C_s (B), \dots (31a')^2$

W	-0.779830	0.023675	1.655112
W	-0.779830	0.023675	-1.655112
W	1.780955	-0.157599	0.000000
O	-1.620542	-1.172245	2.566327
O	-0.875233	1.507694	2.515560
O	-1.733163	0.191353	0.000000
O	1.093660	-0.614608	1.662417
O	-0.875233	1.507694	-2.515560
O	-1.620542	-1.172245	-2.566327
O	1.093660	-0.614608	-1.662417
O	2.490403	1.386774	0.000000

$W_3O_8, {}^3A_2 / C_{2v} (B), \dots (21a_1)^1(8a_2)^1$

W	0.000000	1.771088	-0.940690
W	0.000000	-1.771088	-0.940690
W	0.000000	0.000000	2.075529
O	-1.390968	2.647483	-1.453762
O	1.390968	2.647483	-1.453762
O	0.000000	0.000000	-1.659514
O	0.000000	1.569399	0.949435
O	1.390968	-2.647483	-1.453762
O	-1.390968	-2.647483	-1.453762
O	0.000000	-1.569399	0.949435
O	0.000000	0.000000	3.779815

$W_3O_8, {}^3A' / C_s (B), \dots (31a')^1 (32a')^1$

W	0.819670	-0.184841	1.661117
W	0.819670	-0.184841	-1.661117
W	-1.791500	0.524254	0.000000
O	1.698387	0.816636	2.755833
O	0.819670	-1.795433	2.264422
O	1.787551	-0.158181	0.000000
O	-1.043622	0.465616	1.718316
O	0.819670	-1.795433	-2.264422
O	1.698387	0.816636	-2.755833
O	-1.043622	0.465616	-1.718316
O	-3.328938	-0.245253	0.000000

$W_3O_8, {}^1A_1 / C_{2v} (C), \dots (14b_2)^2 (11b_1)^2 (8a_2)^2 (12b_1)^2 (19a_1)^2$

W	0.000000	1.440379	-1.039524
W	0.000000	-1.440379	-1.039524
W	0.000000	0.000000	2.042948
O	-1.409452	1.945798	-1.881241
O	1.409452	1.945798	-1.881241
O	0.000000	1.521350	0.873236
O	1.409452	-1.945798	-1.881241
O	-1.409452	-1.945798	-1.881241
O	-1.387883	0.000000	3.056207
O	0.000000	-1.521350	0.873236
O	1.387883	0.000000	3.056207

$W_3O_8, {}^3A_1 / C_{2v} (C), \dots (14b_2)^2 (11b_1)^2 (8a_2)^2 (12b_1)^2 (19a_1)^1 (20a_1)^1$

W	0.000000	1.475088	-0.992173
W	0.000000	-1.475088	-0.992173
W	0.000000	0.000000	1.869566
O	-1.419372	2.225888	-1.622419
O	1.419372	2.225888	-1.622419
O	0.000000	1.685372	0.894580
O	1.419372	-2.225888	-1.622419
O	-1.419372	-2.225888	-1.622419
O	-1.391941	0.000000	2.881112
O	0.000000	-1.685372	0.894580
O	1.391941	0.000000	2.881112

$W_3O_8, (^3B_2 \mathbf{a}) / C_{2v} (\mathbf{C}), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^1(15b_2)^1$

W	0.000000	3.214393	-0.655563
W	0.000000	-3.214393	-0.655563
W	0.000000	0.000000	1.390508
O	-1.404292	3.595656	-1.569475
O	1.404292	3.595656	-1.569475
O	0.000000	1.590422	0.356201
O	1.404292	-3.595656	-1.569475
O	-1.404292	-3.595656	-1.569475
O	-1.382013	0.000000	2.415603
O	0.000000	-1.590422	0.356201
O	1.382013	0.000000	2.415603

$W_3O_8, (^3B_2 \mathbf{b}) / C_{2v} (\mathbf{C}), \dots (11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(14b_2)^1(20a_1)^1$

W	0.000000	1.388623	-0.945728
W	0.000000	-1.388623	-0.945728
W	0.000000	0.000000	1.841595
O	-1.461576	1.826430	-1.778645
O	1.461576	1.826430	-1.778645
O	0.000000	1.715272	0.949139
O	1.461576	-1.826430	-1.778645
O	-1.461576	-1.826430	-1.778645
O	-1.426016	0.000000	2.838755
O	0.000000	-1.715272	0.949139
O	1.426016	0.000000	2.838755

$W_3O_8, (^3B_1 \mathbf{b}) / C_{2v} (\mathbf{C}), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^1(13b_1)^1$

W	0.000000	1.462587	-1.054331
W	0.000000	-1.462587	-1.054331
W	0.000000	0.000000	2.034675
O	-1.367885	2.244323	-1.776640
O	1.367885	2.244323	-1.776640
O	0.000000	1.505758	0.846951
O	1.367885	-2.244323	-1.776640
O	-1.367885	-2.244323	-1.776640
O	-1.387316	0.000000	3.048522
O	0.000000	-1.505758	0.846951
O	1.387316	0.000000	3.048522

$W_3O_8, {}^1A_1 / D_{2d}(\mathbf{D}), \dots (12b_2)^2$

O	0.000000	1.300854	1.336851
O	0.000000	-1.300854	1.336851
O	-1.300854	0.000000	-1.336851
O	1.300854	0.000000	-1.336851
O	0.000000	-1.426872	-3.849206
O	1.426872	0.000000	3.849206
O	-1.426872	0.000000	3.849206
O	0.000000	1.426872	-3.849206
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.880969
W	0.000000	0.000000	2.880969

$W_3O_8, {}^3B_2 / D_{2d}(\mathbf{D}), \dots (12b_2)^1(12a_1)^1$

O	0.000000	1.323280	1.321805
O	0.000000	-1.323280	1.321805
O	-1.323280	0.000000	-1.321805
O	1.323280	0.000000	-1.321805
O	0.000000	-1.418647	-3.844691
O	1.418647	0.000000	3.844691
O	-1.418647	0.000000	3.844691
O	0.000000	1.418647	-3.844691
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.868533
W	0.000000	0.000000	2.868533

$W_3O_8, {}^3A_2 / D_{2d}(\mathbf{D}), \dots (12b_2)^1(3b_1)^1$

O	0.000000	1.281886	1.420067
O	0.000000	-1.281886	1.420067
O	-1.281886	0.000000	-1.420067
O	1.281886	0.000000	-1.420067
O	0.000000	-1.415804	-3.887672
O	1.415804	0.000000	3.887672
O	-1.415804	0.000000	3.887672
O	0.000000	1.415804	-3.887672
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.899732
W	0.000000	0.000000	2.899732

$W_3O_8^-, ^2A_1 / C_{2v} (A), \dots (22a_1)^2(23a_1)^1$

W	0.000000	1.248755	-0.953772
W	0.000000	-1.248755	-0.953772
O	1.528101	0.000000	-1.030260
O	-1.528101	0.000000	-1.030260
O	0.000000	1.756713	0.882903
O	0.000000	2.279086	-2.374639
O	0.000000	-1.756713	0.882903
O	0.000000	-2.279086	-2.374639
W	0.000000	0.000000	1.843388
O	-1.444376	0.000000	2.818713
O	1.444376	0.000000	2.818713

$W_3O_8^-, ^4B_2 / C_{2v} (A), \dots (22a_1)^1(15b_2)^1(23a_1)^1$

W	0.000000	1.440656	-1.118825
W	0.000000	-1.440656	-1.118825
O	1.216898	0.000000	-1.638618
O	-1.216898	0.000000	-1.638618
O	0.000000	1.464504	0.733203
O	0.000000	2.914249	-2.049981
O	0.000000	-1.464504	0.733203
O	0.000000	-2.914249	-2.049981
W	0.000000	0.000000	2.193048
O	-1.444884	0.000000	3.161676
O	1.444884	0.000000	3.161676

$W_3O_8^-, ^4B_1 / C_{2v} (A), \dots (22a_1)^1(15b_2)^1(6a_2)^1$

W	0.000000	1.486476	-1.055086
W	0.000000	-1.486476	-1.055086
O	1.229819	0.000000	-1.384035
O	-1.229819	0.000000	-1.384035
O	0.000000	1.547463	0.906670
O	0.000000	2.911770	-2.062219
O	0.000000	-1.547463	0.906670
O	0.000000	-2.911770	-2.062219
W	0.000000	0.000000	2.001408
O	-1.399113	0.000000	3.042622
O	1.399113	0.000000	3.042622

$W_3O_8^-, {}^2A' / C_s (B), \dots (31a')^2(32a')^1$

W	0.167367	-0.768030	1.551318
W	0.167367	-0.768030	-1.551318
W	-0.289279	1.740514	0.000000
O	1.658858	-1.174053	2.352857
O	-1.200508	-1.285666	2.494140
O	0.159721	-1.907772	0.000000
O	0.167367	1.207107	1.734462
O	-1.200508	-1.285666	-2.494140
O	1.658858	-1.174053	-2.352857
O	0.167367	1.207107	-1.734462
O	-1.831615	2.521785	0.000000

$W_3O_8^-, {}^2A'' / C_s (B), \dots (31a')^2(23a'')^1$

W	0.126772	-0.726229	1.636320
W	0.126772	-0.726229	-1.636320
W	-0.351966	1.654629	0.000000
O	1.523292	-0.502034	2.643463
O	-0.954193	-1.866116	2.392492
O	0.648577	-1.605207	0.000000
O	-0.954193	0.897464	1.667414
O	-0.954193	-1.866116	-2.392492
O	1.523292	-0.502034	-2.643463
O	-0.954193	0.897464	-1.667414
O	1.032010	2.676496	0.000000

$W_3O_8^-, {}^4A'' / C_s (B), \dots (31a')^1(23a'')^1(32a')^1$

W	-0.812851	0.025340	1.666930
W	-0.812851	0.025340	-1.666930
W	1.796666	-0.093914	0.000000
O	-1.736618	-1.131246	2.587614
O	-0.818818	1.557644	2.487345
O	-1.766867	0.231709	0.000000
O	0.974151	-0.687702	1.680129
O	-0.818818	1.557644	-2.487345
O	-1.736618	-1.131246	-2.587614
O	0.974151	-0.687702	-1.680129
O	3.348023	0.690812	0.000000

$W_3O_8^-, ^2A_1 / C_{2v} (C), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(20a_1)^1$

W	0.000000	1.398768	-0.954259
W	0.000000	-1.398768	-0.954259
W	0.000000	0.000000	1.845532
O	-1.450464	1.921822	-1.754420
O	1.450464	1.921822	-1.754420
O	0.000000	1.718471	0.946496
O	1.450464	-1.921822	-1.754420
O	-1.450464	-1.921822	-1.754420
O	-1.413744	0.000000	2.853656
O	0.000000	-1.718471	0.946496
O	1.413744	0.000000	2.853656

$W_3O_8^-, ^2A_1 / D_{2d} (D), \dots (12b_2)^2(12a_1)^1$

O	0.000000	1.340380	1.347184
O	0.000000	-1.340380	1.347184
O	-1.340380	0.000000	-1.347184
O	1.340380	0.000000	-1.347184
O	0.000000	-1.448736	-3.813159
O	1.448736	0.000000	3.813159
O	-1.448736	0.000000	3.813159
O	0.000000	1.448736	-3.813159
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.845579
W	0.000000	0.000000	2.845579

$W_3O_8^-, ^4A_2 / D_{2d} (D), \dots (12b_2)^1(12a_1)^1(3b_1)^1$

O	0.000000	1.313639	1.476472
O	0.000000	-1.313639	1.476472
O	-1.313639	0.000000	-1.476472
O	1.313639	0.000000	-1.476472
O	0.000000	-1.434610	-3.883065
O	1.434610	0.000000	3.883065
O	-1.434610	0.000000	3.883065
O	0.000000	1.434610	-3.883065
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.887337
W	0.000000	0.000000	2.887337

$\text{W}_3\text{O}_8^{2-}, {}^1\text{A}_1 / \text{C}_{2v}(\mathbf{C}), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(20a_1)^2$

W	0.000000	1.356276	-0.918952
W	0.000000	-1.356276	-0.918952
W	0.000000	0.000000	1.759532
O	-1.488866	1.907242	-1.675689
O	1.488866	1.907242	-1.675689
O	0.000000	1.783166	0.975786
O	1.488866	-1.907242	-1.675689
O	-1.488866	-1.907242	-1.675689
O	-1.464407	0.000000	2.738062
O	0.000000	-1.783166	0.975786
O	1.464407	0.000000	2.738062

Table S15: Equilibrium Geometries Optimized at the PW91/aVDZ Level.

$\text{Cr}_3\text{O}_8, ({}^1\text{A}_1 \text{a}) / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(15\text{b}_2)^2$

CR	0.000000	1.310016	-0.985160
CR	0.000000	-1.310016	-0.985160
O	1.116029	0.000000	-1.435334
O	-1.116029	0.000000	-1.435334
O	0.000000	1.409092	0.777418
O	0.000000	2.542047	-1.948895
O	0.000000	-1.409092	0.777418
O	0.000000	-2.542047	-1.948895
CR	0.000000	0.000000	1.866713
O	1.298832	0.000000	2.762221
O	-1.298832	0.000000	2.762221

$\text{Cr}_3\text{O}_8, ({}^1\text{A}_1 \text{b}) / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(22\text{a}_1)^2$

CR	0.000000	1.176876	-0.958908
CR	0.000000	-1.176876	-0.958908
O	1.340837	0.000000	-1.027028
O	-1.340837	0.000000	-1.027028
O	0.000000	1.540515	0.761166
O	0.000000	2.258918	-2.092926
O	0.000000	-1.540515	0.761166
O	0.000000	-2.258918	-2.092926
CR	0.000000	0.000000	1.730941
O	1.283957	0.000000	2.639100
O	-1.283957	0.000000	2.639100

$\text{Cr}_3\text{O}_8, {}^3\text{B}_2 / \text{C}_{2v} (\text{A}), \dots (5\text{a}_2)^2(10\text{b}_1)^2(14\text{b}_2)^2(21\text{a}_1)^2(11\text{b}_1)^2(12\text{b}_1)^2(15\text{b}_2)^1(22\text{a}_1)^1$

CR	0.000000	1.286166	-0.980867
CR	0.000000	-1.286166	-0.980867
O	1.201850	0.000000	-1.313577
O	-1.201850	0.000000	-1.313577
O	0.000000	1.453680	0.780359
O	0.000000	2.498939	-1.976406
O	0.000000	-1.453680	0.780359
O	0.000000	-2.498939	-1.976406
CR	0.000000	0.000000	1.820316
O	1.292327	0.000000	2.721752
O	-1.292327	0.000000	2.721752

$\text{Cr}_3\text{O}_8, {}^3\text{A}_1 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(23a_1)^1$

CR	0.000000	1.213483	-0.965914
CR	0.000000	-1.213483	-0.965914
O	1.290034	0.000000	-1.212125
O	-1.290034	0.000000	-1.212125
O	0.000000	1.563230	0.670170
O	0.000000	2.420645	-1.974882
O	0.000000	-1.563230	0.670170
O	0.000000	-2.420645	-1.974882
CR	0.000000	0.000000	1.833023
O	1.348311	0.000000	2.665044
O	-1.348311	0.000000	2.665044

$\text{Cr}_3\text{O}_8, ({}^3\text{B}_1 \text{a}) / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(6a_2)^1$

CR	0.000000	1.291345	-1.000556
CR	0.000000	-1.291345	-1.000556
O	1.177210	0.000000	-1.363966
O	-1.177210	0.000000	-1.363966
O	0.000000	1.438565	0.767325
O	0.000000	2.617367	-1.844801
O	0.000000	-1.438565	0.767325
O	0.000000	-2.617367	-1.844801
CR	0.000000	0.000000	1.809573
O	1.284946	0.000000	2.728751
O	-1.284946	0.000000	2.728751

$\text{Cr}_3\text{O}_8, ({}^3\text{A}_2 \text{a}) / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(6a_2)^1$

CR	0.000000	1.231407	-0.991424
CR	0.000000	-1.231407	-0.991424
O	1.285961	0.000000	-1.139964
O	-1.285961	0.000000	-1.139964
O	0.000000	1.506543	0.759500
O	0.000000	2.505136	-1.910207
O	0.000000	-1.506543	0.759500
O	0.000000	-2.505136	-1.910207
CR	0.000000	0.000000	1.735258
O	1.277508	0.000000	2.662057
O	-1.277508	0.000000	2.662057

$\text{Cr}_3\text{O}_8, (^3\text{A}_2 \text{ } b) / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(13b_1)^1$

CR	0.000000	1.293487	-1.001189
CR	0.000000	-1.293487	-1.001189
O	1.171292	0.000000	-1.446044
O	-1.171292	0.000000	-1.446044
O	0.000000	1.412277	0.772273
O	0.000000	2.631452	-1.822328
O	0.000000	-1.412277	0.772273
O	0.000000	-2.631452	-1.822328
CR	0.000000	0.000000	1.838295
O	1.293502	0.000000	2.742224
O	-1.293502	0.000000	2.742224

$\text{Cr}_3\text{O}_8, (^3\text{B}_1 \text{ } b) / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^1(13b_1)^1$

CR	0.000000	1.253015	-0.996919
CR	0.000000	-1.253015	-0.996919
O	1.277958	0.000000	-1.239979
O	-1.277958	0.000000	-1.239979
O	0.000000	1.476695	0.756681
O	0.000000	2.566869	-1.858188
O	0.000000	-1.476695	0.756681
O	0.000000	-2.566869	-1.858188
CR	0.000000	0.000000	1.769762
O	1.288378	0.000000	2.677600
O	-1.288378	0.000000	2.677600

$\text{Cr}_3\text{O}_8, (^3\text{A}_1 \text{ } b) / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(16b_2)^1$

CR	0.000000	1.312913	-0.983279
CR	0.000000	-1.312913	-0.983279
O	1.159091	0.000000	-1.345219
O	-1.159091	0.000000	-1.345219
O	0.000000	1.570844	0.673476
O	0.000000	2.547924	-1.957353
O	0.000000	-1.570844	0.673476
O	0.000000	-2.547924	-1.957353
CR	0.000000	0.000000	1.895756
O	1.345294	0.000000	2.735298
O	-1.345294	0.000000	2.735298

$\text{Cr}_3\text{O}_8, {}^5\text{A}_2 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.291181	-0.992910
CR	0.000000	-1.291181	-0.992910
O	1.206271	0.000000	-1.365961
O	-1.206271	0.000000	-1.365961
O	0.000000	1.446767	0.749213
O	0.000000	2.513304	-1.979872
O	0.000000	-1.446767	0.749213
O	0.000000	-2.513304	-1.979872
CR	0.000000	0.000000	1.890835
O	1.373297	0.000000	2.739098
O	-1.373297	0.000000	2.739098

$\text{Cr}_3\text{O}_8, {}^5\text{A}_1 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(21a_1)^2(11b_1)^2(12b_1)^2(14b_2)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.267911	-1.022634
CR	0.000000	-1.267911	-1.022634
O	1.208306	0.000000	-1.395918
O	-1.208306	0.000000	-1.395918
O	0.000000	1.380480	0.730655
O	0.000000	2.520527	-1.988543
O	0.000000	-1.380480	0.730655
O	0.000000	-2.520527	-1.988543
CR	0.000000	0.000000	1.965996
O	1.394923	0.000000	2.772715
O	-1.394923	0.000000	2.772715

$\text{Cr}_3\text{O}_8, {}^5\text{B}_2 / \text{C}_{2v} (\text{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(11b_1)^2(12b_1)^2(21a_1)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.285023	-0.979896
CR	0.000000	-1.285023	-0.979896
O	1.218886	0.000000	-1.302819
O	-1.218886	0.000000	-1.302819
O	0.000000	1.486196	0.707284
O	0.000000	2.494757	-2.037937
O	0.000000	-1.486196	0.707284
O	0.000000	-2.494757	-2.037937
CR	0.000000	0.000000	1.900778
O	1.365808	0.000000	2.721991
O	-1.365808	0.000000	2.721991

$\text{Cr}_3\text{O}_8, {}^5\text{B}_1 / \text{C}_{2v}(\mathbf{A}), \dots (10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(5a_2)^1(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.279532	-0.988121
CR	0.000000	-1.279532	-0.988121
O	1.203794	0.000000	-1.336758
O	-1.203794	0.000000	-1.336758
O	0.000000	1.473741	0.805223
O	0.000000	2.461286	-2.025440
O	0.000000	-1.473741	0.805223
O	0.000000	-2.461286	-2.025440
CR	0.000000	0.000000	1.876079
O	1.398244	0.000000	2.707218
O	-1.398244	0.000000	2.707218

$\text{Cr}_3\text{O}_8, ({}^1\text{A}'\mathbf{a}) / \text{C}_s(\mathbf{B}), \dots (31a')^2$

CR	-0.752051	-0.006609	1.566304
CR	1.835402	0.199315	0.000000
CR	-0.752051	-0.006609	-1.566304
O	-1.376656	1.023995	2.584485
O	-0.991632	-1.479514	2.072748
O	1.022039	0.284408	1.517511
O	-1.551278	0.233557	0.000000
O	3.249877	-0.449625	0.000000
O	-1.376656	1.023995	-2.584485
O	1.022039	0.284408	-1.517511
O	-0.991632	-1.479514	-2.072748

$\text{Cr}_3\text{O}_8, ({}^1\text{A}'\mathbf{b}) / \text{C}_s(\mathbf{B}), \dots (23a'')^2$

CR	-0.769751	0.029970	1.551462
CR	1.743771	0.005450	0.000000
CR	-0.769751	0.029970	-1.551462
O	-1.530037	0.631568	2.796888
O	-0.653060	-1.558344	1.566041
O	0.938667	0.577230	1.445217
O	-1.420160	0.579731	0.000000
O	3.296216	-0.076808	0.000000
O	-1.530037	0.631568	-2.796888
O	0.938667	0.577230	-1.445217
O	-0.653060	-1.558344	-1.566041

$\text{Cr}_3\text{O}_8, {}^3\text{A}'' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (23a'')^1$

CR	-0.782943	0.031678	1.543663
CR	1.912192	0.057850	0.000000
CR	-0.782943	0.031678	-1.543663
O	-1.448824	0.797640	2.748980
O	-1.036483	-1.523683	1.664340
O	0.955030	0.352083	1.476053
O	-1.427724	0.620949	0.000000
O	3.449362	-0.236643	0.000000
O	-1.448824	0.797640	-2.748980
O	0.955030	0.352083	-1.476053
O	-1.036483	-1.523683	-1.664340

$\text{Cr}_3\text{O}_8, {}^3\text{A}' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (32a')^1$

CR	-0.782943	0.031678	1.543663
CR	1.912192	0.057850	0.000000
CR	-0.782943	0.031678	-1.543663
O	-1.448824	0.797640	2.748980
O	-1.036483	-1.523683	1.664340
O	0.955030	0.352083	1.476053
O	-1.427724	0.620949	0.000000
O	3.449362	-0.236643	0.000000
O	-1.448824	0.797640	-2.748980
O	0.955030	0.352083	-1.476053
O	-1.036483	-1.523683	-1.664340

$\text{Cr}_3\text{O}_8, ({}^3\text{A}' \mathbf{b}) / \text{C}_s (\mathbf{B}), \dots (23a'')^1 (24a'')^1$

CR	-0.782943	0.031678	1.543663
CR	1.912192	0.057850	0.000000
CR	-0.782943	0.031678	-1.543663
O	-1.448824	0.797640	2.748980
O	-1.036483	-1.523683	1.664340
O	0.955030	0.352083	1.476053
O	-1.427724	0.620949	0.000000
O	3.449362	-0.236643	0.000000
O	-1.448824	0.797640	-2.748980
O	0.955030	0.352083	-1.476053
O	-1.036483	-1.523683	-1.664340

Cr₃O₈, ¹A / C₂ (C), ... (27a)²

CR	-0.510691	1.167151	-0.936662
CR	0.510691	-1.167151	-0.936662
CR	0.000000	0.000000	1.786764
O	-2.004396	0.731703	-1.195747
O	0.096988	2.041027	-2.095689
O	0.000000	1.428184	0.725256
O	2.004396	-0.731703	-1.195747
O	-0.096988	-2.041027	-2.095689
O	-1.283724	-0.032981	2.696022
O	0.000000	-1.428184	0.725256
O	1.283724	0.032981	2.696022

Cr₃O₈, ³B / C₂ (C), ... (27a)¹(27b)¹

CR	-0.451002	2.247738	-0.884004
CR	0.451002	-2.247738	-0.884004
CR	0.000000	0.000000	1.624469
O	-1.144541	1.418781	-2.043810
O	-0.761281	3.800832	-0.884702
O	0.000000	1.440133	0.617162
O	1.144541	-1.418781	-2.043810
O	0.761281	-3.800832	-0.884702
O	-1.292487	-0.013524	2.526659
O	0.000000	-1.440133	0.617162
O	1.292487	0.013524	2.526659

Cr₃O₈, ¹A₁ / D_{2d} (D), ... (12b₂)²

O	0.000000	1.239012	1.188399
O	0.000000	-1.239012	1.188399
O	-1.239012	0.000000	-1.188399
O	1.239012	0.000000	-1.188399
O	0.000000	-1.323148	-3.412506
O	1.323148	0.000000	3.412506
O	-1.323148	0.000000	3.412506
O	0.000000	1.323148	-3.412506
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.550676
CR	0.000000	0.000000	2.550676

$\text{Cr}_3\text{O}_8, {}^3\text{B}_2 / \text{D}_{2d} (\mathbf{D}), \dots (12b_2)^1(12a_1)^1$

O	0.000000	1.266981	1.201963
O	0.000000	-1.266981	1.201963
O	-1.266981	0.000000	-1.201963
O	1.266981	0.000000	-1.201963
O	0.000000	-1.312076	-3.397580
O	1.312076	0.000000	3.397580
O	-1.312076	0.000000	3.397580
O	0.000000	1.312076	-3.397580
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.520959
CR	0.000000	0.000000	2.520959

$\text{Cr}_3\text{O}_8, {}^3\text{A}_2 / \text{D}_{2d} (\mathbf{D}), \dots (12b_2)^1(3b_1)^1$

O	0.000000	1.226631	1.257253
O	0.000000	-1.226631	1.257253
O	-1.226631	0.000000	-1.257253
O	1.226631	0.000000	-1.257253
O	0.000000	-1.305521	-3.467169
O	1.305521	0.000000	3.467169
O	-1.305521	0.000000	3.467169
O	0.000000	1.305521	-3.467169
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.579091
CR	0.000000	0.000000	2.579091

$\text{Cr}_3\text{O}_8^-, {}^2\text{A}_1 / \text{C}_{2v} (\mathbf{A}), \dots (5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^2(23a_1)^1$

CR	0.000000	1.154456	-0.954137
CR	0.000000	-1.154456	-0.954137
O	1.369323	0.000000	-1.082469
O	-1.369323	0.000000	-1.082469
O	0.000000	1.571032	0.705085
O	0.000000	2.245005	-2.119274
O	0.000000	-1.571032	0.705085
O	0.000000	-2.245005	-2.119274
CR	0.000000	0.000000	1.806800
O	1.358726	0.000000	2.648867
O	-1.358726	0.000000	2.648867

Cr_3O_8^- , (${}^2\text{A}_2 \mathbf{a}$) / $\text{C}_{2v}(\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(22a_1)^2(6a_2)^1$

CR	0.000000	1.154456	-0.954137
CR	0.000000	-1.154456	-0.954137
O	1.369323	0.000000	-1.082469
O	-1.369323	0.000000	-1.082469
O	0.000000	1.571032	0.705085
O	0.000000	2.245005	-2.119274
O	0.000000	-1.571032	0.705085
O	0.000000	-2.245005	-2.119274
CR	0.000000	0.000000	1.806800
O	1.358726	0.000000	2.648867
O	-1.358726	0.000000	2.648867

Cr_3O_8^- , (${}^2\text{A}_2 \mathbf{b}$) / $\text{C}_{2v}(\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^2(6a_2)^1$

CR	0.000000	1.154456	-0.954137
CR	0.000000	-1.154456	-0.954137
O	1.369323	0.000000	-1.082469
O	-1.369323	0.000000	-1.082469
O	0.000000	1.571032	0.705085
O	0.000000	2.245005	-2.119274
O	0.000000	-1.571032	0.705085
O	0.000000	-2.245005	-2.119274
CR	0.000000	0.000000	1.806800
O	1.358726	0.000000	2.648867
O	-1.358726	0.000000	2.648867

Cr_3O_8^- , (${}^4\text{B}_2$) / $\text{C}_{2v}(\mathbf{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(23a_1)^1$

CR	0.000000	1.277792	-0.986485
CR	0.000000	-1.277792	-0.986485
O	1.219177	0.000000	-1.350722
O	-1.219177	0.000000	-1.350722
O	0.000000	1.479464	0.718089
O	0.000000	2.529617	-1.975606
O	0.000000	-1.479464	0.718089
O	0.000000	-2.529617	-1.975606
CR	0.000000	0.000000	1.894968
O	1.370679	0.000000	2.725243
O	-1.370679	0.000000	2.725243

Cr_3O_8^- , ${}^4\text{B}_1 / \text{C}_{2v}(\text{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(6a_2)^1$

CR	0.000000	1.291565	-1.007957
CR	0.000000	-1.291565	-1.007957
O	1.223664	0.000000	-1.288027
O	-1.223664	0.000000	-1.288027
O	0.000000	1.441524	0.799150
O	0.000000	2.587124	-1.943370
O	0.000000	-1.441524	0.799150
O	0.000000	-2.587124	-1.943370
CR	0.000000	0.000000	1.808695
O	1.299830	0.000000	2.743074
O	-1.299830	0.000000	2.743074

Cr_3O_8^- , ${}^4\text{A}_2 / \text{C}_{2v}(\text{A})$, ... $(5a_2)^2(10b_1)^2(14b_2)^2(21a_1)^2(11b_1)^2(12b_1)^2(15b_2)^1(22a_1)^1(13b_1)^1$

CR	0.000000	1.303381	-1.010289
CR	0.000000	-1.303381	-1.010289
O	1.209197	0.000000	-1.392854
O	-1.209197	0.000000	-1.392854
O	0.000000	1.415664	0.796992
O	0.000000	2.641882	-1.882039
O	0.000000	-1.415664	0.796992
O	0.000000	-2.641882	-1.882039
CR	0.000000	0.000000	1.841212
O	1.315936	0.000000	2.746951
O	-1.315936	0.000000	2.746951

Cr_3O_8^- , ${}^2\text{A}' / \text{C}_s(\text{B})$, ... $(23a'')^2(31a')^1$

CR	-0.785588	0.026875	1.602730
CR	1.823079	-0.035604	0.000000
CR	-0.785588	0.026875	-1.602730
O	-1.432145	0.894733	2.778757
O	-1.011752	-1.551662	1.737284
O	0.993873	0.360973	1.486444
O	-1.259935	0.600929	0.000000
O	3.404272	-0.063452	0.000000
O	-1.432145	0.894733	-2.778757
O	0.993873	0.360973	-1.486444
O	-1.011752	-1.551662	-1.737284

$\text{Cr}_3\text{O}_8^-, (^2A'' a) / C_s (B), \dots (31a')^2(23a'')^1$

CR	0.659190	-0.026572	1.544853
CR	-1.668965	-0.057701	0.000000
CR	0.659190	-0.026572	-1.544853
O	1.505523	-1.191190	2.245745
O	0.659190	1.303679	2.420920
O	-1.024150	-0.677634	1.509961
O	1.480675	0.324333	0.000000
O	-2.710052	1.138489	0.000000
O	1.505523	-1.191190	-2.245745
O	-1.024150	-0.677634	-1.509961
O	0.659190	1.303679	-2.420920

$\text{Cr}_3\text{O}_8^-, (^2A' b) / C_s (B), \dots (31a')^2(32a')^1$

CR	0.695663	-0.139731	1.476913
CR	-1.712943	0.225442	0.000000
CR	0.695663	-0.139731	-1.476913
O	1.098729	-1.513983	2.188184
O	1.098729	1.135949	2.345121
O	-1.139971	-0.182572	1.564493
O	1.688873	-0.072920	0.000000
O	-2.838996	1.356189	0.000000
O	1.098729	-1.513983	-2.188184
O	-1.139971	-0.182572	-1.564493
O	1.098729	1.135949	-2.345121

$\text{Cr}_3\text{O}_8^-, (^2A'' b) / C_s (B), \dots (23a'')^2(24a'')^1$

CR	0.596989	-0.052770	1.732092
CR	-1.375057	0.060219	0.000000
CR	0.596989	-0.052770	-1.732092
O	1.723864	-1.169665	1.922406
O	0.596989	1.110237	2.829164
O	-1.049095	-0.806404	1.510584
O	0.444377	0.634828	0.000000
O	-2.444658	1.232802	0.000000
O	1.723864	-1.169665	-1.922406
O	-1.049095	-0.806404	-1.510584
O	0.596989	1.110237	-2.829164

$\text{Cr}_3\text{O}_8^-, {}^4\text{A}' / \text{C}_s (\mathbf{B}), \dots (23a'')^1 (31a')^1 (24a'')^1$

CR	-0.649145	0.083640	1.691838
CR	1.511484	-0.230834	0.000000
CR	-0.649145	0.083640	-1.691838
O	-0.555498	1.265389	2.765179
O	-1.918593	-0.864178	1.891358
O	0.849937	-0.871505	1.574366
O	-0.366083	0.724808	0.000000
O	2.974808	0.406444	0.000000
O	-0.555498	1.265389	-2.765179
O	0.849937	-0.871505	-1.574366
O	-1.918593	-0.864178	-1.891358

$\text{Cr}_3\text{O}_8^-, {}^4\text{A}'' / \text{C}_s (\mathbf{B}), \dots (31a')^1 (23a'')^1 (32a')^1$

CR	-0.775282	0.024018	1.564861
CR	1.854428	-0.013628	0.000000
CR	-0.775282	0.024018	-1.564861
O	-1.456785	0.851441	2.749096
O	-0.873050	-1.558304	1.788589
O	0.923747	0.498536	1.440712
O	-1.552902	0.410703	0.000000
O	3.453487	-0.097275	0.000000
O	-1.456785	0.851441	-2.749096
O	0.923747	0.498536	-1.440712
O	-0.873050	-1.558304	-1.788589

$\text{Cr}_3\text{O}_8^-, {}^2\text{A} / \text{C}_2 (\mathbf{C}), \dots (27a)^2 (28a)^1$

CR	-0.587342	1.123707	-0.986344
CR	0.587342	-1.123707	-0.986344
CR	0.000000	0.000000	1.924314
O	-2.092010	0.658389	-1.218339
O	-0.004559	2.098425	-2.103173
O	0.000000	1.312018	0.619969
O	2.092010	-0.658389	-1.218339
O	0.004559	-2.098425	-2.103173
O	-1.349638	-0.108788	2.774104
O	0.000000	-1.312018	0.619969
O	1.349638	0.108788	2.774104

$\text{Cr}_3\text{O}_8^-, {}^2\text{B} / \text{C}_2(\text{C}), \dots(27a)^2(27b)^1$

CR	-0.518158	1.227137	-0.938173
CR	0.518158	-1.227137	-0.938173
CR	0.000000	0.000000	1.763852
O	-2.079238	0.985460	-1.158428
O	0.248137	2.003776	-2.101070
O	0.000000	1.445236	0.753039
O	2.079238	-0.985460	-1.158428
O	-0.248137	-2.003776	-2.101070
O	-1.306743	-0.008174	2.675200
O	0.000000	-1.445236	0.753039
O	1.306743	0.008174	2.675200

$\text{Cr}_3\text{O}_8^-, {}^4\text{B} / \text{C}_2(\text{C}), \dots(27a)^1(27b)^1(28a)^1$

CR	-0.402153	2.883945	-0.679703
CR	0.402153	-2.883945	-0.679703
CR	0.000000	0.000000	1.240851
O	-1.924617	3.342251	-0.892532
O	0.762593	3.853197	-1.209357
O	0.000000	1.394140	0.147616
O	1.924617	-3.342251	-0.892532
O	-0.762593	-3.853197	-1.209357
O	-1.322611	-0.010963	2.132107
O	0.000000	-1.394140	0.147616
O	1.322611	0.010963	2.132107

$\text{Cr}_3\text{O}_8^-, {}^2\text{A}_1 / \text{D}_{2d}(\text{D}), \dots(12b_2)^2(12a_1)^1$

O	0.000000	1.286466	1.199733
O	0.000000	-1.286466	1.199733
O	-1.286466	0.000000	-1.199733
O	1.286466	0.000000	-1.199733
O	0.000000	-1.346006	-3.356840
O	1.346006	0.000000	3.356840
O	-1.346006	0.000000	3.356840
O	0.000000	1.346006	-3.356840
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.494526
CR	0.000000	0.000000	2.494526

$\text{Cr}_3\text{O}_8^-, {}^4\text{B}_2 / \text{D}_{2d}(\mathbf{D}), \dots(12b_2)^1(12a_1)^1(13a_1)^1$

O	0.000000	1.241162	1.225170
O	0.000000	-1.241162	1.225170
O	-1.241162	0.000000	-1.225170
O	1.241162	0.000000	-1.225170
O	0.000000	-1.361688	-3.461812
O	1.361688	0.000000	3.461812
O	-1.361688	0.000000	3.461812
O	0.000000	1.361688	-3.461812
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.619089
CR	0.000000	0.000000	2.619089

$\text{Cr}_3\text{O}_8^-, {}^4\text{A}_2 / \text{D}_{2d}(\mathbf{D}), \dots(12b_2)^1(12a_1)^1(3b_1)^1$

O	0.000000	1.266398	1.323344
O	0.000000	-1.266398	1.323344
O	-1.266398	0.000000	-1.323344
O	1.266398	0.000000	-1.323344
O	0.000000	-1.322247	-3.458330
O	1.322247	0.000000	3.458330
O	-1.322247	0.000000	3.458330
O	0.000000	1.322247	-3.458330
CR	0.000000	0.000000	0.000000
CR	0.000000	0.000000	-2.556905
CR	0.000000	0.000000	2.556905

$\text{W}_3\text{O}_8, {}^1\text{A}_1 / \text{C}_{2v}(\mathbf{A}), \dots(22a_1)^2$

W	0.000000	1.268436	-1.016171
W	0.000000	-1.268436	-1.016171
O	1.481029	0.000000	-0.954880
O	-1.481029	0.000000	-0.954880
O	0.000000	1.641132	0.877469
O	0.000000	2.275262	-2.406975
O	0.000000	-1.641132	0.877469
O	0.000000	-2.275262	-2.406975
W	0.000000	0.000000	1.931712
O	-1.380199	0.000000	2.949797
O	1.380199	0.000000	2.949797

$W_3O_8, ({}^1A_1 \text{ } b) / C_{2v} (A), \dots (15b_2)^2$

W	0.000000	1.475971	-1.050803
W	0.000000	-1.475971	-1.050803
O	1.125977	0.000000	-1.549091
O	-1.125977	0.000000	-1.549091
O	0.000000	1.512724	0.881515
O	0.000000	2.779180	-2.158984
O	0.000000	-1.512724	0.881515
O	0.000000	-2.779180	-2.158984
W	0.000000	0.000000	2.052760
O	-1.401080	0.000000	3.052476
O	1.401080	0.000000	3.052476

$W_3O_8, {}^3B_2 / C_{2v} (A), \dots (15b_2)^1 (22a_1)^1$

W	0.000000	1.460682	-1.039774
W	0.000000	-1.460682	-1.039774
O	1.210874	0.000000	-1.450715
O	-1.210874	0.000000	-1.450715
O	0.000000	1.551828	0.878482
O	0.000000	2.771808	-2.145629
O	0.000000	-1.551828	0.878482
O	0.000000	-2.771808	-2.145629
W	0.000000	0.000000	2.014114
O	-1.392387	0.000000	3.020497
O	1.392387	0.000000	3.020497

$W_3O_8, {}^3A_2 / C_{2v} (A), \dots (22a_1)^1 (6a_2)^1$

W	0.000000	1.404346	-1.041464
W	0.000000	-1.404346	-1.041464
O	1.340224	0.000000	-1.189803
O	-1.340224	0.000000	-1.189803
O	0.000000	1.602111	0.861684
O	0.000000	2.838899	-1.988764
O	0.000000	-1.602111	0.861684
O	0.000000	-2.838899	-1.988764
W	0.000000	0.000000	1.941471
O	-1.377418	0.000000	2.971125
O	1.377418	0.000000	2.971125

$W_3O_8, {}^3A_1 / C_{2v} (A), \dots (22a_1)^1(23a_1)^1$

W	0.000000	1.352046	-0.934418
W	0.000000	-1.352046	-0.934418
O	1.356561	0.000000	-1.302587
O	-1.356561	0.000000	-1.302587
O	0.000000	1.796382	0.857604
O	0.000000	2.674520	-2.044444
O	0.000000	-1.796382	0.857604
O	0.000000	-2.674520	-2.044444
W	0.000000	0.000000	1.810679
O	-1.443117	0.000000	2.758405
O	1.443117	0.000000	2.758405

$W_3O_8, {}^1A' / C_s (B), \dots (31a')^2$

W	-0.776499	0.022297	1.649650
W	-0.776499	0.022297	-1.649650
W	1.775162	-0.157331	0.000000
O	-1.614134	-1.159663	2.578376
O	-0.864269	1.515765	2.490295
O	-1.738090	0.169805	0.000000
O	1.094305	-0.619411	1.661234
O	-0.864269	1.515765	-2.490295
O	-1.614134	-1.159663	-2.578376
O	1.094305	-0.619411	-1.661234
O	2.451266	1.399624	0.000000

$W_3O_8, {}^3A_2 / C_{2v} (B), \dots (21a_1)^1(8a_2)^1$

W	0.000000	1.768696	-0.940863
W	0.000000	-1.768696	-0.940863
W	0.000000	0.000000	2.076117
O	-1.389512	2.644423	-1.452362
O	1.389512	2.644423	-1.452362
O	0.000000	0.000000	-1.660298
O	0.000000	1.565219	0.946531
O	1.389512	-2.644423	-1.452362
O	-1.389512	-2.644423	-1.452362
O	0.000000	-1.565219	0.946531
O	0.000000	0.000000	3.778568

$W_3O_8, {}^3A' / C_s (B), \dots (31a')^1 (32a')^1$

W	0.818293	-0.182324	1.655513
W	0.818293	-0.182324	-1.655513
W	-1.789831	0.522055	0.000000
O	1.693739	0.812918	2.755500
O	0.818293	-1.794126	2.249527
O	1.790854	-0.148392	0.000000
O	-1.043168	0.464247	1.716704
O	0.818293	-1.794126	-2.249527
O	1.693739	0.812918	-2.755500
O	-1.043168	0.464247	-1.716704
O	-3.311074	-0.273703	0.000000

$W_3O_8, {}^1A_1 / C_{2v} (C), \dots (14b_2)^2 (11b_1)^2 (8a_2)^2 (12b_1)^2 (19a_1)^2$

W	0.000000	1.437968	-1.037565
W	0.000000	-1.437968	-1.037565
W	0.000000	0.000000	2.039857
O	-1.407851	1.938256	-1.881028
O	1.407851	1.938256	-1.881028
O	0.000000	1.520977	0.873166
O	1.407851	-1.938256	-1.881028
O	-1.407851	-1.938256	-1.881028
O	-1.386215	0.000000	3.052031
O	0.000000	-1.520977	0.873166
O	1.386215	0.000000	3.052031

$W_3O_8, ({}^3B_2 a) / C_{2v} (C), \dots (14b_2)^2 (11b_1)^2 (8a_2)^2 (12b_1)^2 (19a_1)^1 (15b_2)^1$

W	0.000000	3.193760	-0.662902
W	0.000000	-3.193760	-0.662902
W	0.000000	0.000000	1.406781
O	-1.401134	3.545108	-1.589277
O	1.401134	3.545108	-1.589277
O	0.000000	1.588030	0.372936
O	1.401134	-3.545108	-1.589277
O	-1.401134	-3.545108	-1.589277
O	-1.379998	0.000000	2.431095
O	0.000000	-1.588030	0.372936
O	1.379998	0.000000	2.431095

$W_3O_8, (^3B_2 \text{ } b) / C_{2v} (C), \dots (11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(14b_2)^1(19a_1)^1$

W	0.000000	1.386345	-0.942689
W	0.000000	-1.386345	-0.942689
W	0.000000	0.000000	1.837340
O	-1.458583	1.817845	-1.779834
O	1.458583	1.817845	-1.779834
O	0.000000	1.715388	0.949355
O	1.458583	-1.817845	-1.779834
O	-1.458583	-1.817845	-1.779834
O	-1.424984	0.000000	2.832484
O	0.000000	-1.715388	0.949355
O	1.424984	0.000000	2.832484

$W_3O_8, (^3B_1 \text{ } b) / C_{2v} (C), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^1(13b_1)^1$

W	0.000000	1.460126	-1.053003
W	0.000000	-1.460126	-1.053003
W	0.000000	0.000000	2.032306
O	-1.365367	2.241768	-1.775108
O	1.365367	2.241768	-1.775108
O	0.000000	1.504075	0.846030
O	1.365367	-2.241768	-1.775108
O	-1.365367	-2.241768	-1.775108
O	-1.385618	0.000000	3.045051
O	0.000000	-1.504075	0.846030
O	1.385618	0.000000	3.045051

$W_3O_8, ^1A_1 / D_{2d} (D), \dots (12b_2)^2$

O	0.000000	1.299361	1.335922
O	0.000000	-1.299361	1.335922
O	-1.299361	0.000000	-1.335922
O	1.299361	0.000000	-1.335922
O	0.000000	-1.425638	-3.843504
O	1.425638	0.000000	3.843504
O	-1.425638	0.000000	3.843504
O	0.000000	1.425638	-3.843504
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.876895
W	0.000000	0.000000	2.876895

$W_3O_8, {}^3B_2 / D_{2d} (D), \dots (12b_2)^1(12a_1)^1$

O	0.000000	1.321878	1.321124
O	0.000000	-1.321878	1.321124
O	-1.321878	0.000000	-1.321124
O	1.321878	0.000000	-1.321124
O	0.000000	-1.417166	-3.839215
O	1.417166	0.000000	3.839215
O	-1.417166	0.000000	3.839215
O	0.000000	1.417166	-3.839215
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.864319
W	0.000000	0.000000	2.864319

$W_3O_8, {}^3A_2 / D_{2d} (D), \dots (12b_2)^1(3b_1)^1$

O	0.000000	1.280180	1.419574
O	0.000000	-1.280180	1.419574
O	-1.280180	0.000000	-1.419574
O	1.280180	0.000000	-1.419574
O	0.000000	-1.414319	-3.883213
O	1.414319	0.000000	3.883213
O	-1.414319	0.000000	3.883213
O	0.000000	1.414319	-3.883213
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.896544
W	0.000000	0.000000	2.896544

$W_3O_8^-, {}^2A_1 / C_{2v} (A), \dots (22a_1)^2(23a_1)^1$

W	0.000000	1.246049	-0.950605
W	0.000000	-1.246049	-0.950605
O	1.527379	0.000000	-1.023429
O	-1.527379	0.000000	-1.023429
O	0.000000	1.756705	0.883889
O	0.000000	2.265489	-2.377038
O	0.000000	-1.756705	0.883889
O	0.000000	-2.265489	-2.377038
W	0.000000	0.000000	1.837607
O	-1.443646	0.000000	2.810741
O	1.443646	0.000000	2.810741

$W_3O_8^-, ^4B_2 / C_{2v} (A), \dots (22a_1)^1 (15b_2)^1 (23a_1)^1$

W	0.000000	1.438901	-1.117464
W	0.000000	-1.438901	-1.117464
O	1.215158	0.000000	-1.636538
O	-1.215158	0.000000	-1.636538
O	0.000000	1.461309	0.732352
O	0.000000	2.910240	-2.048626
O	0.000000	-1.461309	0.732352
O	0.000000	-2.910240	-2.048626
W	0.000000	0.000000	2.190638
O	-1.443580	0.000000	3.157654
O	1.443580	0.000000	3.157654

$W_3O_8^-, ^4B_1 / C_{2v} (A), \dots (22a_1)^1 (15b_2)^1 (6a_2)^1$

W	0.000000	1.485312	-1.053237
W	0.000000	-1.485312	-1.053237
O	1.227891	0.000000	-1.380034
O	-1.227891	0.000000	-1.380034
O	0.000000	1.546270	0.905765
O	0.000000	2.907806	-2.061028
O	0.000000	-1.546270	0.905765
O	0.000000	-2.907806	-2.061028
W	0.000000	0.000000	1.997839
O	-1.397510	0.000000	3.037733
O	1.397510	0.000000	3.037733

$W_3O_8^-, ^2A' / C_s (B), \dots (31a')^2 (32a')^1$

W	0.166407	-0.766368	1.547826
W	0.166407	-0.766368	-1.547826
W	-0.286569	1.738064	0.000000
O	1.659644	-1.172560	2.341438
O	-1.197322	-1.281234	2.494644
O	0.149063	-1.906566	0.000000
O	0.166407	1.205663	1.733694
O	-1.197322	-1.281234	-2.494644
O	1.659644	-1.172560	-2.341438
O	0.166407	1.205663	-1.733694
O	-1.834287	2.503537	0.000000

$W_3O_8^-, {}^2A'' / C_s (B), \dots (31a')^2(23a'')^1$

W	0.126030	-0.723938	1.631535
W	0.126030	-0.723938	-1.631535
W	-0.350521	1.650247	0.000000
O	1.519765	-0.497999	2.638773
O	-0.955174	-1.862271	2.385206
O	0.650897	-1.605051	0.000000
O	-0.955174	0.897673	1.665972
O	-0.955174	-1.862271	-2.385206
O	1.519765	-0.497999	-2.638773
O	-0.955174	0.897673	-1.665972
O	1.041030	2.658311	0.000000

$W_3O_8^-, {}^4A'' / C_s (B), \dots (31a')^1(23a'')^1(32a')^1$

W	-0.811123	0.023971	1.662873
W	-0.811123	0.023971	-1.662873
W	1.792083	-0.094314	0.000000
O	-1.727100	-1.107855	2.618350
O	-0.812041	1.575095	2.442037
O	-1.776345	0.180497	0.000000
O	0.972063	-0.689801	1.679558
O	-0.812041	1.575095	-2.442037
O	-1.727100	-1.107855	-2.618350
O	0.972063	-0.689801	-1.679558
O	3.339515	0.693560	0.000000

$W_3O_8^-, {}^2A_1 / C_{2v} (C), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(20a_1)^1$

W	0.000000	1.397374	-0.951781
W	0.000000	-1.397374	-0.951781
W	0.000000	0.000000	1.841063
O	-1.449168	1.916985	-1.752037
O	1.449168	1.916985	-1.752037
O	0.000000	1.718158	0.945970
O	1.449168	-1.916985	-1.752037
O	-1.449168	-1.916985	-1.752037
O	-1.412669	0.000000	2.847165
O	0.000000	-1.718158	0.945970
O	1.412669	0.000000	2.847165

$W_3O_8^-, {}^2A_1 / D_{2d}(\mathbf{D}), \dots (12b_2)^2(12a_1)^1$

O	0.000000	1.339343	1.346074
O	0.000000	-1.339343	1.346074
O	-1.339343	0.000000	-1.346074
O	1.339343	0.000000	-1.346074
O	0.000000	-1.447714	-3.806343
O	1.447714	0.000000	3.806343
O	-1.447714	0.000000	3.806343
O	0.000000	1.447714	-3.806343
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.840787
W	0.000000	0.000000	2.840787

$W_3O_8^-, {}^4A_2 / D_{2d}(\mathbf{D}), \dots (12b_2)^1(12a_1)^1(3b_1)^1$

O	0.000000	1.311949	1.478083
O	0.000000	-1.311949	1.478083
O	-1.311949	0.000000	-1.478083
O	1.311949	0.000000	-1.478083
O	0.000000	-1.433247	-3.877943
O	1.433247	0.000000	3.877943
O	-1.433247	0.000000	3.877943
O	0.000000	1.433247	-3.877943
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	-2.883464
W	0.000000	0.000000	2.883464

$W_3O_8^{2-}, {}^1A_1 / C_{2v}(\mathbf{C}), \dots (14b_2)^2(11b_1)^2(8a_2)^2(12b_1)^2(19a_1)^2(20a_1)^2$

W	0.000000	1.354064	-0.917157
W	0.000000	-1.354064	-0.917157
W	0.000000	0.000000	1.756397
O	-1.487465	1.902313	-1.673870
O	1.487465	1.902313	-1.673870
O	0.000000	1.781762	0.975187
O	1.487465	-1.902313	-1.673870
O	-1.487465	-1.902313	-1.673870
O	-1.463302	0.000000	2.732922
O	0.000000	-1.781762	0.975187
O	1.463302	0.000000	2.732922