Structural and Electronic Properties of Reduced Transition Metal Oxide Clusters, M_4O_{10} and $M_4O_{10}^-$ ($M = Cr, W$), from Photoelectron Spectroscopy and Quantum Chemical Calculations

Shenggang Li,[†] Hua-Jin Zhai,[‡] Lai-Sheng Wang,^{‡,*} and David A. Dixon^{†,*}

Contribution from the Chemistry Department, The University of Alabama, Shelby Hall, Box 870336, Tuscaloosa, Alabama 35487-0336, USA, and Department of Chemistry, Brown University, Providence, Rhode Island 02912, USA

*E-mail: lai-sheng_wang@brown.edu; dadixon@bama.ua.edu

Supporting Information: Discussion of additional spin states and performance of DFT. Complete author lists for references 56, 58, 59, and 68 (a). Tables: calculated energetic properties at the CCSD(T)/aVDZ//BP86/aVDZ level; calculated relative energies for additional electronic states of W_4O_{10} and $W_4O_{10}^-$; calculated clustering energies and heats of formation for Cr_4O_{10} and W_4O_{10} ; zero-point energies and electronic energies calculated at the DFT and CCSD(T) levels. Figures: additional structures and relative energies for Cr_4O_{10} , $Cr_4O_{10}^-$, W_4O_{10} , and $W_4O_{10}^-$; the lowest few unoccupied and highest few occupied molecular orbitals for the $^1A_1/T_d$ (**A**) state of Cr_4O_{10} , the $^1A_1/C_{2v}$ (**B**), $^1A_g/C_{2h}$ (**C**), and $^1A_1/T_d$ (**A**) states of W_4O_{10} . Cartesian coordinates for the equilibrium geometries optimized at the B3LYP/aVDZ and BP86/aVDZ levels.

[†] The University of Alabama.

[‡] Brown University.

Additional Cr₄O₁₀ Spin States. We first discuss the states obtained by exciting one electron (Table 2), with the point group lowered to D_{2d} only, as the 6e orbital remains doubly degenerate in the C_{3v} point group. The ³B₂/D_{2d} (A) state with an electron configuration of ... (14a₁)²(6b₁)¹(5a₂)¹(17e)⁰... has no imaginary frequency at the B3LYP/aVDZ level, but has an imaginary frequency of 593*i* (e) at the BP86/aVDZ level. This state is predicted to lie 0.4, ~13, and ~40 kcal/mol higher in energy than the ¹A₁/T_d (A) state at the B3LYP, BP86 and CCSD(T) levels, respectively. Inclusion of the ZPEs, calculated at the B3LYP/aVDZ level, leads to the ³B₂/D_{2d} (A) state being higher in energy by ~4, ~17, and ~43 kcal/mol at the B3LYP, BP86 and CCSD(T) levels, respectively. The ³A₂/D_{2d} (A) state with an electron configuration of ... (6b₁)²(14a₁)¹(5a₂)¹(17e)⁰... has an imaginary frequency of 446*i* (e) at the B3LYP/aVDZ level, but has no imaginary frequency at the BP86/aVDZ level. This state is predicted to lie ~7, ~18, and ~40 kcal/mol higher in energy than the ¹A₁/T_d (A) state at the B3LYP, BP86 and CCSD(T) levels, respectively. At the B3LYP and BP86 levels, the expectation values of the S² operator for the two triplet states are 2.15 and 2.04, respectively, in contrast to the expected value of 2 for a pure triplet state, so there is modest spin contamination with more at the B3LYP level. Both of these triplet D_{2d} states are predicted to lie higher in energy than the singlet T_d state. Even though the HOMO-LUMO gap for the ¹A₁/T_d (A) state is calculated to be larger at the B3LYP level (~2.5 eV) than that at the BP86 level (~1.3 eV), the relative energies for the triplet states from the singlet state calculated at the B3LYP level are considerably lower than those at the BP86 level, due in part to the higher spin contamination at the B3LYP level than that at the BP86 level. The larger amount of spin contamination at the B3LYP level is most likely due to the presence of the HF component in B3LYP. The B3LYP and BP86 relative energies are also substantially smaller than the CCSD(T) values. This appears to be a general trend for Cr₄O₁₀ and its anion.

We next discuss the states obtained by exciting two electrons, where the point group can be lowered to either D_{2d} or C_{3v} . The ${}^5B_1/D_{2d}$ (**A**) state with an electron configuration of $\dots(14a_1)^1(6b_1)^1(17e)^2(5a_2)^0\dots$ has an imaginary frequency of $363i$ (e) at the B3LYP/aVDZ level, and an imaginary frequency of $303i$ (e) at the BP86/aVDZ level, showing that it wants to undergo a further reduction in symmetry. This state is predicted to lie ~ 9 kcal/mol lower in energy at the B3LYP level, but ~ 22 and ~ 60 kcal/mol higher in energy at the BP86 and CCSD(T) levels than the ${}^1A_1/T_d$ (**A**) state, respectively. The ${}^5A_1/C_{3v}$ (**A**) state with an electron configuration of $\dots(22e)^2(23e)^2(5a_2)^0\dots$ has two imaginary frequencies of $1011i$ and $999i$ at the B3LYP/aVDZ level, but it has no imaginary frequency at the BP86/aVDZ level. This state is predicted to lie ~ 15 kcal/mol lower in energy at the B3LYP level, but ~ 22 kcal/mol higher in energy at the BP86 level than the ${}^1A_1/T_d$ (**A**) state. The expectation values of S^2 for these two quintet states are 6.2 to 6.3 at the B3LYP level and 6.1 at the BP86 level as compared to the expected value of 6 for a pure quintet state. Both quintet states are predicted to be lower in energy than the singlet state at the B3LYP level, but higher in energy at the BP86 level. At the CCSD(T) level, the ${}^5B_1/D_{2d}$ (**A**) state is predicted to be much higher in energy than the singlet state by >60 kcal/mol, so we expect the ${}^5A_1/C_{3v}$ (**A**) state to be also substantially higher in energy than the singlet state at this level.

As shown in Table 2, the ${}^1A_1/C_{2v}$ (**B**) state is predicted to lie significantly higher in energy than the ${}^1A_1/T_d$ (**A**) state by ~ 63 , ~ 66 , and ~ 104 kcal/mol at the B3LYP, BP86, and CCSD(T) levels, respectively. Relative energies at the BP86/aVDZ for additional structures/states are given as Figure S1, which are predicted to lie higher in energy than the ${}^1A_1/T_d$ (**A**) state by >60 kcal/mol.

Additional Cr₄O₁₀⁻ Spin States. The ⁴B₁/D_{2d} (A) state of Cr₄O₁₀⁻ (Table 2) derived from the triplet states of Cr₄O₁₀ with an electron configuration of ... (14a₁)²(6b₁)¹(17e)²(5a₂)⁰... has no imaginary frequency at the B3LYP/aVDZ and BP86/aVDZ levels. This state is predicted to lie ~24 kcal/mol lower in energy than the ²A₁/T_d (A) state at the B3LYP level, but is essentially the same energy as the ²A₁/T_d (A) state at the BP86 level. At the CCSD(T) level, it is predicted to lie higher in energy than the ²A₁/T_d (A) state by ~31 kcal/mol. The ⁴A₁/D_{2d} (A) state with an electron configuration of ... (6b₁)²(14a₁)²(17e)²(5a₂)⁰... has no imaginary frequency at the B3LYP/aVDZ level, but has an imaginary frequency of 213i (e) at the BP86/aVDZ level. This state is predicted to lie ~39 and ~9 kcal/mol lower in energy than the ²A₁/T_d (A) state at the B3LYP and BP86 levels, respectively. At the CCSD(T) level, the ⁴A₁/D_{2d} (A) state is predicted to lie higher in energy than the ²A₁/T_d (A) state by ~28 kcal/mol. The two quartet states have relatively small spin contamination with <S²> values less than 4.0 (the expected value is 3.75) at the B3LYP and BP86 levels.

The ⁶A₁/T_d (A) state derived from the quintet states of the neutral has an electron configuration of ... (6e)²(5t₁)³... with an imaginary frequency of 212i (t) at the B3LYP/aVDZ level, but no imaginary frequency at the BP86/aVDZ level. This state is predicted to lie 45 to 47 kcal/mol higher in energy than the ²A₁/T_d (A) state at the CCSD(T) level, but ~47 and ~4 kcal/mol lower in energy than the latter at the B3LYP and BP86 levels, respectively. This sextet state also has relatively small spin contamination with <S²> values of <9.05 at the B3LYP and BP86 levels as compared to an expected value of 8.75.

As shown in Figure S2, additional structures/states for Cr₄O₁₀⁻ are predicted to lie higher in energy than the ²A₂/C_{3v} (A) state by >40 kcal/mol at the BP86/aVDZ level.

Additional W₄O₁₀ Spin States. For the ¹A₁/T_d (**A**) state of W₄O₁₀ (Table 3), similar to the case of Cr₄O₁₀ both the highest occupied molecular orbital (HOMO) (6e) and lowest unoccupied orbital (LUMO) (5t₁) are degenerate orbitals. All of these five orbitals can be considered as non-bonding orbitals involving the d orbitals on the four metal centers, similar to the case of Cr₄O₁₀. The 5t₁ orbital lies higher in energy than the 6e orbital by ~2.4 eV and ~1.4 eV at the B3LYP and BP86 levels, also very similar to that for Cr₄O₁₀. The difference between Cr₄O₁₀ and W₄O₁₀ lies in the energies of the LUMOs. For Cr₄O₁₀, the 9a₁ virtual orbital is slightly higher in energy than the 13t₂ virtual orbital, and both are higher in energy than the 5t₁ orbital by > 0.6 eV. For W₄O₁₀, the 9a₁ virtual orbital lies below the 13t₂ virtual orbital and is close in energy to the 5t₁ orbital (the 9a₁ orbital is higher in energy than the 5t₁ orbital by ~0.2 eV at the B3LYP level, but lower in energy by ~0.1 eV at the BP86 level). The high spin electronic states arising from the six orbitals (6e, 5t₁, 9a₁) in W₄O₁₀ are calculated to be higher in energy than the ¹A₁/T_d (**A**) state by at least 25, 15, and 20 kcal/mol at the CCSD(T), B3LYP, and BP86 levels.

Relative energies of the various spin states for structure **A** at the equilibrium geometries of the ¹A₁/T_d state are also calculated with the MRSCF method. The active space is chosen to be the same as in the case of Cr₄O₁₀, and consists of the same set of orbitals (6e, 5t₁, and 13t₂). For the ¹A₁/T_d (**A**) state, the total occupation number for the doubly degenerate 6e orbitals is 2.8 electrons, which is much higher than that of 1.8 electrons for Cr₄O₁₀. The total occupation numbers for the triply degenerate 5t₁ and 13t₂ orbitals are again rather similar, ~0.6 electron each. The coefficient for the CI vector for the (6e)⁴ configuration is ~0.74. At the MRSCF level, we predict the ¹T, ³A₁, ³T, ⁵A₁, and ⁵T states to lie higher in energy than the ¹A₁ state by 18.3, 28.8, 16.8, 30.5, and 29.9 kcal/mol, respectively. The MRSCF relative energies for the various spin states of structure **A** are in qualitative agreement with the B3LYP and BP86 relative

energies (see Figure S3). As shown in Figure S3, additional structures/states of W_4O_{10} are predicted to lie higher in energy than the $^1A_1/C_{2v}$ (**B**) state by > 30 kcal/mol at the B3LYP/aVDZ level.

Additional $W_4O_{10}^-$ Spin States. Different doublet states can arise upon the addition of one electron to the virtual orbitals ($5t_1$ and $9a_1$) of the neutral singlet state of structure **A**. When the electron is added to the LUMO ($5t_1$), the resulting doublet states have lower symmetries due to the Jahn-Teller effect. The $^2A_2/D_{2d}$ (**A**) and $^2A_2/C_{3v}$ (**A**) states have imaginary frequencies at both the B3LYP and BP86 levels, whereas the $^2A/C_3$ (**A**) state has no imaginary frequency at both DFT levels. When the electron is added to the LUMO+1 orbital ($9a_1$), the resulting doublet state ($^2A_1/T_d$) has the same symmetry as the neutral singlet state. The $^2A_1/T_d$ (**A**) state has no imaginary frequency at both DFT levels. The energy of the above three doublet states are within 10 kcal/mol from each other at the CCSD(T), B3LYP, and BP86 levels, and all lie much higher in energy than the ground state of $W_4O_{10}^-$ by at least ~ 60 kcal/mol. Higher spin states for the anion were also calculated, and they are predicted to lie higher in energy than the ground state by > 80 kcal/mol.

The MRSCF calculations for the various spin states of structure **A** of $W_4O_{10}^-$ are carried out with the same active space as that for W_4O_{10} plus an additional electron at the equilibrium geometries of the $^2A_1/T_d$ (**A**) state. A 2A_1 state is calculated to have the lowest MRSCF energy, with the 2T , 4A_1 , 4T , 6A_1 , and 6T states being higher in energy by 6.5, 17.2, 2.4, 9.5, and 31.9 kcal/mol, respectively. The configuration with the largest coefficient for the CI vector for the 2A_1 state has three electrons in the $6e$ orbitals and 2 electrons in the $5t_1$ orbitals, again indicating that it may not be the same electronic state as the $^2A_1/T_d$ (**A**) state calculated at the DFT and CCSD(T) levels. The MRSCF relative energies for the various spin states are in reasonable

agreement with the B3LYP and BP86 results as shown in Figure S4. As shown in Figure S4, additional structures/states for $W_4O_{10}^-$ are predicted to lie higher in energy than the $^2A_1/C_{2v}$ (**B**) state by > 30 kcal/mol at the B3LYP/aVDZ level.

Performance of DFT. In our previous study (Ref. 21), we evaluated the performance of different DFT exchange-correlation functionals for the different properties of M_3O_8 and its anion. Here we examine the performance of the two DFT functionals for similar properties of M_4O_{10} and its anion, in order to draw some general conclusions for these reduced TMO clusters. Tables 2 and 3 compare the calculated relative energies for the various structures/states for M_4O_{10} and its anion at the B3LYP, BP86 and CCSD(T) levels. In order to help evaluate the accuracy of the CCSD(T) results, the T_1 diagnostics are also listed. In our comparison, we exclude those data where the T_1 diagnostics are larger than 0.05. For $M = W$, no data in Table 3 are excluded as all the T_1 diagnostics are below 0.035, with the exception of the $^2A/C_3$ (**A**) state of the anion, where we did not calculate a CCSD(T) relative energy due to its low symmetry. For M_4O_{10} and its anion, we can draw two conclusions: (1) For both $M = Cr$ and W , the BP86 relative energies are usually closer to the CCSD(T) values than the B3LYP relative energies. (2) The accuracy of the DFT relative energies depends strongly on the multireference character of the relevant electronic states. The multireference character will of course affect the accuracy of the relative energies calculated at the CCSD(T) level as well. In the case of $M = W$, the relative energies calculated at both the B3LYP and BP86 levels are rather close to the CCSD(T) values, and both DFT methods predict the same ground electronic states. However, for $M = Cr$, the relative energies do not agree as well. The presence of multireference character can greatly affect the accuracy of the DFT results, especially for hybrid functionals with some fraction of HF exchange such as B3LYP.

We previously studied (Ref. 21) the performance of these two functionals in calculating the relative energies of the different structures/states for M_3O_8 and its anion. Here we update our previous assessment by excluding those data where the T_1 diagnostics are larger than 0.05. For the selected data, the T_1 diagnostics for Cr_3O_8 and its anion are slightly below 0.05, similar to those for Cr_4O_{10} and its anion, whereas those for $M = W$ are also similar at around 0.03. For the B3LYP functional, the relative energies for Cr_3O_8 to its ground state differ from the CCSD(T) values by 1 to 9 kcal/mol, those for $Cr_3O_8^-$ differ by up to 3 kcal/mol, those for W_3O_8 differ by up to 7 kcal/mol, and those for $W_3O_8^-$ differ by up to 2 kcal/mol. For the BP86 functional, the relative energies for Cr_3O_8 differ from the CCSD(T) values by up to 7 kcal/mol, those for $Cr_3O_8^-$ differ by 3 to 16 kcal/mol, those for W_3O_8 differ by up to 3 kcal/mol, and those for $W_3O_8^-$ differ by 3 to 4 kcal/mol.

From the comparisons of the relative energies for M_3O_8 , M_4O_{10} , and their anions, we reach two conclusions. (1) For $M = Cr$, even though the T_1 diagnostics for the few selected electronic states for the above comparisons are rather similar at around 0.05, the agreement between the DFT and CCSD(T) relative energies are far better for Cr_3O_8 than that for Cr_4O_{10} . Even though the T_1 diagnostics for the selected electronic states for structure **A** of Cr_4O_{10} are not too large, these electronic states still have strong multireference character as indicated by our MRSCF calculations for even the $^1A_1/T_d$ (**A**) state, which has a reasonable T_1 diagnostic of 0.041. As discussed above, a number of configurations contribute significantly to the $^1A_1/T_d$ (**A**) state at the MRSCF level. (2) For $M = W$, relative energies calculated by both the B3LYP and BP86 methods are in good agreement with those calculated by the CCSD(T) method, with the B3LYP method having somewhat larger maximum deviations than the BP86 method for both M_3O_8 , M_4O_{10} , and their anions.

For $\text{Cr}_4\text{O}_{10}^-$, the B3LYP method significantly overestimates the electron detachment energies for $\text{Cr}_4\text{O}_{10}^-$ (by 1.6-1.9 eV; Table 4). For $\text{W}_4\text{O}_{10}^-$, the ADE and the VDE calculated at the B3LYP level (Table 5) are within 0.1-0.2 eV of the experimental values for band X. The VDEs for bands A and C for $\text{W}_4\text{O}_{10}^-$ calculated at the B3LYP level are also within ~ 0.2 eV from the experimental values (Table 6), so the B3LYP method yields quite accurate electron detachment energies for $\text{W}_4\text{O}_{10}^-$. In our previous study (Ref. 21), we showed that the B3LYP method significantly overestimates the VDEs for Cr_3O_8^- by 0.7 to 1.1 eV for bands X and A, but yields accurate VDEs for W_3O_8^- with deviations of ≤ 0.2 eV from the experimental values for bands X–C. Thus, the B3LYP method is suitable for calculating anion electron detachment energies for the third row transition metal compounds, but not for the first row transition metal compounds. This arises because the bonding in the heavier atoms has more ionic character where the atomic correlation energy is easier to treat.

For the BP86 method, the calculated ADE and VDE for band X of $\text{Cr}_4\text{O}_{10}^-$ are within 0.2 eV of the experimental values (Table 4), and those for $\text{W}_4\text{O}_{10}^-$ for bands X and A are also within 0.1-0.3 eV from the experimental values (Tables 5 and 6), so the BP86 method yields accurate ADEs and VDEs for both $\text{Cr}_4\text{O}_{10}^-$ and $\text{W}_4\text{O}_{10}^-$. In our previous study (Ref. 21), we showed that the VDEs calculated at the BP86 level are within 0.3 eV from the experimental values for bands X, A, B for Cr_3O_8^- , and within 0.1 eV from the experimental value for band X for W_3O_8^- . Thus the BP86 method is suitable for calculating anion electron detachment energies for the third row as well as the first row transition metal compounds, although the errors can increase somewhat for the higher energy band systems.

As shown in Table 7, the triplet excitation energy calculated at the TD-DFT level with the B3LYP functional for the $^3\text{E} \leftarrow ^1\text{A}_1$ excitation for Cr_4O_{10} is within 0.2 eV of the

experimental ΔE_{vert} value for band A. For W_4O_{10} , the triplet excitation energies at the above level of theory for the four lowest energy excitations are within 0.2-0.3 eV from the experimental ΔE_{vert} values for bands A and C. The $(^3\text{B}_2 \text{ } \boldsymbol{b}) \leftarrow ^1\text{A}_1$, $(^3\text{A}_1 \text{ } \boldsymbol{a}) \leftarrow ^1\text{A}_1$, and $(^3\text{A}_1 \text{ } \boldsymbol{b}) \leftarrow ^1\text{A}_1$ transitions are predicted to have similar TD-DFT triplet excitation energies with the B3LYP functional, consistent with calculated self-consistent excitation energies at the CCSD(T) level.

For the BP86 functional, the TD-DFT triplet excitation energy for the $^3\text{E} \leftarrow ^1\text{A}_1$ excitation for Cr_4O_{10} is lower than the experimental ΔE_{vert} value by ~ 0.4 eV. For W_4O_{10} , the TD-DFT triplet excitation energy for the $^3\text{B}_2 \leftarrow ^1\text{A}_1$ transition calculated at the BP86 level is within 0.3 eV of the experimental ΔE_{vert} value for band A. However, those calculated for the $(^3\text{B}_2 \text{ } \boldsymbol{b}) \leftarrow ^1\text{A}_1$ and $(^3\text{A}_1 \text{ } \boldsymbol{a}) \leftarrow ^1\text{A}_1$ transitions are substantially lower than the experimental ΔE_{vert} value for band C by > 1.3 eV, whereas those for the $(^3\text{A}_1 \text{ } \boldsymbol{b}) \leftarrow ^1\text{A}_1$, $^3\text{A}_2 \leftarrow ^1\text{A}_1$, and $^3\text{B}_1 \leftarrow ^1\text{A}_1$ transitions also deviate from experimental band C by ~ 0.5 eV. Thus, the TD-DFT excitation energies calculated with the B3LYP functional appear to be in better agreement with the experimental ΔE_{vert} value than those with the BP86 functional.

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Table S1. Calculated Relative Energies at 0 K in kcal/mol for Different Electronic States of Cr_4O_{10} and $\text{Cr}_4\text{O}_{10}^-$ at the CCSD(T)/aVDZ//BP86/aVDZ Level

Cr_4O_{10}	Relative Energy	$\text{Cr}_4\text{O}_{10}^-$	Relative Energy
$^1\text{A}_1/\text{T}_d (\text{A})$	0.0	$^2\text{A}_1/\text{T}_d (\text{A})$	0.0
$^3\text{B}_2/\text{D}_{2d} (\text{A})$	38.6	$^2\text{A}_2/\text{D}_{2d} (\text{A})$	1.7
$^3\text{A}_2/\text{D}_{2d} (\text{A})$	39.5	$^2\text{A}_2/\text{C}_{3v} (\text{A})$	29.2
$^5\text{B}_1/\text{D}_{2d} (\text{A})$	61.0	$^4\text{B}_1/\text{D}_{2d} (\text{A})$	–
$^5\text{A}_1/\text{C}_{3v} (\text{A})$	–	$^4\text{A}_1/\text{D}_{2d} (\text{A})$	27.9
$^1\text{A}_1/\text{C}_{2v} (\text{B})$	104.1	$^6\text{A}_1/\text{T}_d (\text{A})$	45.0

Table S2. Calculated Relative Energies at 0 K in kcal/mol for Different Electronic States of W_4O_{10} and $\text{W}_4\text{O}_{10}^-$ at the CCSD(T)/aVDZ//BP86/aVDZ Level

W_4O_{10}	Relative Energy	$\text{W}_4\text{O}_{10}^-$	Relative Energy
$^1\text{A}_1/\text{C}_{2v}$ (B)	0.0	$^2\text{A}_1/\text{C}_{2v}$ (B)	0.0
$^1\text{A}_1/\text{T}_d$ (A)	10.8	$^2\text{B}_u/\text{C}_{2h}$ (C)	22.1
$^1\text{A}_g/\text{C}_{2h}$ (C)	12.1	$^2\text{A}_1/\text{T}_d$ (A)	59.7
$^3\text{B}_2/\text{C}_{2v}$ (B)	29.3	$^2\text{A}/\text{C}_3$ (A)	–
$^3\text{B}_g/\text{C}_{2h}$ (C)	39.7		

Table S3: Calculated Relative Energies at 0 K in kcal/mol for the Various Electronic States of W_4O_{10} and $W_4O_{10}^-$

State	CCSD(T) ^a	CCSD(T) ^b	B3LYP ^c	BP86 ^d	$\langle S^2 \rangle$ ^e	T_1 ^f
W_4O_{10}						
$^3A_1/D_{2d}$ (A)	35.1	35.0	40.7	35.0	2.01	0.030
$^3B_1/D_{2d}$ (A)	62.0	57.6	40.5	34.9	2.01	0.033
$^3A_2/D_{2d}$ (A)	–	–	37.2	38.7	2.01	–
$^3B_2/D_{2d}$ (A)	–	–	36.0	38.1	2.01	–
$^5B_1/D_{2d}$ (A)	52.7	52.6	45.9	53.2	6.03	0.035
$^5B_2/D_{2d}$ (A)	64.2	63.9	60.6	59.0	6.02	0.032
$^5A_1/C_{3v}$ (A)	–	–	43.4	55.3	6.02	–
$^5A_2/C_{3v}$ (A)	–	–	44.8	51.8	6.02	–
$W_4O_{10}^-$						
$^2A_2/D_{2d}$ (A)	66.5	66.8	73.5	71.4	0.75	0.029
$^2A_2/C_{3v}$ (A)	65.8	–	67.2	68.8	0.78	0.070
$^4B_1/D_{2d}$ (A)	–	–	82.7	85.2	3.78	–
$^4B_2/D_{2d}$ (A)	–	–	91.4	87.0	3.76	–
$^6A_1/T_d$ (A)	104.5	105.1	93.1	104.0	8.77	0.031

^a CCSD(T)/aVDZ//B3LYP/aVDZ with ZPEs from BP86/aVDZ.

^b CCSD(T)/aVDZ//BP86/aVDZ.

^c B3LYP/aVTZ//B3LYP/aVDZ with ZPEs from BP86/aVDZ.

^d BP86/aVTZ//BP86/aVDZ.

^e B3LYP/aVDZ.

^f CCSD(T)/aVDZ//BP86/aVDZ.

Table S4. Calculated Adiabatic and Vertical Electron Detachment Energies (ADEs and VDEs in eV) for Different Electronic States of $\text{Cr}_4\text{O}_{10}^-$ at the CCSD(T)/aVDZ//BP86/aVDZ Level

Transition	ADEs	VDEs
$^1\text{A}_1/\text{T}_d \leftarrow ^2\text{A}_2/\text{C}_{3v} (\text{A})$	3.35	3.36
$^3\text{B}_2/\text{D}_{2d} \leftarrow ^2\text{A}_2/\text{C}_{3v} (\text{A})$	5.07	—
$^3\text{A}_2/\text{D}_{2d} \leftarrow ^2\text{A}_2/\text{C}_{3v} (\text{A})$	5.09	—
$^1\text{A}_1/\text{T}_d \leftarrow ^2\text{A}_2/\text{D}_{2d} (\text{A})$	2.97	3.09
$^3\text{B}_2/\text{D}_{2d} \leftarrow ^2\text{A}_2/\text{D}_{2d} (\text{A})$	4.69	—
$^3\text{A}_2/\text{D}_{2d} \leftarrow ^2\text{A}_2/\text{D}_{2d} (\text{A})$	4.71	—
$^1\text{A}_1/\text{T}_d \leftarrow ^2\text{A}_1/\text{T}_d (\text{A})$	3.06	3.39
$^3\text{B}_2/\text{D}_{2d} \leftarrow ^2\text{A}_1/\text{T}_d (\text{A})$	4.78	—
$^3\text{A}_2/\text{D}_{2d} \leftarrow ^2\text{A}_1/\text{T}_d (\text{A})$	4.80	—
$^3\text{B}_2/\text{D}_{2d} \leftarrow ^4\text{A}_1/\text{D}_{2d} (\text{A})$	3.52	—
$^3\text{A}_2/\text{D}_{2d} \leftarrow ^4\text{A}_1/\text{D}_{2d} (\text{A})$	3.55	—
$^5\text{B}_1/\text{D}_{2d} \leftarrow ^4\text{A}_1/\text{D}_{2d} (\text{A})$	4.53	—
$^5\text{A}_1/\text{C}_{3v} \leftarrow ^4\text{A}_1/\text{D}_{2d} (\text{A})$	—	—
$^3\text{B}_2/\text{D}_{2d} \leftarrow ^4\text{B}_1/\text{D}_{2d} (\text{A})$	3.44	—
$^3\text{A}_2/\text{D}_{2d} \leftarrow ^4\text{B}_1/\text{D}_{2d} (\text{A})$	3.46	—
$^5\text{B}_1/\text{D}_{2d} \leftarrow ^4\text{B}_1/\text{D}_{2d} (\text{A})$	4.44	—
$^5\text{A}_1/\text{C}_{3v} \leftarrow ^4\text{B}_1/\text{D}_{2d} (\text{A})$	—	—
$^5\text{B}_1/\text{D}_{2d} \leftarrow ^6\text{A}_1/\text{T}_d (\text{A})$	3.75	—
$^5\text{A}_1/\text{C}_{3v} \leftarrow ^6\text{A}_1/\text{T}_d (\text{A})$	—	—

Table S5. Calculated Adiabatic and Vertical Electron Detachment Energies (ADEs and VDEs in eV) for Different Electronic States of $W_4O_{10}^-$ at the CCSD(T)/aVDZ//BP86/aVDZ Level

Transition	ADEs	VDEs
$^1A_1/C_{2v} \leftarrow ^2A_1/C_{2v}$ (B)	4.17	4.52
$^1A_g/C_{2h} \leftarrow ^2B_u/C_{2h}$ (C)	3.74	4.19
$^1A_1/T_d \leftarrow ^2A_1/T_d$ (A)	2.05	2.87

Table S6. Calculated Vertical Electron Detachment Energies (VDEs in eV) to the Excited States of the Neutral Cluster for the Ground State of $\text{W}_4\text{O}_{10}^-$ at the CCSD(T)/aVDZ//BP86/aVDZ Level ^a

Transition	VDEs
$^3\text{B}_2 \leftarrow ^2\text{A}_1/\text{C}_{2v} (\text{B})$	5.91
$^1\text{B}_2 \leftarrow ^2\text{A}_1/\text{C}_{2v} (\text{B})$ ^b	6.53
$(^3\text{B}_2 \text{ b}) \leftarrow ^2\text{A}_1/\text{C}_{2v} (\text{B})$	7.28
$(^3\text{A}_1 \text{ a}) \leftarrow ^2\text{A}_1/\text{C}_{2v} (\text{B})$	7.29 (7.32)
$(^3\text{A}_1 \text{ b}) \leftarrow ^2\text{A}_1/\text{C}_{2v} (\text{B})$	7.42 (7.86)
$^3\text{A}_2 \leftarrow ^2\text{A}_1/\text{C}_{2v} (\text{B})$	7.57 (7.25)
$^3\text{B}_1 \leftarrow ^2\text{A}_1/\text{C}_{2v} (\text{B})$	7.73 (7.78)

^a Those in the parentheses are for the transitions to the corresponding open-shell singlet states.

^b The $^1\text{B}_2$ state is an open-shell singlet state corresponding to the $^3\text{B}_2$ state.

Table S7. Calculated Vertical Excitation Energies in eV of W₄O₁₀ at the Self-Consistent Level at the Ground State Geometries of the Anion with the CCSD(T)/aVDZ//BP86/aVDZ Method ^a

Excitation	ΔE_{vert}
$^3\text{B}_2 \leftarrow ^1\text{A}_1$	1.39
$^1\text{B}_2 \leftarrow ^1\text{A}_1$ ^b	2.01
$(^3\text{B}_2 \textit{b}) \leftarrow ^1\text{A}_1$	2.76
$(^3\text{A}_1 \textit{a}) \leftarrow ^1\text{A}_1$	2.77 (2.80)
$(^3\text{A}_1 \textit{b}) \leftarrow ^1\text{A}_1$	2.89 (3.33)
$^3\text{A}_2 \leftarrow ^1\text{A}_1$	3.05 (2.73)
$^3\text{B}_1 \leftarrow ^1\text{A}_1$	3.21 (3.26)

^a Defined as the difference between the vertical electron detachment energies to the excited and ground states of the neutral. Numbers in the parentheses are for the corresponding open-shell singlet states.

^b The $^1\text{B}_2$ state is an open-shell singlet state corresponding to the $^3\text{B}_2$ state.

Table S8: Clustering Energies ^a at 0 K (ΔE_{0K}) and Heats of Formation ^b at 0 and 298 K ($\Delta_f H_{0K}$ and $\Delta_f H_{298K}$) in kcal/mol for the Ground States of Cr_4O_{10} ($^1A_1/T_d$ (**A**)) and W_4O_{10} ($^1A_1/C_{2v}$ (**B**)) Calculated at the CCSD(T) Level

	$\Delta E_{n=D}^c$	$\Delta E_{n=T}^c$	$\Delta E_{CV,wCVTZ}^c$	ΔE_{ZPE}^d	ΔE_{0K}^e	$\Delta_f H_{0K}^f$	$\Delta_f H_{298K}^g$
Cr_4O_{10}	340.34	349.10	+0.88	-7.01	343.0	-499.6	-504.4
W_4O_{10}	346.34	350.45	+1.69	-3.93	348.2	-509.8	-513.5

^a Equation (1): $\Delta E(M_4O_{10}) = 2 E(MO_2) + 2 E(MO_3) - E(M_4O_{10})$.

^b Error bars due to errors in the experimental heats of formation of the atoms are ± 4 kcal/mol for Cr_4O_{10} and ± 6 kcal/mol for W_4O_{10} .

^c Geometries from B3LYP/aVDZ.

^d BP86/aVDZ.

^e $\Delta E_{0K} = \Delta E_{n=T} + \Delta E_{CV,wCVTZ} + \Delta E_{ZPE}$.

^f Equation (2): $\Delta_f H_{0K} (M_4O_{10}) = 2 \Delta_f H_{0K} (MO_2) + 2 \Delta_f H_{0K} (MO_3) - \Delta E_{0K} (M_4O_{10})$, using calculated heats of formation of the monomers from Table 9 and calculated clustering energies.

^g $\Delta_f H_{298K} [M_mO_n] = \Delta_f H_{0K} [M_mO_n] + \Delta H_{0K \rightarrow 298K} [M_mO_n] - m \Delta H_{0K \rightarrow 298K} (M) - n \Delta H_{0K \rightarrow 298K} (O)$. $\Delta H_{0K \rightarrow 298K}$ 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 level.

Table S9: Zero-point energies (ZPE) at the BP86/aVDZ level, electronic energies (E_e) at the B3LYP/aVTZ//B3LYP/aVDZ, BP86/aVTZ//BP86/aVDZ, CCSD(T)/aVDZ//B3LYP/aVDZ, and CCSD(T)/aVDZ//BP86/aVDZ levels. All energies are shown in Hartree.

State	ZPE ^a	E_e^b	E_e^c	E_e^d	E_e^e
Cr₄O₁₀					
¹ A ₁ /T _d (A)	0.03982	-1099.05342	-1099.58713	-1095.30843	-1095.31172
³ B ₂ /D _{2d} (A)	0.03512	-1099.04806	-1099.56230	-1095.24218	-1095.24394
³ A ₂ /D _{2d} (A)	0.03867	-1099.04192	-1099.55805	-1095.24425	-1095.24655
⁵ B ₁ /D _{2d} (A)	0.03362	-1099.06217	-1099.54644	-1095.20498	-1095.20551
⁵ A ₁ /C _{3v} (A)	0.03544	-1099.07355	-1099.54839	–	–
¹ A ₁ /C _{2v} (B)	0.03827	-1098.95222	-1099.47977	-1095.14094	-1095.14454
Cr₄O₁₀[–]					
² A ₁ /T _d (A)	0.03698	-1099.14829	-1099.68863	-1095.41816	-1095.42139
² A ₂ /D _{2d} (A)	0.04120	-1099.18472	-1099.70820	-1095.41966	-1095.42235
² A ₂ /C _{3v} (A)	0.03647	-1099.24521	-1099.71407	-1095.37111	-1095.43151
⁴ B ₁ /D _{2d} (A)	0.04232	-1099.19215	-1099.69359	–	-1095.37753
⁴ A ₁ /D _{2d} (A)	0.03414	-1099.20745	-1099.70040	-1095.37085	-1095.37243
⁶ A ₁ /T _d (A)	0.03468	-1099.22155	-1099.69204	-1095.34408	-1095.34434
W₄O₁₀					
¹ A ₁ /C _{2v} (B)	0.03428	-1023.25004	-1023.72995	-1019.32259	-1019.32419
¹ A ₁ /T _d (A)	0.03396	-1023.21934	-1023.70440	-1019.30568	-1019.30671
¹ A _g /C _{2h} (C)	0.03426	-1023.22206	-1023.70572	-1019.30325	-1019.30491
³ B ₂ /C _{2v} (B)	0.03359	-1023.21043	-1023.68987	-1019.27483	-1019.27677
³ B _g /C _{2h} (C)	0.03351	-1023.19305	-1023.67195	-1019.25851	-1019.26015
W₄O₁₀[–]					
² A ₁ /C _{2v} (B)	0.03408	-1023.40614	-1023.88670	-1019.47572	-1019.47725
² B _u /C _{2h} (C)	0.03388	-1023.37035	-1023.85301	-1019.44026	-1019.44183
² A ₁ /T _d (A)	0.03240	-1023.28962	-1023.78413	-1019.37879	-1019.38045
² A/C ₃ (A)	0.03186	-1023.30036	-1023.77792	–	–

^a BP86/aVDZ. ^b B3LYP/aVTZ//B3LYP/aVDZ. ^c BP86/aVTZ//BP86/aVDZ.

^e CCSD(T)/aVDZ//B3LYP/aVDZ. ^f CCSD(T)/aVDZ//BP86/aVDZ.

Figure S1. Additional structures for Cr_4O_{10} with relative energies in kcal/mol calculated at the BP86/aVDZ level. This figure compliments Figure 3

Figure S2. Additional structures for $\text{Cr}_4\text{O}_{10}^-$ with relative energies in kcal/mol calculated at the BP86/aVDZ level. This figure compliments Figure 4

Figure S3. Additional structures for W_4O_{10} with relative energies in kcal/mol calculated at the B3LYP/aVDZ level. This figure compliments Figure 5

${}^3B_{3g} / D_{2h} (E), 66.2$

${}^3A'' / C_s (E), 66.3$

${}^1A_1 / C_{2v} (K), 68.0$

${}^3A_u / D_{2h} (E), 72.5$

${}^1A' / C_s (E), 97.4$

${}^1A_1 / C_{2v} (E), 97.4$

Figure S4. Additional structures for $W_4O_{10}^-$ with relative energies in kcal/mol calculated at the BP86/aVDZ level. This figure compliments Figure 6

${}^2A_u / D_{2h} (E), 71.1$

${}^2B_{3g} / D_{2h} (E), 77.2$

${}^4A'' / C_s (E), 104.4$

Figure S5. Lowest few unoccupied and highest few occupied molecular orbitals (LUMOs and HOMOs) for the $^1A_1/T_d$ (**A**) state of Cr_4O_{10}

Figure S6. Lowest few unoccupied and highest few occupied molecular orbitals (LUMOs and HOMOs) for the $^1A_1/C_{2v}$ (**B**) state of W_4O_{10}

HOMO-6, $23a_1$

HOMO-7, $14b_1$

Figure S7. Lowest few unoccupied and highest few occupied molecular orbitals (LUMOs and HOMOs) for the $^1A_g/C_{2h}$ (*C*) state of W_4O_{10} at the B3LYP/aVDZ level

HOMO-5, $20a_g$

HOMO-6, $14a_u$

HOMO-7, $19a_g$

Figure S8. Lowest few unoccupied and highest few occupied molecular orbitals (LUMOs and HOMOs) for the $^1A_1/T_d$ (*A*) state of W_4O_{10} at the B3LYP/aVDZ level

Equilibrium Geometries Optimized at the B3LYP/aVDZ and BP86/aVDZ Levels for Cr_4O_{10} and $\text{Cr}_4\text{O}_{10}^-$.

Cr_4O_{10} , $^1\text{A}_1 / \text{T}_d (\text{A})$, ... $(8\text{a}_1)^2(4\text{t}_1)^6(12\text{t}_2)^6(5\text{e})^4(6\text{e})^4(5\text{t}_1)^0(13\text{t}_2)^0(9\text{a}_1)^0$

B3LYP

CR	-1.074660	1.074660	1.074660
CR	1.074660	-1.074660	1.074660
CR	-1.074660	-1.074660	-1.074660
O	-1.964725	1.964725	1.964725
O	0.000000	1.943001	0.000000
O	0.000000	0.000000	1.943001
O	-1.943001	0.000000	0.000000
O	1.943001	0.000000	0.000000
O	1.964725	-1.964725	1.964725
O	-1.964725	-1.964725	-1.964725
O	0.000000	-1.943001	0.000000
O	0.000000	0.000000	-1.943001
CR	1.074660	1.074660	-1.074660
O	1.964725	1.964725	-1.964725

BP86

CR	-1.075943	1.075943	1.075943
CR	1.075943	-1.075943	1.075943
CR	-1.075943	-1.075943	-1.075943
O	-1.977421	1.977421	1.977421
O	0.000000	1.962477	0.000000
O	0.000000	0.000000	1.962477
O	-1.962477	0.000000	0.000000
O	1.962477	0.000000	0.000000
O	1.977421	-1.977421	1.977421
O	-1.977421	-1.977421	-1.977421
O	0.000000	-1.962477	0.000000
O	0.000000	0.000000	-1.962477
CR	1.075943	1.075943	-1.075943
O	1.977421	1.977421	-1.977421

Cr_4O_{10} , $^3\text{B}_2 / \text{D}_{2d} (\text{A})$, ... $(14\text{a}_1)^2(6\text{b}_1)^1(5\text{a}_2)^1(17\text{e})^0$

B3LYP

CR	1.522659	0.000000	1.092025
CR	0.000000	-1.522659	-1.092025
CR	-1.522659	0.000000	1.092025

O	2.763235	0.000000	2.017392
O	1.373622	1.373622	0.000000
O	1.373622	-1.373622	0.000000
O	0.000000	0.000000	1.963908
O	0.000000	0.000000	-1.963908
O	0.000000	-2.763235	-2.017392
O	-2.763235	0.000000	2.017392
O	-1.373622	-1.373622	0.000000
O	-1.373622	1.373622	0.000000
CR	0.000000	1.522659	-1.092025
O	0.000000	2.763235	-2.017392

BP86

CR	1.521272	0.000000	1.091514
CR	0.000000	-1.521272	-1.091514
CR	-1.521272	0.000000	1.091514
O	2.784978	0.000000	2.018252
O	1.386086	1.386086	0.000000
O	1.386086	-1.386086	0.000000
O	0.000000	0.000000	1.980572
O	0.000000	0.000000	-1.980572
O	0.000000	-2.784978	-2.018252
O	-2.784978	0.000000	2.018252
O	-1.386086	-1.386086	0.000000
O	-1.386086	1.386086	0.000000
CR	0.000000	1.521272	-1.091514
O	0.000000	2.784978	-2.018252

Cr₄O₁₀, ³A₂ / D_{2d} (A), ... (6b₁)²(14a₁)¹(5a₂)¹(17e)⁰

B3LYP

CR	1.537096	0.000000	1.068912
CR	0.000000	-1.537096	-1.068912
CR	-1.537096	0.000000	1.068912
O	2.722817	0.000000	2.063396
O	1.397148	1.397148	0.000000
O	1.397148	-1.397148	0.000000
O	0.000000	0.000000	1.894623
O	0.000000	0.000000	-1.894623
O	0.000000	-2.722817	-2.063396
O	-2.722817	0.000000	2.063396
O	-1.397148	-1.397148	0.000000

O	-1.397148	1.397148	0.000000
CR	0.000000	1.537096	-1.068912
O	0.000000	2.722817	-2.063396
BP86			
CR	1.542340	0.000000	1.058698
CR	0.000000	-1.542340	-1.058698
CR	-1.542340	0.000000	1.058698
O	2.734107	0.000000	2.076543
O	1.416291	1.416291	0.000000
O	1.416291	-1.416291	0.000000
O	0.000000	0.000000	1.893842
O	0.000000	0.000000	-1.893842
O	0.000000	-2.734107	-2.076543
O	-2.734107	0.000000	2.076543
O	-1.416291	-1.416291	0.000000
O	-1.416291	1.416291	0.000000
CR	0.000000	1.542340	-1.058698
O	0.000000	2.734107	-2.076543

Cr_4O_{10} , ${}^5\text{B}_1 / \text{D}_{2d}(\text{A})$, ... $(14\text{a}_1)^1(6\text{b}_1)^1(17\text{e})^2(5\text{a}_2)^0$

B3LYP

CR	1.525556	0.000000	1.103474
CR	0.000000	-1.525556	-1.103474
CR	-1.525556	0.000000	1.103474
O	2.868172	0.000000	1.882939
O	1.376911	1.376911	0.000000
O	1.376911	-1.376911	0.000000
O	0.000000	0.000000	1.995897
O	0.000000	0.000000	-1.995897
O	0.000000	-2.868172	-1.882939
O	-2.868172	0.000000	1.882939
O	-1.376911	-1.376911	0.000000
O	-1.376911	1.376911	0.000000
CR	0.000000	1.525556	-1.103474
O	0.000000	2.868172	-1.882939

BP86

CR	1.519965	0.000000	1.104978
CR	0.000000	-1.519965	-1.104978
CR	-1.519965	0.000000	1.104978
O	2.877067	0.000000	1.897950

O	1.378715	1.378715	0.000000
O	1.378715	-1.378715	0.000000
O	0.000000	0.000000	2.028432
O	0.000000	0.000000	-2.028432
O	0.000000	-2.877067	-1.897950
O	-2.877067	0.000000	1.897950
O	-1.378715	-1.378715	0.000000
O	-1.378715	1.378715	0.000000
CR	0.000000	1.519965	-1.104978
O	0.000000	2.877067	-1.897950

Cr₄O₁₀, ⁵A₁ / C_{3v} (A), ...(22e)²(23e)²(5a₂)⁰

B3LYP

CR	0.000000	0.000000	1.993979
CR	0.000000	1.761001	-0.612501
CR	1.525071	-0.880500	-0.612501
O	0.000000	0.000000	3.548612
O	-1.431249	-0.826332	1.071890
O	0.000000	1.652664	1.071890
O	1.431249	-0.826332	1.071890
O	-1.373230	0.792835	-1.157974
O	0.000000	3.173548	-1.253264
O	2.748373	-1.586774	-1.253264
O	1.373230	0.792835	-1.157974
O	0.000000	-1.585670	-1.157974
CR	-1.525071	-0.880500	-0.612501
O	-2.748373	-1.586774	-1.253264

BP86

CR	0.000000	0.000000	1.943183
CR	0.000000	1.760881	-0.610403
CR	1.524968	-0.880440	-0.610403
O	0.000000	0.000000	3.517019
O	-1.407625	-0.812692	1.112360
O	0.000000	1.625385	1.112360
O	1.407625	-0.812692	1.112360
O	-1.383209	0.798596	-1.173141
O	0.000000	3.206668	-1.223532
O	2.777056	-1.603334	-1.223532
O	1.383209	0.798596	-1.173141
O	0.000000	-1.597193	-1.173141

CR	-1.524968	-0.880440	-0.610403
O	-2.777056	-1.603334	-1.223532

$\text{Cr}_4\text{O}_{10}^-, {}^2\text{A}_1 / \text{T}_d (\text{A}), \dots (6\text{e})^4 (9\text{a}_1)^1 (5\text{t}_1)^0 (13\text{t}_2)^0$

B3LYP

CR	-1.052053	1.052053	1.052053
CR	1.052053	-1.052053	1.052053
CR	-1.052053	-1.052053	-1.052053
O	-1.963194	1.963194	1.963194
O	0.000000	1.989892	0.000000
O	0.000000	0.000000	1.989892
O	-1.989892	0.000000	0.000000
O	1.989892	0.000000	0.000000
O	1.963194	-1.963194	1.963194
O	-1.963194	-1.963194	-1.963194
O	0.000000	-1.989892	0.000000
O	0.000000	0.000000	-1.989892
CR	1.052053	1.052053	-1.052053
O	1.963194	1.963194	-1.963194

BP86

CR	-1.053815	1.053815	1.053815
CR	1.053815	-1.053815	1.053815
CR	-1.053815	-1.053815	-1.053815
O	-1.975850	1.975850	1.975850
O	0.000000	2.008016	0.000000
O	0.000000	0.000000	2.008016
O	-2.008016	0.000000	0.000000
O	2.008016	0.000000	0.000000
O	1.975850	-1.975850	1.975850
O	-1.975850	-1.975850	-1.975850
O	0.000000	-2.008016	0.000000
O	0.000000	0.000000	-2.008016
CR	1.053815	1.053815	-1.053815
O	1.975850	1.975850	-1.975850

$\text{Cr}_4\text{O}_{10}^-, {}^2\text{A}_2 / \text{D}_{2d} (\text{A}), \dots (14\text{a}_1)^2 (6\text{b}_1)^2 (5\text{a}_2)^1 (17\text{e})^0$

B3LYP

CR	1.529694	0.000000	1.084951
CR	0.000000	-1.529694	-1.084951
CR	-1.529694	0.000000	1.084951

O	2.766164	0.000000	2.048646
O	1.383812	1.383812	0.000000
O	1.383812	-1.383812	0.000000
O	0.000000	0.000000	1.935195
O	0.000000	0.000000	-1.935195
O	0.000000	-2.766164	-2.048646
O	-2.766164	0.000000	2.048646
O	-1.383812	-1.383812	0.000000
O	-1.383812	1.383812	0.000000
CR	0.000000	1.529694	-1.084951
O	0.000000	2.766164	-2.048646

BP86

CR	1.535307	0.000000	1.081462
CR	0.000000	-1.535307	-1.081462
CR	-1.535307	0.000000	1.081462
O	2.788716	0.000000	2.054357
O	1.398359	1.398359	0.000000
O	1.398359	-1.398359	0.000000
O	0.000000	0.000000	1.944475
O	0.000000	0.000000	-1.944475
O	0.000000	-2.788716	-2.054357
O	-2.788716	0.000000	2.054357
O	-1.398359	-1.398359	0.000000
O	-1.398359	1.398359	0.000000
CR	0.000000	1.535307	-1.081462
O	0.000000	2.788716	-2.054357

Cr₄O₁₀⁻, ²A₂ / C_{3v} (A), ... (22e)⁴(5a₂)¹(23e)⁰

B3LYP

CR	0.000000	1.780338	-0.652820
CR	-1.541818	-0.890169	-0.652820
CR	1.541818	-0.890169	-0.652820
O	0.000000	3.302252	-1.033521
O	0.000000	1.643563	1.077791
O	-1.393398	0.804479	-1.157091
O	1.393398	0.804479	-1.157091
O	-1.423367	-0.821781	1.077791
O	-2.859834	-1.651126	-1.033521
O	2.859834	-1.651126	-1.033521
O	0.000000	-1.608958	-1.157091

O	1.423367	-0.821781	1.077791
CR	0.000000	0.000000	1.909315
O	0.000000	0.000000	3.485901
BP86			
CR	0.000000	1.777157	-0.640923
CR	-1.539063	-0.888578	-0.640923
CR	1.539063	-0.888578	-0.640923
O	0.000000	3.297072	-1.099274
O	0.000000	1.620131	1.138777
O	-1.397830	0.807038	-1.117446
O	1.397830	0.807038	-1.117446
O	-1.403075	-0.810066	1.138777
O	-2.855348	-1.648536	-1.099274
O	2.855348	-1.648536	-1.099274
O	0.000000	-1.614075	-1.117446
O	1.403075	-0.810066	1.138777
CR	0.000000	0.000000	1.854721
O	0.000000	0.000000	3.437976

$\text{Cr}_4\text{O}_{10}^-, {}^4\text{B}_1 / \text{D}_{2d}(\text{A}), \dots (14a_1)^2(6b_1)^2(17e)^2(5a_2)^0$

B3LYP

CR	1.540850	0.000000	1.092383
CR	0.000000	-1.540850	-1.092383
CR	-1.540850	0.000000	1.092383
O	2.808848	0.000000	2.018864
O	1.370856	1.370856	0.000000
O	1.370856	-1.370856	0.000000
O	0.000000	0.000000	2.027493
O	0.000000	0.000000	-2.027493
O	0.000000	-2.808848	-2.018864
O	-2.808848	0.000000	2.018864
O	-1.370856	-1.370856	0.000000
O	-1.370856	1.370856	0.000000
CR	0.000000	1.540850	-1.092383
O	0.000000	2.808848	-2.018864

BP86

CR	1.521098	0.000000	1.110152
CR	0.000000	-1.521098	-1.110152
CR	-1.521098	0.000000	1.110152
O	2.886612	0.000000	1.929451

O	1.368176	1.368176	0.000000
O	1.368176	-1.368176	0.000000
O	0.000000	0.000000	2.050661
O	0.000000	0.000000	-2.050661
O	0.000000	-2.886612	-1.929451
O	-2.886612	0.000000	1.929451
O	-1.368176	-1.368176	0.000000
O	-1.368176	1.368176	0.000000
CR	0.000000	1.521098	-1.110152
O	0.000000	2.886612	-1.929451

$\text{Cr}_4\text{O}_{10}^-, {}^4\text{A}_1 / \text{D}_{2d}(\text{A}), \dots (6b_1)^2(14a_1)^2(17e)^2(5a_2)^0$

B3LYP

CR	1.543495	0.000000	1.078979
CR	0.000000	-1.543495	-1.078979
CR	-1.543495	0.000000	1.078979
O	2.867888	0.000000	1.926686
O	1.400334	1.400334	0.000000
O	1.400334	-1.400334	0.000000
O	0.000000	0.000000	1.927329
O	0.000000	0.000000	-1.927329
O	0.000000	-2.867888	-1.926686
O	-2.867888	0.000000	1.926686
O	-1.400334	-1.400334	0.000000
O	-1.400334	1.400334	0.000000
CR	0.000000	1.543495	-1.078979
O	0.000000	2.867888	-1.926686

BP86

CR	1.543421	0.000000	1.083219
CR	0.000000	-1.543421	-1.083219
CR	-1.543421	0.000000	1.083219
O	2.878547	0.000000	1.949060
O	1.402412	1.402412	0.000000
O	1.402412	-1.402412	0.000000
O	0.000000	0.000000	1.957451
O	0.000000	0.000000	-1.957451
O	0.000000	-2.878547	-1.949060
O	-2.878547	0.000000	1.949060
O	-1.402412	-1.402412	0.000000
O	-1.402412	1.402412	0.000000

CR	0.000000	1.543421	-1.083219
O	0.000000	2.878547	-1.949060

Cr₄O₁₀⁻, ⁶A₁ / T_d (**A**), ...(6e)²(5t₁)³

B3LYP

CR	-1.091643	1.091643	1.091643
CR	1.091643	-1.091643	1.091643
CR	-1.091643	-1.091643	-1.091643
O	-2.003918	2.003918	2.003918
O	0.000000	1.973301	0.000000
O	0.000000	0.000000	1.973301
O	-1.973301	0.000000	0.000000
O	1.973301	0.000000	0.000000
O	2.003918	-2.003918	2.003918
O	-2.003918	-2.003918	-2.003918
O	0.000000	-1.973301	0.000000
O	0.000000	0.000000	-1.973301
CR	1.091643	1.091643	-1.091643
O	2.003918	2.003918	-2.003918

BP86

CR	-1.090639	1.090639	1.090639
CR	1.090639	-1.090639	1.090639
CR	-1.090639	-1.090639	-1.090639
O	-2.012684	2.012684	2.012684
O	0.000000	1.984968	0.000000
O	0.000000	0.000000	1.984968
O	-1.984968	0.000000	0.000000
O	1.984968	0.000000	0.000000
O	2.012684	-2.012684	2.012684
O	-2.012684	-2.012684	-2.012684
O	0.000000	-1.984968	0.000000
O	0.000000	0.000000	-1.984968
CR	1.090639	1.090639	-1.090639
O	2.012684	2.012684	-2.012684

Cr₄O₁₀, ¹A₁ / C_{2v} (**B**), ...(15b₁)²(23a₁)²(10a₂)²(24a₁)²(18b₂)²(19b₂)²(25a₁)⁰

B3LYP

O	0.000000	2.726811	-2.079714
O	0.000000	3.659252	0.288493
O	1.519180	1.460412	-0.243096

O	-1.519180	1.460412	-0.243096
O	0.000000	-3.659252	0.288493
O	0.000000	-2.726811	-2.079714
O	-1.519180	-1.460412	-0.243096
O	-1.539127	0.000000	2.112595
O	1.539127	0.000000	2.112595
O	1.519180	-1.460412	-0.243096
CR	1.161655	0.000000	0.619958
CR	-1.161655	0.000000	0.619958
CR	0.000000	2.357410	-0.565019
CR	0.000000	-2.357410	-0.565019
BP86			
O	0.000000	2.650936	-2.103923
O	0.000000	3.657881	0.275727
O	1.563124	1.462046	-0.233841
O	-1.563124	1.462046	-0.233841
O	0.000000	-3.657881	0.275727
O	0.000000	-2.650936	-2.103923
O	-1.563124	-1.462046	-0.233841
O	-1.559711	0.000000	2.129421
O	1.559711	0.000000	2.129421
O	1.563124	-1.462046	-0.233841
CR	1.186603	0.000000	0.614615
CR	-1.186603	0.000000	0.614615
CR	0.000000	2.320205	-0.559130
CR	0.000000	-2.320205	-0.559130

Equilibrium Geometries Optimized at the B3LYP/aVDZ and BP86/aVDZ Levels for W_4O_{10} and $W_4O_{10}^-$.

W_4O_{10} , $^1A_1 / C_{2v} (B)$, ... $(15b_1)^2(10a_2)^2(24a_1)^2(18b_2)^2(19b_2)^2(25a_1)^0$

B3LYP

W	0.000000	2.546614	-0.601237
W	0.000000	-2.546614	-0.601237
W	-1.317311	0.000000	0.628565
O	0.000000	2.958130	-2.260569
O	0.000000	3.980331	0.323389
O	1.684519	1.605287	-0.294456
O	-1.684519	1.605287	-0.294456
O	0.000000	-3.980331	0.323389
O	0.000000	-2.958130	-2.260569
O	-1.684519	-1.605287	-0.294456
O	-1.707726	0.000000	2.273309
W	1.317311	0.000000	0.628565
O	1.707726	0.000000	2.273309
O	1.684519	-1.605287	-0.294456

BP86

W	0.000000	2.512319	-0.592592
W	0.000000	-2.512319	-0.592592
W	-1.320671	0.000000	0.619839
O	0.000000	2.888099	-2.273876
O	0.000000	3.982576	0.299412
O	1.719123	1.613640	-0.279058
O	-1.719123	1.613640	-0.279058
O	0.000000	-3.982576	0.299412
O	0.000000	-2.888099	-2.273876
O	-1.719123	-1.613640	-0.279058
O	-1.701108	0.000000	2.280551
W	1.320671	0.000000	0.619839
O	1.701108	0.000000	2.280551
O	1.719123	-1.613640	-0.279058

W_4O_{10} , $^3B_2 / C_{2v} (B)$, ... $(19b_2)^1(25a_1)^1$

B3LYP

W	0.000000	2.532628	-0.673845
W	0.000000	-2.532628	-0.673845
W	-1.325919	0.000000	0.707006

O	0.000000	2.702728	-2.371235
O	0.000000	4.089269	0.025643
O	1.653541	1.643041	-0.154670
O	-1.653541	1.643041	-0.154670
O	0.000000	-4.089269	0.025643
O	0.000000	-2.702728	-2.371235
O	-1.653541	-1.643041	-0.154670
O	-1.798491	0.000000	2.348186
W	1.325919	0.000000	0.707006
O	1.798491	0.000000	2.348186
O	1.653541	-1.643041	-0.154670

BP86

W	0.000000	2.480761	0.664496
W	0.000000	-2.480761	0.664496
W	1.335269	0.000000	-0.697984
O	0.000000	2.655555	2.374632
O	0.000000	4.052389	-0.035269
O	-1.697068	1.638845	0.159673
O	1.697068	1.638845	0.159673
O	0.000000	-4.052389	-0.035269
O	0.000000	-2.655555	2.374632
O	1.697068	-1.638845	0.159673
O	1.815291	0.000000	-2.348949
W	-1.335269	0.000000	-0.697984
O	-1.815291	0.000000	-2.348949
O	-1.697068	-1.638845	0.159673

W₄O₁₀⁻, ²A₁ / C_{2v} (**B**), ... (19b₂)²(25a₁)¹

B3LYP

W	0.000000	2.412202	-0.626434
W	0.000000	-2.412202	-0.626434
W	-1.290490	0.000000	0.658737
O	0.000000	2.657494	-2.332934
O	0.000000	3.927170	0.196677
O	1.734894	1.613479	-0.238289
O	-1.734894	1.613479	-0.238289
O	0.000000	-3.927170	0.196677
O	0.000000	-2.657494	-2.332934
O	-1.734894	-1.613479	-0.238289
O	-1.752335	0.000000	2.314027

W	1.290490	0.000000	0.658737
O	1.752335	0.000000	2.314027
O	1.734894	-1.613479	-0.238289

BP86

W	0.000000	2.402210	-0.619256
W	0.000000	-2.402210	-0.619256
W	-1.293040	0.000000	0.650031
O	0.000000	2.656471	-2.337448
O	0.000000	3.929797	0.208527
O	1.753587	1.620402	-0.237319
O	-1.753587	1.620402	-0.237319
O	0.000000	-3.929797	0.208527
O	0.000000	-2.656471	-2.337448
O	-1.753587	-1.620402	-0.237319
O	-1.749984	0.000000	2.318891
W	1.293040	0.000000	0.650031
O	1.749984	0.000000	2.318891
O	1.753587	-1.620402	-0.237319

$W_4O_{10}^{2-}, {}^1A_1 / C_{2v} (B), \dots (19b_2)^2(25a_1)^2$

B3LYP

W	0.000000	2.297806	0.663877
W	0.000000	-2.297806	0.663877
W	1.273451	0.000000	-0.701089
O	0.000000	2.496209	2.394193
O	0.000000	3.827629	-0.177392
O	-1.766287	1.587982	0.240710
O	1.766287	1.587982	0.240710
O	0.000000	-3.827629	-0.177392
O	0.000000	-2.496209	2.394193
O	1.766287	-1.587982	0.240710
O	1.838221	0.000000	-2.354004
W	-1.273451	0.000000	-0.701089
O	-1.838221	0.000000	-2.354004
O	-1.766287	-1.587982	0.240710

BP86

W	0.000000	2.303076	0.655252
W	0.000000	-2.303076	0.655252
W	1.275510	0.000000	-0.690359
O	0.000000	2.524543	2.395699

O	0.000000	3.838006	-0.203106
O	-1.778699	1.597550	0.245384
O	1.778699	1.597550	0.245384
O	0.000000	-3.838006	-0.203106
O	0.000000	-2.524543	2.395699
O	1.778699	-1.597550	0.245384
O	1.827907	0.000000	-2.358622
W	-1.275510	0.000000	-0.690359
O	-1.827907	0.000000	-2.358622
O	-1.778699	-1.597550	0.245384

W₄O₁₀, ¹A_g / C_{2h} (C), ... (20a_g)²(18b_u)²(13b_g)²(14b_g)²(19b_u)²(15a_u)²(20b_u)⁰

B3LYP

W	0.447050	1.206175	0.000000
W	-0.447050	-1.206175	0.000000
O	2.075131	0.740808	0.000000
O	-2.075131	-0.740808	0.000000
O	0.000000	1.722464	1.772535
O	0.000000	1.722464	-1.772535
O	0.000000	-1.722464	1.772535
O	0.000000	-1.722464	-1.772535
W	0.000000	0.000000	2.733620
W	0.000000	0.000000	-2.733620
O	1.388857	0.009636	3.727778
O	-1.388857	-0.009636	3.727778
O	1.388857	0.009636	-3.727778
O	-1.388857	-0.009636	-3.727778

BP86

W	0.449610	1.210747	0.000000
W	-0.449610	-1.210747	0.000000
O	2.092556	0.748803	0.000000
O	-2.092556	-0.748803	0.000000
O	0.000000	1.744709	1.770945
O	0.000000	1.744709	-1.770945
O	0.000000	-1.744709	1.770945
O	0.000000	-1.744709	-1.770945
W	0.000000	0.000000	2.707752
W	0.000000	0.000000	-2.707752
O	1.397237	0.007900	3.713344
O	-1.397237	-0.007900	3.713344

O	1.397237	0.007900	-3.713344
O	-1.397237	-0.007900	-3.713344

W₄O₁₀, ³B_g / C_{2h} (C), ... (15a_u)¹ (20b_u)¹

B3LYP

W	0.505187	1.223362	0.000000
W	-0.505187	-1.223362	0.000000
O	2.193497	1.016635	0.000000
O	-2.193497	-1.016635	0.000000
O	0.000000	1.605552	1.801805
O	0.000000	1.605552	-1.801805
O	0.000000	-1.605552	1.801805
O	0.000000	-1.605552	-1.801805
W	0.000000	0.000000	2.886057
W	0.000000	0.000000	-2.886057
O	1.382495	-0.017225	3.886527
O	-1.382495	0.017225	3.886527
O	1.382495	-0.017225	-3.886527
O	-1.382495	0.017225	-3.886527

BP86

W	0.504181	1.230855	0.000000
W	-0.504181	-1.230855	0.000000
O	2.206980	1.025168	0.000000
O	-2.206980	-1.025168	0.000000
O	0.000000	1.650891	1.792486
O	0.000000	1.650891	-1.792486
O	0.000000	-1.650891	1.792486
O	0.000000	-1.650891	-1.792486
W	0.000000	0.000000	2.828447
W	0.000000	0.000000	-2.828447
O	1.390397	-0.024524	3.840447
O	-1.390397	0.024524	3.840447
O	1.390397	-0.024524	-3.840447
O	-1.390397	0.024524	-3.840447

W₄O₁₀⁻, ²B_u / C_{2h} (C), ... (15a_u)² (20b_u)¹

B3LYP

W	0.450282	1.199178	0.000000
W	-0.450282	-1.199178	0.000000
O	2.159472	1.053337	0.000000

O	-2.159472	-1.053337	0.000000
O	0.000000	1.705427	1.803806
O	0.000000	1.705427	-1.803806
O	0.000000	-1.705427	1.803806
O	0.000000	-1.705427	-1.803806
W	0.000000	0.000000	2.728278
W	0.000000	0.000000	-2.728278
O	1.405531	-0.009981	3.725900
O	-1.405531	0.009981	3.725900
O	1.405531	-0.009981	-3.725900
O	-1.405531	0.009981	-3.725900

BP86

W	0.449117	1.205063	0.000000
W	-0.449117	-1.205063	0.000000
O	2.170665	1.057539	0.000000
O	-2.170665	-1.057539	0.000000
O	0.000000	1.725533	1.802813
O	0.000000	1.725533	-1.802813
O	0.000000	-1.725533	1.802813
O	0.000000	-1.725533	-1.802813
W	0.000000	0.000000	2.708116
W	0.000000	0.000000	-2.708116
O	1.414378	-0.012319	3.715923
O	-1.414378	0.012319	3.715923
O	1.414378	-0.012319	-3.715923
O	-1.414378	0.012319	-3.715923

W₄O₁₀²⁻, ¹A_g / C_{2h} (C), ... (15a_u)² (20b_u)²

B3LYP

W	0.441836	1.211306	0.000000
W	-0.441836	-1.211306	0.000000
O	2.174692	1.322223	0.000000
O	-2.174692	-1.322223	0.000000
O	0.000000	1.695442	1.836581
O	0.000000	1.695442	-1.836581
O	0.000000	-1.695442	1.836581
O	0.000000	-1.695442	-1.836581
W	0.000000	0.000000	2.725245
W	0.000000	0.000000	-2.725245
O	1.422465	-0.033657	3.730074

O	-1.422465	0.033657	3.730074
O	1.422465	-0.033657	-3.730074
O	-1.422465	0.033657	-3.730074
BP86			
W	0.439868	1.219577	0.000000
W	-0.439868	-1.219577	0.000000
O	2.184792	1.324375	0.000000
O	-2.184792	-1.324375	0.000000
O	0.000000	1.714394	1.834945
O	0.000000	1.714394	-1.834945
O	0.000000	-1.714394	1.834945
O	0.000000	-1.714394	-1.834945
W	0.000000	0.000000	2.709911
W	0.000000	0.000000	-2.709911
O	1.432390	-0.038158	3.723229
O	-1.432390	0.038158	3.723229
O	1.432390	-0.038158	-3.723229
O	-1.432390	0.038158	-3.723229

$W_4O_{10}, {}^1A_1 / T_d(A), \dots (4t_1)^6(8a_1)^2(12t_2)^6(5e)^4(6e)^4(5t_1)^0(9a_1)^0$

B3LYP

W	-1.197103	1.197103	1.197103
W	1.197103	-1.197103	1.197103
W	-1.197103	-1.197103	-1.197103
O	-2.177995	2.177995	2.177995
O	0.000000	2.073024	0.000000
O	0.000000	0.000000	2.073024
O	-2.073024	0.000000	0.000000
O	2.073024	0.000000	0.000000
O	2.177995	-2.177995	2.177995
O	-2.177995	-2.177995	-2.177995
O	0.000000	-2.073024	0.000000
O	0.000000	0.000000	-2.073024
W	1.197103	1.197103	-1.197103
O	2.177995	2.177995	-2.177995

BP86

W	-1.193985	1.193985	1.193985
W	1.193985	-1.193985	1.193985
W	-1.193985	-1.193985	-1.193985
O	-2.181837	2.181837	2.181837

O	0.000000	2.092165	0.000000
O	0.000000	0.000000	2.092165
O	-2.092165	0.000000	0.000000
O	2.092165	0.000000	0.000000
O	2.181837	-2.181837	2.181837
O	-2.181837	-2.181837	-2.181837
O	0.000000	-2.092165	0.000000
O	0.000000	0.000000	-2.092165
W	1.193985	1.193985	-1.193985
O	2.181837	2.181837	-2.181837

$W_4O_{10}, {}^3A_1 / D_{2d} (A), \dots (6b_1)^2(14a_1)^1(15a_1)^1$

B3LYP

W	1.634633	0.000000	1.125149
W	0.000000	1.634633	-1.125149
W	0.000000	-1.634633	-1.125149
O	2.988457	0.000000	2.170599
O	0.000000	0.000000	2.105314
O	1.540287	1.540287	0.000000
O	1.540287	-1.540287	0.000000
O	-1.540287	1.540287	0.000000
O	0.000000	2.988457	-2.170599
O	0.000000	-2.988457	-2.170599
O	0.000000	0.000000	-2.105314
O	-1.540287	-1.540287	0.000000
W	-1.634633	0.000000	1.125149
O	-2.988457	0.000000	2.170599

BP86

W	1.632890	0.000000	1.114987
W	0.000000	1.632890	-1.114987
W	0.000000	-1.632890	-1.114987
O	2.987527	0.000000	2.180119
O	0.000000	0.000000	2.110824
O	1.557682	1.557682	0.000000
O	1.557682	-1.557682	0.000000
O	-1.557682	1.557682	0.000000
O	0.000000	2.987527	-2.180119
O	0.000000	-2.987527	-2.180119
O	0.000000	0.000000	-2.110824
O	-1.557682	-1.557682	0.000000

W	-1.632890	0.000000	1.114987
O	-2.987527	0.000000	2.180119

W₄O₁₀, ³B₁ / D_{2d} (A), ...(14a₁)²(6b₁)¹(15a₁)¹

B3LYP

W	1.600154	0.000000	1.171596
W	0.000000	1.600154	-1.171596
W	0.000000	-1.600154	-1.171596
O	3.040515	0.000000	2.092848
O	0.000000	0.000000	2.213952
O	1.501571	1.501571	0.000000
O	1.501571	-1.501571	0.000000
O	-1.501571	1.501571	0.000000
O	0.000000	3.040515	-2.092848
O	0.000000	-3.040515	-2.092848
O	0.000000	0.000000	-2.213952
O	-1.501571	-1.501571	0.000000
W	-1.600154	0.000000	1.171596
O	-3.040515	0.000000	2.092848

BP86

W	1.592656	0.000000	1.171456
W	0.000000	1.592656	-1.171456
W	0.000000	-1.592656	-1.171456
O	3.045842	0.000000	2.097721
O	0.000000	0.000000	2.239008
O	1.512309	1.512309	0.000000
O	1.512309	-1.512309	0.000000
O	-1.512309	1.512309	0.000000
O	0.000000	3.045842	-2.097721
O	0.000000	-3.045842	-2.097721
O	0.000000	0.000000	-2.239008
O	-1.512309	-1.512309	0.000000
W	-1.592656	0.000000	1.171456
O	-3.045842	0.000000	2.097721

W₄O₁₀, ³B₂ / D_{2d} (A), ...(14a₁)²(6b₁)¹(5a₂)¹(17e)⁰

B3LYP

W	1.687015	0.000000	1.230950
W	0.000000	1.687015	-1.230950
W	0.000000	-1.687015	-1.230950

O	3.028397	0.000000	2.281245
O	0.000000	0.000000	2.101118
O	1.448772	1.448772	0.000000
O	1.448772	-1.448772	0.000000
O	-1.448772	1.448772	0.000000
O	0.000000	3.028397	-2.281245
O	0.000000	-3.028397	-2.281245
O	0.000000	0.000000	-2.101118
O	-1.448772	-1.448772	0.000000
W	-1.687015	0.000000	1.230950
O	-3.028397	0.000000	2.281245

BP86

W	1.683310	0.000000	1.225063
W	0.000000	1.683310	-1.225063
W	0.000000	-1.683310	-1.225063
O	3.041629	0.000000	2.274389
O	0.000000	0.000000	2.121297
O	1.462860	1.462860	0.000000
O	1.462860	-1.462860	0.000000
O	-1.462860	1.462860	0.000000
O	0.000000	3.041629	-2.274389
O	0.000000	-3.041629	-2.274389
O	0.000000	0.000000	-2.121297
O	-1.462860	-1.462860	0.000000
W	-1.683310	0.000000	1.225063
O	-3.041629	0.000000	2.274389

W₄O₁₀, ³A₂ / D_{2d} (A), ... (6b₁)²(14a₁)¹(5a₂)¹(17e)⁰

B3LYP

W	1.718210	0.000000	1.183066
W	0.000000	1.718210	-1.183066
W	0.000000	-1.718210	-1.183066
O	2.973635	0.000000	2.334941
O	0.000000	0.000000	1.971347
O	1.495100	1.495100	0.000000
O	1.495100	-1.495100	0.000000
O	-1.495100	1.495100	0.000000
O	0.000000	2.973635	-2.334941
O	0.000000	-2.973635	-2.334941
O	0.000000	0.000000	-1.971347

O	-1.495100	-1.495100	0.000000
W	-1.718210	0.000000	1.183066
O	-2.973635	0.000000	2.334941
BP86			
W	1.721048	0.000000	1.165177
W	0.000000	1.721048	-1.165177
W	0.000000	-1.721048	-1.165177
O	2.977409	0.000000	2.334420
O	0.000000	0.000000	1.964836
O	1.518377	1.518377	0.000000
O	1.518377	-1.518377	0.000000
O	-1.518377	1.518377	0.000000
O	0.000000	2.977409	-2.334420
O	0.000000	-2.977409	-2.334420
O	0.000000	0.000000	-1.964836
O	-1.518377	-1.518377	0.000000
W	-1.721048	0.000000	1.165177
O	-2.977409	0.000000	2.334420

$\text{W}_4\text{O}_{10}, {}^5\text{B}_1 / \text{D}_{2d}(\text{A}), \dots (6b_1)^1(14a_1)^1(17e)^2(5a_2)^0$

B3LYP

W	1.838040	0.000000	0.982153
W	0.000000	1.838040	-0.982153
W	0.000000	-1.838040	-0.982153
O	3.250299	0.000000	1.940919
O	0.000000	0.000000	1.563063
O	1.626299	1.626299	0.000000
O	1.626299	-1.626299	0.000000
O	-1.626299	1.626299	0.000000
O	0.000000	3.250299	-1.940919
O	0.000000	-3.250299	-1.940919
O	0.000000	0.000000	-1.563063
O	-1.626299	-1.626299	0.000000
W	-1.838040	0.000000	0.982153
O	-3.250299	0.000000	1.940919

BP86

W	1.851133	0.000000	0.939097
W	0.000000	1.851133	-0.939097
W	0.000000	-1.851133	-0.939097
O	3.245179	0.000000	1.942607

O	0.000000	0.000000	1.506706
O	1.662570	1.662570	0.000000
O	1.662570	-1.662570	0.000000
O	-1.662570	1.662570	0.000000
O	0.000000	3.245179	-1.942607
O	0.000000	-3.245179	-1.942607
O	0.000000	0.000000	-1.506706
O	-1.662570	-1.662570	0.000000
W	-1.851133	0.000000	0.939097
O	-3.245179	0.000000	1.942607

W₄O₁₀, ⁵A₁ / C_{3v} (A), ... (22e)²(23e)²(5a₂)⁰

B3LYP

W	0.000000	0.000000	2.205158
W	0.000000	1.952336	-0.707467
W	1.690772	-0.976168	-0.707467
O	0.000000	0.000000	3.911100
O	-1.467954	-0.847524	1.124887
O	0.000000	1.695048	1.124887
O	1.467954	-0.847524	1.124887
O	-1.427609	0.824231	-1.297570
O	0.000000	3.519182	-1.386185
O	3.047701	-1.759591	-1.386185
O	1.427609	0.824231	-1.297570
O	0.000000	-1.648461	-1.297570
W	-1.690772	-0.976168	-0.707467
O	-3.047701	-1.759591	-1.386185

BP86

W	0.000000	0.000000	2.166911
W	0.000000	1.953467	-0.698720
W	1.691752	-0.976734	-0.698720
O	0.000000	0.000000	3.888446
O	-1.464705	-0.845648	1.163254
O	0.000000	1.691296	1.163254
O	1.464705	-0.845648	1.163254
O	-1.435759	0.828936	-1.302105
O	0.000000	3.534229	-1.375448
O	3.060732	-1.767115	-1.375448
O	1.435759	0.828936	-1.302105
O	0.000000	-1.657872	-1.302105

W	-1.691752	-0.976734	-0.698720
O	-3.060732	-1.767115	-1.375448

W₄O₁₀, ⁵B₂ / D_{2d} (A), ... (6b₁)¹(14a₁)¹(5a₂)¹(14a₁)¹(17e)⁰

B3LYP

W	1.640450	0.000000	1.165849
W	0.000000	1.640450	-1.165849
W	0.000000	-1.640450	-1.165849
O	2.947422	0.000000	2.276909
O	0.000000	0.000000	2.127850
O	1.522000	1.522000	0.000000
O	1.522000	-1.522000	0.000000
O	-1.522000	1.522000	0.000000
O	0.000000	2.947422	-2.276909
O	0.000000	-2.947422	-2.276909
O	0.000000	0.000000	-2.127850
O	-1.522000	-1.522000	0.000000
W	-1.640450	0.000000	1.165849
O	-2.947422	0.000000	2.276909

BP86

W	1.633471	0.000000	1.159439
W	0.000000	1.633471	-1.159439
W	0.000000	-1.633471	-1.159439
O	2.956262	0.000000	2.272963
O	0.000000	0.000000	2.147839
O	1.535326	1.535326	0.000000
O	1.535326	-1.535326	0.000000
O	-1.535326	1.535326	0.000000
O	0.000000	2.956262	-2.272963
O	0.000000	-2.956262	-2.272963
O	0.000000	0.000000	-2.147839
O	-1.535326	-1.535326	0.000000
W	-1.633471	0.000000	1.159439
O	-2.956262	0.000000	2.272963

W₄O₁₀, ⁵A₂ / C_{3v} (A), ... (22e)²(5a₂)¹(21a₁)¹(23e)⁰

B3LYP

W	0.000000	0.000000	2.073911
W	0.000000	1.950556	-0.715594
W	1.689231	-0.975278	-0.715594

O	0.000000	0.000000	3.780739
O	-1.453593	-0.839232	1.336756
O	0.000000	1.678464	1.336756
O	1.453593	-0.839232	1.336756
O	-1.615101	0.932479	-0.828176
O	0.000000	3.435298	-1.544141
O	2.975056	-1.717649	-1.544141
O	1.615101	0.932479	-0.828176
O	0.000000	-1.864958	-0.828176
W	-1.689231	-0.975278	-0.715594
O	-2.975056	-1.717649	-1.544141

BP86

W	0.000000	0.000000	2.049873
W	0.000000	1.916416	-0.711673
W	1.659665	-0.958208	-0.711673
O	0.000000	0.000000	3.765645
O	-1.476766	-0.852611	1.305457
O	0.000000	1.705223	1.305457
O	1.476766	-0.852611	1.305457
O	-1.658939	0.957789	-0.844660
O	0.000000	3.458758	-1.453484
O	2.995372	-1.729379	-1.453484
O	1.658939	0.957789	-0.844660
O	0.000000	-1.915578	-0.844660
W	-1.659665	-0.958208	-0.711673
O	-2.995372	-1.729379	-1.453484

W₄O₁₀⁻, ²A₁ / T_d (A), ... (6e)⁴(9a₁)¹(5t₁)⁰

B3LYP

W	-1.151616	1.151616	1.151616
W	1.151616	-1.151616	1.151616
W	-1.151616	-1.151616	-1.151616
O	-2.149986	2.149986	2.149986
O	0.000000	2.157685	0.000000
O	0.000000	0.000000	2.157685
O	-2.157685	0.000000	0.000000
O	2.157685	0.000000	0.000000
O	2.149986	-2.149986	2.149986
O	-2.149986	-2.149986	-2.149986
O	0.000000	-2.157685	0.000000

O	0.000000	0.000000	-2.157685
W	1.151616	1.151616	-1.151616
O	2.149986	2.149986	-2.149986
BP86			
W	-1.151004	1.151004	1.151004
W	1.151004	-1.151004	1.151004
W	-1.151004	-1.151004	-1.151004
O	-2.156364	2.156364	2.156364
O	0.000000	2.172522	0.000000
O	0.000000	0.000000	2.172522
O	-2.172522	0.000000	0.000000
O	2.172522	0.000000	0.000000
O	2.156364	-2.156364	2.156364
O	-2.156364	-2.156364	-2.156364
O	0.000000	-2.172522	0.000000
O	0.000000	0.000000	-2.172522
W	1.151004	1.151004	-1.151004
O	2.156364	2.156364	-2.156364

$\text{W}_4\text{O}_{10}^{-}, {}^2\text{A}_2 / \text{D}_{2d}(\text{A}), \dots (6b_1)^2(14a_1)^2(5a_2)^1(17e)^0$

B3LYP

W	1.707418	0.000000	1.215773
W	0.000000	1.707418	-1.215773
W	0.000000	-1.707418	-1.215773
O	3.040486	0.000000	2.309158
O	0.000000	0.000000	2.050944
O	1.469142	1.469142	0.000000
O	1.469142	-1.469142	0.000000
O	-1.469142	1.469142	0.000000
O	0.000000	3.040486	-2.309158
O	0.000000	-3.040486	-2.309158
O	0.000000	0.000000	-2.050944
O	-1.469142	-1.469142	0.000000
W	-1.707418	0.000000	1.215773
O	-3.040486	0.000000	2.309158

BP86

W	1.707233	0.000000	1.208641
W	0.000000	1.707233	-1.208641
W	0.000000	-1.707233	-1.208641
O	3.051958	0.000000	2.306331

O	0.000000	0.000000	2.062922
O	1.483162	1.483162	0.000000
O	1.483162	-1.483162	0.000000
O	-1.483162	1.483162	0.000000
O	0.000000	3.051958	-2.306331
O	0.000000	-3.051958	-2.306331
O	0.000000	0.000000	-2.062922
O	-1.483162	-1.483162	0.000000
W	-1.707233	0.000000	1.208641
O	-3.051958	0.000000	2.306331

$\text{W}_4\text{O}_{10}^-, {}^2\text{A}_2 / \text{C}_{3v}(\text{A}), \dots (22\text{e})^2(5\text{a}_2)^1(23\text{e})^0$

B3LYP

W	0.000000	0.000000	2.049435
W	0.000000	1.993888	-0.706296
W	1.726757	-0.996944	-0.706296
O	0.000000	0.000000	3.769277
O	-1.468247	-0.847693	1.224580
O	0.000000	1.695386	1.224580
O	1.468247	-0.847693	1.224580
O	-1.478811	0.853792	-1.135544
O	0.000000	3.664554	-1.131317
O	3.173597	-1.832277	-1.131317
O	1.478811	0.853792	-1.135544
O	0.000000	-1.707584	-1.135544
W	-1.726757	-0.996944	-0.706296
O	-3.173597	-1.832277	-1.131317

BP86

W	0.000000	0.000000	2.041463
W	0.000000	1.988917	-0.700184
W	1.722453	-0.994459	-0.700184
O	0.000000	0.000000	3.771263
O	-1.489203	-0.859792	1.236986
O	0.000000	1.719583	1.236986
O	1.489203	-0.859792	1.236986
O	-1.487577	0.858853	-1.130206
O	0.000000	3.657261	-1.181680
O	3.167281	-1.828630	-1.181680
O	1.487577	0.858853	-1.130206
O	0.000000	-1.717706	-1.130206

W	-1.722453	-0.994459	-0.700184
O	-3.167281	-1.828630	-1.181680

$\text{W}_4\text{O}_{10}^-, {}^2\text{A} / \text{C}_3 (\text{A}), \dots (22\text{e})^4 (25\text{a})^1 (23\text{e})^0$

B3LYP

W	0.000000	0.000000	2.037353
W	0.000000	1.988888	-0.697607
W	1.722428	-0.994444	-0.697607
O	0.000000	0.000000	3.759284
O	-1.266251	-1.116244	1.199143
O	-0.333570	1.654728	1.199143
O	1.599822	-0.538483	1.199143
O	-1.512393	0.811632	-1.142233
O	-0.015949	3.653015	-1.138977
O	3.171578	-1.812695	-1.138977
O	1.459090	0.903955	-1.142233
O	0.053303	-1.715587	-1.142233
W	-1.722428	-0.994444	-0.697607
O	-3.155629	-1.840320	-1.138977

BP86

W	0.000000	0.000000	2.024197
W	0.000000	1.981638	-0.688877
W	1.716149	-0.990819	-0.688877
O	0.000000	0.000000	3.754718
O	-1.295565	-1.127233	1.207748
O	-0.328430	1.685609	1.207748
O	1.623995	-0.558376	1.207748
O	-1.506078	0.828196	-1.150560
O	0.036968	3.644175	-1.177922
O	3.137464	-1.854102	-1.177922
O	1.470278	0.890204	-1.150560
O	0.035800	-1.718400	-1.150560
W	-1.716149	-0.990819	-0.688877
O	-3.174432	-1.790072	-1.177922

$\text{W}_4\text{O}_{10}^-, {}^4\text{B}_1 / \text{D}_{2d} (\text{A}), \dots (14\text{a}_1)^2 (6\text{b}_1)^1 (17\text{e})^2 (5\text{a}_2)^0$

B3LYP

W	1.631486	0.000000	1.321592
W	0.000000	1.631486	-1.321592
W	0.000000	-1.631486	-1.321592

O	3.154556	0.000000	2.133494
O	0.000000	0.000000	2.337094
O	1.366520	1.366520	0.000000
O	1.366520	-1.366520	0.000000
O	-1.366520	1.366520	0.000000
O	0.000000	3.154556	-2.133494
O	0.000000	-3.154556	-2.133494
O	0.000000	0.000000	-2.337094
O	-1.366520	-1.366520	0.000000
W	-1.631486	0.000000	1.321592
O	-3.154556	0.000000	2.133494

BP86

W	1.606889	0.000000	1.336710
W	0.000000	1.606889	-1.336710
W	0.000000	-1.606889	-1.336710
O	3.139466	0.000000	2.158278
O	0.000000	0.000000	2.402381
O	1.359617	1.359617	0.000000
O	1.359617	-1.359617	0.000000
O	-1.359617	1.359617	0.000000
O	0.000000	3.139466	-2.158278
O	0.000000	-3.139466	-2.158278
O	0.000000	0.000000	-2.402381
O	-1.359617	-1.359617	0.000000
W	-1.606889	0.000000	1.336710
O	-3.139466	0.000000	2.158278

W₄O₁₀⁻, ⁴B₂ / D_{2d} (A), ... (14a₁)²(6b₁)¹(5a₂)¹(15a₁)¹(17e)⁰

B3LYP

W	1.632552	0.000000	1.200468
W	0.000000	1.632552	-1.200468
W	0.000000	-1.632552	-1.200468
O	3.009944	0.000000	2.255978
O	0.000000	0.000000	2.189376
O	1.498125	1.498125	0.000000
O	1.498125	-1.498125	0.000000
O	-1.498125	1.498125	0.000000
O	0.000000	3.009944	-2.255978
O	0.000000	-3.009944	-2.255978
O	0.000000	0.000000	-2.189376

O	-1.498125	-1.498125	0.000000
W	-1.632552	0.000000	1.200468
O	-3.009944	0.000000	2.255978
BP86			
W	1.635361	0.000000	1.199867
W	0.000000	1.635361	-1.199867
W	0.000000	-1.635361	-1.199867
O	3.028150	0.000000	2.255282
O	0.000000	0.000000	2.201150
O	1.505595	1.505595	0.000000
O	1.505595	-1.505595	0.000000
O	-1.505595	1.505595	0.000000
O	0.000000	3.028150	-2.255282
O	0.000000	-3.028150	-2.255282
O	0.000000	0.000000	-2.201150
O	-1.505595	-1.505595	0.000000
W	-1.635361	0.000000	1.199867
O	-3.028150	0.000000	2.255282

$W_4O_{10}^{-}, {}^6A_1 / T_d(A), \dots (6e)^2(5t_1)^3(9a_1)^0$

B3LYP

W	-1.224024	1.224024	1.224024
W	1.224024	-1.224024	1.224024
W	-1.224024	-1.224024	-1.224024
O	-2.226309	2.226309	2.226309
O	0.000000	2.063989	0.000000
O	0.000000	0.000000	2.063989
O	-2.063989	0.000000	0.000000
O	2.063989	0.000000	0.000000
O	2.226309	-2.226309	2.226309
O	-2.226309	-2.226309	-2.226309
O	0.000000	-2.063989	0.000000
O	0.000000	0.000000	-2.063989
W	1.224024	1.224024	-1.224024
O	2.226309	2.226309	-2.226309

BP86

W	-1.221855	1.221855	1.221855
W	1.221855	-1.221855	1.221855
W	-1.221855	-1.221855	-1.221855
O	-2.230841	2.230841	2.230841

O	0.000000	2.080205	0.000000
O	0.000000	0.000000	2.080205
O	-2.080205	0.000000	0.000000
O	2.080205	0.000000	0.000000
O	2.230841	-2.230841	2.230841
O	-2.230841	-2.230841	-2.230841
O	0.000000	-2.080205	0.000000
O	0.000000	0.000000	-2.080205
W	1.221855	1.221855	-1.221855
O	2.230841	2.230841	-2.230841

$W_4O_{10}^{2-}, {}^1A_1 / T_d(A), \dots (6e)^4(9a_1)^2(5t_1)^0$

B3LYP

W	-1.119856	1.119856	1.119856
W	1.119856	-1.119856	1.119856
W	-1.119856	-1.119856	-1.119856
O	-2.140694	2.140694	2.140694
O	0.000000	2.205370	0.000000
O	0.000000	0.000000	2.205370
O	-2.205370	0.000000	0.000000
O	2.205370	0.000000	0.000000
O	2.140694	-2.140694	2.140694
O	-2.140694	-2.140694	-2.140694
O	0.000000	-2.205370	0.000000
O	0.000000	0.000000	-2.205370
W	1.119856	1.119856	-1.119856
O	2.140694	2.140694	-2.140694

BP86

W	-1.123614	1.123614	1.123614
W	1.123614	-1.123614	1.123614
W	-1.123614	-1.123614	-1.123614
O	-2.151388	2.151388	2.151388
O	0.000000	2.215346	0.000000
O	0.000000	0.000000	2.215346
O	-2.215346	0.000000	0.000000
O	2.215346	0.000000	0.000000
O	2.151388	-2.151388	2.151388
O	-2.151388	-2.151388	-2.151388
O	0.000000	-2.215346	0.000000
O	0.000000	0.000000	-2.215346

W	1.123614	1.123614	-1.123614
O	2.151388	2.151388	-2.151388

Additional Structures Optimized at the B3LYP/aVDZ Levels for Cr_4O_{10} and $\text{Cr}_4\text{O}_{10}^-$.

Cr_4O_{10} , $^1\text{A}_1 / \text{C}_{2v} (\mathbf{B})$

O	0.000000	2.704710	-2.157209
O	0.000000	3.823884	0.149765
O	1.432696	1.514908	-0.162497
O	-1.432696	1.514908	-0.162497
O	0.000000	-3.823884	0.149765
O	0.000000	-2.704710	-2.157209
O	-1.432696	-1.514908	-0.162497
O	-1.648917	0.000000	2.183420
O	1.648917	0.000000	2.183420
O	1.432696	-1.514908	-0.162497
CR	1.387855	0.000000	0.664600
CR	-1.387855	0.000000	0.664600
CR	0.000000	2.464796	-0.614928
CR	0.000000	-2.464796	-0.614928

Cr_4O_{10} , $^1\text{A}_1 / \text{C}_{2v} (\mathbf{B})$

O	0.000000	1.367809	-2.252557
O	0.000000	3.681340	-1.024260
O	1.326976	1.480693	0.224017
O	-1.326976	1.480693	0.224017
O	0.000000	-3.681340	-1.024260
O	0.000000	-1.367809	-2.252557
O	-1.326976	-1.480693	0.224017
O	-1.959027	0.000000	2.423517
O	1.959027	0.000000	2.423517
O	1.326976	-1.480693	0.224017
CR	1.288874	0.000000	1.018934
CR	-1.288874	0.000000	1.018934
CR	0.000000	2.129499	-0.883845
CR	0.000000	-2.129499	-0.883845

Cr_4O_{10} , $^3\text{B}_2 / \text{C}_{2v} (\mathbf{B})$

O	0.000000	2.878218	-2.086366
O	0.000000	3.793673	0.277206
O	1.438687	1.526640	-0.210607
O	-1.438687	1.526640	-0.210607
O	0.000000	-3.793673	0.277206

O	0.000000	-2.878218	-2.086366
O	-1.438687	-1.526640	-0.210607
O	-1.484044	0.000000	2.138041
O	1.484044	0.000000	2.138041
O	1.438687	-1.526640	-0.210607
CR	1.169733	0.000000	0.608422
CR	-1.169733	0.000000	0.608422
CR	0.000000	2.492459	-0.577644
CR	0.000000	-2.492459	-0.577644

$\text{Cr}_4\text{O}_{10}, {}^3\text{A}_2 / \text{C}_{2v} (\mathbf{B})$

O	0.000000	3.220608	-1.919344
O	0.000000	3.598023	0.592806
O	1.431180	1.491876	-0.380991
O	-1.431180	1.491876	-0.380991
O	0.000000	-3.598023	0.592806
O	0.000000	-3.220608	-1.919344
O	-1.431180	-1.491876	-0.380991
O	-1.800597	0.000000	2.017981
O	1.800597	0.000000	2.017981
O	1.431180	-1.491876	-0.380991
CR	1.308268	0.000000	0.553291
CR	-1.308268	0.000000	0.553291
CR	0.000000	2.515949	-0.529778
CR	0.000000	-2.515949	-0.529778

$\text{Cr}_4\text{O}_{10}, {}^3\text{B}_1 / \text{C}_{2v} (\mathbf{B})$

O	0.000000	2.851496	-2.136949
O	0.000000	3.807063	0.223259
O	1.403844	1.511944	-0.224405
O	-1.403844	1.511944	-0.224405
O	0.000000	-3.807063	0.223259
O	0.000000	-2.851496	-2.136949
O	-1.403844	-1.511944	-0.224405
O	-1.576056	0.000000	2.194909
O	1.576056	0.000000	2.194909
O	1.403844	-1.511944	-0.224405
CR	1.303924	0.000000	0.675658
CR	-1.303924	0.000000	0.675658
CR	0.000000	2.495723	-0.619794

CR	0.000000	-2.495723	-0.619794
Cr₄O₁₀, ¹A_g / C_{2h} (C)			
CR	0.464205	1.038613	0.000000
CR	-0.464205	-1.038613	0.000000
O	1.928724	0.532398	0.000000
O	-1.928724	-0.532398	0.000000
O	0.000000	1.568393	1.582184
O	0.000000	1.568393	-1.582184
O	0.000000	-1.568393	1.582184
O	0.000000	-1.568393	-1.582184
CR	0.000000	0.000000	2.516773
CR	0.000000	0.000000	-2.516773
O	1.272336	0.010853	3.414201
O	-1.272336	-0.010853	3.414201
O	1.272336	0.010853	-3.414201
O	-1.272336	-0.010853	-3.414201
Cr₄O₁₀, ³B_u / C_{2h} (C)			
CR	0.641072	1.087978	0.000000
CR	-0.641072	-1.087978	0.000000
O	2.069712	0.507667	0.000000
O	-2.069712	-0.507667	0.000000
O	0.000000	1.414321	1.626375
O	0.000000	1.414321	-1.626375
O	0.000000	-1.414321	1.626375
O	0.000000	-1.414321	-1.626375
CR	0.000000	0.000000	2.691669
CR	0.000000	0.000000	-2.691669
O	1.271828	-0.017971	3.592120
O	-1.271828	0.017971	3.592120
O	1.271828	-0.017971	-3.592120
O	-1.271828	0.017971	-3.592120
Cr₄O₁₀, ¹A₁ / C_{2v} (G)			
CR	0.000000	2.523798	0.006831
O	0.000000	3.489785	-1.215674
O	0.000000	3.348936	1.328597
O	1.426605	1.508701	-0.049303
CR	2.312134	0.000000	-0.033256

CR	0.000000	-2.523798	0.006831
O	3.851398	0.000000	0.064957
O	1.426605	-1.508701	-0.049303
O	0.000000	-3.489785	-1.215674
O	0.000000	-3.348936	1.328597
O	-1.426605	-1.508701	-0.049303
CR	-2.312134	0.000000	-0.033256
O	-1.426605	1.508701	-0.049303
O	-3.851398	0.000000	0.064957

$\text{Cr}_4\text{O}_{10}, {}^3\text{B}_1 / \text{C}_{2v} (\text{G})$

CR	0.000000	2.482006	-0.146793
O	0.000000	3.665451	-1.175991
O	0.000000	3.064193	1.302839
O	1.423392	1.488304	-0.394933
CR	2.248379	0.000000	0.050473
CR	0.000000	-2.482006	-0.146793
O	3.505583	0.000000	0.951977
O	1.423392	-1.488304	-0.394933
O	0.000000	-3.665451	-1.175991
O	0.000000	-3.064193	1.302839
O	-1.423392	-1.488304	-0.394933
CR	-2.248379	0.000000	0.050473
O	-1.423392	1.488304	-0.394933
O	-3.505583	0.000000	0.951977

$\text{Cr}_4\text{O}_{10}^-, {}^2\text{A}_1 / \text{C}_{2v} (\text{B})$

O	0.000000	2.461322	-2.145086
O	0.000000	3.603959	0.230026
O	1.601191	1.428307	-0.198649
O	-1.601191	1.428307	-0.198649
O	0.000000	-3.603959	0.230026
O	0.000000	-2.461322	-2.145086
O	-1.601191	-1.428307	-0.198649
O	-1.560665	0.000000	2.148029
O	1.560665	0.000000	2.148029
O	1.601191	-1.428307	-0.198649
CR	1.162833	0.000000	0.637079
CR	-1.162833	0.000000	0.637079
CR	0.000000	2.252773	-0.582303

CR	0.000000	-2.252773	-0.582303
Cr₄O₁₀⁻, ²A₂ / C_{2v} (B)			
O	0.000000	2.904943	-2.144911
O	0.000000	3.764353	0.345379
O	1.425605	1.473743	-0.261247
O	-1.425605	1.473743	-0.261247
O	0.000000	-3.764353	0.345379
O	0.000000	-2.904943	-2.144911
O	-1.425605	-1.473743	-0.261247
O	-1.650494	0.000000	2.185049
O	1.650494	0.000000	2.185049
O	1.425605	-1.473743	-0.261247
CR	1.297131	0.000000	0.661953
CR	-1.297131	0.000000	0.661953
CR	0.000000	2.511928	-0.616293
CR	0.000000	-2.511928	-0.616293

Cr₄O₁₀⁻, ²B₁ / C_{2v} (B)			
O	0.000000	2.774132	-2.051945
O	0.000000	3.585750	0.409307
O	1.548296	1.470726	-0.309046
O	-1.548296	1.470726	-0.309046
O	0.000000	-3.585750	0.409307
O	0.000000	-2.774132	-2.051945
O	-1.548296	-1.470726	-0.309046
O	-1.714486	0.000000	2.075685
O	1.714486	0.000000	2.075685
O	1.548296	-1.470726	-0.309046
CR	1.226219	0.000000	0.598153
CR	-1.226219	0.000000	0.598153
CR	0.000000	2.330602	-0.536471
CR	0.000000	-2.330602	-0.536471

Cr₄O₁₀⁻, ²B_u / C_{2h} (C)			
CR	0.501217	1.038711	0.000000
CR	-0.501217	-1.038711	0.000000
O	2.041706	0.761714	0.000000
O	-2.041706	-0.761714	0.000000
O	0.000000	1.568914	1.598844

O	0.000000	1.568914	-1.598844
O	0.000000	-1.568914	1.598844
O	0.000000	-1.568914	-1.598844
CR	0.000000	0.000000	2.493383
CR	0.000000	0.000000	-2.493383
O	1.294206	0.001283	3.388334
O	-1.294206	-0.001283	3.388334
O	1.294206	0.001283	-3.388334
O	-1.294206	-0.001283	-3.388334

Additional Structures Optimized at the B3LYP/aVDZ Levels for W_4O_{10} and $W_4O_{10}^-$.

$W_4O_{10}, {}^1A_1 / C_{2v} (B)$

W	0.000000	2.333769	-0.812295
W	0.000000	-2.333769	-0.812295
W	-1.366883	0.000000	0.857188
O	0.000000	2.019173	-2.486901
O	0.000000	4.028276	-0.577457
O	1.609288	1.681596	0.079588
O	-1.609288	1.681596	0.079588
O	0.000000	-4.028276	-0.577457
O	0.000000	-2.019173	-2.486901
O	-1.609288	-1.681596	0.079588
O	-1.917270	0.000000	2.489926
W	1.366883	0.000000	0.857188
O	1.917270	0.000000	2.489926
O	1.609288	-1.681596	0.079588

$W_4O_{10}, {}^1A_g / D_{2h} (D)$

O	0.000000	2.140911	0.000000
O	-1.591040	0.000000	1.448119
O	-1.591040	0.000000	-1.448119
O	1.591040	0.000000	1.448119
O	1.591040	0.000000	-1.448119
O	-3.223995	-2.101268	0.000000
O	0.000000	-2.140911	0.000000
O	3.223995	-2.101268	0.000000
W	1.731542	1.284632	0.000000
W	-1.731542	1.284632	0.000000
W	-1.731542	-1.284632	0.000000
W	1.731542	-1.284632	0.000000
O	3.223995	2.101268	0.000000
O	-3.223995	2.101268	0.000000

$W_4O_{10}, {}^1A_1 / C_{2v} (E)$

W	0.000000	1.469282	-0.114664
W	0.000000	-1.469282	-0.114664
O	-1.218958	0.000000	-0.530991
O	1.218958	0.000000	-0.530991
O	0.000000	1.911205	-1.903395

O	0.000000	1.524562	1.823879
O	0.000000	-1.911205	-1.903395
O	0.000000	-1.524562	1.823879
W	0.000000	0.000000	-2.673703
W	0.000000	0.000000	2.974718
O	-1.364380	0.000000	-3.691353
O	1.364380	0.000000	-3.691353
O	-1.390143	0.000000	3.970306
O	1.390143	0.000000	3.970306

$W_4O_{10}, {}^1A_g / D_{2h} (E)$

W	0.000000	1.152719	0.000000
W	0.000000	-1.152719	0.000000
O	0.000000	0.000000	1.588078
O	0.000000	0.000000	-1.588078
O	-1.829187	1.677438	0.000000
O	1.829187	1.677438	0.000000
O	-1.829187	-1.677438	0.000000
O	1.829187	-1.677438	0.000000
W	-2.848805	0.000000	0.000000
W	2.848805	0.000000	0.000000
O	-3.847333	0.000000	1.385578
O	-3.847333	0.000000	-1.385578
O	3.847333	0.000000	1.385578
O	3.847333	0.000000	-1.385578

$W_4O_{10}, {}^3A_u / D_{2h} (E)$

W	0.000000	1.189937	0.000000
W	0.000000	-1.189937	0.000000
O	0.000000	0.000000	1.568786
O	0.000000	0.000000	-1.568786
O	-1.859360	1.620379	0.000000
O	1.859360	1.620379	0.000000
O	-1.859360	-1.620379	0.000000
O	1.859360	-1.620379	0.000000
W	-2.933595	0.000000	0.000000
W	2.933595	0.000000	0.000000
O	-3.941187	0.000000	1.377329
O	-3.941187	0.000000	-1.377329
O	3.941187	0.000000	1.377329

O	3.941187	0.000000	-1.377329
$W_4O_{10}, {}^3A_{3g} / D_{2h} (E)$			
W	0.000000	1.189396	0.000000
W	0.000000	-1.189396	0.000000
O	0.000000	0.000000	1.545471
O	0.000000	0.000000	-1.545471
O	-1.877338	1.659280	0.000000
O	1.877338	1.659280	0.000000
O	-1.877338	-1.659280	0.000000
O	1.877338	-1.659280	0.000000
W	-2.906193	0.000000	0.000000
W	2.906193	0.000000	0.000000
O	-3.933381	0.000000	1.383108
O	-3.933381	0.000000	-1.383108
O	3.933381	0.000000	1.383108
O	3.933381	0.000000	-1.383108
$W_4O_{10}, {}^1A' / C_s (E)$			
W	0.104095	0.107980	1.471875
W	0.104095	0.107980	-1.471875
O	-1.090658	0.594503	0.000000
O	1.344568	0.426470	0.000000
O	0.104095	1.900083	1.904530
O	-0.096474	-1.819634	1.524804
O	0.104095	1.900083	-1.904530
O	-0.096474	-1.819634	-1.524804
W	0.043454	2.675667	0.000000
W	-0.222770	-2.963052	0.000000
O	-1.303664	3.715226	0.000000
O	1.426006	3.669971	0.000000
O	-1.711075	-3.804310	0.000000
O	1.052495	-4.102077	0.000000
$W_4O_{10}, {}^3A'' / C_s (E)$			
W	-1.216438	-0.088180	0.000000
W	1.161123	-0.018109	0.000000
O	0.046856	0.054640	1.539728
O	0.046856	0.054640	-1.539728
O	-1.690028	-1.943197	0.000000

O	-1.532121	1.891391	0.000000
O	1.680549	-1.836202	0.000000
O	1.602034	1.841687	0.000000
W	0.013389	-2.903424	0.000000
W	0.011105	2.982974	0.000000
O	0.046856	-3.903826	1.382385
O	0.046856	-3.903826	-1.382385
O	0.018616	3.996011	1.379324
O	0.018616	3.996011	-1.379324

$W_4O_{10}, {}^1A_g / C_{2h} (F)$

W	0.623086	2.048559	0.000000
W	-0.623086	-2.048559	0.000000
O	2.154574	2.747479	0.000000
O	-2.154574	-2.747479	0.000000
O	0.000000	1.622219	1.709014
O	0.000000	1.622219	-1.709014
O	0.000000	-1.622219	1.709014
O	0.000000	-1.622219	-1.709014
W	0.000000	0.000000	2.729342
W	0.000000	0.000000	-2.729342
O	1.372712	-0.021533	3.738509
O	-1.372712	0.021533	3.738509
O	1.372712	-0.021533	-3.738509
O	-1.372712	0.021533	-3.738509

$W_4O_{10}, {}^1A_1 / C_{2v} (G)$

W	0.000000	2.731336	-0.163810
W	0.000000	-2.731336	-0.163810
W	-2.204593	0.000000	0.097694
O	0.000000	3.984615	-1.319090
O	0.000000	3.453585	1.379194
O	1.585079	1.691655	-0.416323
O	-1.585079	1.691655	-0.416323
O	0.000000	-3.453585	1.379194
O	0.000000	-3.984615	-1.319090
O	-1.585079	-1.691655	-0.416323
O	-3.289407	0.000000	1.384114
W	2.204593	0.000000	0.097694
O	3.289407	0.000000	1.384114

O	1.585079	-1.691655	-0.416323
$W_4O_{10}, {}^1A_1 / C_{2v} (H)$			
O	0.000000	2.985514	3.065802
O	0.000000	2.384364	0.114944
O	1.379246	2.532582	-2.499973
O	0.000000	0.000000	-1.836545
O	-1.379246	-2.532582	-2.499973
O	0.000000	-2.384364	0.114944
O	0.000000	0.000000	2.509331
O	0.000000	-2.985514	3.065802
W	0.000000	-1.894548	-1.727919
W	0.000000	-1.783758	1.888223
W	0.000000	1.894548	-1.727919
W	0.000000	1.783758	1.888223
O	1.379246	-2.532582	-2.499973
O	-1.379246	2.532582	-2.499973

$W_4O_{10}, {}^1A_g / C_{2h} (I)$			
W	-0.427953	1.380806	1.792711
W	0.427953	-1.380806	-1.792711
W	0.427953	-1.380806	1.792711
O	-2.070715	1.213296	2.212260
O	0.427953	2.143321	3.053670
O	-0.099958	1.945284	0.000000
O	2.070715	-1.213296	-2.212260
O	-0.427953	-2.143321	-3.053670
O	-0.427953	-2.143321	3.053670
O	0.099958	-1.945284	0.000000
O	2.070715	-1.213296	2.212260
W	-0.427953	1.380806	-1.792711
O	-2.070715	1.213296	-2.212260
O	0.427953	2.143321	-3.053670

$W_4O_{10}, {}^1A_g / D_{2h} (I)$			
W	1.852357	1.456106	0.000000
W	-1.852357	-1.456106	0.000000
W	1.852357	-1.456106	0.000000
O	2.736664	1.874317	1.394243
O	2.736664	1.874317	-1.394243

O	0.000000	1.888509	0.000000
O	-2.736664	-1.874317	-1.394243
O	-2.736664	-1.874317	1.394243
O	2.736664	-1.874317	1.394243
O	0.000000	-1.888509	0.000000
O	2.736664	-1.874317	-1.394243
W	-1.852357	1.456106	0.000000
O	-2.736664	1.874317	1.394243
O	-2.736664	1.874317	-1.394243

$W_4O_{10}, {}^1A_1 / C_{2v} (J)$

W	0.000000	0.000000	-2.008039
W	0.000000	0.000000	2.546788
W	0.000000	2.368693	-0.303205
O	-1.384905	0.000000	-2.982949
O	1.384905	0.000000	-2.982949
O	1.378595	0.000000	3.550205
O	-1.378595	0.000000	3.550205
O	-1.405370	3.180929	-0.830968
O	0.000000	1.521478	1.407609
O	1.405370	3.180929	-0.830968
W	0.000000	-2.368693	-0.303205
O	-1.405370	-3.180929	-0.830968
O	1.405370	-3.180929	-0.830968
O	0.000000	-1.521478	1.407609

$W_4O_{10}, {}^1A_1 / C_{2v} (K)$

W	0.000000	2.675555	-0.264848
W	0.000000	-2.675555	-0.264848
W	0.000000	0.000000	2.370635
O	-1.375457	3.678829	-0.178728
O	1.375457	3.678829	-0.178728
O	0.000000	1.821689	-1.992648
O	0.000000	1.514483	1.237716
O	1.375457	-3.678829	-0.178728
O	-1.375457	-3.678829	-0.178728
O	-1.382191	0.000000	3.372871
O	0.000000	-1.514483	1.237716
O	1.382191	0.000000	3.372871
W	0.000000	0.000000	-2.329693

O	0.000000	-1.821689	-1.992648
$W_4O_{10}^-, ^2A_u / C_{2h} (C)$			
W	0.494050	1.242447	0.000000
W	-0.494050	-1.242447	0.000000
O	2.209237	1.336952	0.000000
O	-2.209237	-1.336952	0.000000
O	0.000000	1.617544	1.828291
O	0.000000	1.617544	-1.828291
O	0.000000	-1.617544	1.828291
O	0.000000	-1.617544	-1.828291
W	0.000000	0.000000	2.847216
W	0.000000	0.000000	-2.847216
O	1.398461	-0.034344	3.851656
O	-1.398461	0.034344	3.851656
O	1.398461	-0.034344	-3.851656
O	-1.398461	0.034344	-3.851656
$W_4O_{10}^-, ^2A_1 / C_{2v} (J)$			
W	0.000000	0.000000	-2.152200
W	0.000000	0.000000	2.621279
W	0.000000	2.140140	-0.298397
O	-1.462805	0.000000	-3.060303
O	1.462805	0.000000	-3.060303
O	1.390162	0.000000	3.631126
O	-1.390162	0.000000	3.631126
O	-1.415800	2.991911	-0.759833
O	0.000000	1.531933	1.539529
O	1.415800	2.991911	-0.759833
W	0.000000	-2.140140	-0.298397
O	-1.415800	-2.991911	-0.759833
O	1.415800	-2.991911	-0.759833
O	0.000000	-1.531933	1.539529
$W_4O_{10}^-, ^2A_u / D_{2h} (E)$			
W	0.000000	1.148843	0.000000
W	0.000000	-1.148843	0.000000
O	0.000000	0.000000	1.595050
O	0.000000	0.000000	-1.595050
O	-1.902407	1.660208	0.000000

O	1.902407	1.660208	0.000000
O	-1.902407	-1.660208	0.000000
O	1.902407	-1.660208	0.000000
W	-2.871256	0.000000	0.000000
W	2.871256	0.000000	0.000000
O	-3.892154	0.000000	1.393040
O	-3.892154	0.000000	-1.393040
O	3.892154	0.000000	1.393040
O	3.892154	0.000000	-1.393040

$W_4O_{10}^-, ^2B_{3g} / D_{2h} (E)$

W	0.000000	1.164279	0.000000
W	0.000000	-1.164279	0.000000
O	0.000000	0.000000	1.616387
O	0.000000	0.000000	-1.616387
O	-1.864519	1.671227	0.000000
O	1.864519	1.671227	0.000000
O	-1.864519	-1.671227	0.000000
O	1.864519	-1.671227	0.000000
W	-2.831998	0.000000	0.000000
W	2.831998	0.000000	0.000000
O	-3.846290	0.000000	1.394055
O	-3.846290	0.000000	-1.394055
O	3.846290	0.000000	1.394055
O	3.846290	0.000000	-1.394055

$W_4O_{10}^-, ^2A_u / C_{2h} (I)$

W	0.087126	1.406009	1.883966
W	-0.087126	-1.406009	-1.883966
W	-0.087126	-1.406009	1.883966
O	-1.426830	1.943107	2.500429
O	1.426830	1.867039	2.863724
O	0.330071	1.544325	0.000000
O	1.426830	-1.943107	-2.500429
O	-1.426830	-1.867039	-2.863724
O	-1.426830	-1.867039	2.863724
O	-0.330071	-1.544325	0.000000
O	1.426830	-1.943107	2.500429
W	0.087126	1.406009	-1.883966
O	-1.426830	1.943107	-2.500429

O	1.426830	1.867039	-2.863724
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$W_4O_{10}^-, ^2B_{3u} / D_{2h} (I)$

W	1.895707	1.411166	0.000000
W	-1.895707	-1.411166	0.000000
W	1.895707	-1.411166	0.000000
O	2.702040	1.906190	1.438119
O	2.702040	1.906190	-1.438119
O	0.000000	1.570298	0.000000
O	-2.702040	-1.906190	-1.438119
O	-2.702040	-1.906190	1.438119
O	2.702040	-1.906190	1.438119
O	0.000000	-1.570298	0.000000
O	2.702040	-1.906190	-1.438119
W	-1.895707	1.411166	0.000000
O	-2.702040	1.906190	1.438119
O	-2.702040	1.906190	-1.438119

$W_4O_{10}^-, ^2A_g / C_{2h} (I)$

W	0.070682	1.421078	1.711448
W	-0.070682	-1.421078	-1.711448
W	-0.070682	-1.421078	1.711448
O	-1.407909	1.852139	2.467848
O	1.407909	1.738386	2.741409
O	0.266115	2.243578	0.000000
O	1.407909	-1.852139	-2.467848
O	-1.407909	-1.738386	-2.741409
O	-1.407909	-1.738386	2.741409
O	-0.266115	-2.243578	0.000000
O	1.407909	-1.852139	2.467848
W	0.070682	1.421078	-1.711448
O	-1.407909	1.852139	-2.467848
O	1.407909	1.738386	-2.741409

$W_4O_{10}^-, ^2A_g / D_{2h} (I)$

W	1.715566	1.424296	0.000000
W	-1.715566	-1.424296	0.000000
W	1.715566	-1.424296	0.000000
O	2.614015	1.794752	1.414978
O	2.614015	1.794752	-1.414978

O	0.000000	2.259610	0.000000
O	-2.614015	-1.794752	-1.414978
O	-2.614015	-1.794752	1.414978
O	2.614015	-1.794752	1.414978
O	0.000000	-2.259610	0.000000
O	2.614015	-1.794752	-1.414978
W	-1.715566	1.424296	0.000000
O	-2.614015	1.794752	1.414978
O	-2.614015	1.794752	-1.414978

$W_4O_{10}^-, {}^2A_2 / C_{2v} (B)$

W	0.000000	2.535764	-0.591652
W	0.000000	-2.535764	-0.591652
W	-1.395636	0.000000	0.620437
O	0.000000	3.108626	-2.220853
O	0.000000	3.886454	0.479775
O	1.673950	1.609277	-0.409265
O	-1.673950	1.609277	-0.409265
O	0.000000	-3.886454	0.479775
O	0.000000	-3.108626	-2.220853
O	-1.673950	-1.609277	-0.409265
O	-1.725087	0.000000	2.293344
W	1.395636	0.000000	0.620437
O	1.725087	0.000000	2.293344
O	1.673950	-1.609277	-0.409265

$W_4O_{10}^-, {}^2B_2 / C_{2v} (B)$

W	0.000000	2.278713	0.739480
W	0.000000	-2.278713	0.739480
W	1.320888	0.000000	-0.786659
O	0.000000	2.308134	2.458884
O	0.000000	3.888240	0.112417
O	-1.730184	1.590732	0.139141
O	1.730184	1.590732	0.139141
O	0.000000	-3.888240	0.112417
O	0.000000	-2.308134	2.458884
O	1.730184	-1.590732	0.139141
O	1.920541	0.000000	-2.413182
W	-1.320888	0.000000	-0.786659
O	-1.920541	0.000000	-2.413182

O	-1.730184	-1.590732	0.139141
W₄O₁₀⁻, ⁴A₂ / C_{2v} (B)			
W	0.000000	2.543721	0.595120
W	0.000000	-2.543721	0.595120
W	1.440566	0.000000	-0.619436
O	0.000000	2.861511	2.289538
O	0.000000	4.039010	-0.259145
O	-1.685877	1.699630	0.211224
O	1.685877	1.699630	0.211224
O	0.000000	-4.039010	-0.259145
O	0.000000	-2.861511	2.289538
O	1.685877	-1.699630	0.211224
O	2.039807	0.000000	-2.227913
W	-1.440566	0.000000	-0.619436
O	-2.039807	0.000000	-2.227913
O	-1.685877	-1.699630	0.211224

W₄O₁₀⁻, ²A'' / C_s (E)			
W	1.180123	0.162936	0.000000
W	-1.139728	0.028219	0.000000
O	-0.101459	-0.054126	1.595788
O	-0.101459	-0.054126	-1.595788
O	1.741553	1.976763	0.000000
O	1.573499	-1.854552	0.000000
O	-1.781891	1.821226	0.000000
O	-1.557578	-1.892035	0.000000
W	-0.060382	2.793987	0.000000
W	0.051009	-2.938314	0.000000
O	-0.101459	3.775478	1.419704
O	-0.101459	3.775478	-1.419704
O	0.071648	-3.963630	1.390282
O	0.071648	-3.963630	-1.390282

W₄O₁₀⁻, ⁴A'' / C_s (E)			
W	-1.276468	-0.116267	0.000000
W	1.196693	-0.052757	0.000000
O	0.044759	0.060593	1.518010
O	0.044759	0.060593	-1.518010
O	-1.719417	-2.001095	0.000000

O	-1.486884	1.926911	0.000000
O	1.713233	-1.871658	0.000000
O	1.581825	1.872129	0.000000
W	0.008608	-2.865781	0.000000
W	0.030239	2.996405	0.000000
O	0.055398	-3.861057	1.406292
O	0.055398	-3.861057	-1.406292
O	0.044759	4.014919	1.397612
O	0.044759	4.014919	-1.397612