Electronic Supplementary Material (ESI) for ChemComm.


Supporting Information for:

# Not all Density Functionals are Created Equal: The Case of the Missing Electron in the Oxidized $[W–W{\equiv}O]^{7+}$ Core

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**Materials and Methods.**

Reactions were carried out under a dry $N_2$ atmosphere using Schlenk techniques and glovebox methods. Hexanes were purified using a Vacuum Atmospheres solvent purification system. Dichloromethane was freshly distilled under an $N_2$ atmosphere over $CaH_2$ prior to use. Silver trifluoromethanesulfonate, Ag(OTf), was purchased from Strem Chemicals and used as received. $(W_2O(dpa)_4)(OTf)(BPh_4)$ (**1**) was prepared according to literature procedures.[1] Elemental analysis was carried out by Midwest Microlab, LLC (Indianapolis, IN, USA). The IR spectrum was taken on a Bruker TENSOR 27 FTIR spectrometer using an attenuated total reflectance (ATR) adapter. The EPR measurement was carried out at 15 K using a Bruker EleXsys EPR spectrometer (E-500-A console with ER 049SX SuperX bridge and SuperX cavity). The parameters were as follows: frequency = 9.3818 GHz, microwave power = 0.5024 mW, field center = 3700 G, field width = 600 G, modulation amplitude = 4 G, modulation frequency = 100 kHz, time constant = 163.84 ms.

**X-ray Structure Determination**. Crystallographic data were measured at the Molecular Structure Laboratory of the Chemistry Department of the University of Wisconsin-Madison. The crystal was selected under oil under ambient conditions and attached to the tip of a MiTeGen MicroMount. The crystal was mounted in a stream of cold nitrogen at 100(1) K and centered in the X-ray beam using a video camera. The crystal evaluation and data collection were performed on a Bruker Quazar SMART APEX II diffractometer with Mo $K_\alpha$ ($\lambda$ = 0.71073 Å) radiation at a detector to crystal distance of 5.00 cm. The data were collected using a routine to survey an entire sphere of reciprocal space and were indexed using the SMART program.[2] The structure was solved using direct methods and refined by least-squares refinement on $F^2$ followed by difference Fourier synthesis.[3]. All of the hydrogen atoms were included in the final structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

**Computational Methods**.

The initial coordinates for all calculations were obtained from the crystallographic data for **2** with the solvent molecules of crystallization and counter triflate ions removed. All of the geometry optimizations were carried out with ORCA version 2.9.1.[4] The functionals used were BP86,[5, 6] B3LYP,[7-10] TPSS,[11] and TPSSh.[11] Geometry optimization calculations were performed with the def2-SV(P) basis set[12] for C and H atoms and the def2-SVP/J auxiliary basis set.[13, 14] The def2-TZVP(-f) basis set[15] was used for O and N atoms with the def2-TZVP/J auxiliary basis set.[13, 14] The def2-TZVPP basis set was used for W atoms with the def2-TZVPP/J auxiliary basis set,[13, 14] along with the ZORA approximation.[16] Tight optimization and tight self-consistent field convergence were employed along with grid4 for all geometry optimization calculations. The integration grid was increased to grid5 for single point calculations. The RI approximation was used for BP86 and TPSS calculations. The RIJONX approximation was used for B3LYP and TPSSh calculations. For potential energy surface calculations the def2-SV(P) basis set[12] was used for C, H, N, and O atoms along with the def2-SVP/J auxiliary basis set.[13, 14] The def2-TZVPP and def2-TZVPP/J basis set and auxiliary basis set[13, 14] was used for W atoms, along with the ZORA approximation to take relativistic effects into account.[16] Molecular graphics and analyses were performed with the UCSF Chimera package.[17]

**Synthesis**

**$(W_2O(dpa)_4)(SO_3CF_3)_3$** (**2**). Black crystals of **1** (150.5 mg, 0.0982 mmol) were dissolved in 20 mL of dichloromethane and cooled to 0 °C. In a separate flask, solid white Ag(OTf) (52.0 mg, 0.202 mmol) was suspended in 5 mL of dichloromethane and cooled to 0 °C. The brown/yellow solution of **1** was quickly transferred to the flask containing the suspension of Ag(OTf), upon which a color change to dark green was observed along with the appearance of a silver precipitate. The mixture was allowed to stir for 30 min at 0 °C. The green solution was filtered through a fine porosity frit and the filtrate was layered with cold hexanes (30 mL). The reaction

solution was set to crystalize at –20 °C. X-ray quality plate crystals were obtained after 5 days. Yield: 80.8 mg, 54.4 %. Anal. Calcd. for $[W_2OC_{40}H_{32}N_{12}][SO_3CF_3]_{2.9}[BC_{24}H_{20}]_{0.1}$:‡ C 35.59 %, H 2.25 %, N 11.00 %. Found C 35.71 %, H 2.37 %, N 11.22 %. IR (ATR, $cm^{-1}$): 1595 m, 1461 s, 1437 m, 1383 w, 1314 w, 1259 s, 1223 m, 1152 m, 1124 w, 1029 s, 955 w, 839 w, 763 m, 741 w, 692 w, 636 s. UV-Vis (0 $^0$C $CH_2Cl_2$, nm): 408 (18,659 L $mol^{-1}$ $cm^{-1}$), 440 (15,590 L $mol^{-1}$ $cm^{-1}$), 711 (3654 L $mol^{-1}$ $cm^{-1}$).

**Table S1**. Experimental and Calculated Bond Distances and Angles for **1**.

| | W–W, Å | W–O, Å | W–W-O, ° |
|---|---|---|---|
| $[W_2O(dpa)_4]^{2+}$ (**1**) | 3.0735(3) | 1.692(4) | 178.0(1) |
| BP86 DFT | 3.108 | 1.704 | 179.9 |
| B3LYP DFT | 3.149 | 1.689 | 179.9 |
| TPSS DFT | 3.061 | 1.704 | 179.5 |
| TPSSh DFT | 3.064 | 1.693 | 179.7 |

**Table S2**. Alpha and beta orbital occupation numbers for **1**.

| | $W_{distal}$ | $W_{oxo}$ | Oxo |
|---|---|---|---|
| alpha HOMO-1 | 12 % | 88 % | 0 % |
| alpha HOMO | 87 % | 7 % | 6 % |
| beta HOMO | 89 % | 6 % | 5 % |
| beta LUMO | 8 % | 92 % | 0 % |

**Table S3**. Crystallographic data for $(W_2O(dpa)_4)(SO_3CF_3)_3$ at 100 K

| compound | **2** |
|---|---|
| formula | $(W_2OC_{40}H_{32}N_{12})(SO_3CF_3)_3 \bullet CH_2Cl_2$ |
| crystal system | monoclinic |
| space group | P $2_1/n$ |
| *a* (Å) | 13.3770(4) |
| *b* (Å) | 15.6886(4) |
| *c* (Å) | 25.1243(7) |
| *α* (deg) | 90.00 |
| *β* (deg) | 102.4021(15) |
| *γ* (deg) | 90.00 |
| V (Å$^3$) | 5149.7(2) |
| *Z* | 4 |
| ρ (Mg m$^{-3}$) | 2.059 |
| $R_1$[a], $wR_2$[b] [I > 2σ(*I*)] | 0.0202, 0.0445 |
| $R_1$[a], $wR_2$[b] (all data) | 0.0249, 0.0460 |

[a] $R_1 = \Sigma||F_o| - |F_c||/ \Sigma|F_o|$.

[b] $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/ \Sigma[w(F_o^2)^2]]^{1/2}$, $w = 1/\sigma^2(F_o^2) + (aP)^2 + bP$, where $P = [\max(0 \text{ or } F_o^2) + 2(F_c^2)]/3$.

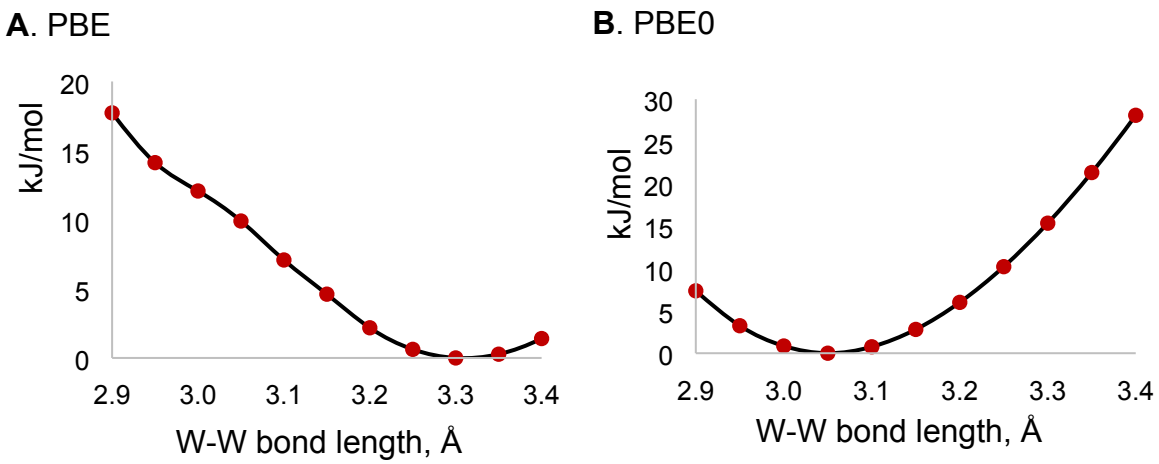


**Figure S1**. Potential energy surface scans for the (A) PBE functional, (B) PBE0 functional with fixed W–W bond distance from 2.90 to 3.50 Å.

**References**

‡ Although tetraphenylborate was not present as a counter anion in the X-ray crystallographic analysis, the elemental analysis suggests there is a small amount of tetraphenylborate anions in the bulk sample.


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BP86 XYZ Coordinates for $[W_2(dpa)_4]^{3+}$ (**2**)

| | | | |
|---|---|---|---|
| W | 0.079465 | 0.034742 | 3.082532 |
| W | -0.076658 | -0.212393 | -0.216598 |
| O | -0.157794 | -0.337642 | -1.894669 |
| N | -1.068259 | -1.407290 | 4.297526 |
| N | -1.775599 | -0.774185 | 2.320009 |
| N | -2.176858 | -0.026934 | 0.153887 |
| N | 1.654852 | -1.087435 | 4.147874 |
| N | 0.788829 | -1.844282 | 2.280216 |
| N | -0.216758 | -2.301007 | 0.232405 |
| N | 1.324187 | 1.628917 | 3.964396 |
| N | 1.849349 | 0.713431 | 2.041741 |
| N | 2.051222 | -0.350425 | -0.017873 |
| N | -1.396350 | 1.310661 | 4.114198 |
| N | -0.712795 | 1.781722 | 2.084516 |
| N | 0.091084 | 1.919137 | -0.094794 |
| C | -1.022544 | -2.094526 | 5.456497 |
| H | -0.171744 | -1.892420 | 6.124078 |
| C | -2.021810 | -3.020319 | 5.773410 |
| H | -1.981375 | -3.568504 | 6.726638 |
| C | -3.059134 | -3.242742 | 4.843197 |
| H | -3.844012 | -3.984866 | 5.062811 |
| C | -3.097183 | -2.535399 | 3.631243 |
| H | -3.886798 | -2.723587 | 2.890537 |
| C | -2.073669 | -1.597326 | 3.395077 |
| C | -2.705613 | -0.362708 | 1.375516 |
| C | -4.090519 | -0.236482 | 1.624612 |
| H | -4.484622 | -0.446177 | 2.629059 |
| C | -4.947571 | 0.174808 | 0.600050 |
| H | -6.030293 | 0.263211 | 0.782579 |
| C | -4.399751 | 0.496222 | -0.657846 |
| H | -5.031513 | 0.827219 | -1.495990 |
| C | -3.022299 | 0.411318 | -0.831818 |
| H | -2.547318 | 0.680742 | -1.785337 |
| C | 2.476459 | -1.013534 | 5.214247 |
| H | 2.355813 | -0.145109 | 5.878841 |
| C | 3.433871 | -2.006781 | 5.443891 |
| H | 4.092512 | -1.943020 | 6.323048 |
| C | 3.543489 | -3.068588 | 4.521202 |
| H | 4.307073 | -3.849412 | 4.670476 |
| C | 2.695685 | -3.136100 | 3.404388 |
| H | 2.794079 | -3.944985 | 2.667102 |
| C | 1.735330 | -2.116700 | 3.256111 |
| C | 0.266421 | -2.797714 | 1.417669 |
| C | 0.173800 | -4.175309 | 1.717045 |
| H | 0.504943 | -4.542674 | 2.698679 |
| C | -0.357557 | -5.058848 | 0.773514 |
| H | -0.421006 | -6.136204 | 0.994202 |
| C | -0.831052 | -4.544194 | -0.449843 |
| H | -1.260738 | -5.197560 | -1.224213 |
| C | -0.770497 | -3.171957 | -0.669488 |
| H | -1.155213 | -2.722245 | -1.595315 |
| C | 1.379894 | 2.475768 | 5.011739 |
| H | 0.596550 | 2.375252 | 5.777652 |

| | | | |
|---|---|---|---|
| C | 2.395802 | 3.433037 | 5.098067 |
| H | 2.439195 | 4.112805 | 5.962250 |
| C | 3.339873 | 3.514827 | 4.052713 |
| H | 4.134826 | 4.277567 | 4.089032 |
| C | 3.271766 | 2.640273 | 2.956621 |
| H | 3.987396 | 2.717337 | 2.126274 |
| C | 2.239610 | 1.681992 | 2.954107 |
| C | 2.689577 | 0.163521 | 1.083845 |
| C | 4.093352 | 0.072829 | 1.215120 |
| H | 4.578598 | 0.429325 | 2.134688 |
| C | 4.854271 | -0.489222 | 0.186294 |
| H | 5.950433 | -0.551626 | 0.275618 |
| C | 4.193507 | -0.994712 | -0.951010 |
| H | 4.746823 | -1.449419 | -1.786622 |
| C | 2.804773 | -0.933750 | -1.002975 |
| H | 2.244879 | -1.342548 | -1.855515 |
| C | -2.113134 | 1.398512 | 5.252578 |
| H | -1.927087 | 0.632970 | 6.020510 |
| C | -3.047881 | 2.424134 | 5.426181 |
| H | -3.620553 | 2.493610 | 6.363194 |
| C | -3.246844 | 3.344417 | 4.375333 |
| H | -3.994959 | 4.146868 | 4.482225 |
| C | -2.508585 | 3.242778 | 3.185628 |
| H | -2.678830 | 3.939350 | 2.352968 |
| C | -1.563933 | 2.202066 | 3.094980 |
| C | -0.280453 | 2.591199 | 1.043480 |
| C | -0.167661 | 3.997211 | 1.123547 |
| H | -0.405252 | 4.509780 | 2.066412 |
| C | 0.265949 | 4.725750 | 0.012408 |
| H | 0.343837 | 5.823388 | 0.062837 |
| C | 0.623767 | 4.030450 | -1.159786 |
| H | 0.973877 | 4.557270 | -2.060374 |
| C | 0.551227 | 2.641334 | -1.164979 |
| H | 0.849443 | 2.055471 | -2.045462 |

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B3LYP XYZ Coordinates for $[W_2(dpa)_4]^{3+}$ (**2**)

| | | | |
|---|---|---|---|
| W | 0.077498 | 0.032031 | 3.025103 |
| W | -0.069938 | -0.200815 | -0.069728 |
| O | -0.149849 | -0.321451 | -1.748935 |
| N | -1.072481 | -1.415097 | 4.267129 |
| N | -1.842160 | -0.781149 | 2.328307 |
| N | -2.205423 | -0.028378 | 0.180915 |
| N | 1.662874 | -1.095258 | 4.111975 |
| N | 0.796220 | -1.910493 | 2.284911 |
| N | -0.213618 | -2.327603 | 0.255739 |
| N | 1.328681 | 1.634067 | 3.932705 |
| N | 1.917465 | 0.724154 | 2.041130 |
| N | 2.081349 | -0.343713 | 0.004881 |
| N | -1.404694 | 1.315604 | 4.082449 |
| N | -0.719727 | 1.850897 | 2.083671 |
| N | 0.086945 | 1.951617 | -0.073447 |
| C | -1.005347 | -2.072560 | 5.432801 |

| | | | |
|---|---|---|---|
| H | -0.130676 | -1.884522 | 6.058197 |
| C | -2.009119 | -2.957529 | 5.811850 |
| H | -1.946511 | -3.483532 | 6.766755 |
| C | -3.081566 | -3.166478 | 4.930409 |
| H | -3.871358 | -3.877599 | 5.190474 |
| C | -3.148221 | -2.480561 | 3.715432 |
| H | -3.965692 | -2.664373 | 3.018491 |
| C | -2.114370 | -1.579697 | 3.420881 |
| C | -2.749672 | -0.398853 | 1.375594 |
| C | -4.145254 | -0.323702 | 1.561724 |
| H | -4.578073 | -0.563252 | 2.532442 |
| C | -4.959491 | 0.097740 | 0.518348 |
| H | -6.042196 | 0.159618 | 0.662041 |
| C | -4.383131 | 0.464172 | -0.710064 |
| H | -4.990537 | 0.798637 | -1.553615 |
| C | -3.009260 | 0.402315 | -0.830736 |
| H | -2.504450 | 0.684639 | -1.755261 |
| C | 2.457369 | -1.003105 | 5.187181 |
| H | 2.348575 | -0.112605 | 5.809033 |
| C | 3.379826 | -2.001724 | 5.480871 |
| H | 4.017750 | -1.918496 | 6.363233 |
| C | 3.478517 | -3.096292 | 4.607417 |
| H | 4.214571 | -3.882877 | 4.798730 |
| C | 2.650282 | -3.188815 | 3.486540 |
| H | 2.746816 | -4.023422 | 2.792328 |
| C | 1.721632 | -2.158528 | 3.278558 |
| C | 0.299874 | -2.841267 | 1.410505 |
| C | 0.247335 | -4.231259 | 1.641473 |
| H | 0.603313 | -4.639304 | 2.586869 |
| C | -0.298768 | -5.071158 | 0.679499 |
| H | -0.343290 | -6.149431 | 0.858659 |
| C | -0.812109 | -4.526256 | -0.510108 |
| H | -1.247288 | -5.154619 | -1.289956 |
| C | -0.764915 | -3.156328 | -0.674066 |
| H | -1.157802 | -2.675021 | -1.570334 |
| C | 1.366795 | 2.450292 | 4.994559 |
| H | 0.556026 | 2.358260 | 5.719588 |
| C | 2.395465 | 3.373565 | 5.148272 |
| H | 2.419276 | 4.029986 | 6.020610 |
| C | 3.378432 | 3.448773 | 4.148909 |
| H | 4.183952 | 4.184763 | 4.229824 |
| C | 3.335496 | 2.597073 | 3.042591 |
| H | 4.082367 | 2.675591 | 2.252775 |
| C | 2.285406 | 1.669501 | 2.977443 |
| C | 2.733135 | 0.200563 | 1.072958 |
| C | 4.140973 | 0.148723 | 1.133135 |
| H | 4.662082 | 0.529992 | 2.010629 |
| C | 4.856397 | -0.429159 | 0.092340 |
| H | 5.948435 | -0.473391 | 0.139634 |
| C | 4.169570 | -0.974648 | -1.005902 |
| H | 4.697223 | -1.435631 | -1.843427 |
| C | 2.789953 | -0.925387 | -1.002509 |
| H | 2.202514 | -1.341817 | -1.821528 |
| C | -2.093042 | 1.385227 | 5.229991 |

| | | | |
|---|---|---|---|
| H | -1.920970 | 0.592204 | 5.960114 |
| C | -2.988929 | 2.423211 | 5.462884 |
| H | -3.540208 | 2.472661 | 6.404201 |
| C | -3.175370 | 3.382045 | 4.454587 |
| H | -3.894045 | 4.194158 | 4.599703 |
| C | -2.457362 | 3.306158 | 3.258893 |
| H | -2.623331 | 4.033684 | 2.464571 |
| C | -1.547610 | 2.248484 | 3.113822 |
| C | -0.316625 | 2.635966 | 1.035676 |
| C | -0.251986 | 4.044425 | 1.050264 |
| H | -0.517411 | 4.591419 | 1.954336 |
| C | 0.192137 | 4.727565 | -0.074537 |
| H | 0.245875 | 5.820132 | -0.063447 |
| C | 0.591748 | 4.007417 | -1.213366 |
| H | 0.944847 | 4.508888 | -2.116816 |
| C | 0.539152 | 2.628725 | -1.165358 |
| H | 0.847344 | 2.016570 | -2.013602 |

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TPSS XYZ Coordinates for $[W_2(dpa)_4]^{3+}$ (**2**)

| | | | |
|---|---|---|---|
| W | 0.079364 | 0.032628 | 3.071308 |
| W | -0.074466 | -0.207726 | -0.158893 |
| O | -0.156349 | -0.333149 | -1.836117 |
| N | -1.052726 | -1.415385 | 4.282177 |
| N | -1.770426 | -0.778421 | 2.311842 |
| N | -2.181637 | -0.007593 | 0.166886 |
| N | 1.659050 | -1.073652 | 4.131251 |
| N | 0.790130 | -1.841297 | 2.271591 |
| N | -0.233514 | -2.305022 | 0.245813 |
| N | 1.307199 | 1.633350 | 3.947151 |
| N | 1.844278 | 0.712846 | 2.032877 |
| N | 2.056508 | -0.367363 | -0.005388 |
| N | -1.403765 | 1.292540 | 4.097377 |
| N | -0.714313 | 1.773910 | 2.074093 |
| N | 0.109550 | 1.925400 | -0.085604 |
| C | -0.998932 | -2.108067 | 5.438100 |
| H | -0.149199 | -1.906726 | 6.096840 |
| C | -1.993058 | -3.034547 | 5.754824 |
| H | -1.946801 | -3.584336 | 6.700101 |
| C | -3.035230 | -3.253343 | 4.832591 |
| H | -3.814155 | -3.992232 | 5.054321 |
| C | -3.082108 | -2.543846 | 3.625244 |
| H | -3.873181 | -2.726312 | 2.893311 |
| C | -2.062652 | -1.606630 | 3.386736 |
| C | -2.712113 | -0.354834 | 1.380819 |
| C | -4.092324 | -0.228107 | 1.634206 |
| H | -4.486107 | -0.451442 | 2.629473 |
| C | -4.944336 | 0.200713 | 0.615181 |
| H | -6.021034 | 0.290299 | 0.797109 |
| C | -4.396619 | 0.535230 | -0.636622 |
| H | -5.025451 | 0.877425 | -1.464681 |
| C | -3.022445 | 0.444803 | -0.814160 |
| H | -2.544707 | 0.717170 | -1.758374 |

| | | | |
|---|---|---|---|
| C | 2.485963 | -0.990446 | 5.193354 |
| H | 2.364614 | -0.122963 | 5.848562 |
| C | 3.444853 | -1.977718 | 5.422665 |
| H | 4.104375 | -1.907628 | 6.293351 |
| C | 3.552290 | -3.044218 | 4.508681 |
| H | 4.313663 | -3.818318 | 4.660191 |
| C | 2.702634 | -3.121664 | 3.397229 |
| H | 2.797452 | -3.931867 | 2.669668 |
| C | 1.741931 | -2.107343 | 3.246395 |
| C | 0.259129 | -2.805031 | 1.421920 |
| C | 0.167556 | -4.178406 | 1.723160 |
| H | 0.510602 | -4.546982 | 2.693717 |
| C | -0.378667 | -5.055721 | 0.785120 |
| H | -0.442606 | -6.127456 | 1.003487 |
| C | -0.863465 | -4.539593 | -0.430394 |
| H | -1.301591 | -5.188884 | -1.195032 |
| C | -0.798781 | -3.170384 | -0.651946 |
| H | -1.184616 | -2.716714 | -1.568058 |
| C | 1.353278 | 2.486429 | 4.990530 |
| H | 0.569695 | 2.385732 | 5.747100 |
| C | 2.363358 | 3.445183 | 5.076418 |
| H | 2.399370 | 4.126330 | 5.932416 |
| C | 3.313330 | 3.524050 | 4.039209 |
| H | 4.102022 | 4.284523 | 4.078252 |
| C | 3.255594 | 2.646802 | 2.947956 |
| H | 3.973850 | 2.719401 | 2.127254 |
| C | 2.227991 | 1.688180 | 2.943289 |
| C | 2.696802 | 0.155102 | 1.086901 |
| C | 4.096572 | 0.065536 | 1.220667 |
| H | 4.581618 | 0.433220 | 2.128973 |
| C | 4.851999 | -0.510916 | 0.198327 |
| H | 5.942295 | -0.573896 | 0.286175 |
| C | 4.190831 | -1.027208 | -0.930889 |
| H | 4.741444 | -1.489899 | -1.756075 |
| C | 2.804863 | -0.961996 | -0.985458 |
| H | 2.242037 | -1.371045 | -1.828013 |
| C | -2.128304 | 1.371589 | 5.232083 |
| H | -1.943867 | 0.606267 | 5.991558 |
| C | -3.064912 | 2.391391 | 5.403882 |
| H | -3.641003 | 2.453881 | 6.332419 |
| C | -3.258904 | 3.317150 | 4.359938 |
| H | -4.004580 | 4.113465 | 4.468245 |
| C | -2.516252 | 3.225105 | 3.175287 |
| H | -2.679528 | 3.923980 | 2.350836 |
| C | -1.571865 | 2.188549 | 3.083763 |
| C | -0.270028 | 2.597480 | 1.045872 |
| C | -0.154355 | 3.999047 | 1.132342 |
| H | -0.402736 | 4.509377 | 2.066911 |
| C | 0.295237 | 4.723827 | 0.027492 |
| H | 0.376399 | 5.815232 | 0.079273 |
| C | 0.661284 | 4.030286 | -1.140350 |
| H | 1.020232 | 4.556149 | -2.030751 |
| C | 0.581377 | 2.644044 | -1.151042 |
| H | 0.878701 | 2.057060 | -2.023426 |

**********

TPSSh XYZ Coordinates for $[W_2(dpa)_4]^{3+}$ (**2**)

| | | | |
|---|---|---|---|
| W | 0.064533 | 0.009155 | 3.015541 |
| W | -0.012416 | -0.141093 | 0.003011 |
| O | -0.200433 | -0.328413 | -1.668434 |
| N | -1.038825 | -1.425026 | 4.274859 |
| N | -1.832850 | -0.790828 | 2.356709 |
| N | -2.157460 | 0.025777 | 0.230377 |
| N | 1.664586 | -1.064583 | 4.089619 |
| N | 0.789046 | -1.895564 | 2.282645 |
| N | -0.217074 | -2.277122 | 0.258846 |
| N | 1.290831 | 1.632811 | 3.872793 |
| N | 1.872137 | 0.700127 | 1.982818 |
| N | 2.105644 | -0.380081 | -0.020572 |
| N | -1.406383 | 1.271505 | 4.072343 |
| N | -0.727448 | 1.822269 | 2.072534 |
| N | 0.147800 | 1.984190 | -0.046319 |
| C | -0.947852 | -2.080007 | 5.443071 |
| H | -0.058102 | -1.892520 | 6.046498 |
| C | -1.948206 | -2.960573 | 5.842393 |
| H | -1.867417 | -3.486577 | 6.795520 |
| C | -3.040399 | -3.166697 | 4.984280 |
| H | -3.826073 | -3.874428 | 5.263574 |
| C | -3.134694 | -2.484174 | 3.768488 |
| H | -3.967978 | -2.667892 | 3.090603 |
| C | -2.103771 | -1.588561 | 3.450039 |
| C | -2.729271 | -0.393480 | 1.396999 |
| C | -4.128004 | -0.348820 | 1.555921 |
| H | -4.577549 | -0.627274 | 2.508580 |
| C | -4.925648 | 0.091904 | 0.505971 |
| H | -6.011867 | 0.130360 | 0.625680 |
| C | -4.326789 | 0.504134 | -0.695704 |
| H | -4.919419 | 0.854742 | -1.542706 |
| C | -2.947870 | 0.467055 | -0.787135 |
| H | -2.424448 | 0.780467 | -1.690655 |
| C | 2.465645 | -0.954990 | 5.161209 |
| H | 2.361813 | -0.051960 | 5.765149 |
| C | 3.384849 | -1.954591 | 5.464798 |
| H | 4.029933 | -1.858609 | 6.340243 |
| C | 3.470458 | -3.067859 | 4.613243 |
| H | 4.201437 | -3.855141 | 4.818310 |
| C | 2.637112 | -3.180243 | 3.497066 |
| H | 2.721069 | -4.030625 | 2.820251 |
| C | 1.717656 | -2.146068 | 3.273550 |
| C | 0.278834 | -2.822171 | 1.405040 |
| C | 0.202718 | -4.209190 | 1.625270 |
| H | 0.552946 | -4.633672 | 2.566151 |
| C | -0.360199 | -5.025619 | 0.649052 |
| H | -0.426122 | -6.104810 | 0.812445 |
| C | -0.859791 | -4.453689 | -0.532112 |
| H | -1.307512 | -5.062945 | -1.319559 |
| C | -0.781844 | -3.080832 | -0.683049 |

| | | | |
|---|---|---|---|
| H | -1.157542 | -2.575462 | -1.572980 |
| C | 1.327340 | 2.476551 | 4.916388 |
| H | 0.527243 | 2.385196 | 5.652762 |
| C | 2.344495 | 3.419381 | 5.032256 |
| H | 2.369419 | 4.095399 | 5.889167 |
| C | 3.314872 | 3.488225 | 4.020217 |
| H | 4.109649 | 4.237403 | 4.076776 |
| C | 3.270401 | 2.614299 | 2.930284 |
| H | 4.004866 | 2.682076 | 2.127189 |
| C | 2.233761 | 1.672267 | 2.902119 |
| C | 2.738353 | 0.146736 | 1.065029 |
| C | 4.136878 | 0.058728 | 1.179686 |
| H | 4.640743 | 0.438977 | 2.068576 |
| C | 4.863993 | -0.549827 | 0.160425 |
| H | 5.952058 | -0.625009 | 0.239323 |
| C | 4.196817 | -1.083228 | -0.956192 |
| H | 4.740761 | -1.562979 | -1.772126 |
| C | 2.817845 | -0.994703 | -1.003764 |
| H | 2.235128 | -1.393349 | -1.835023 |
| C | -2.104573 | 1.324774 | 5.217983 |
| H | -1.918765 | 0.533819 | 5.946379 |
| C | -3.022894 | 2.345317 | 5.443981 |
| H | -3.579859 | 2.383377 | 6.382130 |
| C | -3.225851 | 3.300005 | 4.435045 |
| H | -3.963521 | 4.094899 | 4.576888 |
| C | -2.502285 | 3.240542 | 3.241099 |
| H | -2.681554 | 3.961753 | 2.443571 |
| C | -1.568958 | 2.203918 | 3.102522 |
| C | -0.302609 | 2.647114 | 1.059499 |
| C | -0.259578 | 4.054631 | 1.099040 |
| H | -0.563125 | 4.586512 | 2.000515 |
| C | 0.207534 | 4.756657 | -0.006384 |
| H | 0.243751 | 5.849248 | 0.019517 |
| C | 0.650107 | 4.059151 | -1.144625 |
| H | 1.017599 | 4.581033 | -2.030157 |
| C | 0.620598 | 2.678435 | -1.119294 |
| H | 0.959192 | 2.074724 | -1.962254 |