Electronic Supplementary Material (ESI) for CrystEngComm.


# Supplementary Information

# Assembly of Organic−Inorganic Hybrid Materials Constructed from Polyoxometalate and Metal–1,2,4-triazole units: Synthesis, Structures, Magnetic, Electrochemical and Photocatalysis Properties

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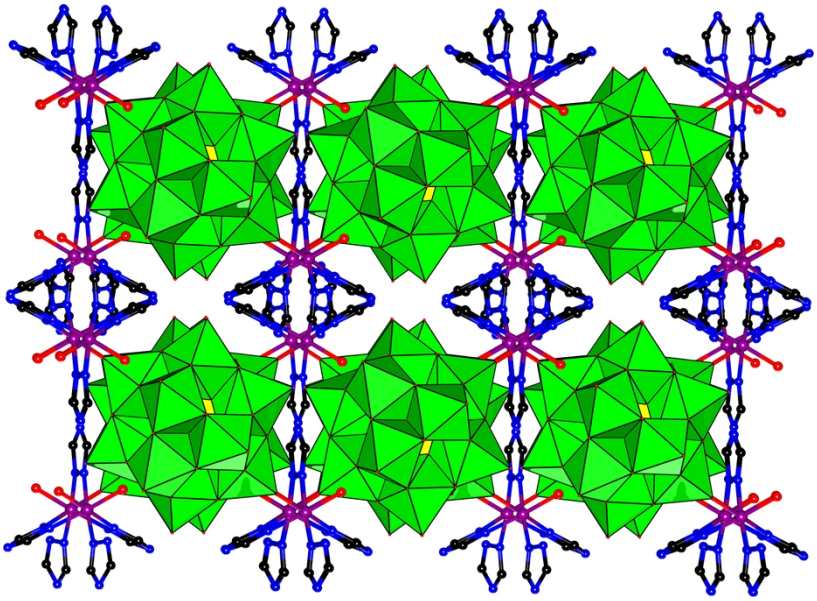

**Fig. S1** The 3D supramolecular framework formed by the hydrogen bonding interactions in **1**. Color legend: gray, C; black, N; red, O; violet, Co.

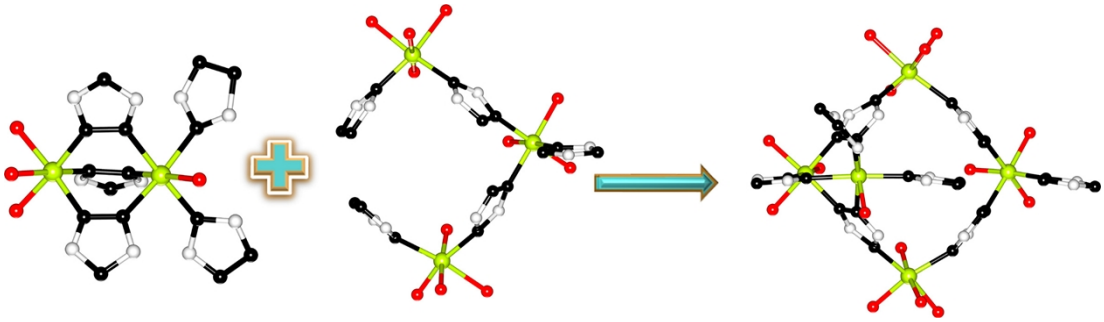

**Fig. S2** Structural representations of [$Co_5$] fragment built from {$Co_2$} dimer and one {$Co_3$} triad in **5**. Color legend: gray, C; black, N; red, O; lime, Co.

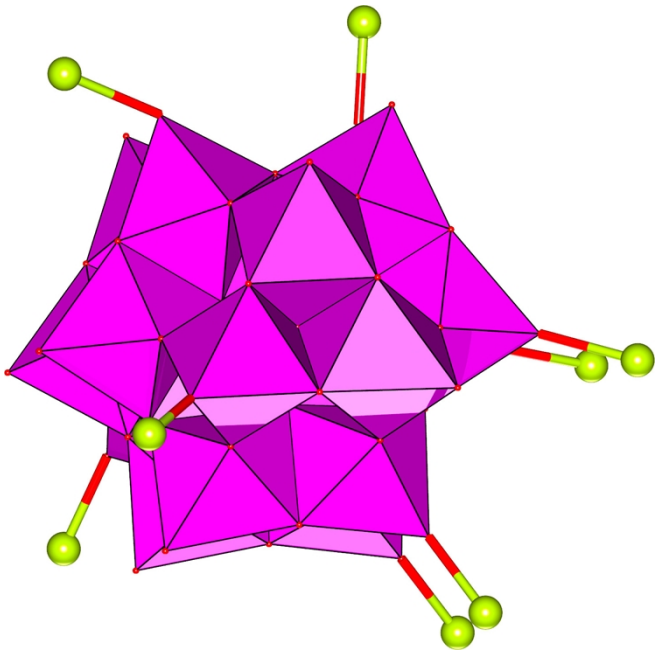

**Fig. S3** The coordination mode of $P_2W_{18}$ in **5**. Color legend: red, O; lime, Co; purple, W; yellow, P.

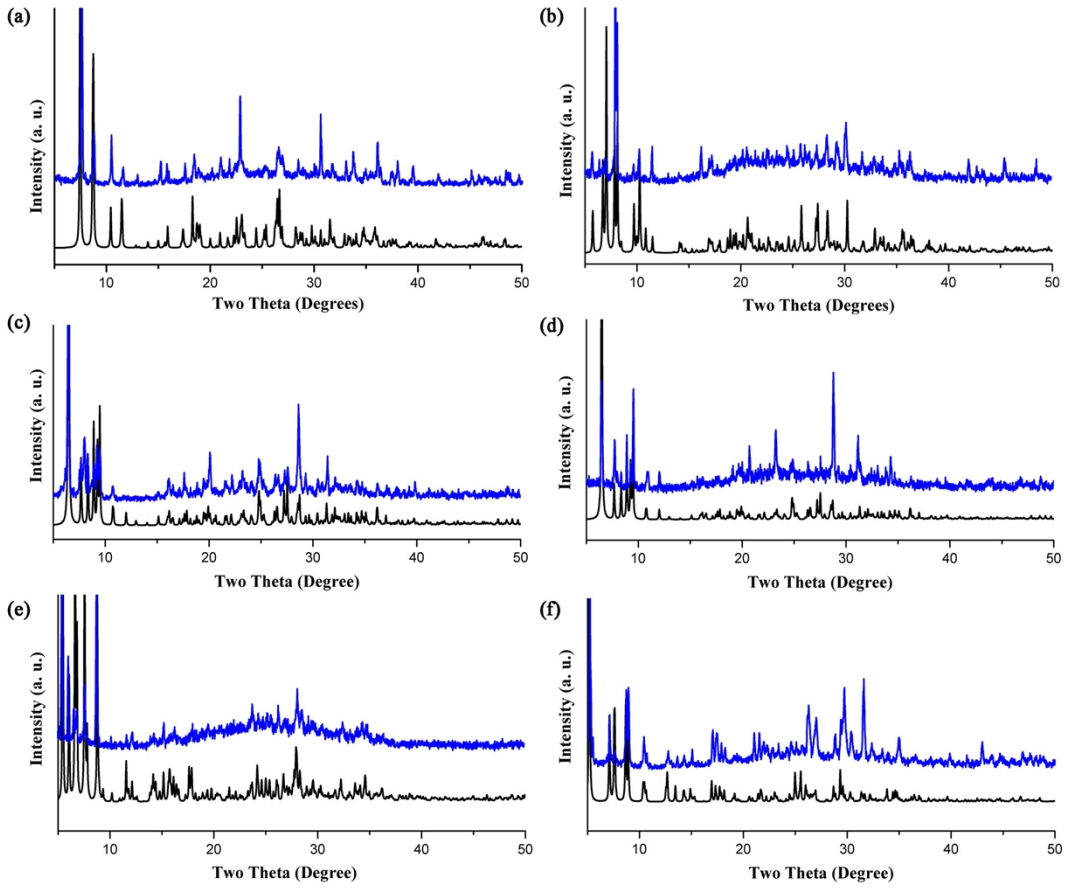


**Fig. S4** The XRD pattern of the as-synthesized (blue line) and simulated pattern (black line) of **1** (a), **2** (b), **3** (c), **4** (d), **5** (e) and **6** (f).

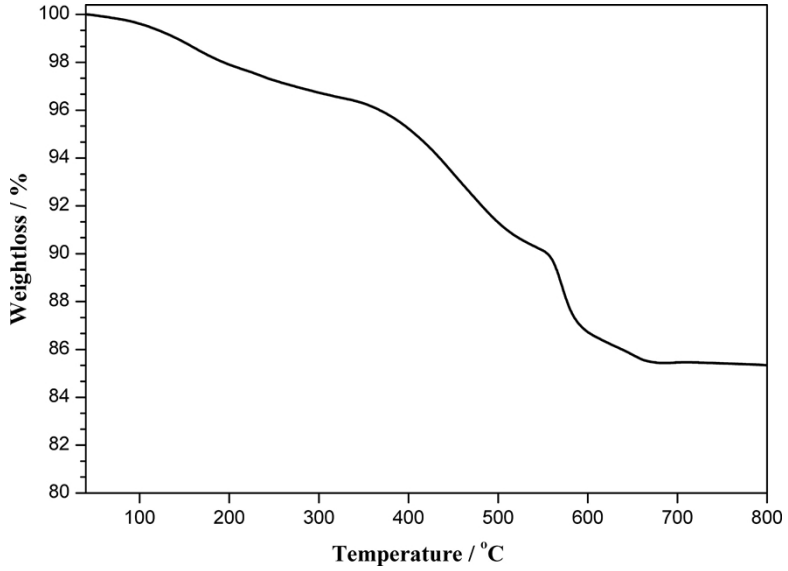


**Fig. S5** The TG curve of compound **1**.

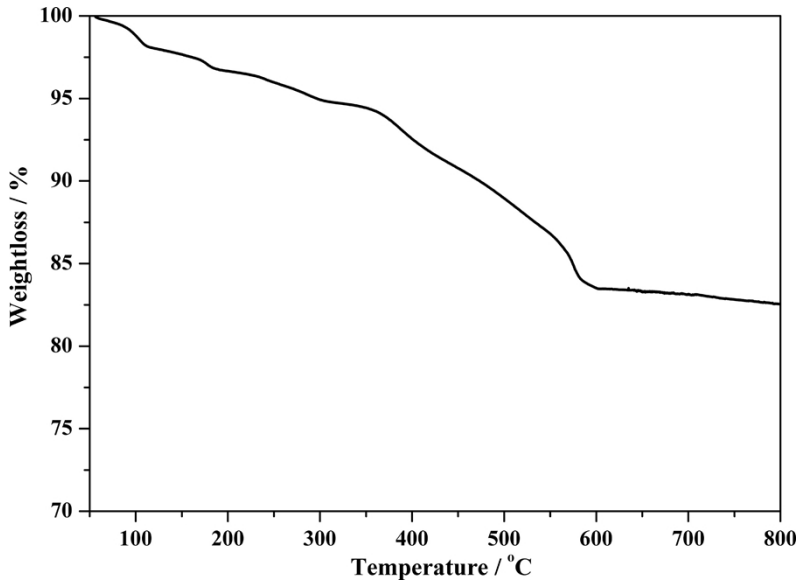


**Fig. S6** The TG curve of compound **2**.

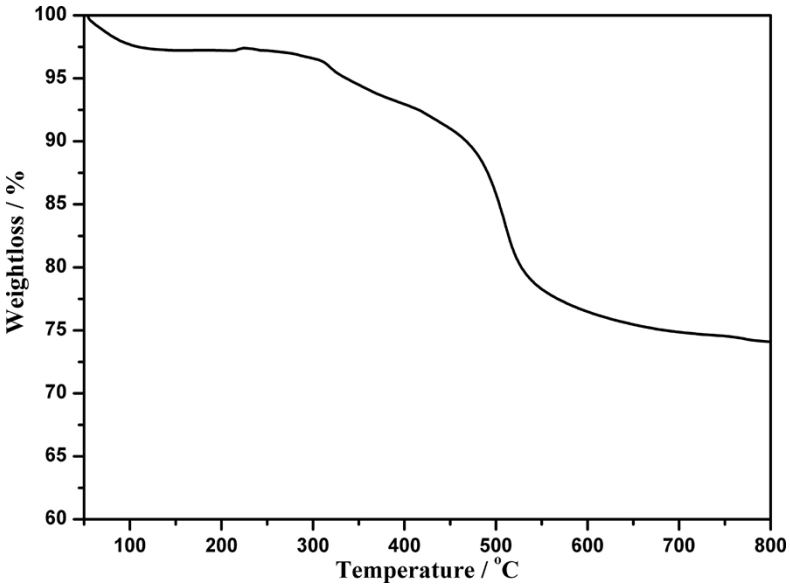


**Fig. S7** The TG curve of compound **3**.

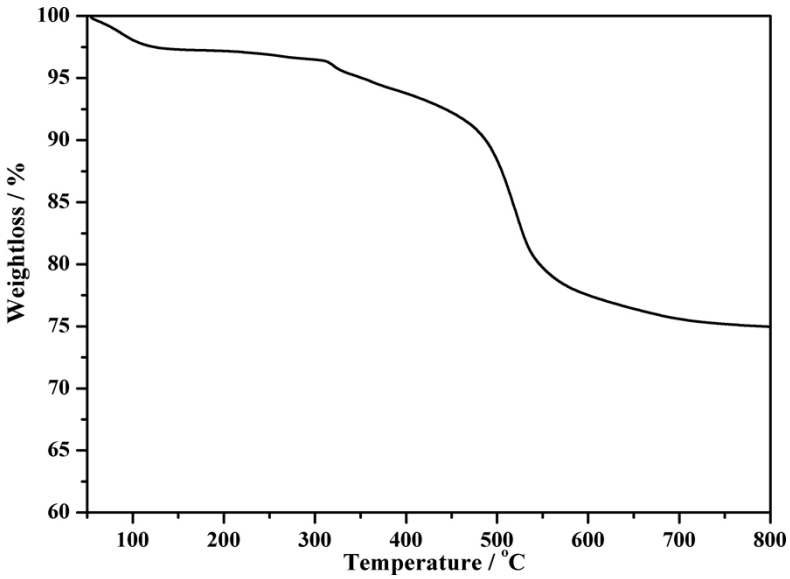


**Fig. S8** The TG curve of compound **4**.

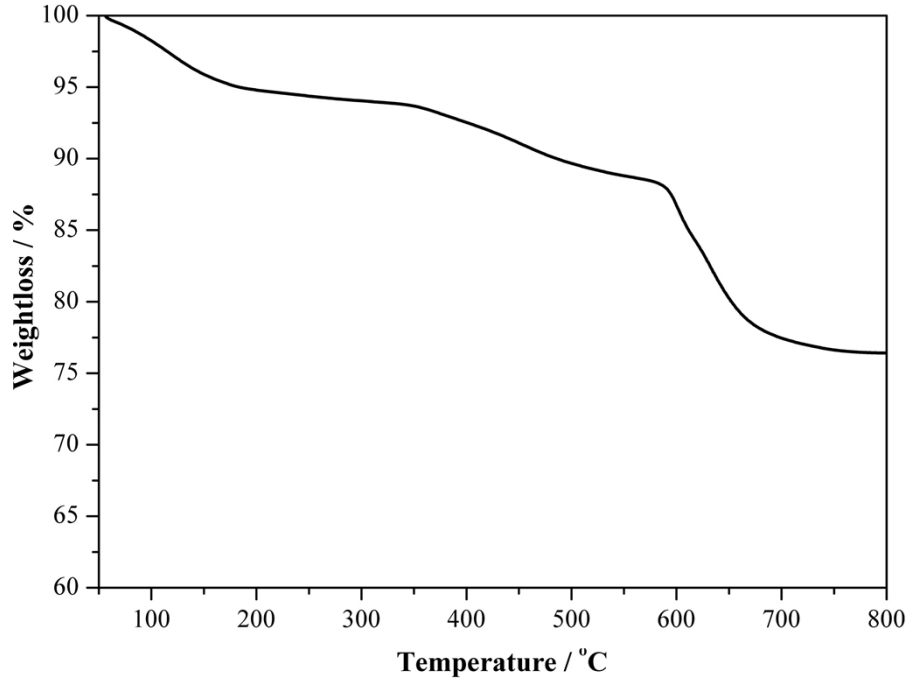


**Fig. S9** The TG curve of compound **5**.

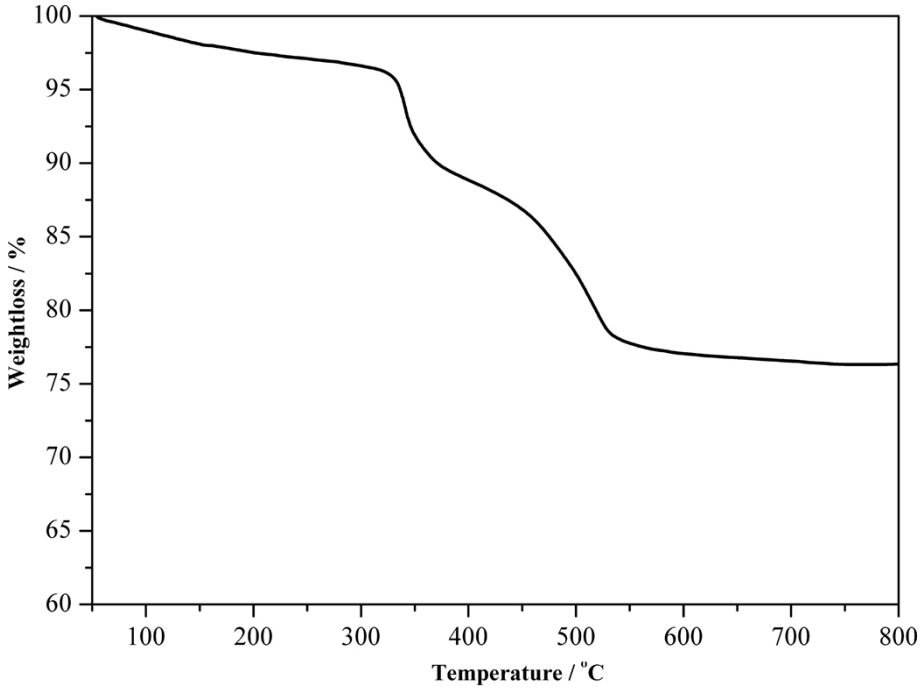


**Fig. S10** The TG curve of compound **6**.

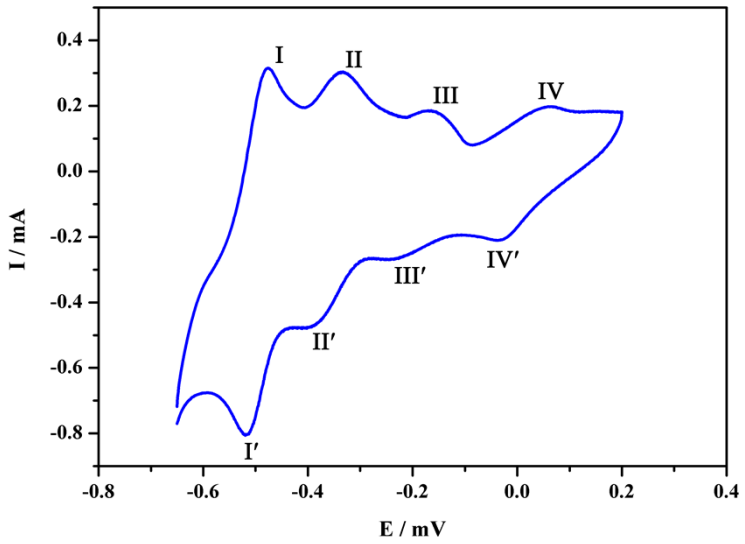


**Fig. S11** Cyclic voltammograms of **3** in the potential region of +0.2 to −0.65 V at scan rates of 150 mV $s^{-1}$.

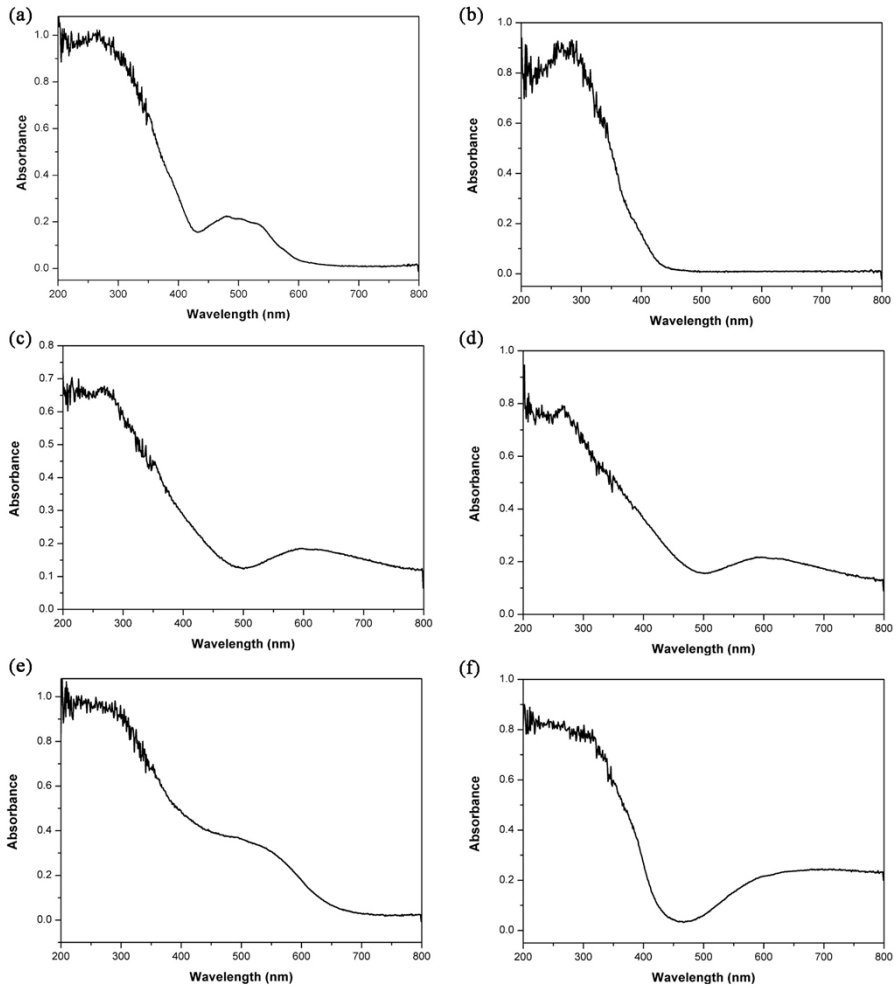


**Fig. S12** The diffuse reflectance UV-vis absorption spectra of compounds **1**(a), **2** (b), **3** (c), **4** (d), **5** (e) and **6** (f).

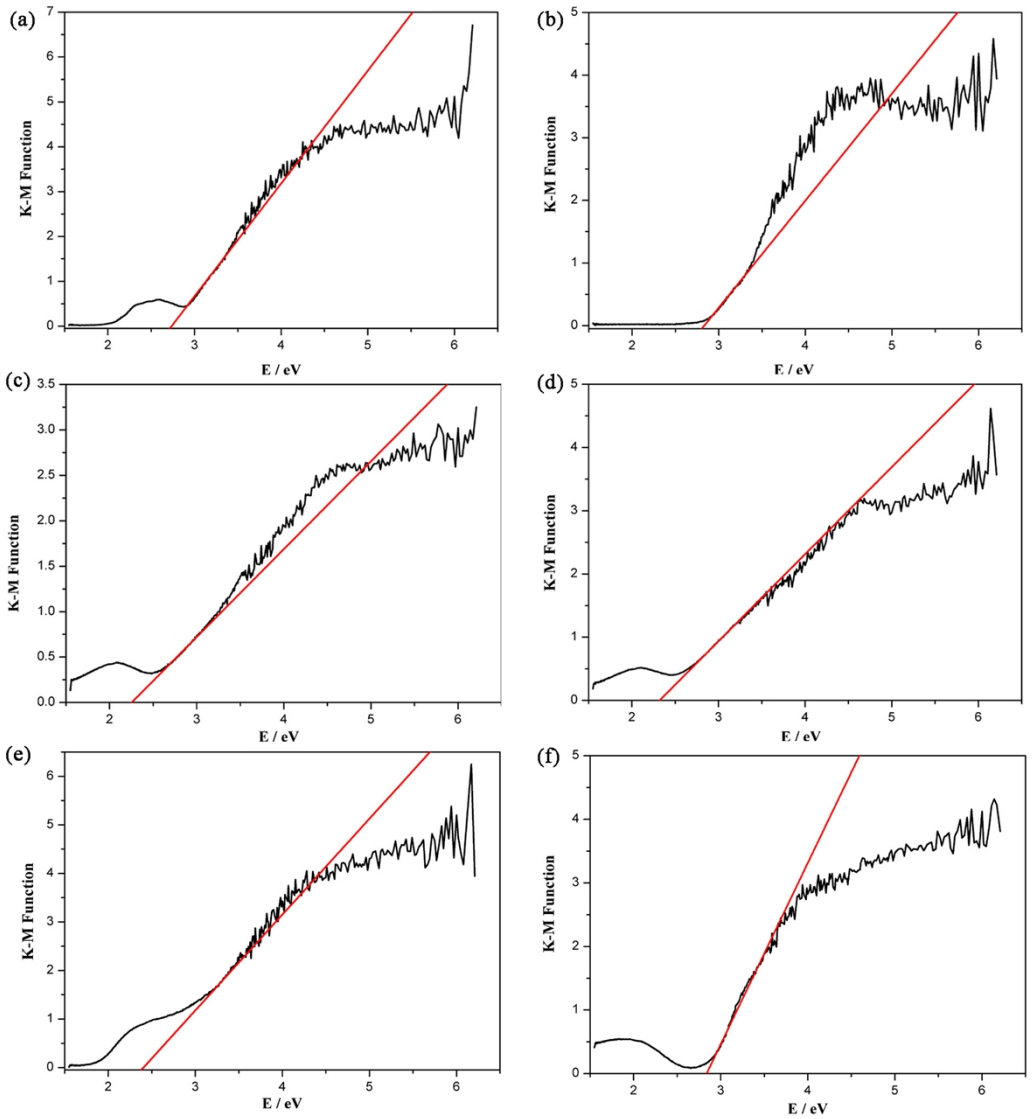


**Fig. S13** The diffuse reflectance UV-vis-NIR spectra of K-M function *vs.* energy (eV) of compounds **1** (a), **2** (b), **3** (c), **4** (d), **5** (e) and **6** (f).

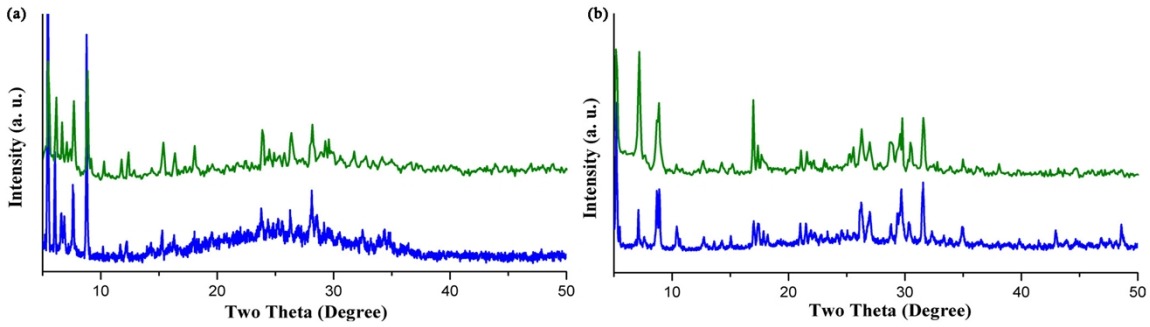


**Fig. S14** The XRD pattern of the as-synthesized (blue line) and after-photocatalytic (green line) pattern of **5** (a) and **6** (b).

**Table S1** Selected bond distances (Å) and angles (°) for compounds **1**–**6**.

| **1** | | | |
|---|---|---|---|
| W(1)-O(18) | 1.700(15) | W(2)-O(20) | 1.906(16) |
| W(1)-O(3) | 1.860(18) | W(2)-O(3) | 1.922(17) |
| W(1)-O(17) | 1.876(6) | W(2)-O(16)#1 | 2.42(2) |
| W(1)-O(21) | 1.898(16) | W(2)-O(4) | 2.48(2) |
| W(1)-O(14) | 1.940(16) | W(3)-O(11) | 1.690(13) |
| W(1)-O(13)#1 | 2.37(2) | W(3)-O(12) | 1.864(16) |
| W(1)-O(4) | 2.37(2) | W(3)-O(9) | 1.866(14) |
| W(2)-O(22) | 1.651(11) | W(3)-O(7) | 1.902(16) |
| W(2)-O(2) | 1.872(18) | W(3)-O(15) | 1.904(16) |
| W(2)-O(12)#1 | 1.876(16) | W(3)-O(16) | 2.30(2) |
| W(4)-O(6) | 1.656(14) | W(5)-O(5) | 1.927(14) |
| W(4)-O(21) | 1.857(15) | W(5)-O(16) | 2.35(3) |
| W(4)-O(5) | 1.857(16) | W(6)-O(10) | 1.652(13) |
| W(4)-O(7)#1 | 1.862(15) | W(6)-O(20) | 1.846(17) |
| W(4)-O(8)#1 | 1.892(15) | W(6)-O(8) | 1.896(16) |
| W(4)-O(13)#1 | 2.39(2) | W(6)-O(17) | 1.902(16) |
| W(5)-O(1) | 1.620(18) | W(6)-O(9) | 1.931(15) |
| W(5)-O(14) | 1.837(16) | W(6)-O(4) | 2.36(2) |
| W(5)-O(15) | 1.894(15) | Co(1)-N(4) | 2.066(18) |
| W(5)-O(2)#1 | 1.910(16) | Co(1)-N(2) | 2.076(18) |
| Co(1)-N(7) | 2.099(16) | Si(1)-O(19) | 1.57(2) |
| Co(1)-O(1W) | 2.134(14) | Si(1)-O(13) | 1.60(2) |
| Co(1)-N(1) | 2.149(16) | Si(1)-O(4) | 1.61(2) |
| Co(1)-O(11) | 2.167(12) | Si(1)-O(16) | 1.69(3) |
| O(18)-W(1)-O(3) | 102.2(8) | O(18)-W(1)-O(13)#1 | 156.3(9) |
| O(18)-W(1)-O(17) | 101.3(8) | O(3)-W(1)-O(13)#1 | 94.7(9) |
| O(3)-W(1)-O(17) | 89.2(7) | O(17)-W(1)-O(13)#1 | 95.3(8) |
| O(18)-W(1)-O(21) | 101.4(8) | O(21)-W(1)-O(13)#1 | 61.7(8) |
| O(3)-W(1)-O(21) | 90.1(8) | O(14)-W(1)-O(13)#1 | 64.1(9) |
| O(17)-W(1)-O(21) | 156.8(9) | O(18)-W(1)-O(4) | 159.3(8) |
| O(18)-W(1)-O(14) | 100.0(9) | O(3)-W(1)-O(4) | 66.5(8) |
| O(3)-W(1)-O(14) | 157.8(9) | O(17)-W(1)-O(4) | 62.6(8) |

| | | | |
|---|---|---|---|
| O(17)-W(1)-O(14) | 86.4(7) | O(21)-W(1)-O(4) | 96.1(8) |
| O(13)#1-W(1)-O(4) | 44.3(8) | O(22)-W(2)-O(2) | 100.6(8) |
| O(2)-W(2)-O(16)#1 | 62.1(8) | O(22)-W(2)-O(12)#1 | 101.1(7) |
| O(12)#1-W(2)-O(16)#1 | 59.5(8) | O(2)-W(2)-O(12)#1 | 88.0(7) |
| O(20)-W(2)-O(16)#1 | 96.8(8) | O(22)-W(2)-O(20) | 104.6(7) |
| O(3)-W(2)-O(16)#1 | 96.8(9) | O(2)-W(2)-O(20) | 88.8(8) |
| O(22)-W(2)-O(4) | 158.4(8) | O(12)#1-W(2)-O(20) | 154.3(8) |
| O(2)-W(2)-O(4) | 95.9(8) | O(22)-W(2)-O(3) | 101.3(8) |
| O(12)#1-W(2)-O(4) | 93.2(8) | O(2)-W(2)-O(3) | 158.0(8) |
| O(20)-W(2)-O(4) | 61.8(8) | O(12)#1-W(2)-O(3) | 86.0(8) |
| O(3)-W(2)-O(4) | 63.4(7) | O(20)-W(2)-O(3) | 87.5(7) |
| O(16)#1-W(2)-O(4) | 49.1(8) | O(22)-W(2)-O(16)#1 | 152.4(8) |
| O(11)-W(3)-O(12) | 99.6(7) | O(12)-W(3)-O(16) | 62.2(8) |
| O(11)-W(3)-O(9) | 103.3(7) | O(9)-W(3)-O(16) | 96.1(8) |
| O(12)-W(3)-O(9) | 157.1(8) | O(7)-W(3)-O(16) | 96.8(9) |
| O(11)-W(3)-O(7) | 99.4(7) | O(15)-W(3)-O(16) | 62.7(9) |
| O(12)-W(3)-O(7) | 86.4(8) | O(11)-W(3)-O(19)#1 | 158.1(7) |
| O(9)-W(3)-O(7) | 89.5(6) | O(12)-W(3)-O(19)#1 | 93.6(8) |
| O(11)-W(3)-O(15) | 101.6(8) | O(9)-W(3)-O(19)#1 | 64.5(7) |
| O(12)-W(3)-O(15) | 87.8(7) | O(7)-W(3)-O(19)#1 | 63.9(7) |
| O(9)-W(3)-O(15) | 87.9(7) | O(15)-W(3)-O(19)#1 | 96.3(8) |
| O(7)-W(3)-O(15) | 158.9(8) | O(16)-W(3)-O(19)#1 | 46.8(8) |
| O(11)-W(3)-O(16) | 154.8(8) | O(6)-W(4)-O(21) | 101.8(9) |
| O(21)-W(4)-O(13)#1 | 61.8(8) | O(6)-W(4)-O(5) | 102.1(9) |
| O(5)-W(4)-O(13)#1 | 66.0(8) | O(21)-W(4)-O(5) | 88.1(6) |
| O(7)#1-W(4)-O(13)#1 | 92.9(8) | O(6)-W(4)-O(7)#1 | 100.1(8) |
| O(8)#1-W(4)-O(13)#1 | 95.8(8) | O(21)-W(4)-O(7)#1 | 87.7(7) |
| O(6)-W(4)-O(19) | 156.9(9) | O(5)-W(4)-O(7)#1 | 157.7(8) |
| O(21)-W(4)-O(19) | 95.4(8) | O(6)-W(4)-O(8)#1 | 101.1(8) |
| O(5)-W(4)-O(19) | 93.7(9) | O(21)-W(4)-O(8)#1 | 157.2(8) |
| O(7)#1-W(4)-O(19) | 64.9(8) | O(5)-W(4)-O(8)#1 | 86.4(7) |
| O(8)#1-W(4)-O(19) | 62.9(8) | O(7)#1-W(4)-O(8)#1 | 88.9(6) |
| O(13)#1-W(4)-O(19) | 44.2(8) | O(6)-W(4)-O(13)#1 | 158.8(9) |
| O(1)-W(5)-O(14) | 103.1(9) | O(14)-W(5)-O(16) | 95.3(9) |
| O(1)-W(5)-O(15) | 101.0(8) | O(15)-W(5)-O(16) | 61.7(8) |

| | | | |
|---|---|---|---|
| O(14)-W(5)-O(15) | 89.2(7) | O(2)#1-W(5)-O(16) | 63.1(8) |
| O(1)-W(5)-O(2)#1 | 99.6(9) | O(5)-W(5)-O(16) | 96.2(9) |
| O(14)-W(5)-O(2)#1 | 157.3(9) | O(1)-W(5)-O(13)#1 | 157.5(8) |
| O(15)-W(5)-O(2)#1 | 86.4(6) | O(14)-W(5)-O(13)#1 | 63.0(8) |
| O(1)-W(5)-O(5) | 101.0(8) | O(15)-W(5)-O(13)#1 | 96.6(8) |
| O(14)-W(5)-O(5) | 89.6(6) | O(2)#1-W(5)-O(13)#1 | 95.4(8) |
| O(15)-W(5)-O(5) | 157.7(9) | O(5)-W(5)-O(13)#1 | 63.2(8) |
| O(2)#1-W(5)-O(5) | 86.2(7) | O(16)-W(5)-O(13)#1 | 47.7(8) |
| O(1)-W(5)-O(16) | 154.7(8) | O(10)-W(6)-O(20) | 102.3(8) |
| O(20)-W(6)-O(4) | 65.1(8) | O(10)-W(6)-O(8) | 99.9(8) |
| O(8)-W(6)-O(4) | 94.9(8) | O(20)-W(6)-O(8) | 86.7(7) |
| O(17)-W(6)-O(4) | 62.6(8) | O(10)-W(6)-O(17) | 103.3(8) |
| O(9)-W(6)-O(4) | 93.0(8) | O(20)-W(6)-O(17) | 88.7(7) |
| O(10)-W(6)-O(19)#1 | 156.6(7) | O(8)-W(6)-O(17) | 156.7(9) |
| O(20)-W(6)-O(19)#1 | 93.1(9) | O(10)-W(6)-O(9) | 100.7(8) |
| O(8)-W(6)-O(19)#1 | 63.1(8) | O(20)-W(6)-O(9) | 156.9(8) |
| O(17)-W(6)-O(19)#1 | 94.4(9) | O(8)-W(6)-O(9) | 87.9(6) |
| O(9)-W(6)-O(19)#1 | 64.5(8) | O(17)-W(6)-O(9) | 87.4(7) |
| O(4)-W(6)-O(19)#1 | 43.4(7) | O(10)-W(6)-O(4) | 160.0(7) |
| N(4)-Co(1)-N(2) | 172.5(7) | O(19)-Si(1)-O(13) | 110.6(12) |
| N(4)-Co(1)-N(7) | 90.0(6) | O(19)#1-Si(1)-O(13) | 69.4(12) |
| N(2)-Co(1)-N(7) | 92.4(7) | O(19)-Si(1)-O(4) | 112.8(11) |
| N(4)-Co(1)-O(1W) | 86.4(6) | O(19)#1-Si(1)-O(4) | 67.2(11) |
| N(2)-Co(1)-O(1W) | 86.4(7) | O(13)-Si(1)-O(4) | 112.5(12) |
| N(7)-Co(1)-O(1W) | 90.7(6) | O(13)#1-Si(1)-O(4) | 67.5(12) |
| N(4)-Co(1)-N(1) | 93.3(6) | O(13)-Si(1)-O(16)#1 | 72.7(11) |
| N(2)-Co(1)-N(1) | 93.7(7) | O(19)-Si(1)-O(16) | 109.4(12) |
| N(7)-Co(1)-N(1) | 92.5(6) | O(13)-Si(1)-O(16) | 107.3(11) |
| O(1W)-Co(1)-N(1) | 176.7(6) | O(13)#1-Si(1)-O(16) | 72.7(11) |
| N(4)-Co(1)-O(11) | 90.7(6) | O(4)-Si(1)-O(16) | 104.1(12) |
| N(2)-Co(1)-O(11) | 87.0(6) | O(4)#1-Si(1)-O(16) | 75.9(12) |
| N(7)-Co(1)-O(11) | 179.1(6) | N(1)-Co(1)-O(11) | 86.7(6) |
| O(1W)-Co(1)-O(11) | 90.0(5) | | |

Symmetry codes: #1 -x, -y, -z+2; #2 -x-1/2, y, -z+5/2.

| **2** | | | |
|---|---|---|---|
| O(1)-W(1) | 1.696(17) | O(7)-W(2) | 1.883(16) |
| O(2)-W(3) | 1.716(16) | O(7)-W(8) | 1.951(16) |
| O(3)-W(1) | 1.895(17) | O(6W)-Zn(1) | 2.134(19) |
| O(3)-W(3) | 1.912(17) | O(8)-W(1) | 1.920(15) |
| O(4)-W(1) | 1.885(15) | O(8)-W(5) | 1.925(15) |
| O(4)-W(2) | 1.926(15) | O(7W)-Zn(1) | 2.17(2) |
| O(5)-W(3) | 1.844(16) | O(9)-W(3) | 1.887(16) |
| O(5)-W(2) | 1.941(16) | O(9)-W(7) | 1.923(16) |
| O(6)-W(2) | 1.909(17) | O(8W)-Zn(2) | 2.155(18) |
| O(6)-W(9) | 1.924(17) | O(10)-W(4) | 1.906(17) |
| O(10)-W(1) | 1.942(17) | O(16)-Si(1) | 1.647(17) |
| O(9W)-Zn(2) | 2.080(19) | O(16)-W(4) | 2.310(15) |
| O(11)-W(9) | 1.674(18) | O(16)-W(1) | 2.335(15) |
| O(12)-W(4) | 1.695(17) | O(16)-W(5) | 2.358(15) |
| O(13)-W(4) | 1.886(15) | O(17)-W(8) | 1.880(17) |
| O(13)-W(9) | 1.921(15) | O(17)-W(7) | 1.918(16) |
| O(14)-W(9) | 1.908(16) | O(18)-W(7) | 1.730(17) |
| O(14)-W(8) | 1.928(17) | O(19)-W(8) | 1.701(17) |
| O(15)-W(5) | 1.905(17) | O(20)-W(6) | 1.901(15) |
| O(15)-W(4) | 1.928(16) | O(20)-W(5) | 1.914(15) |
| O(21)-Si(1) | 1.637(16) | O(24)-W(11) | 1.880(15) |
| O(21)-W(6) | 2.305(15) | O(24)-W(9) | 1.923(16) |
| O(21)-W(7) | 2.341(15) | O(25)-Si(1) | 1.627(17) |
| O(21)-W(3) | 2.363(15) | O(25)-W(12) | 2.313(15) |
| O(22)-Si(1) | 1.624(17) | O(25)-W(11) | 2.348(15) |
| O(22)-W(2) | 2.352(16) | O(25)-W(10) | 2.357(16) |
| O(22)-W(8) | 2.339(17) | O(26)-W(5) | 1.899(18) |
| O(22)-W(9) | 2.361(17) | O(26)-W(12) | 1.913(18) |
| O(23)-W(4) | 1.888(17) | O(27)-W(10) | 1.894(17) |
| O(23)-W(11) | 1.912(18) | O(27)-W(7) | 1.900(16) |
| O(28)-W(6) | 1.884(17) | O(33)-W(10) | 1.921(15) |
| O(28)-W(12) | 1.907(17) | O(34)-W(5) | 1.721(18) |
| O(29)-W(10) | 1.888(15) | O(35)-W(2) | 1.696(16) |

| | | | |
|---|---|---|---|
| O(29)-W(8) | 1.895(15) | O(36)-W(10) | 1.680(18) |
| O(30)-W(11) | 1.713(19) | O(37)-W(12) | 1.719(15) |
| O(31)-W(11) | 1.922(16) | O(37)-Zn(2) | 2.253(16) |
| O(31)-W(10) | 1.942(16) | O(38)-W(7) | 1.911(15) |
| O(32)-W(12) | 1.904(17) | O(38)-W(6) | 1.918(15) |
| O(32)-W(11) | 1.921(16) | O(39)-W(6) | 1.915(15) |
| O(33)-W(12) | 1.906(16) | O(39)-W(3) | 1.966(14) |
| O(40)-W(6) | 1.726(15) | Zn(2)-N(8) | 2.05(2) |
| O(40)-Zn(3) | 2.166(15) | Zn(2)-N(5) | 2.12(2) |
| Zn(1)-N(10) | 2.09(2) | Zn(2)-N(2) | 2.19(2) |
| Zn(1)-N(7) | 2.09(2) | Zn(3)-N(9) | 2.01(2) |
| Zn(1)-N(1) | 2.15(2) | Zn(3)-N(16) | 2.34(2) |
| Zn(1)-N(4) | 2.15(2) | O(25)-Si(1)-O(22) | 110.3(9) |
| O(25)-Si(1)-O(16) | 108.6(8) | O(25)-Si(1)-O(21) | 108.9(8) |
| O(22)-Si(1)-O(16) | 108.5(9) | O(22)-Si(1)-O(21) | 109.9(8) |
| O(21)-Si(1)-O(16) | 110.7(9) | O(1)-W(1)-O(3) | 101.8(8) |
| O(4)-W(1)-O(10) | 89.1(7) | O(1)-W(1)-O(4) | 103.7(8) |
| O(8)-W(1)-O(10) | 87.4(7) | O(3)-W(1)-O(4) | 86.7(7) |
| O(1)-W(1)-O(16) | 169.2(7) | O(1)-W(1)-O(8) | 97.9(8) |
| O(3)-W(1)-O(16) | 84.8(6) | O(3)-W(1)-O(8) | 88.1(7) |
| O(4)-W(1)-O(16) | 85.2(6) | O(4)-W(1)-O(8) | 158.4(7) |
| O(8)-W(1)-O(16) | 73.5(6) | O(1)-W(1)-O(10) | 101.3(8) |
| O(10)-W(1)-O(16) | 72.2(6) | O(3)-W(1)-O(10) | 156.9(7) |
| O(35)-W(2)-O(7) | 100.9(8) | O(6)-W(2)-O(5) | 156.9(6) |
| O(35)-W(2)-O(6) | 100.9(8) | O(4)-W(2)-O(5) | 83.2(7) |
| O(7)-W(2)-O(6) | 89.2(7) | O(35)-W(2)-O(22) | 172.2(8) |
| O(35)-W(2)-O(4) | 102.2(8) | O(7)-W(2)-O(22) | 73.7(6) |
| O(7)-W(2)-O(4) | 156.8(7) | O(6)-W(2)-O(22) | 73.7(7) |
| O(6)-W(2)-O(4) | 88.6(7) | O(4)-W(2)-O(22) | 83.5(6) |
| O(35)-W(2)-O(5) | 101.9(7) | O(5)-W(2)-O(22) | 83.9(6) |
| O(7)-W(2)-O(5) | 90.0(7) | O(2)-W(3)-O(5) | 102.1(7) |
| O(2)-W(3)-O(9) | 102.2(7) | O(3)-W(3)-O(39) | 87.1(7) |
| O(5)-W(3)-O(9) | 91.9(7) | O(2)-W(3)-O(21) | 171.1(7) |
| O(2)-W(3)-O(3) | 100.9(7) | O(5)-W(3)-O(21) | 86.1(6) |
| O(5)-W(3)-O(3) | 85.3(7) | O(9)-W(3)-O(21) | 73.6(6) |

| | | | |
|---|---|---|---|
| O(9)-W(3)-O(3) | 156.8(7) | O(3)-W(3)-O(21) | 83.2(6) |
| O(2)-W(3)-O(39) | 99.8(7) | O(39)-W(3)-O(21) | 72.3(6) |
| O(5)-W(3)-O(39) | 157.8(6) | O(9)-W(3)-O(39) | 86.9(7) |
| O(12)-W(4)-O(23) | 103.8(8) | O(13)-W(4)-O(15) | 158.2(7) |
| O(12)-W(4)-O(13) | 102.8(7) | O(10)-W(4)-O(15) | 86.8(7) |
| O(23)-W(4)-O(13) | 85.4(7) | O(12)-W(4)-O(16) | 169.0(7) |
| O(12)-W(4)-O(10) | 98.7(8) | O(23)-W(4)-O(16) | 84.4(6) |
| O(23)-W(4)-O(10) | 157.6(7) | O(13)-W(4)-O(16) | 84.9(6) |
| O(13)-W(4)-O(10) | 89.1(7) | O(10)-W(4)-O(16) | 73.4(6) |
| O(12)-W(4)-O(15) | 98.9(7) | O(15)-W(4)-O(16) | 73.4(6) |
| O(23)-W(4)-O(15) | 90.3(7) | O(34)-W(5)-O(26) | 102.2(8) |
| O(34)-W(5)-O(15) | 101.9(8) | O(15)-W(5)-O(8) | 87.7(7) |
| O(26)-W(5)-O(15) | 90.2(7) | O(20)-W(5)-O(8) | 87.7(6) |
| O(34)-W(5)-O(20) | 100.6(8) | O(34)-W(5)-O(16) | 172.0(7) |
| O(26)-W(5)-O(20) | 85.2(7) | O(26)-W(5)-O(16) | 83.9(6) |
| O(15)-W(5)-O(20) | 157.5(7) | O(15)-W(5)-O(16) | 72.7(6) |
| O(34)-W(5)-O(8) | 101.3(8) | O(20)-W(5)-O(16) | 84.9(6) |
| O(26)-W(5)-O(8) | 156.2(7) | O(8)-W(5)-O(16) | 72.9(6) |
| O(40)-W(6)-O(28) | 102.8(8) | O(28)-W(6)-O(38) | 90.3(7) |
| O(40)-W(6)-O(20) | 99.8(7) | O(20)-W(6)-O(38) | 159.1(7) |
| O(28)-W(6)-O(20) | 85.3(7) | O(39)-W(6)-O(38) | 86.6(7) |
| O(40)-W(6)-O(39) | 99.4(7) | O(40)-W(6)-O(21) | 171.6(7) |
| O(28)-W(6)-O(39) | 157.8(7) | O(28)-W(6)-O(21) | 83.5(6) |
| O(20)-W(6)-O(39) | 89.7(6) | O(20)-W(6)-O(21) | 86.0(6) |
| O(40)-W(6)-O(38) | 101.0(7) | O(39)-W(6)-O(21) | 74.5(6) |
| O(18)-W(7)-O(27) | 102.5(8) | O(38)-W(6)-O(21) | 73.2(6) |
| O(18)-W(7)-O(38) | 100.6(7) | O(38)-W(7)-O(9) | 87.7(7) |
| O(27)-W(7)-O(38) | 88.2(7) | O(17)-W(7)-O(9) | 90.0(7) |
| O(18)-W(7)-O(17) | 102.7(8) | O(18)-W(7)-O(21) | 171.4(7) |
| O(27)-W(7)-O(17) | 84.5(7) | O(27)-W(7)-O(21) | 82.7(6) |
| O(38)-W(7)-O(17) | 156.6(7) | O(38)-W(7)-O(21) | 72.4(6) |
| O(18)-W(7)-O(9) | 101.5(7) | O(17)-W(7)-O(21) | 84.5(6) |
| O(27)-W(7)-O(9) | 156.0(7) | O(9)-W(7)-O(21) | 73.6(6) |
| O(19)-W(8)-O(17) | 102.7(8) | O(17)-W(8)-O(7) | 89.8(7) |
| O(19)-W(8)-O(29) | 103.6(7) | O(29)-W(8)-O(7) | 156.4(7) |

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|---|---|---|---|
| O(17)-W(8)-O(29) | 85.0(7) | O(14)-W(8)-O(7) | 87.4(7) |
| O(19)-W(8)-O(14) | 99.2(8) | O(19)-W(8)-O(22) | 169.4(7) |
| O(17)-W(8)-O(14) | 158.1(7) | O(17)-W(8)-O(22) | 85.4(7) |
| O(29)-W(8)-O(14) | 88.9(7) | O(29)-W(8)-O(22) | 83.8(6) |
| O(19)-W(8)-O(7) | 100.0(7) | O(14)-W(8)-O(22) | 73.0(6) |
| O(7)-W(8)-O(22) | 72.9(6) | O(14)-W(9)-O(24) | 88.7(7) |
| O(11)-W(9)-O(14) | 99.4(8) | O(13)-W(9)-O(24) | 85.0(7) |
| O(11)-W(9)-O(13) | 104.1(8) | O(6)-W(9)-O(24) | 157.8(7) |
| O(14)-W(9)-O(13) | 156.5(7) | O(11)-W(9)-O(22) | 168.6(7) |
| O(11)-W(9)-O(6) | 98.7(8) | O(14)-W(9)-O(22) | 72.8(7) |
| O(14)-W(9)-O(6) | 88.5(7) | O(13)-W(9)-O(22) | 84.1(6) |
| O(13)-W(9)-O(6) | 88.8(7) | O(6)-W(9)-O(22) | 73.2(6) |
| O(11)-W(9)-O(24) | 103.4(8) | O(24)-W(9)-O(22) | 85.0(7) |
| O(36)-W(10)-O(29) | 102.9(8) | O(27)-W(10)-O(31) | 156.5(7) |
| O(36)-W(10)-O(27) | 104.8(8) | O(33)-W(10)-O(31) | 87.0(6) |
| O(29)-W(10)-O(27) | 85.9(7) | O(36)-W(10)-O(25) | 169.4(7) |
| O(36)-W(10)-O(33) | 100.8(8) | O(29)-W(10)-O(25) | 82.8(6) |
| O(29)-W(10)-O(33) | 156.2(7) | O(27)-W(10)-O(25) | 84.3(6) |
| O(27)-W(10)-O(33) | 90.1(7) | O(33)-W(10)-O(25) | 73.4(6) |
| O(36)-W(10)-O(31) | 98.6(8) | O(31)-W(10)-O(25) | 72.5(6) |
| O(29)-W(10)-O(31) | 87.5(6) | O(30)-W(11)-O(24) | 102.4(8) |
| O(30)-W(11)-O(23) | 102.5(8) | O(23)-W(11)-O(32) | 87.9(7) |
| O(24)-W(11)-O(23) | 85.1(7) | O(31)-W(11)-O(32) | 88.0(7) |
| O(30)-W(11)-O(31) | 100.9(8) | O(30)-W(11)-O(25) | 169.9(7) |
| O(24)-W(11)-O(31) | 90.2(7) | O(24)-W(11)-O(25) | 85.9(7) |
| O(23)-W(11)-O(31) | 156.6(7) | O(23)-W(11)-O(25) | 83.7(7) |
| O(30)-W(11)-O(32) | 99.4(8) | O(31)-W(11)-O(25) | 73.0(6) |
| O(24)-W(11)-O(32) | 158.0(7) | O(32)-W(11)-O(25) | 72.6(6) |
| O(37)-W(12)-O(28) | 102.7(7) | O(28)-W(12)-O(26) | 83.3(7) |
| O(37)-W(12)-O(32) | 100.6(7) | O(32)-W(12)-O(26) | 89.0(7) |
| O(28)-W(12)-O(32) | 156.4(7) | O(33)-W(12)-O(26) | 158.8(6) |
| O(37)-W(12)-O(33) | 100.0(7) | O(37)-W(12)-O(25) | 172.2(7) |
| O(28)-W(12)-O(33) | 89.7(7) | O(28)-W(12)-O(25) | 83.3(6) |
| O(32)-W(12)-O(33) | 89.5(7) | O(32)-W(12)-O(25) | 73.7(6) |
| O(37)-W(12)-O(26) | 101.1(7) | O(33)-W(12)-O(25) | 74.8(6) |

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|---|---|---|---|
| O(26)-W(12)-O(25) | 84.5(6) | N(7)-Zn(1)-O(6W) | 89.4(8) |
| N(10)-Zn(1)-N(7) | 174.4(9) | N(1)-Zn(1)-O(6W) | 171.3(8) |
| N(10)-Zn(1)-N(1) | 97.4(9) | N(4)-Zn(1)-O(6W) | 95.9(8) |
| N(7)-Zn(1)-N(1) | 87.4(9) | N(10)-Zn(1)-O(7W) | 90.5(9) |
| N(10)-Zn(1)-N(4) | 88.5(9) | N(7)-Zn(1)-O(7W) | 86.9(9) |
| N(7)-Zn(1)-N(4) | 94.0(9) | N(1)-Zn(1)-O(7W) | 88.1(9) |
| N(1)-Zn(1)-N(4) | 92.4(9) | N(4)-Zn(1)-O(7W) | 179.0(9) |
| N(10)-Zn(1)-O(6W) | 85.4(8) | O(6W)-Zn(1)-O(7W) | 83.7(9) |
| N(8)-Zn(2)-O(9W) | 169.5(8) | N(5)-Zn(2)-N(2) | 92.6(8) |
| N(8)-Zn(2)-N(5) | 95.1(9) | O(8W)-Zn(2)-N(2) | 176.6(7) |
| O(9W)-Zn(2)-N(5) | 94.5(8) | N(8)-Zn(2)-O(37) | 82.9(7) |
| N(8)-Zn(2)-O(8W) | 86.4(8) | O(9W)-Zn(2)-O(37) | 87.3(7) |
| O(9W)-Zn(2)-O(8W) | 89.1(7) | N(5)-Zn(2)-O(37) | 175.7(8) |
| N(5)-Zn(2)-O(8W) | 90.7(8) | O(8W)-Zn(2)-O(37) | 85.3(7) |
| N(8)-Zn(2)-N(2) | 92.7(9) | N(2)-Zn(2)-O(37) | 91.3(7) |
| O(9W)-Zn(2)-N(2) | 91.2(8) | N(9)-Zn(3)-O(40) | 91.5(8) |
| O(40)-Zn(3)-N(16)#1 | 88.2(8) | N(9)#1-Zn(3)-O(40) | 88.5(9) |
| O(40)#1-Zn(3)-N(16)#1 | 91.8(8) | N(9)-Zn(3)-O(40)#1 | 88.5(9) |
| N(9)-Zn(3)-N(16) | 87.3(10) | N(9)#1-Zn(3)-O(40)#1 | 91.5(8) |
| N(9)#1-Zn(3)-N(16) | 92.7(10) | N(9)-Zn(3)-N(16)#1 | 92.7(10) |
| O(40)-Zn(3)-N(16) | 91.8(8) | N(9)#1-Zn(3)-N(16)#1 | 87.3(10) |
| O(40)#1-Zn(3)-N(16) | 88.2(8) | | |
| Symmetry codes: #1 -x, -y+1, -z+2. | | | |
| **3** | | | |
| O(1)-W(4) | 1.67(2) | O(5A)-W(5) | 2.02(5) |
| O(2)-W(5) | 1.85(2) | O(5A)-W(2) | 2.05(4) |
| O(2)-W(3) | 1.92(2) | O(6)-W(6)#1 | 1.92(2) |
| O(3)-Ge(1) | 1.69(4) | O(6)-W(2) | 1.93(2) |
| O(3)-W(4) | 2.30(4) | O(7)-Ge(1) | 1.71(5) |
| O(3)-W(3) | 2.36(5) | O(7)-O(14) | 1.73(6) |
| O(3)-W(5) | 2.48(4) | O(7)-W(1) | 2.27(4) |
| O(4)-W(3) | 1.61(2) | O(7)-W(3)#1 | 2.38(4) |
| O(5)-W(5) | 1.81(5) | O(7)-W(2) | 2.44(4) |
| O(5)-W(2) | 1.88(5) | O(8)-W(1) | 1.68(2) |

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|---|---|---|---|
| O(9)-W(4) | 1.89(2) | O(12B)-W(5) | 2.05(4) |
| O(9)-W(6) | 1.90(2) | O(13)-W(1) | 1.87(2) |
| O(10)-W(6) | 1.64(2) | O(13)-W(6) | 1.88(2) |
| O(11)-W(5) | 1.673(19) | O(14)-Ge(1) | 1.61(4) |
| O(11)-Cu(1) | 2.425(18) | O(14)-W(1) | 2.33(5) |
| O(12A)-O(12B) | 0.93(5) | O(14)-W(4) | 2.44(4) |
| O(12A)-O(19) | 1.71(6) | O(14)-W(6) | 2.48(4) |
| O(12A)-W(5) | 1.72(4) | O(15)-W(1) | 1.82(2) |
| O(12A)-W(6)#1 | 1.87(4) | O(15)-W(4) | 1.92(3) |
| O(12B)-W(6)#1 | 2.05(4) | O(16)-W(2) | 1.68(2) |
| O(17)-W(3) | 1.87(2) | O(21)-W(2) | 1.87(2) |
| O(17)-W(4) | 1.91(2) | O(21)-W(1) | 1.89(2) |
| O(18)-W(4) | 1.88(2) | O(22)-W(3)#1 | 1.90(2) |
| O(18)-W(5) | 1.92(2) | O(22)-W(2) | 1.93(2) |
| O(19)-Ge(1) | 1.79(4) | Ge(1)-O(14)#1 | 1.61(4) |
| O(19)-W(5) | 2.25(4) | Ge(1)-O(3)#1 | 1.69(4) |
| O(19)-W(6)#1 | 2.32(4) | Ge(1)-O(7)#1 | 1.71(5) |
| O(19)-W(2) | 2.37(4) | Ge(1)-O(19)#1 | 1.79(4) |
| O(20)-W(3)#1 | 1.88(2) | W(3)-O(20)#1 | 1.88(2) |
| O(20)-W(1) | 1.89(2) | W(3)-O(22)#1 | 1.90(2) |
| W(3)-O(7)#1 | 2.38(4) | Cu(2)-N(4) | 1.97(2) |
| W(6)-O(12A)#1 | 1.87(4) | Cu(2)-N(6) | 2.05(3) |
| W(6)-O(6)#1 | 1.92(2) | Cu(2)-Cl(1) | 2.548(8) |
| W(6)-O(12B)#1 | 2.05(4) | Cu(3)-N(8) | 1.993(16) |
| W(6)-O(19)#1 | 2.32(4) | Cu(3)-N(5) | 2.01(2) |
| Cu(1)-N(1) | 2.039(17) | N(11)-Cu(4) | 1.848(18) |
| Cu(1)-N(3) | 2.06(2) | Cu(4)-N(10)#4 | 1.870(18) |
| Cu(1)-O(11)#2 | 2.425(19) | N(10)-Cu(4)#5 | 1.870(17) |
| Cu(2)-N(2) | 1.950(18) | Cu(2)-N(7) | 1.968(19) |
| O(14)#1-Ge(1)-O(3) | 111(2) | O(8)-W(1)-O(15) | 104.4(11) |
| O(14)-Ge(1)-O(3) | 69(2) | O(8)-W(1)-O(13) | 104.8(11) |
| O(14)#1-Ge(1)-O(7) | 117(2) | O(15)-W(1)-O(13) | 88.1(10) |
| O(14)-Ge(1)-O(7) | 63(2) | O(8)-W(1)-O(21) | 101.3(11) |
| O(3)-Ge(1)-O(7) | 111(2) | O(15)-W(1)-O(21) | 86.6(10) |
| O(3)#1-Ge(1)-O(7) | 69(2) | O(13)-W(1)-O(21) | 153.9(11) |

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|---|---|---|---|
| O(14)#1-Ge(1)-O(19) | 72.8(19) | O(8)-W(1)-O(20) | 101.1(12) |
| O(14)-Ge(1)-O(19) | 107.2(19) | O(15)-W(1)-O(20) | 154.5(11) |
| O(3)-Ge(1)-O(19) | 73(2) | O(13)-W(1)-O(20) | 85.9(10) |
| O(3)#1-Ge(1)-O(19) | 106.7(19) | O(21)-W(1)-O(20) | 88.0(9) |
| O(7)-Ge(1)-O(19) | 77(2) | O(8)-W(1)-O(7) | 155.0(15) |
| O(7)#1-Ge(1)-O(19) | 103(2) | O(15)-W(1)-O(7) | 94.4(14) |
| O(7)-W(1)-O(14) | 44.2(15) | O(13)-W(1)-O(7) | 91.9(12) |
| O(16)-W(2)-O(21) | 103.4(10) | O(21)-W(1)-O(7) | 63.2(12) |
| O(16)-W(2)-O(5) | 112.7(15) | O(20)-W(1)-O(7) | 61.1(13) |
| O(21)-W(2)-O(5) | 79.2(15) | O(8)-W(1)-O(14) | 160.8(14) |
| O(16)-W(2)-O(22) | 100.5(11) | O(15)-W(1)-O(14) | 62.0(12) |
| O(21)-W(2)-O(22) | 88.0(10) | O(13)-W(1)-O(14) | 63.4(12) |
| O(5)-W(2)-O(22) | 146.3(15) | O(21)-W(1)-O(14) | 91.8(12) |
| O(16)-W(2)-O(6) | 96.1(10) | O(20)-W(1)-O(14) | 93.3(13) |
| O(21)-W(2)-O(6) | 160.1(10) | O(22)-W(2)-O(6) | 92.0(10) |
| O(5)-W(2)-O(6) | 90.1(15) | O(16)-W(2)-O(5A) | 89.1(15) |
| O(6)-W(2)-O(19) | 62.5(12) | O(21)-W(2)-O(5A) | 95.7(14) |
| O(5A)-W(2)-O(19) | 68.0(16) | O(5)-W(2)-O(5A) | 26.3(14) |
| O(16)-W(2)-O(7) | 156.2(14) | O(22)-W(2)-O(5A) | 168.7(14) |
| O(21)-W(2)-O(7) | 59.8(12) | O(6)-W(2)-O(5A) | 80.9(14) |
| O(5)-W(2)-O(7) | 82.2(17) | O(16)-W(2)-O(19) | 150.1(13) |
| O(22)-W(2)-O(7) | 64.5(12) | O(21)-W(2)-O(19) | 98.0(12) |
| O(6)-W(2)-O(7) | 102.5(12) | O(5)-W(2)-O(19) | 51.3(16) |
| O(5A)-W(2)-O(7) | 108.3(17) | O(22)-W(2)-O(19) | 100.9(12) |
| O(19)-W(2)-O(7) | 53.7(15) | O(4)-W(3)-O(20)#1 | 103.6(12) |
| O(4)-W(3)-O(17) | 101.5(12) | O(17)-W(3)-O(20)#1 | 154.9(11) |
| O(17)-W(3)-O(3) | 59.1(12) | O(4)-W(3)-O(22)#1 | 100.5(11) |
| O(20)#1-W(3)-O(3) | 96.4(13) | O(17)-W(3)-O(22)#1 | 88.3(9) |
| O(22)#1-W(3)-O(3) | 95.0(12) | O(20)#1-W(3)-O(22)#1 | 88.5(9) |
| O(2)-W(3)-O(3) | 63.7(12) | O(4)-W(3)-O(2) | 102.8(11) |
| O(4)-W(3)-O(7)#1 | 156.9(14) | O(17)-W(3)-O(2) | 88.3(9) |
| O(17)-W(3)-O(7)#1 | 97.1(13) | O(20)#1-W(3)-O(2) | 84.8(9) |
| O(20)#1-W(3)-O(7)#1 | 59.1(13) | O(22)#1-W(3)-O(2) | 156.7(10) |
| O(22)#1-W(3)-O(7)#1 | 66.2(12) | O(4)-W(3)-O(3) | 154.9(14) |
| O(2)-W(3)-O(7)#1 | 91.4(12) | O(1)-W(4)-O(18) | 102.3(10) |

| | | | |
|---|---|---|---|
| O(3)-W(3)-O(7)#1 | 48.3(14) | O(1)-W(4)-O(9) | 99.4(10) |
| O(1)-W(4)-O(3) | 159.1(15) | O(18)-W(4)-O(9) | 158.1(10) |
| O(18)-W(4)-O(3) | 65.3(11) | O(1)-W(4)-O(17) | 104.3(12) |
| O(9)-W(4)-O(3) | 93.3(12) | O(18)-W(4)-O(17) | 86.3(9) |
| O(17)-W(4)-O(3) | 59.8(13) | O(9)-W(4)-O(17) | 86.4(10) |
| O(15)-W(4)-O(3) | 95.0(13) | O(1)-W(4)-O(15) | 102.1(12) |
| O(1)-W(4)-O(14) | 154.5(14) | O(18)-W(4)-O(15) | 89.7(9) |
| O(18)-W(4)-O(14) | 94.5(11) | O(9)-W(4)-O(15) | 87.7(10) |
| O(9)-W(4)-O(14) | 65.8(12) | O(17)-W(4)-O(15) | 153.6(10) |
| O(17)-W(4)-O(14) | 95.7(13) | O(3)-W(4)-O(14) | 46.4(15) |
| O(15)-W(4)-O(14) | 58.6(12) | O(11)-W(5)-O(12A) | 116.7(16) |
| O(2)-W(5)-O(18) | 88.2(9) | O(11)-W(5)-O(5) | 111.8(15) |
| O(11)-W(5)-O(5A) | 88.7(14) | O(12A)-W(5)-O(5) | 90(2) |
| O(12A)-W(5)-O(5A) | 88.4(19) | O(11)-W(5)-O(2) | 103.6(10) |
| O(5)-W(5)-O(5A) | 26.8(15) | O(12A)-W(5)-O(2) | 81.7(16) |
| O(2)-W(5)-O(5A) | 166.8(14) | O(5)-W(5)-O(2) | 143.5(15) |
| O(18)-W(5)-O(5A) | 94.9(14) | O(11)-W(5)-O(18) | 99.0(9) |
| O(11)-W(5)-O(12B) | 90.7(14) | O(12A)-W(5)-O(18) | 144.2(16) |
| O(12A)-W(5)-O(12B) | 26.8(15) | O(5)-W(5)-O(18) | 78.1(15) |
| O(5)-W(5)-O(12B) | 94.5(19) | O(18)-W(5)-O(12B) | 169.5(14) |
| O(2)-W(5)-O(12B) | 93.6(14) | O(5A)-W(5)-O(12B) | 81.1(17) |
| O(12A)-W(5)-O(3) | 84.0(17) | O(11)-W(5)-O(19) | 154.0(13) |
| O(5)-W(5)-O(3) | 82.1(18) | O(12A)-W(5)-O(19) | 48.8(18) |
| O(2)-W(5)-O(3) | 61.8(13) | O(5)-W(5)-O(19) | 54.3(17) |
| O(18)-W(5)-O(3) | 61.2(11) | O(2)-W(5)-O(19) | 95.8(13) |
| O(5A)-W(5)-O(3) | 108.5(17) | O(18)-W(5)-O(19) | 98.9(13) |
| O(12B)-W(5)-O(3) | 110.7(15) | O(5A)-W(5)-O(19) | 71.1(16) |
| O(19)-W(5)-O(3) | 51.8(15) | O(12B)-W(5)-O(19) | 70.7(16) |
| O(10)-W(6)-O(12A)#1 | 116.0(16) | O(11)-W(5)-O(3) | 154.0(12) |
| O(10)-W(6)-O(13) | 103.2(11) | O(10)-W(6)-O(9) | 101.3(10) |
| O(12A)#1-W(6)-O(13) | 80.7(15) | O(12A)#1-W(6)-O(9) | 142.6(15) |
| O(9)-W(6)-O(12B)#1 | 167.9(14) | O(13)-W(6)-O(9) | 89.9(10) |
| O(6)#1-W(6)-O(12B)#1 | 82.1(14) | O(10)-W(6)-O(6)#1 | 98.6(11) |
| O(10)-W(6)-O(19)#1 | 153.7(13) | O(12A)#1-W(6)-O(6)#1 | 84.7(15) |
| O(12A)#1-W(6)-O(19)#1 | 46.8(17) | O(13)-W(6)-O(6)#1 | 157.5(9) |

| | | | |
|---|---|---|---|
| O(13)-W(6)-O(19)#1 | 93.8(13) | O(9)-W(6)-O(6)#1 | 91.4(10) |
| O(9)-W(6)-O(19)#1 | 98.6(12) | O(10)-W(6)-O(12B)#1 | 89.7(15) |
| O(6)#1-W(6)-O(19)#1 | 63.8(13) | O(12A)#1-W(6)-O(12B)#1 | 27.0(14) |
| O(12B)#1-W(6)-O(19)#1 | 69.4(16) | O(13)-W(6)-O(12B)#1 | 92.3(14) |
| O(10)-W(6)-O(14) | 156.5(13) | O(13)-W(6)-O(14) | 60.0(13) |
| O(12A)#1-W(6)-O(14) | 79.5(16) | O(9)-W(6)-O(14) | 64.7(12) |
| N(3)-Cu(1)-O(11) | 85.9(7) | O(6)#1-W(6)-O(14) | 100.5(12) |
| N(2)-Cu(2)-N(7) | 168.4(8) | O(12B)#1-W(6)-O(14) | 106.3(15) |
| N(2)-Cu(2)-N(4) | 86.5(9) | O(19)#1-W(6)-O(14) | 49.7(14) |
| N(7)-Cu(2)-N(4) | 89.4(9) | N(1)#2-Cu(1)-N(3) | 88.3(7) |
| N(2)-Cu(2)-N(6) | 91.4(9) | N(1)-Cu(1)-N(3) | 91.7(7) |
| N(7)-Cu(2)-N(6) | 91.9(9) | N(1)-Cu(1)-O(11)#2 | 91.7(7) |
| N(4)-Cu(2)-N(6) | 175.5(8) | N(3)-Cu(1)-O(11)#2 | 94.1(7) |
| N(2)-Cu(2)-Cl(1) | 101.0(6) | N(1)-Cu(1)-O(11) | 88.3(7) |
| N(7)-Cu(2)-Cl(1) | 90.1(6) | N(6)-Cu(2)-Cl(1) | 89.9(7) |
| N(4)-Cu(2)-Cl(1) | 94.4(6) | N(8)-Cu(3)-N(5)#3 | 91.8(8) |
| N(11)-Cu(4)-N(10)#4 | 173.3(8) | N(8)-Cu(3)-N(5) | 88.2(8) |
| Symmetry codes: #1 -x, -y+1, -z+2; #2 -x+1, -y+2, -z+2; #3 -x+1, -y+2, -z+3; #4 x+1, y, z; #5 x-1, y, z. | | | |
| **4** | | | |
| O(1)-W(6) | 1.901(18) | O(4B)-W(4) | 2.01(3) |
| O(1)-W(5) | 1.908(18) | O(4B)-W(2) | 2.03(3) |
| O(2)-W(5) | 1.859(17) | O(5)-W(1) | 1.858(19) |
| O(2)-W(4) | 1.957(18) | O(5)-W(2) | 1.865(19) |
| O(3)-Si(1) | 1.697(14) | O(6)-W(2) | 1.701(19) |
| O(3)-W(4) | 2.326(13) | O(7)-W(2) | 1.899(17) |
| O(3)-W(1) | 2.352(14) | O(7)-W(6)#1 | 1.899(17) |
| O(3)-W(2) | 2.357(14) | O(8)-Si(1) | 1.642(15) |
| O(4A)-W(2) | 1.82(3) | O(8)-W(3) | 2.351(15) |
| O(4A)-W(4) | 1.89(3) | O(8)-W(6)#1 | 2.395(16) |
| O(8)-W(2) | 2.410(16) | O(15)-Si(1) | 1.620(14) |
| O(9)-W(3) | 1.870(19) | O(15)-W(5) | 2.383(14) |
| O(9)-W(2) | 1.90(2) | O(15)-W(4) | 2.392(15) |
| O(10)-W(6)#1 | 1.87(2) | O(15)-W(6) | 2.410(14) |
| O(10)-W(3) | 1.932(18) | O(16)-W(6) | 1.889(17) |

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|---|---|---|---|
| O(11)-W(3) | 1.654(19) | O(16)-W(4) | 1.913(17) |
| O(12)-Si(1) | 1.587(15) | O(17)-W(4) | 1.693(16) |
| O(12)-W(5) | 2.389(14) | O(17)-Cu(1) | 2.406(15) |
| O(12)-W(3) | 2.411(15) | O(18)-W(6) | 1.689(16) |
| O(12)-W(1)#1 | 2.447(16) | O(19)-W(5) | 1.652(19) |
| O(20)-W(5) | 1.871(19) | O(24)-W(1)#1 | 1.91(2) |
| O(20)-W(3) | 1.925(18) | Si(1)-O(12)#1 | 1.587(15) |
| O(21A)-W(4) | 1.74(3) | Si(1)-O(15)#1 | 1.620(14) |
| O(21A)-W(1) | 1.90(3) | Si(1)-O(8)#1 | 1.642(15) |
| O(21B)-W(1) | 2.03(3) | Si(1)-O(3)#1 | 1.697(15) |
| O(21B)-W(4) | 2.06(3) | Cu(1)-N(4) | 1.980(16) |
| O(22)-W(1) | 1.658(19) | Cu(1)-N(6) | 2.007(17) |
| O(23)-W(5)#1 | 1.885(17) | Cu(1)-O(17)#2 | 2.406(16) |
| O(23)-W(1) | 1.910(17) | Cu(2)-N(3) | 1.936(19) |
| O(24)-W(3) | 1.851(18) | Cu(2)-N(11) | 1.975(17) |
| Cu(2)-N(5) | 2.009(19) | Cu(3)-N(1) | 2.012(18) |
| Cu(2)-N(2) | 2.05(2) | Cu(3)-Cl(1) | 2.769(7) |
| Cu(2)-Cl(1) | 2.543(7) | N(10)-Cu(4) | 1.880(16) |
| Cu(3)-N(1)#5 | 2.012(18) | N(12)-Cu(3)#6 | 1.982(18) |
| O(12)-Si(1)-O(15) | 68.8(7) | N(4)-Cu(1)-N(6)#2 | 90.2(6) |
| O(12)-Si(1)-O(15)#1 | 111.2(7) | N(4)-Cu(1)-N(6) | 89.8(6) |
| O(12)-Si(1)-O(8)#1 | 112.1(8) | N(4)-Cu(1)-O(17)#2 | 90.2(6) |
| O(15)-Si(1)-O(8)#1 | 70.6(7) | N(6)-Cu(1)-O(17)#2 | 95.1(6) |
| O(12)-Si(1)-O(8) | 67.9(8) | N(4)-Cu(1)-O(17) | 89.8(6) |
| O(15)-Si(1)-O(8) | 109.4(7) | N(6)-Cu(1)-O(17) | 84.9(6) |
| O(12)-Si(1)-O(3)#1 | 71.9(7) | N(3)-Cu(2)-N(11) | 166.7(7) |
| O(12)#1-Si(1)-O(3)#1 | 108.1(7) | N(3)-Cu(2)-N(5) | 87.1(8) |
| O(15)-Si(1)-O(3)#1 | 109.1(7) | N(11)-Cu(2)-N(5) | 90.4(7) |
| O(8)-Si(1)-O(3)#1 | 106.8(7) | N(3)-Cu(2)-N(2) | 89.7(8) |
| O(12)-Si(1)-O(3) | 108.1(7) | N(11)-Cu(2)-N(2) | 91.9(7) |
| O(15)-Si(1)-O(3) | 70.9(7) | N(5)-Cu(2)-N(2) | 175.4(8) |
| O(8)-Si(1)-O(3) | 73.2(7) | N(3)-Cu(2)-Cl(1) | 102.1(6) |
| N(12)#3-Cu(3)-N(1)#5 | 90.8(8) | N(11)-Cu(2)-Cl(1) | 91.1(5) |
| N(12)#4-Cu(3)-N(1)#5 | 89.2(8) | N(5)-Cu(2)-Cl(1) | 94.1(6) |
| N(12)#3-Cu(3)-N(1) | 89.2(8) | N(2)-Cu(2)-Cl(1) | 89.7(6) |

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|---|---|---|---|
| N(12)#4-Cu(3)-N(1) | 90.8(8) | O(22)-W(1)-O(5) | 103.6(9) |
| N(12)#3-Cu(3)-Cl(1)#5 | 91.1(6) | O(22)-W(1)-O(21A) | 111.7(13) |
| N(12)#4-Cu(3)-Cl(1)#5 | 88.9(6) | O(5)-W(1)-O(21A) | 87.9(11) |
| N(1)-Cu(3)-Cl(1)#5 | 95.5(5) | O(22)-W(1)-O(23) | 101.1(9) |
| N(12)#3-Cu(3)-Cl(1) | 88.9(6) | O(5)-W(1)-O(23) | 85.3(8) |
| N(12)#4-Cu(3)-Cl(1) | 91.1(6) | O(21A)-W(1)-O(23) | 147.2(13) |
| N(1)-Cu(3)-Cl(1) | 84.5(5) | O(22)-W(1)-O(24)#1 | 103.5(10) |
| O(22)-W(1)-O(21B) | 89.5(12) | O(5)-W(1)-O(24)#1 | 152.8(8) |
| O(5)-W(1)-O(21B) | 88.2(10) | O(21A)-W(1)-O(24)#1 | 80.9(11) |
| O(23)-W(1)-O(21B) | 168.6(11) | O(23)-W(1)-O(24)#1 | 90.8(8) |
| O(24)#1-W(1)-O(21B) | 90.7(10) | O(22)-W(1)-O(12)#1 | 158.6(8) |
| O(22)-W(1)-O(3) | 153.9(8) | O(5)-W(1)-O(12)#1 | 91.2(7) |
| O(5)-W(1)-O(3) | 59.1(7) | O(21A)-W(1)-O(12)#1 | 83.7(12) |
| O(21A)-W(1)-O(3) | 52.9(11) | O(23)-W(1)-O(12)#1 | 64.4(6) |
| O(23)-W(1)-O(3) | 96.8(6) | O(24)#1-W(1)-O(12)#1 | 63.1(7) |
| O(24)#1-W(1)-O(3) | 94.9(7) | O(21B)-W(1)-O(12)#1 | 106.5(11) |
| O(21B)-W(1)-O(3) | 71.8(10) | O(3)-W(1)-O(12)#1 | 47.4(5) |
| O(6)-W(2)-O(7) | 102.4(9) | O(6)-W(2)-O(4A) | 110.4(13) |
| O(4A)-W(2)-O(7) | 146.2(13) | O(6)-W(2)-O(5) | 104.1(9) |
| O(5)-W(2)-O(7) | 85.2(8) | O(4A)-W(2)-O(5) | 93.8(12) |
| O(6)-W(2)-O(9) | 101.7(9) | O(9)-W(2)-O(4B) | 92.5(11) |
| O(4A)-W(2)-O(9) | 75.5(13) | O(6)-W(2)-O(3) | 152.8(8) |
| O(5)-W(2)-O(9) | 154.1(8) | O(4A)-W(2)-O(3) | 55.0(11) |
| O(7)-W(2)-O(9) | 90.8(8) | O(5)-W(2)-O(3) | 58.9(7) |
| O(6)-W(2)-O(4B) | 88.6(12) | O(7)-W(2)-O(3) | 97.4(7) |
| O(5)-W(2)-O(4B) | 86.6(11) | O(9)-W(2)-O(3) | 96.5(7) |
| O(7)-W(2)-O(4B) | 167.7(11) | O(4B)-W(2)-O(3) | 70.4(10) |
| O(7)-W(2)-O(8) | 64.5(7) | O(6)-W(2)-O(8) | 157.7(8) |
| O(9)-W(2)-O(8) | 62.4(7) | O(4A)-W(2)-O(8) | 81.9(12) |
| O(4B)-W(2)-O(8) | 106.8(11) | O(5)-W(2)-O(8) | 93.1(7) |
| O(3)-W(2)-O(8) | 49.4(5) | O(11)-W(3)-O(10) | 102.5(10) |
| O(11)-W(3)-O(24) | 102.8(10) | O(24)-W(3)-O(10) | 84.9(8) |
| O(11)-W(3)-O(9) | 100.9(10) | O(9)-W(3)-O(10) | 91.3(8) |
| O(24)-W(3)-O(9) | 156.2(9) | O(20)-W(3)-O(10) | 157.0(9) |
| O(11)-W(3)-O(20) | 100.5(9) | O(11)-W(3)-O(8) | 157.1(9) |

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|---|---|---|---|
| O(24)-W(3)-O(20) | 89.4(8) | O(24)-W(3)-O(8) | 93.6(7) |
| O(9)-W(3)-O(20) | 84.9(8) | O(9)-W(3)-O(8) | 64.1(8) |
| O(24)-W(3)-O(12) | 64.7(7) | O(20)-W(3)-O(8) | 95.4(7) |
| O(9)-W(3)-O(12) | 92.4(8) | O(10)-W(3)-O(8) | 62.9(7) |
| O(20)-W(3)-O(12) | 63.4(7) | O(11)-W(3)-O(12) | 158.3(9) |
| O(10)-W(3)-O(12) | 94.3(7) | O(4A)-W(4)-O(16) | 146.0(12) |
| O(8)-W(3)-O(12) | 44.5(5) | O(17)-W(4)-O(2) | 97.8(7) |
| O(17)-W(4)-O(21A) | 112.7(13) | O(21A)-W(4)-O(2) | 149.2(13) |
| O(17)-W(4)-O(4A) | 111.0(12) | O(4A)-W(4)-O(2) | 77.4(12) |
| O(21A)-W(4)-O(4A) | 94.4(15) | O(16)-W(4)-O(2) | 88.3(7) |
| O(17)-W(4)-O(16) | 101.3(7) | O(17)-W(4)-O(4B) | 89.0(11) |
| O(21A)-W(4)-O(16) | 82.2(12) | O(21A)-W(4)-O(4B) | 91.1(14) |
| O(4A)-W(4)-O(21B) | 96.9(14) | O(16)-W(4)-O(4B) | 169.3(11) |
| O(16)-W(4)-O(21B) | 92.2(10) | O(2)-W(4)-O(4B) | 93.3(11) |
| O(2)-W(4)-O(21B) | 170.1(10) | O(17)-W(4)-O(21B) | 91.7(11) |
| O(4B)-W(4)-O(21B) | 84.4(13) | O(21B)-W(4)-O(3) | 71.9(10) |
| O(17)-W(4)-O(3) | 155.3(7) | O(17)-W(4)-O(15) | 156.3(7) |
| O(21A)-W(4)-O(3) | 54.7(12) | O(21A)-W(4)-O(15) | 85.7(13) |
| O(4A)-W(4)-O(3) | 55.1(11) | O(4A)-W(4)-O(15) | 81.0(11) |
| O(16)-W(4)-O(3) | 97.8(6) | O(16)-W(4)-O(15) | 65.1(6) |
| O(2)-W(4)-O(3) | 98.2(6) | O(2)-W(4)-O(15) | 63.9(6) |
| O(4B)-W(4)-O(3) | 71.5(10) | O(4B)-W(4)-O(15) | 106.2(11) |
| O(19)-W(5)-O(20) | 101.6(10) | O(21B)-W(4)-O(15) | 107.5(10) |
| O(2)-W(5)-O(20) | 88.8(8) | O(3)-W(4)-O(15) | 48.1(5) |
| O(19)-W(5)-O(23)#1 | 100.9(9) | O(19)-W(5)-O(2) | 98.7(9) |
| O(2)-W(5)-O(23)#1 | 160.1(8) | O(2)-W(5)-O(15) | 65.3(6) |
| O(20)-W(5)-O(23)#1 | 90.7(8) | O(20)-W(5)-O(15) | 96.3(7) |
| O(19)-W(5)-O(1) | 99.5(10) | O(23)#1-W(5)-O(15) | 95.0(7) |
| O(2)-W(5)-O(1) | 88.0(7) | O(1)-W(5)-O(15) | 63.6(6) |
| O(20)-W(5)-O(1) | 159.0(8) | O(19)-W(5)-O(12) | 159.5(9) |
| O(23)#1-W(5)-O(1) | 85.3(8) | O(2)-W(5)-O(12) | 96.0(7) |
| O(19)-W(5)-O(15) | 155.8(9) | O(20)-W(5)-O(12) | 64.5(7) |
| O(18)-W(6)-O(10)#1 | 101.9(10) | O(23)#1-W(5)-O(12) | 66.0(7) |
| O(18)-W(6)-O(16) | 100.8(8) | O(1)-W(5)-O(12) | 95.2(7) |
| O(10)#1-W(6)-O(16) | 84.6(8) | O(15)-W(5)-O(12) | 44.6(5) |

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| O(18)-W(6)-O(7)#1 | 100.4(9) | O(18)-W(6)-O(8)#1 | 156.9(8) |
| O(10)#1-W(6)-O(7)#1 | 91.0(8) | O(10)#1-W(6)-O(8)#1 | 62.7(7) |
| O(16)-W(6)-O(7)#1 | 158.7(8) | O(16)-W(6)-O(8)#1 | 94.9(6) |
| O(18)-W(6)-O(1) | 100.3(9) | O(7)#1-W(6)-O(8)#1 | 64.8(7) |
| O(10)#1-W(6)-O(1) | 157.6(9) | O(1)-W(6)-O(8)#1 | 96.6(7) |
| O(16)-W(6)-O(1) | 89.4(7) | O(18)-W(6)-O(15) | 156.9(8) |
| O(7)#1-W(6)-O(1) | 86.8(8) | O(10)#1-W(6)-O(15) | 95.0(7) |
| O(8)#1-W(6)-O(15) | 46.2(5) | O(16)-W(6)-O(15) | 65.0(6) |
| O(1)-W(6)-O(15) | 63.1(6) | O(7)#1-W(6)-O(15) | 94.8(7) |
| N(8)-Cu(4)-N(10) | 174.2(8) | | |
| Symmetry codes: #1 -x, -y, -z+1; #2 -x+1, -y+1, -z+1; #3 x-1, y, z; #4 -x+2, -y+1, -z+2; #5 -x+1, -y+1, -z+2; #6 x+1, y, z. | | | |
| **5** | | | |
| N(1)-Co(2) | 2.11(2) | N(11)-Co(2) | 2.06(2) |
| N(2)-Co(3) | 2.079(19) | N(12)-Co(3) | 2.13(3) |
| N(3)-Co(1) | 2.080(18) | N(13)-Co(5) | 2.23(3) |
| N(4)-Co(3) | 2.192(18) | N(14)-Co(6) | 2.22(2) |
| N(5)-Co(2) | 2.085(16) | N(15)-Co(4) | 2.079(17) |
| N(6)-Co(1) | 2.075(15) | N(16)-Co(1) | 2.090(19) |
| N(7)-Co(3) | 2.125(14) | N(17)-Co(4) | 2.087(19) |
| N(8)-Co(6) | 2.11(2) | N(19)-Co(5) | 2.06(3) |
| N(9)-Co(3)#2 | 2.182(17) | O(1)-W(1) | 1.718(14) |
| N(10)-Co(4) | 2.058(17) | O(2)-W(1) | 1.923(15) |
| O(2)-W(2) | 1.961(15) | O(6)-W(4) | 1.949(15) |
| O(1W)-Co(2) | 1.865(15) | O(5W)-Co(5) | 2.22(2) |
| O(3)-W(3) | 1.894(15) | O(7)-W(3) | 1.911(15) |
| O(3)-W(1) | 1.961(16) | O(7)-W(5) | 1.923(15) |
| O(2W)-Co(2) | 2.115(19) | O(8)-W(2) | 1.873(16) |
| O(4)-W(3) | 1.724(16) | O(8)-W(9) | 1.965(15) |
| O(3W)-Co(1) | 2.146(17) | O(7W)-Co(5) | 2.16(3) |
| O(5)-W(3) | 1.923(15) | O(9)-P(1) | 1.591(15) |
| O(5)-W(2) | 1.927(16) | O(9)-W(2) | 2.351(15) |
| O(6)-W(2) | 1.862(15) | O(9)-W(1) | 2.368(14) |
| O(9)-W(3) | 2.380(15) | O(14)-W(9) | 1.919(15) |
| O(8W)-Co(6) | 2.07(3) | O(14)-W(8) | 1.922(16) |
| O(10)-W(3) | 1.876(15) | O(15)-W(9) | 1.725(17) |

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|---|---|---|---|
| O(10)-W(6) | 1.941(15) | O(16)-W(4) | 1.874(15) |
| O(11)-W(1) | 1.847(15) | O(16)-W(9) | 1.898(15) |
| O(11)-W(7) | 1.994(15) | O(17)-W(4) | 1.696(16) |
| O(12)-W(1) | 1.881(15) | O(18)-W(5) | 1.881(16) |
| O(12)-W(8) | 1.963(15) | O(18)-W(4) | 1.935(16) |
| O(13)-W(8) | 1.712(15) | O(19)-P(1) | 1.528(15) |
| O(12W)-Co(6) | 1.774(17) | O(19)-W(5) | 2.363(15) |
| O(19)-W(4) | 2.398(15) | O(24)-P(1) | 1.521(15) |
| O(20)-P(1) | 1.508(16) | O(24)-W(7) | 2.353(14) |
| O(20)-W(9) | 2.382(15) | O(24)-W(6) | 2.353(15) |
| O(20)-W(8) | 2.386(15) | O(25)-W(6) | 1.713(16) |
| O(21)-W(8) | 1.878(15) | O(25)-Co(1) | 2.111(16) |
| O(21)-W(7) | 1.902(15) | O(26)-W(6) | 1.886(15) |
| O(22)-W(7) | 1.721(15) | O(26)-W(5) | 1.902(15) |
| O(22)-Co(1)#3 | 2.098(15) | O(27)-W(4) | 1.877(15) |
| O(23)-W(6) | 1.905(15) | O(27)-W(10) | 1.919(16) |
| O(23)-W(7) | 1.911(15) | O(28)-W(5) | 1.881(16) |
| O(28)-W(11) | 1.917(16) | O(34)-W(13) | 1.719(18) |
| O(29)-W(8) | 1.855(15) | O(35)-W(15) | 1.899(12) |
| O(29)-W(14) | 1.955(15) | O(35)-W(14) | 1.901(13) |
| O(30)-W(7) | 1.859(15) | O(36)-W(15) | 1.746(19) |
| O(30)-W(13) | 1.937(15) | O(37)-W(10) | 1.865(16) |
| O(31)-W(9) | 1.859(16) | O(37)-W(15) | 1.899(16) |
| O(31)-W(15) | 1.918(16) | O(38)-W(10) | 1.730(18) |
| O(32)-W(6) | 1.845(15) | O(39)-W(11) | 1.873(18) |
| O(32)-W(12) | 1.961(16) | O(39)-W(10) | 1.954(17) |
| O(33)-W(14) | 1.727(16) | O(40)-W(11) | 1.897(17) |
| O(40)-W(12) | 1.908(16) | O(44)-W(15) | 2.365(17) |
| O(41)-W(12) | 1.891(16) | O(44)-W(14) | 2.375(15) |
| O(41)-W(13) | 1.930(16) | O(45)-W(11) | 1.705(15) |
| O(42)-P(2) | 1.537(17) | O(45)-Co(2) | 2.069(16) |
| O(42)-W(13) | 2.336(16) | O(46)-W(16) | 1.897(18) |
| O(42)-W(12) | 2.350(16) | O(46)-W(10) | 1.928(18) |
| O(43)-P(2) | 1.511(17) | O(47)-W(11) | 1.880(17) |
| O(43)-W(11) | 2.286(15) | O(47)-W(17) | 1.955(17) |

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|---|---|---|---|
| O(43)-W(10) | 2.426(17) | O(48)-W(16) | 1.904(17) |
| O(44)-P(2) | 1.515(16) | O(48)-W(15) | 1.947(17) |
| O(49)-P(2) | 1.613(17) | O(53)-W(18) | 1.929(19) |
| O(49)-W(16) | 2.332(17) | O(53)-W(16) | 1.935(19) |
| O(49)-W(18) | 2.378(17) | O(54)-W(17) | 1.923(17) |
| O(49)-W(17) | 2.385(16) | O(54)-W(18) | 1.938(17) |
| O(50)-W(18) | 1.912(18) | O(55)-W(17) | 1.94(2) |
| O(50)-W(13) | 1.926(17) | O(55)-W(16) | 1.948(18) |
| O(51)-W(18) | 1.908(16) | O(56)-W(17) | 1.699(19) |
| O(51)-W(14) | 1.920(16) | O(57)-W(16) | 1.714(18) |
| O(52)-W(17) | 1.871(18) | O(57)-Co(5)#4 | 2.017(18) |
| O(52)-W(12) | 1.891(17) | O(58)-W(5) | 1.739(16) |
| O(58)-Co(6) | 2.144(17) | Co(3)-O(59)#1 | 2.191(14) |
| O(59)-W(2) | 1.683(12) | Co(4)-N(10)#2 | 2.058(17) |
| O(59)-Co(3)#5 | 2.191(14) | Co(4)-N(15)#2 | 2.079(17) |
| O(60)-W(18) | 1.620(14) | Co(4)-N(17)#2 | 2.087(19) |
| O(61)-W(14) | 1.875(17) | Co(5)-O(57)#6 | 2.017(18) |
| O(61)-W(13) | 1.921(16) | Co(1)-O(22)#3 | 2.098(15) |
| O(62)-W(12) | 1.734(17) | Co(3)-N(9)#2 | 2.182(17) |
| O(62)-Co(5) | 2.148(17) | O(20)-P(1)-O(24) | 111.6(9) |
| N(6)-Co(1)-N(3) | 91.7(7) | O(20)-P(1)-O(19) | 110.8(8) |
| N(6)-Co(1)-N(16) | 91.6(7) | O(24)-P(1)-O(19) | 111.8(8) |
| N(3)-Co(1)-N(16) | 93.7(7) | O(20)-P(1)-O(9) | 107.9(8) |
| N(6)-Co(1)-O(22)#3 | 175.1(6) | O(24)-P(1)-O(9) | 105.9(8) |
| N(3)-Co(1)-O(22)#3 | 92.2(7) | O(19)-P(1)-O(9) | 108.6(8) |
| N(16)-Co(1)-O(22)#3 | 91.2(6) | O(43)-P(2)-O(44) | 112.0(9) |
| N(6)-Co(1)-O(25) | 92.3(6) | O(43)-P(2)-O(42) | 111.3(9) |
| N(3)-Co(1)-O(25) | 88.0(7) | O(44)-P(2)-O(42) | 113.3(9) |
| N(16)-Co(1)-O(25) | 175.7(7) | O(43)-P(2)-O(49) | 106.6(9) |
| O(22)#3-Co(1)-O(25) | 84.8(6) | O(44)-P(2)-O(49) | 106.2(9) |
| N(6)-Co(1)-O(3W) | 90.4(7) | O(42)-P(2)-O(49) | 106.9(9) |
| N(3)-Co(1)-O(3W) | 174.5(7) | O(1W)-Co(2)-N(11) | 172.3(9) |
| N(16)-Co(1)-O(3W) | 91.4(7) | O(1W)-Co(2)-O(45) | 83.8(8) |
| O(22)#3-Co(1)-O(3W) | 85.4(6) | N(11)-Co(2)-O(45) | 88.9(8) |
| O(25)-Co(1)-O(3W) | 86.9(7) | O(1W)-Co(2)-N(5) | 93.3(8) |

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| N(2)-Co(3)-N(7) | 92.4(7) | N(11)-Co(2)-N(5) | 94.1(8) |
| N(2)-Co(3)-N(12) | 91.9(12) | O(45)-Co(2)-N(5) | 175.9(7) |
| N(7)-Co(3)-N(12) | 171.3(11) | O(1W)-Co(2)-N(1) | 92.8(9) |
| N(2)-Co(3)-N(9)#2 | 92.8(8) | N(11)-Co(2)-N(1) | 89.6(8) |
| N(7)-Co(3)-N(9)#2 | 91.4(7) | O(45)-Co(2)-N(1) | 88.4(7) |
| N(12)-Co(3)-N(9)#2 | 95.9(11) | N(5)-Co(2)-N(1) | 88.8(7) |
| N(2)-Co(3)-O(59)#1 | 175.0(7) | O(1W)-Co(2)-O(2W) | 87.1(8) |
| N(7)-Co(3)-O(59)#1 | 89.7(6) | N(11)-Co(2)-O(2W) | 90.2(8) |
| N(12)-Co(3)-O(59)#1 | 86.6(11) | O(45)-Co(2)-O(2W) | 89.1(7) |
| N(9)#2-Co(3)-O(59)#1 | 82.6(6) | N(5)-Co(2)-O(2W) | 93.7(7) |
| N(2)-Co(3)-N(4) | 91.5(8) | N(1)-Co(2)-O(2W) | 177.5(7) |
| N(7)-Co(3)-N(4) | 88.2(6) | N(10)#2-Co(4)-N(15) | 88.9(8) |
| N(12)-Co(3)-N(4) | 84.2(11) | N(10)-Co(4)-N(15) | 91.1(7) |
| N(9)#2-Co(3)-N(4) | 175.7(7) | N(10)-Co(4)-N(17) | 90.2(7) |
| O(59)#1-Co(3)-N(4) | 93.1(6) | N(15)-Co(4)-N(17) | 91.9(7) |
| O(57)#6-Co(5)-N(19) | 97.6(11) | N(15)#2-Co(4)-N(17) | 88.1(7) |
| O(57)#6-Co(5)-O(62) | 173.7(7) | N(10)-Co(4)-N(17)#2 | 89.8(7) |
| N(19)-Co(5)-O(62) | 85.4(10) | O(12W)-Co(6)-O(8W) | 93.9(13) |
| O(57)#6-Co(5)-O(7W) | 88.2(9) | O(12W)-Co(6)-N(8) | 89.5(12) |
| N(19)-Co(5)-O(7W) | 172.1(11) | O(8W)-Co(6)-N(8) | 165.3(10) |
| O(62)-Co(5)-O(7W) | 88.3(8) | O(12W)-Co(6)-O(58) | 175.1(11) |
| O(57)#6-Co(5)-O(5W) | 88.0(8) | O(8W)-Co(6)-O(58) | 89.4(9) |
| N(19)-Co(5)-O(5W) | 85.8(12) | N(8)-Co(6)-O(58) | 86.4(7) |
| O(62)-Co(5)-O(5W) | 86.7(8) | O(12W)-Co(6)-N(14) | 91.3(11) |
| O(7W)-Co(5)-O(5W) | 89.0(10) | O(8W)-Co(6)-N(14) | 91.0(9) |
| O(57)#6-Co(5)-N(13) | 84.2(9) | N(8)-Co(6)-N(14) | 103.2(9) |
| N(19)-Co(5)-N(13) | 97.5(11) | O(58)-Co(6)-N(14) | 92.3(7) |
| O(62)-Co(5)-N(13) | 100.9(9) | O(1)-W(1)-O(11) | 103.2(7) |
| O(7W)-Co(5)-N(13) | 88.5(9) | O(1)-W(1)-O(12) | 103.7(7) |
| O(5W)-Co(5)-N(13) | 171.9(10) | O(11)-W(1)-O(12) | 89.4(7) |
| O(59)-W(2)-O(6) | 101.0(7) | O(1)-W(1)-O(2) | 99.6(7) |
| O(59)-W(2)-O(8) | 105.3(7) | O(11)-W(1)-O(2) | 157.0(6) |
| O(6)-W(2)-O(8) | 87.3(7) | O(12)-W(1)-O(2) | 88.2(7) |
| O(59)-W(2)-O(5) | 96.6(7) | O(1)-W(1)-O(3) | 99.2(7) |
| O(6)-W(2)-O(5) | 89.9(6) | O(11)-W(1)-O(3) | 87.3(6) |

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|---|---|---|---|
| O(8)-W(2)-O(5) | 158.0(7) | O(12)-W(1)-O(3) | 157.0(6) |
| O(59)-W(2)-O(2) | 101.4(7) | O(2)-W(1)-O(3) | 86.1(6) |
| O(6)-W(2)-O(2) | 157.6(6) | O(1)-W(1)-O(9) | 169.0(7) |
| O(8)-W(2)-O(2) | 87.6(6) | O(11)-W(1)-O(9) | 83.9(6) |
| O(5)-W(2)-O(2) | 86.7(6) | O(12)-W(1)-O(9) | 84.5(6) |
| O(59)-W(2)-O(9) | 168.4(7) | O(2)-W(1)-O(9) | 73.1(6) |
| O(6)-W(2)-O(9) | 84.9(6) | O(3)-W(1)-O(9) | 72.5(6) |
| O(8)-W(2)-O(9) | 84.8(6) | O(4)-W(3)-O(10) | 105.1(7) |
| O(5)-W(2)-O(9) | 73.3(6) | O(4)-W(3)-O(3) | 101.1(7) |
| O(2)-W(2)-O(9) | 72.9(5) | O(10)-W(3)-O(3) | 90.6(6) |
| O(17)-W(4)-O(16) | 101.9(7) | O(4)-W(3)-O(7) | 101.3(7) |
| O(17)-W(4)-O(27) | 98.5(7) | O(10)-W(3)-O(7) | 85.4(6) |
| O(16)-W(4)-O(27) | 89.6(7) | O(3)-W(3)-O(7) | 157.5(7) |
| O(17)-W(4)-O(18) | 101.2(7) | O(4)-W(3)-O(5) | 100.0(7) |
| O(16)-W(4)-O(18) | 156.6(7) | O(10)-W(3)-O(5) | 154.8(7) |
| O(27)-W(4)-O(18) | 90.9(7) | O(3)-W(3)-O(5) | 87.5(6) |
| O(17)-W(4)-O(6) | 98.7(7) | O(7)-W(3)-O(5) | 86.8(6) |
| O(16)-W(4)-O(6) | 85.0(6) | O(58)-W(5)-O(18) | 99.9(7) |
| O(27)-W(4)-O(6) | 162.8(7) | O(58)-W(5)-O(28) | 100.0(7) |
| O(18)-W(4)-O(6) | 87.7(6) | O(18)-W(5)-O(28) | 89.8(7) |
| O(17)-W(4)-O(19) | 173.7(7) | O(58)-W(5)-O(26) | 102.2(7) |
| O(16)-W(4)-O(19) | 83.9(6) | O(18)-W(5)-O(26) | 157.9(6) |
| O(27)-W(4)-O(19) | 84.0(6) | O(28)-W(5)-O(26) | 86.8(7) |
| O(18)-W(4)-O(19) | 72.9(6) | O(58)-W(5)-O(7) | 95.3(7) |
| O(6)-W(4)-O(19) | 79.2(6) | O(18)-W(5)-O(7) | 92.2(7) |
| O(25)-W(6)-O(32) | 98.9(7) | O(28)-W(5)-O(7) | 164.0(7) |
| O(25)-W(6)-O(26) | 102.5(7) | O(26)-W(5)-O(7) | 85.3(6) |
| O(32)-W(6)-O(26) | 91.4(7) | O(58)-W(5)-O(19) | 174.4(6) |
| O(25)-W(6)-O(23) | 99.6(7) | O(18)-W(5)-O(19) | 74.6(6) |
| O(32)-W(6)-O(23) | 90.9(7) | O(28)-W(5)-O(19) | 81.1(6) |
| O(26)-W(6)-O(23) | 157.1(6) | O(26)-W(5)-O(19) | 83.3(6) |
| O(25)-W(6)-O(10) | 95.8(7) | O(7)-W(5)-O(19) | 84.1(6) |
| O(32)-W(6)-O(10) | 165.3(7) | O(22)-W(7)-O(30) | 99.8(7) |
| O(26)-W(6)-O(10) | 84.2(6) | O(22)-W(7)-O(21) | 101.6(7) |
| O(23)-W(6)-O(10) | 87.8(6) | O(30)-W(7)-O(21) | 90.5(7) |

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|---|---|---|---|
| O(25)-W(6)-O(24) | 171.9(6) | O(22)-W(7)-O(23) | 101.0(7) |
| O(32)-W(6)-O(24) | 85.1(6) | O(30)-W(7)-O(23) | 90.2(7) |
| O(26)-W(6)-O(24) | 84.2(6) | O(21)-W(7)-O(23) | 156.9(6) |
| O(23)-W(6)-O(24) | 73.2(6) | O(22)-W(7)-O(11) | 94.9(6) |
| O(10)-W(6)-O(24) | 80.4(6) | O(30)-W(7)-O(11) | 165.3(6) |
| O(13)-W(8)-O(29) | 99.0(7) | O(21)-W(7)-O(11) | 85.9(6) |
| O(13)-W(8)-O(21) | 103.5(7) | O(23)-W(7)-O(11) | 87.6(6) |
| O(29)-W(8)-O(21) | 89.1(7) | O(22)-W(7)-O(24) | 173.1(6) |
| O(13)-W(8)-O(14) | 99.5(7) | O(30)-W(7)-O(24) | 84.1(6) |
| O(29)-W(8)-O(14) | 92.5(7) | O(21)-W(7)-O(24) | 84.0(6) |
| O(21)-W(8)-O(14) | 156.5(6) | O(23)-W(7)-O(24) | 73.1(6) |
| O(13)-W(8)-O(12) | 95.3(7) | O(11)-W(7)-O(24) | 81.4(5) |
| O(29)-W(8)-O(12) | 165.4(6) | O(15)-W(9)-O(31) | 98.7(8) |
| O(21)-W(8)-O(12) | 85.2(6) | O(15)-W(9)-O(16) | 102.5(7) |
| O(14)-W(8)-O(12) | 87.5(7) | O(31)-W(9)-O(16) | 89.8(7) |
| O(13)-W(8)-O(20) | 172.2(6) | O(15)-W(9)-O(14) | 99.1(7) |
| O(29)-W(8)-O(20) | 84.8(6) | O(31)-W(9)-O(14) | 90.5(7) |
| O(21)-W(8)-O(20) | 83.3(6) | O(16)-W(9)-O(14) | 158.1(7) |
| O(14)-W(8)-O(20) | 73.5(6) | O(15)-W(9)-O(8) | 98.1(8) |
| O(12)-W(8)-O(20) | 81.2(6) | O(31)-W(9)-O(8) | 163.2(7) |
| O(38)-W(10)-O(37) | 101.7(8) | O(16)-W(9)-O(8) | 86.1(6) |
| O(38)-W(10)-O(27) | 97.4(8) | O(14)-W(9)-O(8) | 87.2(6) |
| O(37)-W(10)-O(27) | 89.2(7) | O(15)-W(9)-O(20) | 172.6(7) |
| O(38)-W(10)-O(46) | 98.1(8) | O(31)-W(9)-O(20) | 82.9(6) |
| O(37)-W(10)-O(46) | 88.0(7) | O(16)-W(9)-O(20) | 84.7(6) |
| O(27)-W(10)-O(46) | 164.5(7) | O(14)-W(9)-O(20) | 73.6(6) |
| O(38)-W(10)-O(39) | 101.9(8) | O(8)-W(9)-O(20) | 80.5(6) |
| O(37)-W(10)-O(39) | 156.4(7) | O(45)-W(11)-O(39) | 97.8(8) |
| O(27)-W(10)-O(39) | 87.8(7) | O(45)-W(11)-O(47) | 95.8(7) |
| O(46)-W(10)-O(39) | 88.6(7) | O(39)-W(11)-O(47) | 89.8(8) |
| O(38)-W(10)-O(43) | 173.6(7) | O(45)-W(11)-O(40) | 101.1(7) |
| O(37)-W(10)-O(43) | 84.5(6) | O(39)-W(11)-O(40) | 161.1(7) |
| O(27)-W(10)-O(43) | 84.0(6) | O(47)-W(11)-O(40) | 86.8(7) |
| O(46)-W(10)-O(43) | 80.6(7) | O(45)-W(11)-O(28) | 96.8(7) |
| O(39)-W(10)-O(43) | 71.8(6) | O(39)-W(11)-O(28) | 91.7(7) |

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|---|---|---|---|
| O(62)-W(12)-O(52) | 97.3(8) | O(47)-W(11)-O(28) | 167.0(7) |
| O(62)-W(12)-O(41) | 101.9(8) | O(40)-W(11)-O(28) | 87.6(7) |
| O(52)-W(12)-O(41) | 91.6(7) | O(45)-W(11)-O(43) | 174.0(7) |
| O(62)-W(12)-O(40) | 101.8(7) | O(39)-W(11)-O(43) | 76.6(6) |
| O(52)-W(12)-O(40) | 87.7(7) | O(47)-W(11)-O(43) | 82.3(6) |
| O(41)-W(12)-O(40) | 156.2(7) | O(40)-W(11)-O(43) | 84.5(6) |
| O(62)-W(12)-O(32) | 98.5(7) | O(28)-W(11)-O(43) | 85.4(6) |
| O(52)-W(12)-O(32) | 164.0(7) | O(32)-W(12)-O(42) | 82.6(6) |
| O(41)-W(12)-O(32) | 88.0(7) | O(34)-W(13)-O(61) | 99.5(7) |
| O(40)-W(12)-O(32) | 86.2(7) | O(34)-W(13)-O(50) | 96.6(8) |
| O(62)-W(12)-O(42) | 175.7(7) | O(61)-W(13)-O(50) | 86.7(7) |
| O(52)-W(12)-O(42) | 81.9(6) | O(34)-W(13)-O(41) | 101.4(8) |
| O(41)-W(12)-O(42) | 74.0(6) | O(61)-W(13)-O(41) | 159.1(7) |
| O(40)-W(12)-O(42) | 82.3(6) | O(50)-W(13)-O(41) | 91.0(7) |
| O(41)-W(13)-O(30) | 89.6(7) | O(34)-W(13)-O(30) | 97.3(8) |
| O(34)-W(13)-O(42) | 175.0(7) | O(61)-W(13)-O(30) | 87.6(7) |
| O(61)-W(13)-O(42) | 85.4(6) | O(50)-W(13)-O(30) | 165.7(7) |
| O(50)-W(13)-O(42) | 82.8(6) | O(61)-W(14)-O(51) | 87.7(7) |
| O(41)-W(13)-O(42) | 73.7(6) | O(35)-W(14)-O(51) | 89.6(7) |
| O(30)-W(13)-O(42) | 83.6(6) | O(33)-W(14)-O(29) | 97.7(7) |
| O(33)-W(14)-O(61) | 103.0(8) | O(61)-W(14)-O(29) | 88.4(7) |
| O(33)-W(14)-O(35) | 100.9(8) | O(35)-W(14)-O(29) | 88.1(7) |
| O(61)-W(14)-O(35) | 156.2(6) | O(51)-W(14)-O(29) | 165.0(7) |
| O(33)-W(14)-O(51) | 97.3(8) | O(33)-W(14)-O(44) | 172.5(7) |
| O(29)-W(14)-O(44) | 83.3(6) | O(61)-W(14)-O(44) | 84.5(6) |
| O(36)-W(15)-O(37) | 102.3(8) | O(35)-W(14)-O(44) | 71.7(6) |
| O(36)-W(15)-O(35) | 100.2(8) | O(51)-W(14)-O(44) | 82.0(6) |
| O(37)-W(15)-O(35) | 157.4(7) | O(31)-W(15)-O(48) | 165.3(7) |
| O(36)-W(15)-O(31) | 97.5(8) | O(36)-W(15)-O(44) | 172.1(7) |
| O(37)-W(15)-O(31) | 87.8(7) | O(37)-W(15)-O(44) | 85.5(6) |
| O(35)-W(15)-O(31) | 90.6(7) | O(35)-W(15)-O(44) | 72.0(6) |
| O(36)-W(15)-O(48) | 97.1(9) | O(31)-W(15)-O(44) | 84.1(6) |
| O(37)-W(15)-O(48) | 87.2(7) | O(48)-W(15)-O(44) | 81.8(7) |
| O(35)-W(15)-O(48) | 88.7(7) | O(57)-W(16)-O(46) | 102.5(8) |
| O(46)-W(16)-O(53) | 157.9(8) | O(57)-W(16)-O(48) | 102.2(8) |

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|---|---|---|---|
| O(48)-W(16)-O(53) | 89.4(8) | O(46)-W(16)-O(48) | 87.1(7) |
| O(57)-W(16)-O(55) | 100.1(8) | O(57)-W(16)-O(53) | 99.6(8) |
| O(46)-W(16)-O(55) | 88.6(8) | O(55)-W(16)-O(49) | 73.0(7) |
| O(48)-W(16)-O(55) | 157.7(8) | O(56)-W(17)-O(52) | 99.9(9) |
| O(53)-W(16)-O(55) | 86.5(8) | O(56)-W(17)-O(54) | 102.0(8) |
| O(57)-W(16)-O(49) | 170.2(8) | O(52)-W(17)-O(54) | 90.0(8) |
| O(46)-W(16)-O(49) | 84.4(7) | O(56)-W(17)-O(55) | 102.6(9) |
| O(48)-W(16)-O(49) | 84.8(7) | O(52)-W(17)-O(55) | 157.5(7) |
| O(53)-W(16)-O(49) | 73.5(7) | O(54)-W(17)-O(55) | 86.5(8) |
| O(55)-W(17)-O(47) | 87.1(8) | O(56)-W(17)-O(47) | 102.3(8) |
| O(56)-W(17)-O(49) | 172.9(8) | O(52)-W(17)-O(47) | 86.9(7) |
| O(52)-W(17)-O(49) | 85.9(7) | O(54)-W(17)-O(47) | 155.7(7) |
| O(54)-W(17)-O(49) | 73.6(7) | O(51)-W(18)-O(53) | 88.8(8) |
| O(55)-W(17)-O(49) | 71.8(7) | O(50)-W(18)-O(53) | 157.9(7) |
| O(47)-W(17)-O(49) | 82.1(6) | O(60)-W(18)-O(54) | 100.1(8) |
| O(60)-W(18)-O(51) | 102.6(8) | O(51)-W(18)-O(54) | 157.3(7) |
| O(60)-W(18)-O(50) | 101.1(9) | O(50)-W(18)-O(54) | 88.5(7) |
| O(51)-W(18)-O(50) | 87.1(7) | O(53)-W(18)-O(54) | 86.9(8) |
| O(60)-W(18)-O(53) | 101.1(9) | O(60)-W(18)-O(49) | 171.0(8) |
| O(50)-W(18)-O(49) | 85.4(7) | O(51)-W(18)-O(49) | 83.9(6) |
| O(53)-W(18)-O(49) | 72.5(7) | | |
| Symmetry codes: #1 -x+3/2, y+1/2, -z+1/2; #2 -x+1, -y+2, -z+1; #3 -x+1, -y+2, -z; #4 -x+1/2, y-1/2, -z+1/2; #5 -x+3/2, y-1/2, -z+1/2; #6 -x+1/2, y+1/2, -z+1/2; #7 x-1/2, -y+3/2, z-1/2; #8 x+1/2, -y+3/2, z+1/2. | | | |
| **6** | | | |
| W(1)-O(4) | 1.678(15) | W(2)-O(11) | 1.892(2) |
| W(1)-O(14) | 1.860(15) | W(2)-O(1) | 1.899(12) |
| W(1)-O(12) | 1.865(14) | W(2)-O(8A) | 2.01(3) |
| W(1)-O(15) | 1.891(2) | W(2)-O(17) | 2.32(3) |
| W(1)-O(3) | 1.922(13) | W(2)-O(19) | 2.37(3) |
| W(1)-O(18)#1 | 2.34(3) | W(3)-O(6) | 1.681(12) |
| W(1)-O(19) | 2.40(3) | W(3)-O(8) | 1.76(3) |
| W(2)-O(5) | 1.694(13) | W(3)-O(14)#1 | 1.835(16) |
| W(2)-O(12) | 1.810(15) | W(3)-O(13) | 1.8804(13) |
| W(2)-O(8) | 1.86(3) | W(3)-O(2) | 1.908(12) |
| W(3)-O(8A) | 2.03(3) | W(4)-O(1)#1 | 2.019(14) |

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|---|---|---|---|
| W(3)-O(17) | 2.41(3) | W(4)-O(7) | 2.347(10) |
| W(3)-O(18) | 2.46(2) | W(5)-O(21) | 0.80(3) |
| W(4)-O(22) | 0.78(3) | W(5)-O(16) | 1.69(3) |
| W(4)-O(10) | 1.73(2) | W(5)-O(20) | 1.93(2) |
| W(4)-O(21) | 1.94(3) | W(5)-O(2)#1 | 1.947(12) |
| W(4)-O(20)#1 | 1.90(3) | W(5)-O(22) | 1.95(3) |
| W(4)-O(2)#1 | 1.934(13) | W(5)-O(3) | 2.012(14) |
| W(5)-O(7) | 2.361(10) | Cu(1)-O(28) | 2.20(4) |
| W(6)-O(20) | 0.87(3) | Cu(1)-O(24) | 2.36(2) |
| W(6)-O(9) | 1.75(3) | Cu(2)-N(9)#3 | 1.983(14) |
| W(6)-O(22)#1 | 1.88(3) | Cu(2)-N(1) | 1.986(13) |
| W(6)-O(21) | 1.91(3) | Cu(2)-O(25) | 2.011(12) |
| W(6)-O(3) | 1.939(13) | Cu(2)-N(6) | 2.025(15) |
| W(6)-O(1) | 1.952(12) | Cu(2)-O(5) | 2.406(14) |
| W(6)-O(7) | 2.433(9) | Cu(3)-N(4) | 1.996(13) |
| Cu(1)-O(23) | 1.95(3) | Cu(3)-O(26) | 2.010(18) |
| Cu(1)-N(2) | 1.957(14) | Cu(3)-O(27) | 2.05(2) |
| Cu(1)-O(25) | 2.042(18) | Cu(3)-N(10) | 2.23(2) |
| S(2)-O(28) | 1.48(4) | Cu(4)-N(7) | 1.962(15) |
| S(2)-O(30) | 1.53(4) | Cu(4)-N(5) | 1.973(16) |
| S(2)-O(29) | 1.56(4) | Cu(4)-N(3)#5 | 1.989(15) |
| P(1)-O(18) | 1.53(3) | Cu(4)-O(26) | 2.036(10) |
| P(1)-O(19) | 1.54(3) | Cu(4)-O(31) | 2.26(3) |
| P(1)-O(17) | 1.56(2) | Cu(4)-O(32) | 2.34(2) |
| P(1)-O(7) | 1.579(17) | S(1)-O(32) | 1.45(3) |
| O(4)-W(1)-O(14) | 103.9(8) | S(1)-O(31) | 1.45(3) |
| O(4)-W(1)-O(12) | 102.6(7) | S(1)-O(33) | 1.71(3) |
| O(14)-W(1)-O(12) | 153.5(8) | O(4)-W(1)-O(19) | 160.9(8) |
| O(4)-W(1)-O(15) | 97.3(9) | O(14)-W(1)-O(19) | 95.1(9) |
| O(14)-W(1)-O(15) | 87.8(8) | O(12)-W(1)-O(19) | 58.5(8) |
| O(12)-W(1)-O(15) | 88.4(8) | O(15)-W(1)-O(19) | 85.9(9) |
| O(4)-W(1)-O(3) | 98.3(6) | O(3)-W(1)-O(19) | 79.1(7) |
| O(14)-W(1)-O(3) | 89.1(6) | O(18)#1-W(1)-O(19) | 34.4(8) |
| O(12)-W(1)-O(3) | 87.5(6) | O(5)-W(2)-O(12) | 102.7(7) |
| O(15)-W(1)-O(3) | 164.4(9) | O(5)-W(2)-O(8) | 114.4(10) |

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|---|---|---|---|
| O(4)-W(1)-O(18)#1 | 164.3(8) | O(12)-W(2)-O(8) | 142.2(9) |
| O(14)-W(1)-O(18)#1 | 60.7(8) | O(5)-W(2)-O(11) | 96.4(7) |
| O(12)-W(1)-O(18)#1 | 92.8(8) | O(12)-W(2)-O(11) | 89.0(8) |
| O(15)-W(1)-O(18)#1 | 85.6(9) | O(8)-W(2)-O(11) | 80.3(11) |
| O(3)-W(1)-O(18)#1 | 79.5(7) | O(5)-W(2)-O(1) | 98.1(6) |
| O(5)-W(2)-O(17) | 162.2(8) | O(12)-W(2)-O(1) | 88.3(6) |
| O(12)-W(2)-O(17) | 94.8(8) | O(8)-W(2)-O(1) | 93.2(9) |
| O(8)-W(2)-O(17) | 48.8(10) | O(11)-W(2)-O(1) | 165.6(7) |
| O(11)-W(2)-O(17) | 87.2(9) | O(6)-W(3)-O(8) | 113.3(10) |
| O(1)-W(2)-O(17) | 78.9(7) | O(6)-W(3)-O(14)#1 | 103.1(8) |
| O(5)-W(2)-O(19) | 162.0(9) | O(8)-W(3)-O(14)#1 | 142.6(10) |
| O(12)-W(2)-O(19) | 59.5(8) | O(6)-W(3)-O(13) | 98.1(7) |
| O(8)-W(2)-O(19) | 83.6(11) | O(8)-W(3)-O(13) | 77.8(11) |
| O(11)-W(2)-O(19) | 87.0(9) | O(14)#1-W(3)-O(13) | 89.4(8) |
| O(1)-W(2)-O(19) | 79.5(7) | O(6)-W(3)-O(2) | 99.2(5) |
| O(6)-W(3)-O(17) | 159.8(8) | O(8)-W(3)-O(2) | 93.0(9) |
| O(8)-W(3)-O(17) | 47.5(10) | O(14)#1-W(3)-O(2) | 89.0(6) |
| O(14)#1-W(3)-O(17) | 96.9(9) | O(13)-W(3)-O(2) | 162.5(7) |
| O(13)-W(3)-O(17) | 84.5(9) | O(22)-W(4)-O(10) | 73(2) |
| O(2)-W(3)-O(17) | 78.3(7) | O(22)-W(4)-O(20)#1 | 45(2) |
| O(6)-W(3)-O(18) | 161.4(8) | O(10)-W(4)-O(20)#1 | 101.8(12) |
| O(8)-W(3)-O(18) | 85.3(11) | W(5)-W(4)-O(20)#1 | 108.0(9) |
| O(14)#1-W(3)-O(18) | 58.4(9) | O(22)-W(4)-O(2)#1 | 145(2) |
| O(13)-W(3)-O(18) | 85.0(8) | O(10)-W(4)-O(2)#1 | 102.2(9) |
| O(2)-W(3)-O(18) | 79.3(7) | O(22)-W(4)-O(21) | 62(2) |
| O(22)-W(4)-O(1)#1 | 123(2) | O(10)-W(4)-O(21) | 102.4(12) |
| O(10)-W(4)-O(1)#1 | 101.4(10) | O(20)#1-W(4)-O(21) | 89.0(13) |
| O(21)-W(4)-O(1)#1 | 156.0(9) | O(2)#1-W(4)-O(21) | 85.7(10) |
| O(22)-W(4)-O(7) | 100.5(19) | O(21)-W(5)-O(20) | 47(2) |
| O(10)-W(4)-O(7) | 174.0(9) | O(16)-W(5)-O(20) | 103.9(12) |
| O(20)#1-W(4)-O(7) | 73.1(8) | O(21)-W(5)-O(2)#1 | 143(2) |
| O(2)#1-W(4)-O(7) | 82.9(4) | O(16)-W(5)-O(2)#1 | 101.6(9) |
| O(21)-W(4)-O(7) | 74.7(8) | O(20)-W(5)-O(2)#1 | 154.4(9) |
| O(1)#1-W(4)-O(7) | 81.3(4) | O(21)-W(5)-O(22) | 61(2) |
| O(21)-W(5)-O(16) | 75(2) | O(16)-W(5)-O(22) | 103.8(12) |

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|---|---|---|---|
| O(16)-W(5)-O(3) | 101.5(10) | O(20)-W(5)-O(22) | 88.9(12) |
| W(4)-W(5)-O(3) | 140.6(4) | O(2)#1-W(5)-O(22) | 84.0(9) |
| O(20)-W(5)-O(3) | 82.3(10) | O(21)-W(5)-O(3) | 124(2) |
| O(2)#1-W(5)-O(3) | 93.6(5) | O(3)-W(5)-O(7) | 80.9(5) |
| O(22)-W(5)-O(3) | 154.5(9) | O(20)-W(6)-O(9) | 86(2) |
| O(21)-W(5)-O(7) | 100(2) | O(20)-W(6)-O(22)#1 | 48.8(19) |
| O(16)-W(5)-O(7) | 175.2(10) | O(9)-W(6)-O(22)#1 | 103.6(12) |
| O(20)-W(5)-O(7) | 72.2(8) | O(20)-W(6)-O(21) | 49.2(18) |
| O(2)#1-W(5)-O(7) | 82.3(4) | O(9)-W(6)-O(21) | 102.3(12) |
| O(22)-W(5)-O(7) | 73.6(8) | O(22)#1-W(6)-O(21) | 89.8(12) |
| O(22)#1-W(6)-O(3) | 153.6(9) | O(20)-W(6)-O(3) | 131.8(17) |
| O(21)-W(6)-O(3) | 82.7(10) | O(9)-W(6)-O(3) | 102.7(10) |
| O(20)-W(6)-O(1) | 131.3(18) | O(22)#1-W(6)-O(7) | 73.1(9) |
| O(9)-W(6)-O(1) | 104.2(9) | O(21)-W(6)-O(7) | 73.0(9) |
| O(22)#1-W(6)-O(1) | 82.7(10) | O(3)-W(6)-O(7) | 80.5(5) |
| O(21)-W(6)-O(1) | 153.5(10) | O(1)-W(6)-O(7) | 80.5(5) |
| O(3)-W(6)-O(1) | 92.8(5) | O(23)-Cu(1)-N(2) | 89.9(5) |
| O(20)-W(6)-O(7) | 87.9(18) | N(2)-Cu(1)-N(2)#2 | 167.5(10) |
| O(9)-W(6)-O(7) | 174.1(9) | O(23)-Cu(1)-O(25) | 173.5(10) |
| N(9)#3-Cu(2)-N(1) | 177.4(7) | N(2)-Cu(1)-O(25) | 90.8(4) |
| N(9)#3-Cu(2)-O(25) | 87.6(7) | O(23)-Cu(1)-O(28) | 91.3(13) |
| N(1)-Cu(2)-O(25) | 90.6(6) | N(2)-Cu(1)-O(28) | 83.8(5) |
| N(9)#3-Cu(2)-N(6) | 92.5(7) | O(25)-Cu(1)-O(28) | 95.2(12) |
| N(1)-Cu(2)-N(6) | 89.6(6) | O(23)-Cu(1)-O(24) | 89.0(10) |
| O(25)-Cu(2)-N(6) | 171.0(7) | N(2)-Cu(1)-O(24) | 96.2(5) |
| N(9)#3-Cu(2)-O(5) | 90.0(6) | O(25)-Cu(1)-O(24) | 84.5(9) |
| N(1)-Cu(2)-O(5) | 87.9(5) | N(4)-Cu(3)-N(4)#4 | 157.7(9) |
| O(25)-Cu(2)-O(5) | 82.8(6) | N(4)-Cu(3)-O(26) | 89.5(5) |
| N(6)-Cu(2)-O(5) | 106.3(6) | N(4)-Cu(3)-O(27) | 89.2(5) |
| N(7)-Cu(4)-N(5) | 175.9(7) | O(26)-Cu(3)-O(27) | 173.2(9) |
| N(7)-Cu(4)-N(3)#5 | 88.8(7) | N(4)-Cu(3)-N(10) | 101.1(4) |
| N(5)-Cu(4)-N(3)#5 | 91.9(7) | O(26)-Cu(3)-N(10) | 94.5(8) |
| N(7)-Cu(4)-O(26) | 89.6(6) | O(27)-Cu(3)-N(10) | 92.3(9) |
| N(5)-Cu(4)-O(26) | 89.7(6) | N(5)-Cu(4)-O(31) | 78.4(10) |
| N(3)#5-Cu(4)-O(26) | 178.3(7) | N(3)#5-Cu(4)-O(31) | 86.2(9) |

| | | | |
|---|---|---|---|
| N(7)-Cu(4)-O(31) | 105.7(9) | O(26)-Cu(4)-O(31) | 93.9(9) |
| O(32)-S(1)-O(31)#5 | 119.2(13) | N(7)-Cu(4)-O(32) | 75.3(9) |
| O(32)-S(1)-O(31) | 60.8(13) | N(5)-Cu(4)-O(32) | 108.3(9) |
| O(31)#5-S(1)-O(31) | 63(3) | N(3)#5-Cu(4)-O(32) | 106.3(7) |
| O(32)-S(1)-O(31)#4 | 60.8(13) | O(26)-Cu(4)-O(32) | 72.9(7) |
| O(31)#5-S(1)-O(31)#6 | 117(3) | O(28)#7-S(2)-O(29) | 83(2) |
| O(32)-S(1)-O(33) | 95.8(17) | O(28)-S(2)-O(29) | 97(2) |
| O(32)#6-S(1)-O(33) | 84.2(17) | O(28)#7-S(2)-O(29)#7 | 97(2) |
| O(31)#5-S(1)-O(33) | 98.1(14) | O(28)-S(2)-O(29)#7 | 83(2) |
| O(31)-S(1)-O(33) | 81.9(14) | O(18)#1-P(1)-O(19) | 54.3(13) |
| O(19)-P(1)-O(17)#1 | 114.5(14) | O(18)-P(1)-O(19) | 113.9(14) |
| O(17)#1-P(1)-O(17) | 148.4(18) | O(18)#1-P(1)-O(17)#1 | 62.5(14) |
| O(18)#1-P(1)-O(7) | 107.4(9) | O(18)-P(1)-O(17)#1 | 107.4(13) |
| O(19)-P(1)-O(7) | 107.3(10) | O(19)#1-P(1)-O(17)#1 | 54.8(14) |
| O(17)-P(1)-O(7) | 105.8(9) | | |
| Symmetry codes: #1 -x, y, -z; #2 x, -y, z; #3 -x+1/2, y-1/2, -z+1; #4 x, -y+1, z; #5 -x+1, y, -z+1; #6 -x+1, -y+1, -z+1; #7 -x+1, -y, -z+1; #8 -x+1/2, y+1/2, -z+1. | | | |