Journal Name

ARTICLE

Supporting Information

# Organically-templated inorganic-organic hybrid Metal (Zn and Cd) Sulphite-Oxalate with layered and three-dimensional structures

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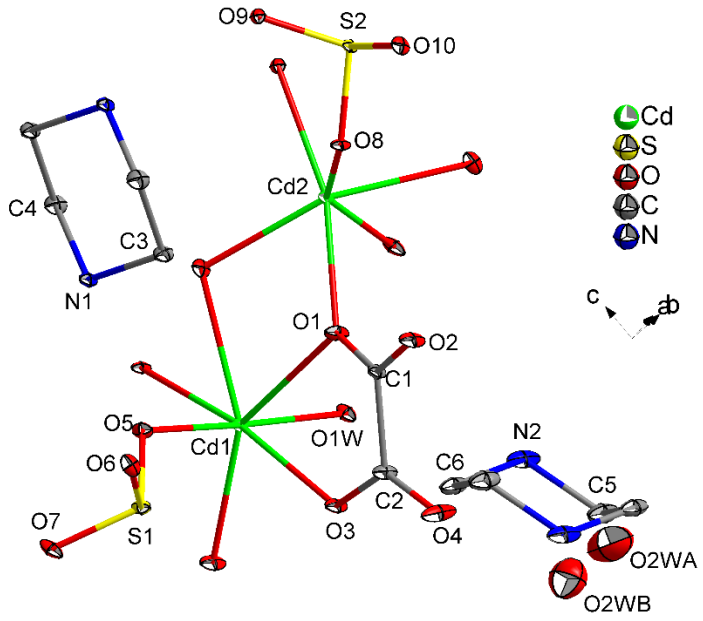


**Fig. S1** Asymmetric unit of **$[C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)]$ 3** with 15% ellipsoidal probability.

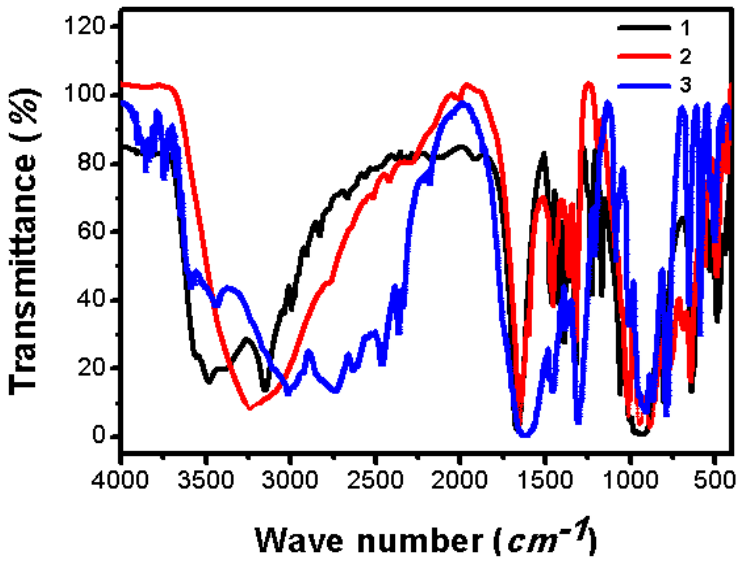


**Fig. S2** FTIR spectra of $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(C_6N_2H_{13})].(H_2O)_2$, **1**; $[C_4N_2H_{12}]_{0.5}[Zn_2(SO_3)_2(C_2O_4)_{0.5}(H_2O)_2]$, **2**; and $[C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)]$ **3**.

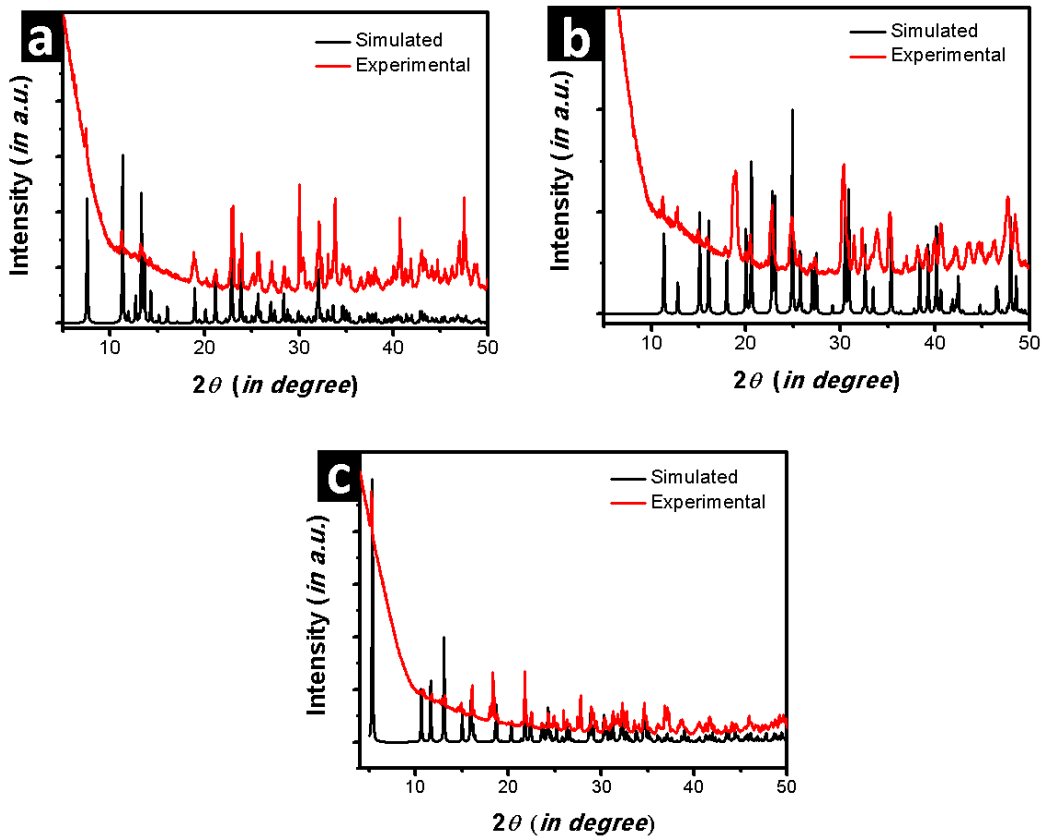


**Fig. S3** PXRD pattern for (a) $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(C_6N_2H_{13})].(H_2O)_2$, **1**; and (b) $[C_4N_2H_{12}]_{0.5}[Zn_2(SO_3)_2(C_2O_4)_{0.5}(H_2O)_2]$ **2**; and (c)$[C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)]$ **3**.

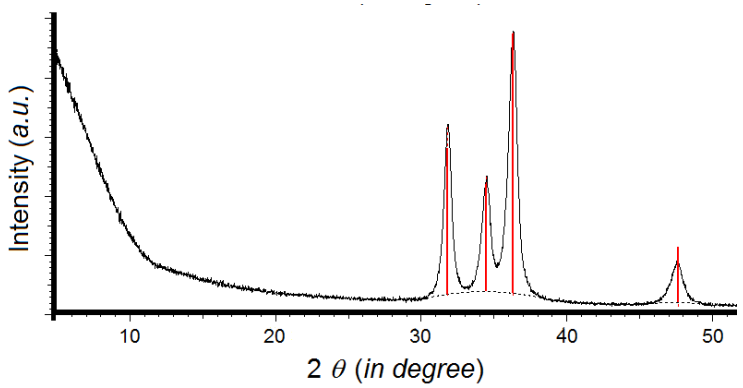


**Fig. S4** Post calcination PXRD analysis of $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(C_6N_2H_{13})].(H_2O)_2$, **1** and $[C_4N_2H_{12}]_{0.5}$ $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(H_2O)_2]$, **2** showing formation of ZnO (PDF-01-075-0576)

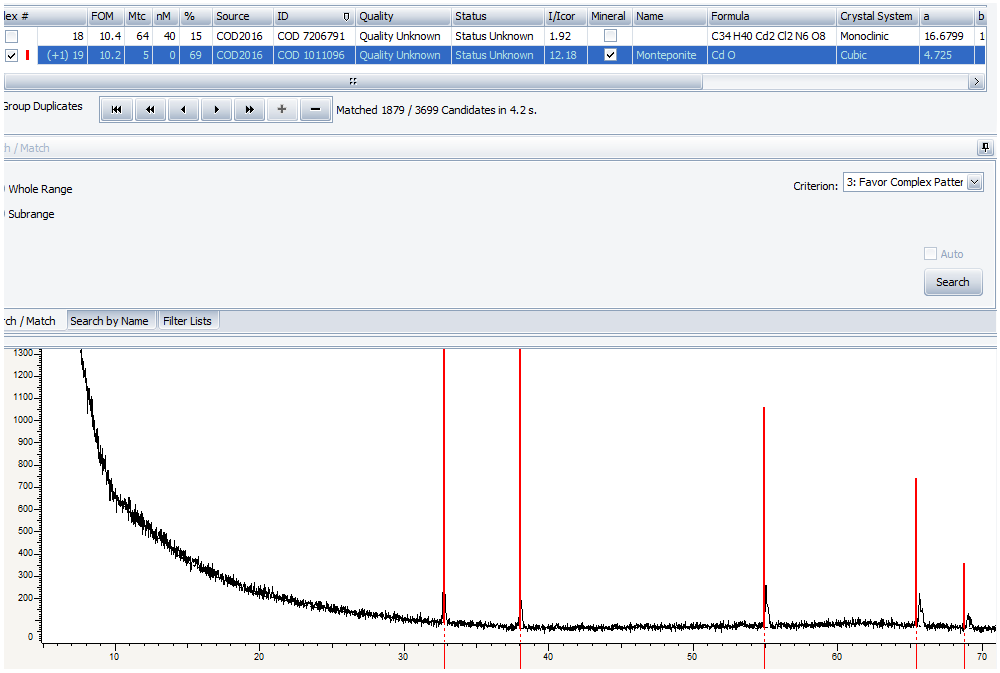


**Fig. S5** Post calcination PXRD analysis of $[C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)]$ **3** showing formation of CdO (COD-1011096)

**Table S1.** Hydrogen bonding table for complexes **1**-**3**.[#]

| D–H···A | Symmetry of A | D–H | H···A | D–A | ∠D–H···A |
|---|---|---|---|---|---|
| | **$[Zn_2(SO_3)_2(C_2O_4)_{0.5}(C_6N_2H_{13})].(H_2O)_2$, 1** | | | | |
| N2–H2···O6 | -1+x,y,-1+z | 0.91 | 2.18 | 2.908(2) | 136 |
| N2–H2···O7 | -1+x,y,-1+z | 0.91 | 2.32 | 2.917(2) | 123 |
| C2–H2B···O4 | | 0.97 | 2.54 | 3.108(3) | 117 |
| C6–H6A···O2 | x,1/2-y,-1/2+z | 0.97 | 2.40 | 3.304(3) | 155 |
| C6–H6B···O2 | | 0.97 | 2.57 | 3.201(3) | 123 |
| | **$[C_4N_2H_{12}]_{0.5}$ $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(H_2O)_2]$, 2** | | | | |
| N1–H1A···O3 | y,x,1-z | 0.90 | 2.28 | 3.146(5) | 161 |
| O1W–H1W···O2 | 1/2+y,1/2-x,1/2-z | 0.78(6) | 2.00(5) | 2.767(5) | 172(6) |
| C2–H2A···O1W | 1/2-x,-1/2+y,1/2-z | 0.97 | 2.49 | 2.879(12) | 104 |
| C2–H2B···O3 | | 0.97 | 2.24 | 3.023(12) | 137 |
| | **$[C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)]$, 3** | | | | |
| O2WA–H2WA···O1W | 2-x,-y,1-z | 0.85 | 2.15 | 2.997(13) | 171 |
| N1–H1A···O9 | 2-x,1-y,-z | 0.89 | 2 | 2.812(4) | 150 |
| N1–H1B···O5 | | 0.89 | 1.91 | 2.777(4) | 164 |
| O2WA–H2WB··· O4 | | 0.85 | 2.06 | 2.901(12) | 168 |
| N2–H2A···O3 | -1+x,y,z | 0.89 | 1.88 | 2.751(5) | 166 |
| N2–H2B···O2 | -1+x,y,z | 0.89 | 2.52 | 3.009(5) | 116 |
| N2–H2B···O4 | | 0.89 | 1.86 | 2.689(5) | 154 |
| O1W–H1WA···O6 | 1+x,-1+y,z | 0.83(5) | 1.91(6) | 2.728(4) | 167(6) |
| O1W–H1WB···O7 | x,-1+y,z | 0.83(6) | 1.88(6) | 2.672(4) | 161(6) |
| C3–H3A···O8 | -1+x,y,z | 0.97 | 2.52 | 3.429(5) | 156 |
| C3–H3B···O7 | -1+x,y,z | 0.97 | 2.56 | 3.334(5) | 137 |
| C4–H4A···O5 | 2-x,1-y,-z | 0.97 | 2.55 | 3.372(6) | 142 |
| C4–H4B···O10 | | 0.97 | 2.56 | 3.295(6) | 133 |
| C6–H6A···O4 | 1-x,1-y,1-z | 0.97 | 2.45 | 3.370(6) | 158 |

[#]Where 'D' is donor and 'A' is acceptor, the bond lengths are in (Å) and angles are in (°).

**Table S2.** Complete list of bond lengths [Å] and bond angles [◦] for complex **1-3**[#]

| $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(C_6N_2H_{13})].(H_2O)_2$, 1 | | | | | | | |
|---|---|---|---|---|---|---|---|
| Zn1-O1 | 1.9766(14) | Zn1-O8 | 2.0528(14) | S2-O6 | 1.5267(14) | N2-C5 | 1.489(3) |
| Zn2-O2$^{a}$ | 1.9406(14) | Zn1-N1 | 2.1601(14) | O7-C1 | 1.241(2) | N2-C7 | 1.490(3) |
| Zn2-O3 | 1.9795(14) | S1-O1 | 1.5213(14) | O8-C1$^{e}$ | 1.258(2) | C1-C1$^{e}$ | 1.540(3) |
| Zn1-O4 | 1.9791(14) | S1-O2 | 1.5254(15) | N1-C2 | 1.472(3) | C3-C2 | 1.529(3) |
| Zn2-O5 | 1.9451(13) | S1-O3$^{b}$ | 1.5318(14) | N1-C4 | 1.480(2) | C5-C4 | 1.529(3) |
| Zn2-O6$^{a}$ | 1.9772(14) | S2-O4 | 1.5293(14) | N1-C6 | 1.476(2) | C6-C7 | 1.515(3) |
| Zn1-O7 | 2.1461(13) | S2-O5 | 1.5156(14) | N2-C3 | 1.492(3) | | |
| O1-Zn1-O4 | 129.22(7) | O2$^{a}$-Zn2-O6$^{a}$ | 111.06(6) | S2-O4-Zn1 | 123.20(9) | C5-N2-C7 | 110.14(17) |
| O1-Zn1-O7 | 91.66(6) | O5-Zn2-O3 | 104.22(6) | S2-O5-Zn2 | 129.43(8) | C7-N2-C3 | 109.60(16) |
| O1-Zn1-O8 | 111.73(6) | O5-Zn2-O6$^{a}$ | 96.20(6) | S2-O6-Zn2$^{d}$ | 127.51(8) | O7-C1-O8$^{e}$ | 126.28(16) |
| O1-Zn1-N1 | 98.42(6) | O6$^{a}$-Zn2-O3 | 112.20(6) | S1-O2-Zn2$^{d}$ | 123.94(8) | O7-C1-C1$^{e}$ | 116.97(19) |
| O4-Zn1-O7 | 91.36(6) | O1-S1-O2 | 104.83(8) | C1-O7-Zn1 | 112.39(11) | O8$^{e}$-C1-C1$^{e}$ | 116.8(2) |
| O4-Zn1-O8 | 118.58(7) | O1-S1-O3$^{b}$ | 105.46(8) | C1$^{e}$-O8-Zn1 | 114.96(12) | N1-C2-C3 | 112.00(16) |
| O4-Zn1-N1 | 90.30(6) | O2-S1-O3$^{b}$ | 104.21(8) | C2-N1-C6 | 108.09(18) | N2-C3-C2 | 107.80(16) |
| O7-Zn1-N1 | 165.50(6) | O5-S2-O6 | 106.38(8) | C2-N1-C4 | 108.19(17) | N1-C4-C5 | 111.44(16) |
| O8-Zn1-O7 | 78.93(5) | O5-S2-O4 | 103.10(8) | C2-N1-Zn1 | 108.93(11) | N2-C5-C4 | 108.30(15) |
| O8-Zn1-N1 | 87.64(5) | O6-S2-O4 | 104.89(8) | C6-N1-Zn1 | 110.51(11) | N1-C6-C7 | 111.96(17) |
| O2$^{a}$-Zn2-O3 | 107.36(6) | S1-O1-Zn1 | 129.96(9) | C6-N1-C4 | 108.09(17) | N2-C7-C6 | 108.34(16) |
| O2$^{a}$-Zn2-O5 | 125.35(6) | S1$^{c}$-O3-Zn2 | 122.34(8) | C5-N2-C3 | 109.49(17) | | |
| $[C_4N_2H_{12}]_{0.5}$ $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(H_2O)_2]$, 2 | | | | | | | |
| Zn1-O1 | 2.056(4) | Zn1-O1W | 2.081(4) | C1-O3 | 1.252(5) | C2-C2$^{n}$ | 1.474(19) |
| Zn2-O2 | 1.978(3) | S1-O1 | 1.506(4) | C1-C1$^{l}$ | 1.518(15) | N1-C2 | 1.457(11) |
| Zn1-O3 | 2.128(4) | S1-O2 | 1.543(3) | | | | |
| O1$^{i}$-Zn1-O1 | 163.3(2) | O1W-Zn1-O3$^{j}$ | 168.50(18) | O2$^{j}$-S1-O2 | 104.9(2) | C2$^{m}$-N1-C2 | 107.5(12) |
| O1-Zn1-O3 | 96.52(9) | O1W$^{j}$-Zn1-O1W | 99.9(3) | S1-O1-Zn1 | 122.6(3) | O3$^{k}$-C1-O3 | 126.5(7) |
| O1-Zn1-O1W | 84.65(8) | O2$^{f}$-Zn2-O2 | 118.93(15) | S1-O2-Zn2 | 123.69(17) | O3-C1-C1$^{l}$ | 116.8(4) |
| O3-Zn1-O3$^{j}$ | 76.9(2) | O2$^{g}$-Zn2-O2 | 104.96(7) | C1-O3-Zn1 | 114.8(4) | N1-C2-C2$^{n}$ | 107.4(9) |
| O1W-Zn1-O3 | 91.63(17) | O1-S1-O2 | 104.41(16) | | | | |
| $[C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)$, 3 | | | | | | | |
| Cd1-O1 | 2.481(3) | Cd2-O6$^{q}$ | 2.335(3) | S1-O7 | 1.534(3) | C2-C1 | 1.566(5) |
| Cd1-O2$^{o}$ | 2.336(3) | Cd2-O7$^{q}$ | 2.317(3) | S2-O8 | 1.545(3) | N1-C3 | 1.490(5) |
| Cd1-O3 | 2.292(3) | Cd2-O8 | 2.261(3) | S2-O9 | 1.525(3) | N1-C4 | 1.490(5) |
| Cd1-O5 | 2.255(3) | Cd2-O9$^{p}$ | 2.268(3) | S2-O10 | 1.533(3) | N2-C6 | 1.480(7) |
| Cd1-O8$^{o}$ | 2.383(3) | Cd2-O10$^{o}$ | 2.279(3) | O3-C2 | 1.263(4) | N2-C5 | 1.487(7) |
| Cd1-O10$^{o}$ | 2.481(3) | Cd2-S1$^{q}$ | 2.9742(10) | O1-C1 | 1.258(5) | C3-C4$^{u}$ | 1.505(6) |
| Cd1-O1W | 2.313(3) | S1-O6 | 1.528(3) | O2-C1 | 1.239(5) | C5-C6$^{t}$ | 1.512(7) |
| Cd2-O1 | 2.284(3) | S1-O5 | 1.529(3) | O4-C2 | 1.240(5) | | |
| O5-Cd1-O3 | 90.32(11) | O10$^{o}$-Cd2-O7$^{q}$ | 91.32(10) | S2-O10-Cd2$^{s}$ | 129.50(16) | N2-C6-C5$^{t}$ | 110.9(4) |
| O5-Cd1-O1W | 175.84(10) | O1-Cd2-O7$^{q}$ | 90.51(11) | S2-O10-Cd1$^{s}$ | 97.98(13) | N2-C6-H6A | 109.5 |
| O3-Cd1-O1W | 87.91(11) | O8-Cd2-O6$^{q}$ | 88.24(10) | Cd2$^{s}$-O10-Cd1$^{s}$ | 104.74(11) | C5$^{t}$-C6-H6A | 109.5 |
| O5-Cd1-O2$^{o}$ | 97.22(11) | O9$^{p}$-Cd2-O6$^{q}$ | 93.69(10) | S2-O8-Cd2 | 120.04(14) | N2-C6-H6B | 109.5 |
| O3-Cd1-O2$^{o}$ | 79.68(10) | O10$^{o}$-Cd2-O6$^{q}$ | 152.27(10) | S2-O8-Cd1$^{s}$ | 101.72(13) | C5$^{t}$-C6-H6B | 109.5 |
| O1W-Cd1-O2$^{o}$ | 86.16(11) | O1-Cd2-O6$^{q}$ | 101.86(11) | Cd2-O8-Cd1$^{s}$ | 123.96(11) | H6A-C6-H6B | 108.1 |
| O5-Cd1-O8$^{o}$ | 95.67(10) | O7$^{q}$-Cd2-O6$^{q}$ | 61.11(10) | S1-O7-Cd2$^{r}$ | 99.10(14) | H2WA-O2WA-H2WB | 109.5 |
| O3-Cd1-O8$^{o}$ | 167.05(9) | O8-Cd2-S1$^{q}$ | 118.53(7) | C1-O2-Cd1$^{s}$ | 137.7(3) | H2WC-O2WB-H2WD | 111.2 |
| O1W-Cd1-O8$^{o}$ | 86.82(10) | O9$^{p}$-Cd2-S1$^{q}$ | 96.94(7) | Cd1-O1W-H1WA | 114(5) | C3-N1-C4 | 111.5(3) |
| O2$^{o}$-Cd1-O8$^{o}$ | 88.16(9) | O10$^{o}$-Cd2-S1$^{q}$ | 121.93(7) | Cd1-O1W-H1WB | 110(5) | C3-N1-H1A | 109.3 |
| O5-Cd1-O10$^{o}$ | 84.11(10) | O1-Cd2-S1$^{q}$ | 98.39(8) | H1WA-O1W-H1WB | 104(4) | C4-N1-H1A | 109.3 |
| O3-Cd1-O10$^{o}$ | 134.18(9) | O7$^{q}$-Cd2-S1$^{q}$ | 30.61(7) | O4-C2-O3 | 124.5(4) | C3-N1-H1B | 109.3 |
| O1W-Cd1-O10$^{o}$ | 94.43(10) | O6$^{q}$-Cd2-S1$^{q}$ | 30.55(7) | O4-C2-C1 | 118.7(3) | C4-N1-H1B | 109.3 |
| O2$^{o}$-Cd1-O10$^{o}$ | 146.13(9) | O9-S2-O10 | 105.51(16) | O3-C2-C1 | 116.8(3) | H1A-N1-H1B | 108 |
| O8$^{o}$-Cd1-O10$^{o}$ | 58.13(8) | O9-S2-O8 | 104.30(15) | C6-N2-C5 | 111.6(4) | N1-C3-C4$^{u}$ | 110.0(3) |
| O5-Cd1-O1 | 89.91(10) | O10-S2-O8 | 100.41(15) | C6-N2-H2A | 109.3 | N1-C3-H3A | 109.7 |
| O3-Cd1-O1 | 67.74(9) | O6-S1-O5 | 104.44(16) | C5-N2-H2A | 109.3 | C4$^{u}$-C3-H3A | 109.7 |
| O1W-Cd1-O1 | 85.94(10) | O6-S1-O7 | 101.14(16) | C6-N2-H2B | 109.3 | N1-C3-H3B | 109.7 |
| O2$^{o}$-Cd1-O1 | 146.70(10) | O5-S1-O7 | 104.67(17) | C5-N2-H2B | 109.3 | C4$^{u}$-C3-H3B | 109.7 |
| O8$^{o}$-Cd1-O1 | 123.58(9) | O6-S1-Cd2$^{r}$ | 50.95(11) | H2A-N2-H2B | 108 | H3A-C3-H3B | 108.2 |
| O10$^{o}$-Cd1-O1 | 66.81(9) | O5-S1-Cd2$^{r}$ | 110.72(11) | O2-C1-O1 | 128.3(3) | N1-C4-C3$^{u}$ | 110.7(3) |
| O8-Cd2-O9$^{p}$ | 89.78(9) | O7-S1-Cd2$^{r}$ | 50.29(11) | O2-C1-C2 | 117.6(3) | N1-C4-H4A | 109.5 |
| O8-Cd2-O10$^{o}$ | 118.27(10) | S1-O5-Cd1 | 120.98(16) | O1-C1-C2 | 114.0(3) | C3$^{u}$-C4-H4A | 109.5 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| O9$^{p}$-Cd2-O10$^{o}$ | 94.38(10) | S1-O6-Cd2$^{r}$ | 98.50(14) | N2-C5-C6$^{t}$ | 109.3(4) | N1-C4-H4B | 109.5 |
| O8-Cd2-O1 | 86.95(10) | C2-O3-Cd1 | 122.1(2) | N2-C5-H5A | 109.8 | C3$^{u}$-C4-H4B | 109.5 |
| O9$^{p}$-Cd2-O1 | 163.99(10) | S2-O9-Cd2$^{p}$ | 120.17(14) | C6$^{t}$-C5-H5A | 109.8 | H4A-C4-H4B | 108.1 |
| O10$^{o}$-Cd2-O1 | 73.54(10) | C1-O1-Cd2 | 139.5(2) | N2-C5-H5B | 109.8 | | |
| O8-Cd2-O7$^{q}$ | 148.01(10) | C1-O1-Cd1 | 115.9(2) | C6$^{t}$-C5-H5B | 109.8 | | |
| O9$^{p}$-Cd2-O7$^{q}$ | 100.43(10) | Cd2-O1-Cd1 | 104.59(11) | H5A-C5-H5B | 108.3 | | |

#Symmetry transformations used to generate equivalent atoms:

(*a*) x, -y+1/2, z-1/2; (*b*) x, y, z+1; (*c*) x, y, z-1; (*d*) x, -y+1/2, z+1/2; (*e*) -x+1, -y, -z+2; (*f*) -x+1, -y, z; (*g*) -y+1/2, x-1/2, -z+1/2; (*h*) y+1/2, -x+1/2, -z+1/2; (*i*) y+1, x-1, z; (*j*) x, y, -z; (*k*) -x+2, -y, z; (*l*) -x+2, -y, -z; (*m*) y, x, z; (*n*) -y+2, -x+2, -z+1; (o) x-1,y,z ; (p) -x+1,-y+2,-z+2; (q) x,y+1,z; (r) x,y-1,z; (s) x+1,y,z; (t) -x+2,-y+1,-z+1; (u) -x+1,-y+1,-z+2

**Table S3.** Atomic coordinates (×10$^4$) and equivalent isotropic displacement parameters (Å×10$^3$) for **1-3** U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | U(eq) | | x | y | z | U(eq) |
|---|---|---|---|---|---|---|---|---|---|
| $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(C_6N_2H_{13})].(H_2O)_2$, **1** | | | | | | | | | |
| Zn1 | 3448(1) | 1022(1) | 8731(1) | 19(1) | O1W | 8490(7) | -230(1) | 8584(6) | 142(2) |
| Zn2 | 5156(1) | 2421(1) | 5152(1) | 20(1) | O2W | 5724(7) | 266(2) | 6399(8) | 165(2) |
| S1 | 2865(1) | 1883(1) | 11465(1) | 20(1) | N1 | 1093(2) | 1164(1) | 6383(2) | 18(1) |
| S2 | 6585(1) | 1598(1) | 8507(1) | 17(1) | N2 | -1603(2) | 1342(1) | 3549(2) | 25(1) |
| O1 | 2727(2) | 1294(1) | 10632(2) | 27(1) | C1 | 5786(2) | 150(1) | 10711(2) | 19(1) |
| O2 | 3014(2) | 2288(1) | 10056(2) | 26(1) | C2 | 1269(3) | 948(1) | 4750(3) | 34(1) |
| O3 | 4623(2) | 1902(1) | 3052(2) | 28(1) | C3 | -352(2) | 1037(1) | 3024(3) | 29(1) |
| O4 | 4713(2) | 1431(1) | 7525(2) | 30(1) | C4 | -373(2) | 874(1) | 6522(3) | 31(1) |
| O5 | 6839(2) | 2009(1) | 7189(2) | 23(1) | C5 | -2017(2) | 984(1) | 4841(3) | 28(1) |
| O6 | 6677(2) | 1951(1) | 10137(2) | 25(1) | C6 | 707(3) | 1778(1) | 6126(3) | 36(1) |
| O7 | 5762(2) | 678(1) | 10739(2) | 25(1) | C7 | -872(3) | 1896(1) | 4413(3) | 33(1) |
| O8 | 3028(2) | 165(1) | 8265(2) | 27(1) | | | | | |
| $[C_4N_2H_{12}]_{0.5}$ $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(H_2O)_2]$, **2** | | | | | | | | | |
| Zn1 | 8225(1) | -1776(1) | 0 | 11(1) | O3 | 9287(3) | -713(3) | 1484(5) | 27(1) |
| Zn2 | 5000 | 0 | 2500 | 12(1) | O1W | 7370(3) | -2630(3) | 1786(5) | 18(1) |
| S1 | 6834(1) | 686(1) | 0 | 12(1) | N1 | 9115(8) | 9115(8) | 5000 | 145(12) |
| O1 | 6737(4) | -668(4) | 0 | 15(1) | C1 | 10000 | 0 | 851(8) | 15(2) |
| O2 | 6086(3) | 1087(3) | 1373(3) | 14(1) | C2 | 8854(10) | 10352(10) | 4558(13) | 64(5) |
| $[C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)$, **3** | | | | | | | | | |
| Cd(1) | -1086(1) | 8084(1) | 7714(1) | 10(1) | O(1W) | -2477(5) | 10939(4) | 7189(2) | 17(1) |
| Cd(2) | 2526(1) | 10389(1) | 8640(1) | 11(1) | O(4) | 3846(6) | 6991(6) | 5728(2) | 37(1) |
| S(2) | 7612(2) | 9613(1) | 9380(1) | 10(1) | C(2) | 2785(6) | 7349(5) | 6374(2) | 16(1) |
| S(1) | 1216(2) | 3777(1) | 7673(1) | 14(1) | N(2) | 8322(6) | 6278(6) | 5438(2) | 30(1) |
| O(5) | 525(5) | 5322(3) | 8217(2) | 16(1) | C(1) | 3994(6) | 7839(5) | 7079(2) | 13(1) |
| O(6) | 3555(5) | 2666(4) | 7954(2) | 18(1) | C(5) | 8718(8) | 6596(8) | 4565(3) | 32(1) |
| O(3) | 762(5) | 7366(4) | 6505(2) | 18(1) | C(6) | 8854(8) | 4383(7) | 5663(3) | 29(1) |
| O(9) | 7648(5) | 8466(3) | 10147(2) | 13(1) | O(2WA) | 3360(30) | 9761(15) | 4481(7) | 91(6) |
| O(1) | 2670(5) | 8564(4) | 7636(2) | 19(1) | O(2WB) | 1520(30) | 9760(17) | 4562(10) | 82(7) |
| O(10) | 9992(4) | 8928(4) | 8998(2) | 15(1) | N(1) | 3392(6) | 4671(4) | 9500(2) | 15(1) |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| O(8) | 6247(4) | 8955(3) | 8797(2) | 12(1) | C(3) | 5532(7) | 4907(6) | 9149(2) | 17(1) |
| | | | | | C(4) | 2648(7) | 5656(6) | 10240(3) | 20(1) |
| O(7) | -228(5) | 2618(4) | 7980(2) | 20(1) | | | | | |
| O(2) | 6072(5) | 7531(4) | 7016(2) | 21(1) | | | | | |

**Table S4.** Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1-3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

| | U11 | U22 | U33 | U23 | U13 | U12 | | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(C_6N_2H_{13})].(H_2O)_2$, **1** | | | | | | | | | | | | | |
| Zn1 | 18(1) | 16(1) | 17(1) | 1(1) | 2(1) | 0(1) | O1W | 287(6) | 52(2) | 192(4) | -6(2) | 204(5) | -18(2) |
| Zn2 | 21(1) | 20(1) | 15(1) | -1(1) | 5(1) | 0(1) | O2W | 209(5) | 101(3) | 256(6) | -17(3) | 167(5) | -7(3) |
| S1 | 21(1) | 20(1) | 18(1) | -3(1) | 8(1) | -1(1) | N1 | 17(1) | 17(1) | 15(1) | 0(1) | 2(1) | 0(1) |
| S2 | 17(1) | 17(1) | 14(1) | 1(1) | 4(1) | 2(1) | N2 | 19(1) | 31(1) | 17(1) | 1(1) | -1(1) | 3(1) |
| O1 | 37(1) | 21(1) | 24(1) | -7(1) | 13(1) | -5(1) | C1 | 17(1) | 19(1) | 17(1) | 1(1) | 2(1) | 0(1) |
| O2 | 25(1) | 28(1) | 23(1) | 4(1) | 6(1) | -3(1) | C2 | 24(1) | 53(2) | 17(1) | -4(1) | 3(1) | 12(1) |
| O3 | 30(1) | 29(1) | 17(1) | -7(1) | 2(1) | 3(1) | C3 | 22(1) | 42(1) | 18(1) | -4(1) | 5(1) | 2(1) |
| O4 | 22(1) | 42(1) | 20(1) | 5(1) | 2(1) | -10(1) | C4 | 20(1) | 40(1) | 28(1) | 13(1) | 5(1) | -2(1) |
| O5 | 22(1) | 28(1) | 18(1) | 6(1) | 7(1) | 0(1) | C5 | 19(1) | 36(1) | 24(1) | -1(1) | 5(1) | -2(1) |
| O6 | 33(1) | 25(1) | 15(1) | -1(1) | 7(1) | 6(1) | C6 | 37(1) | 17(1) | 31(1) | 0(1) | -8(1) | 2(1) |
| O7 | 23(1) | 16(1) | 25(1) | 1(1) | -2(1) | 0(1) | C7 | 33(1) | 22(1) | 31(1) | 5(1) | -1(1) | 6(1) |
| O8 | 22(1) | 18(1) | 27(1) | 1(1) | -5(1) | 1(1) | | | | | | | |
| $[C_4N_2H_{12}]_{0.5}$ $[Zn_2(SO_3)_2(C_2O_4)_{0.5}(H_2O)_2]$, **2** | | | | | | | | | | | | | |
| Zn1 | 11(1) | 11(1) | 10(1) | 0 | 0 | 0(1) | O3 | 35(2) | 35(2) | 11(2) | 1(1) | 1(1) | -20(2) |
| Zn2 | 10(1) | 10(1) | 14(1) | 0 | 0 | 0 | O1W | 17(1) | 17(1) | 20(2) | 7(1) | 7(1) | 3(2) |
| S1 | 11(1) | 11(1) | 13(1) | 0 | 0 | -2(1) | N1 | 198(18) | 198(18) | 38(7) | 0 | 0 | -170(20) |
| O1 | 14(2) | 12(2) | 20(2) | 0 | 0 | 1(2) | C1 | 17(2) | 17(2) | 9(3) | 0 | 0 | 0(3) |
| O2 | 16(1) | 13(1) | 14(1) | -2(1) | 2(1) | -3(1) | C2 | 37(6) | 83(9) | 73(10) | -70(7) | -37(6) | 39(6) |
| $[(C_4N_2H_{12}][Cd_2(SO_3)_2(C_2O_4)(H_2O)].(H_2O)]$, **3** | | | | | | | | | | | | | |
| Cd(1) | 7(1) | 13(1) | 12(1) | -4(1) | 1(1) | -3(1) | O(1W) | 13(1) | 15(1) | 24(2) | -1(1) | -3(1) | -5(1) |
| Cd(2) | 7(1) | 12(1) | 13(1) | -3(1) | 0(1) | -4(1) | O(4) | 13(2) | 80(3) | 24(2) | -28(2) | 7(1) | -19(2) |
| S(2) | 7(1) | 12(1) | 11(1) | -3(1) | 1(1) | -4(1) | C(2) | 6(2) | 26(2) | 18(2) | -12(2) | 1(1) | -3(1) |
| S(1) | 16(1) | 11(1) | 14(1) | -2(1) | -3(1) | -3(1) | N(2) | 7(2) | 58(3) | 28(2) | -23(2) | 3(1) | -10(2) |
| O(5) | 18(1) | 10(1) | 17(1) | -3(1) | -3(1) | -2(1) | C(1) | 10(2) | 17(2) | 15(2) | -4(1) | 0(1) | -7(1) |
| O(6) | 12(1) | 14(1) | 27(2) | -1(1) | 2(1) | -3(1) | C(5) | 20(2) | 51(3) | 29(2) | -13(2) | -2(2) | -11(2) |
| O(3) | 9(1) | 32(2) | 17(1) | -9(1) | 2(1) | -11(1) | C(6) | 19(2) | 52(3) | 21(2) | -13(2) | 0(2) | -16(2) |
| O(9) | 13(1) | 14(1) | 11(1) | -2(1) | 0(1) | -6(1) | O(2WA) | 126(15) | 73(7) | 69(7) | -8(5) | -28(8) | -20(7) |
| O(1) | 11(1) | 28(2) | 19(1) | -14(1) | 5(1) | -7(1) | O(2WB) | 99(17) | 76(10) | 72(10) | 11(8) | -18(10) | -26(10) |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| O(10) | 8(1) | 20(1) | 18(1) | -5(1) | 5(1) | -6(1) | N(1) | 13(2) | 18(2) | 16(2) | 1(1) | -5(1) | -8(1) |
| O(8) | 6(1) | 16(1) | 13(1) | -5(1) | -2(1) | -3(1) | C(3) | 11(2) | 26(2) | 16(2) | -4(2) | 0(1) | -8(2) |
| O(7) | 12(1) | 17(1) | 33(2) | -2(1) | -7(1) | -7(1) | C(4) | 11(2) | 26(2) | 21(2) | -5(2) | 1(2) | -5(2) |
| O(2) | 8(1) | 35(2) | 22(2) | -12(1) | 1(1) | -9(1) | | | | | | | |