

Supporting Information

From zero- to three-dimensional heterobimetallic coordination polymers with the $[\text{Pt}\{\text{SSC-N}(\text{CH}_2\text{COO})_2\}_2]^{4-}$ metalloligand

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1. Powder X-ray diffraction studies

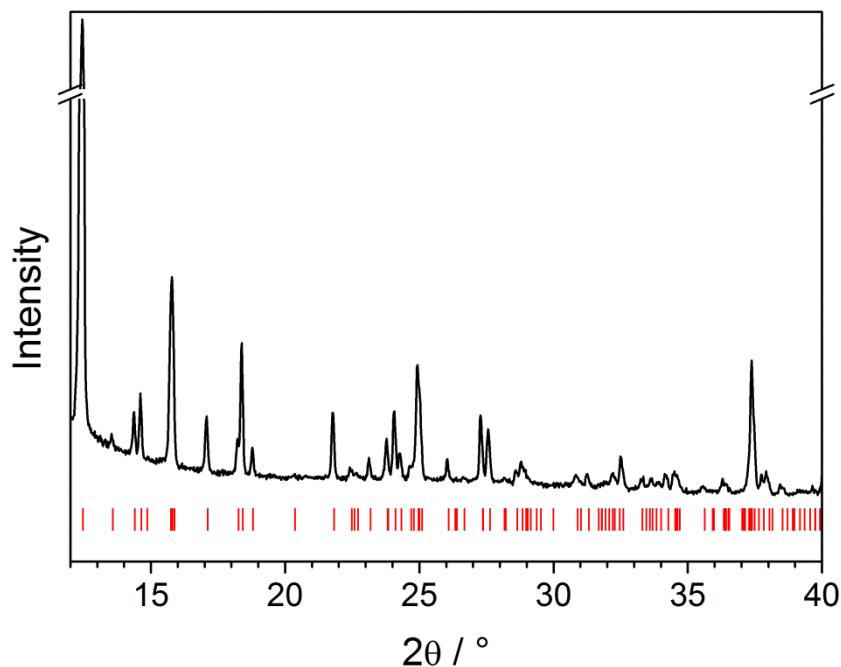


Figure S1. Powder X-ray diffraction pattern of **2-Sr·4H₂O** as compared to the pattern calculated from single-crystal data (red bars). For better comparison, the used unit cell parameters were determined at room temperature: space group $P\bar{1}$ (triclinic), $a = 6.878(2)$ Å, $b = 7.946(2)$ Å, $c = 11.582(2)$ Å, $\alpha = 94.17(2)^\circ$, $\beta = 100.80(2)^\circ$, $\gamma = 114.99(2)^\circ$.

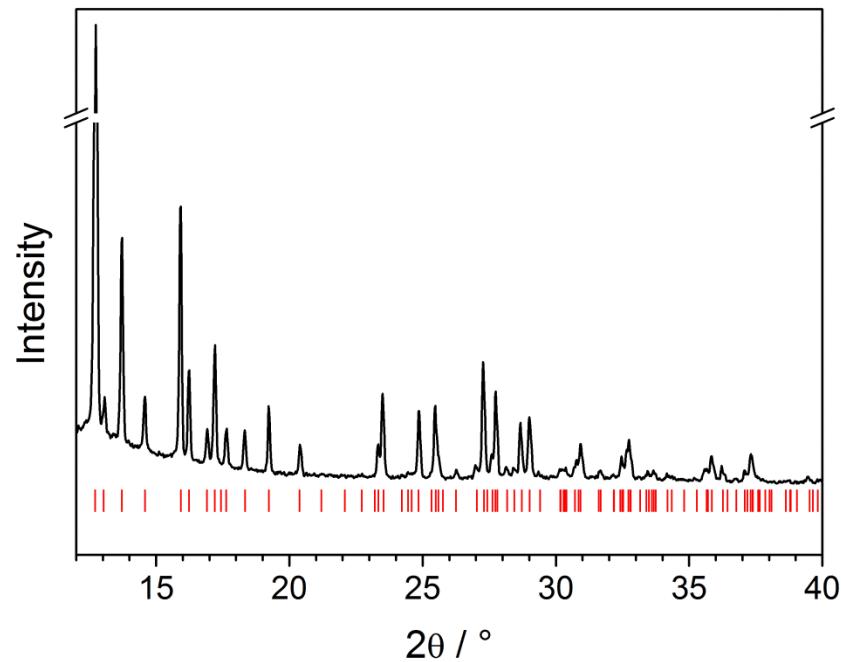


Figure S2. Powder X-ray diffraction pattern of **2-Cd·4H₂O** as compared to the pattern calculated from single-crystal data (red bars). For better comparison, the used unit cell parameters were determined at room temperature: space group $P\bar{1}$ (triclinic), $a = 6.767(1)$ Å, $b = 7.464(2)$ Å, $c = 11.454(1)$ Å, $\alpha = 103.93(1)^\circ$, $\beta = 96.78(1)^\circ$, $\gamma = 103.77(1)^\circ$.

2. Thermal analyses

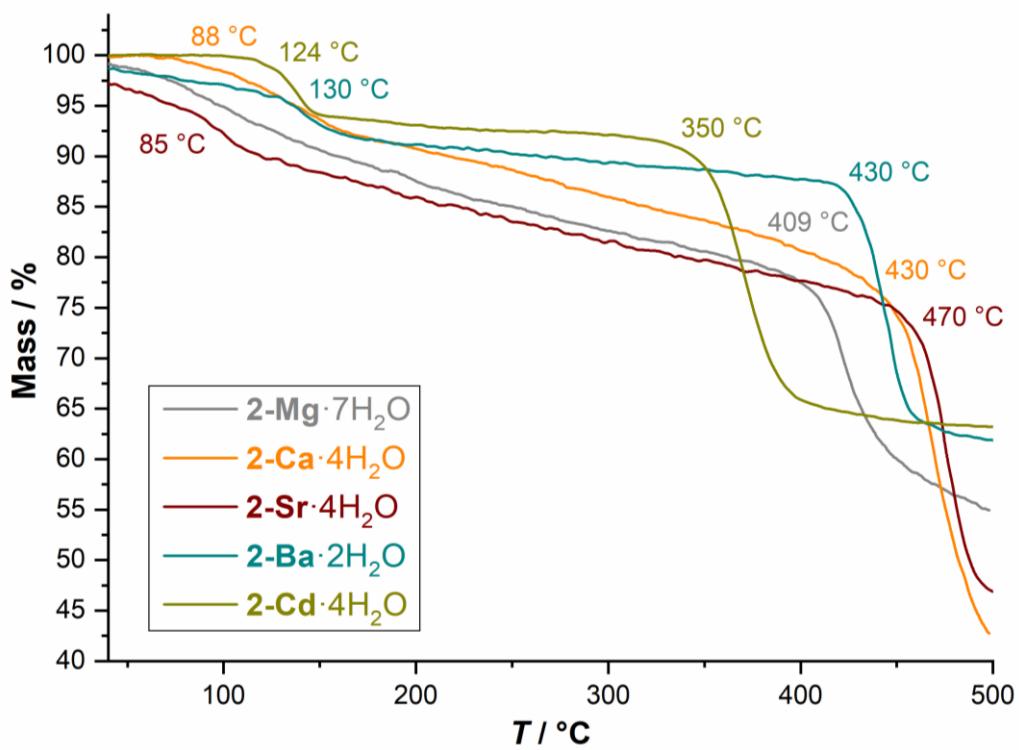


Figure S3. Thermogravimetric (TG) analyses of the isolated hydrates of alkaline earth and cadmium compounds **2** under an inert atmosphere of nitrogen.

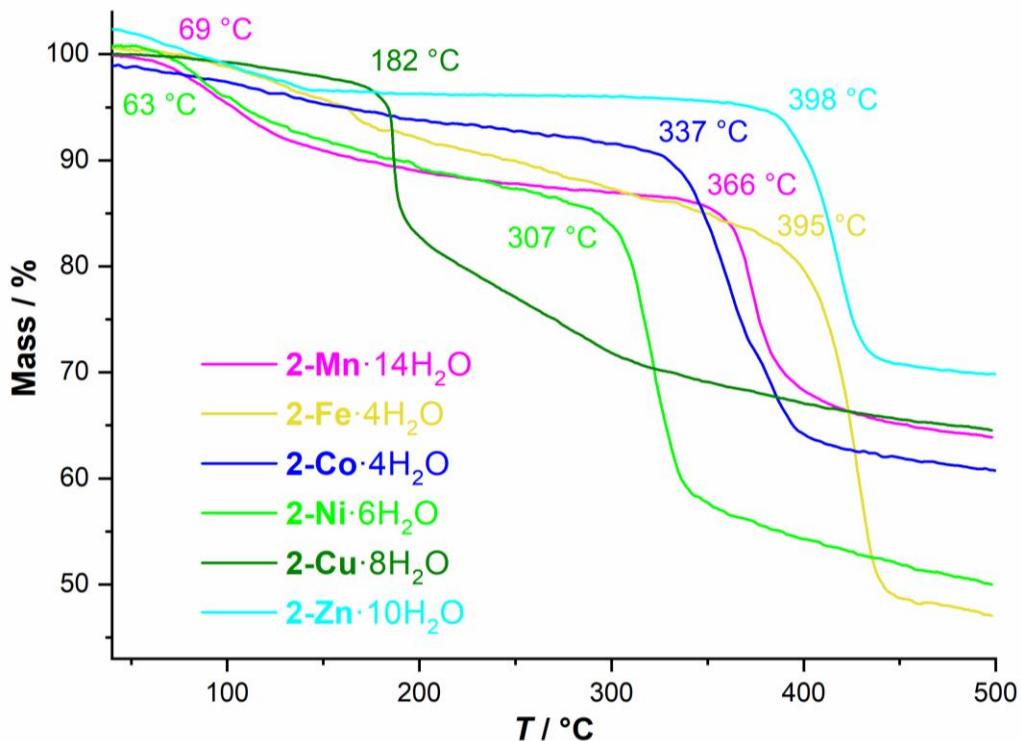


Figure S4. Thermogravimetric (TG) analyses of the isolated hydrates of first-row transition metal compounds **2** under an inert atmosphere of nitrogen.

3. IR spectra

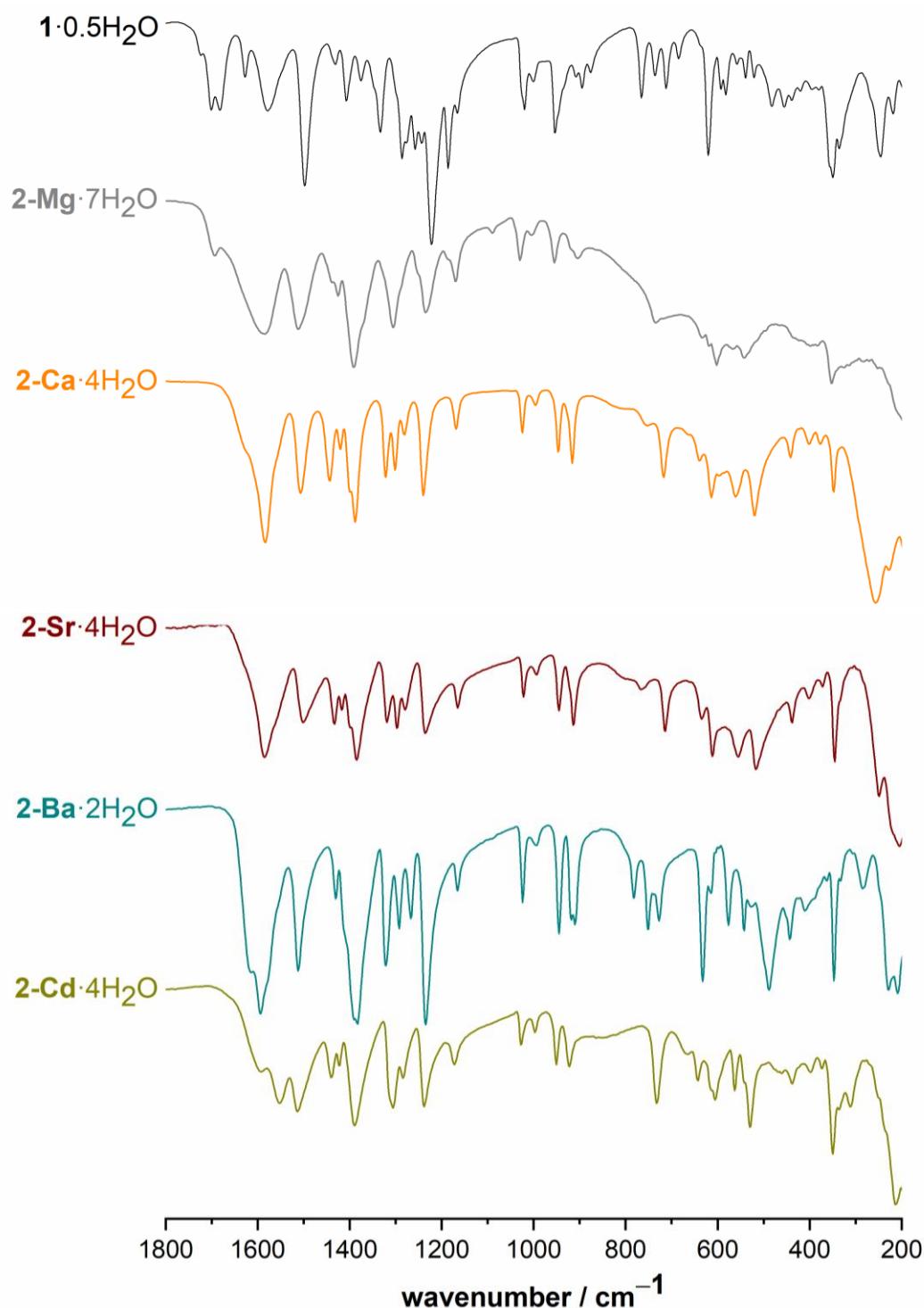


Figure S5. ATR IR spectra of the isolated hydrates of alkaline-earth and cadmium compounds **2**.

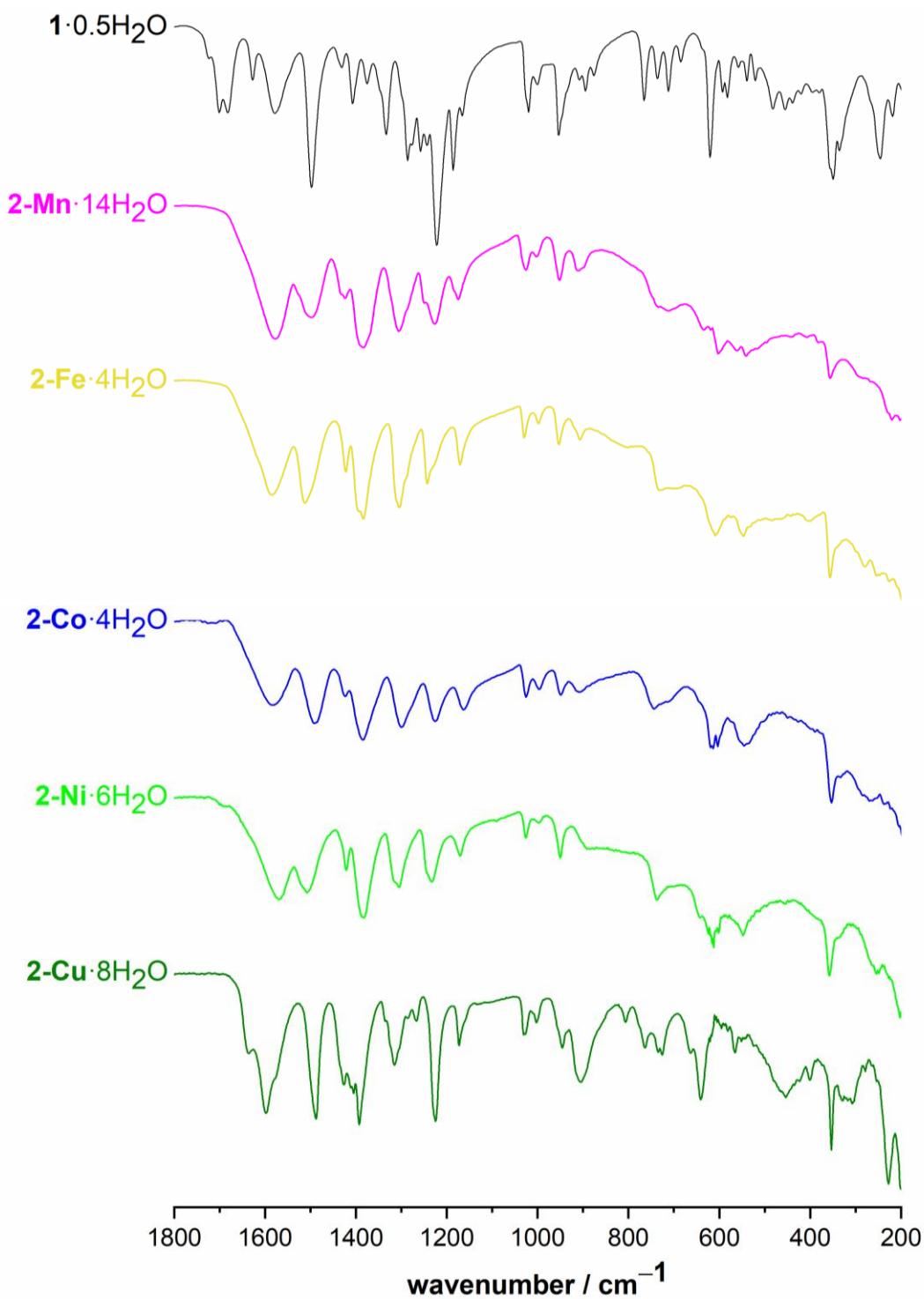


Figure S6. ATR IR spectra of the isolated hydrates of first-row transition-metal compounds **2**.

4. Single-crystal X-ray structural analyses

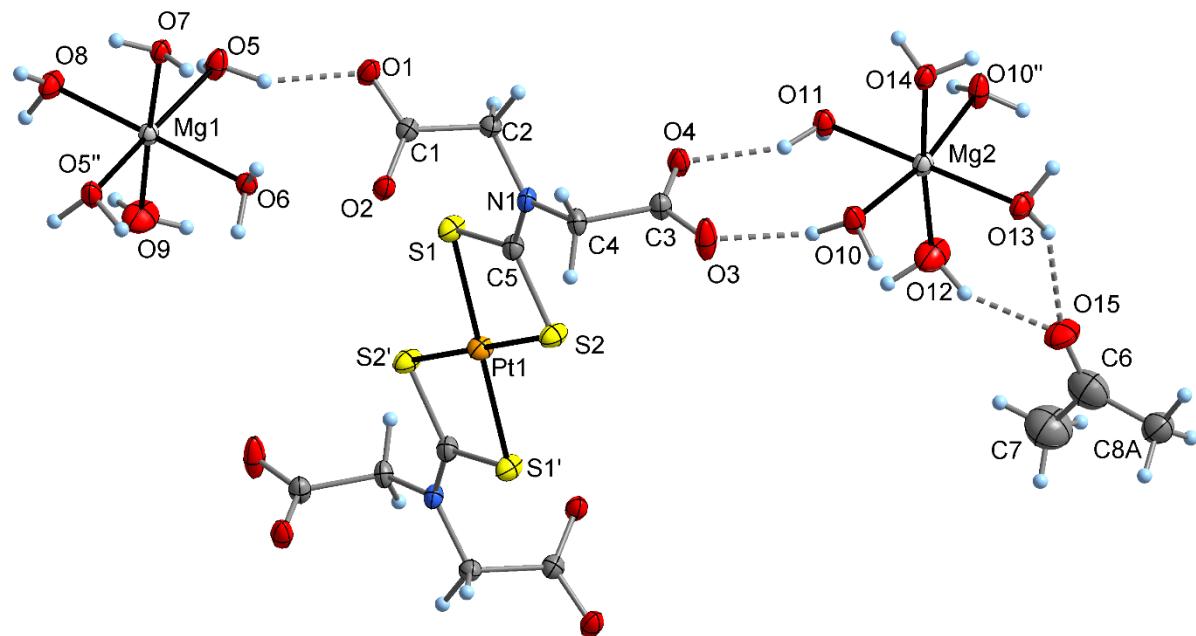


Figure S7. Molecular structure of H_2O - and acetone-solvated $\text{Mg}_2[\text{Pt}(\text{L})_2]$ (**2-Mg**) in the crystal, showing the atom numbering scheme. Displacement ellipsoids drawn at the 50% probability level. The atom Pt1 is situated on a crystallographic centre of inversion, and the atoms Mg1, Mg2, O6–O9 and O11–O15 and C6, C7 and C8A on crystallographic mirror planes. Selected intermolecular distances (pm) and angles (°): Pt1-S1 231.01(8), Pt1-S2 231.62(8), Mg1-O5 204.6(2), Mg1-O6 206.7(3), Mg1-O7 209.9(3), Mg1-O8 205.1(3), Mg1-O9 205.7(4), Mg2-O10 203.0(2), Mg1-O11 207.8(3), Mg1-O12 207.5(4), Mg1-O13 207.3(3), Mg1-O14 210.6(3), C5-S1 172.6(3), C5-S2 171.6(3), C5-N1 131.4(4), S1-Pt1-S2' 75.60(3), S1-Pt1-S2' 104.41(3), S1-C5-S2 110.9(2).

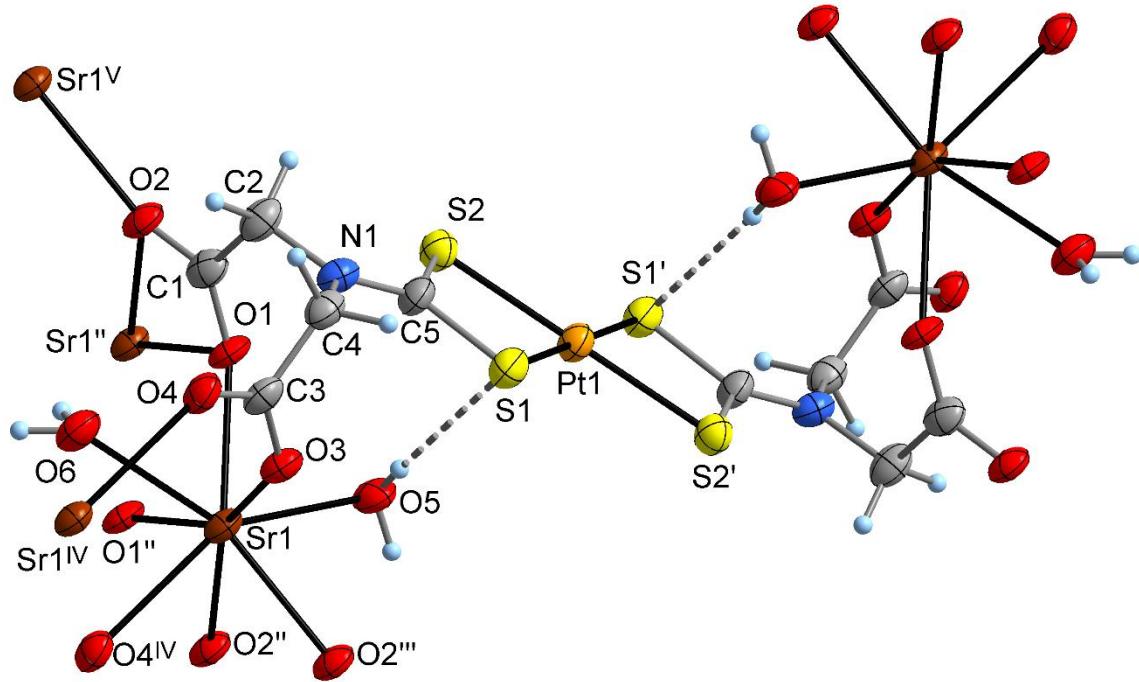


Figure S8. Molecular structure of $\text{Sr}_2[\text{Pt}(\text{L})_2] \cdot 4\text{H}_2\text{O}$ in the crystal, showing the atom numbering scheme. Displacement ellipsoids drawn at the 50% probability level. The Pt atom is situated on a crystallographic centre of inversion. Selected intermolecular distances (pm) and angles ($^\circ$): Pt1-S1 232.2(4), Pt1-S2 231.5(4), Sr1-O1 252(1), Sr1-O1'' 266(1), Sr1-O2'' 268(1), Sr1-O2''' 250(1), Sr1-O3 248(1), Sr1-O4^{IV} 263(1), Sr1-O5 261(1), Sr1-O6 257(1), C5-S1 172(2), C5-S2 172(2), C5-N1 135(2), S1-Pt1-S2 75.4(2), S1-Pt1-S2' 104.6(2), O1-Sr1-O1'' 75.9(4), O1-Sr1-O2'' 115.3(4), O1-Sr1-O2''' 139.6(4), O1-Sr1-O3 83.5(4), O1-Sr1-O4^{IV} 138.1(4), O1-Sr1-O5 70.7(4), O1-Sr1-O6 67.4(4), O1''-Sr1-O2'' 49.1(3), O1''-Sr1-O2''' 120.6(4), O1''-Sr1-O3 155.0(3), O1''-Sr1-O4^{IV} 85.0(4), O1''-Sr1-O5 86.7(4), O1''-Sr1-O6 81.3(4), O2''-Sr1-O2''' 71.5(4), O2''-Sr1-O3 155.8(3), O2''-Sr1-O4^{IV} 74.9(4), O2''-Sr1-O5 74.5(4), O2''-Sr1-O6 122.3(4), O2'''-Sr1-O3 84.3(4), O2'''-Sr1-O4^{IV} 82.1(4), O2'''-Sr1-O5 73.7(4), O2'''-Sr1-O6 145.5(4), O3-Sr1-O4^{IV} 101.7(4), O3-Sr1-O5 99.7(4), O3-Sr1-O6 77.9(4), O4^{IV}-Sr1-O5 145.7(4), O4^{IV}-Sr1-O6 73.1(4), O5-Sr1-O6 138.1(4), S1-C5-S2 111.0(9).

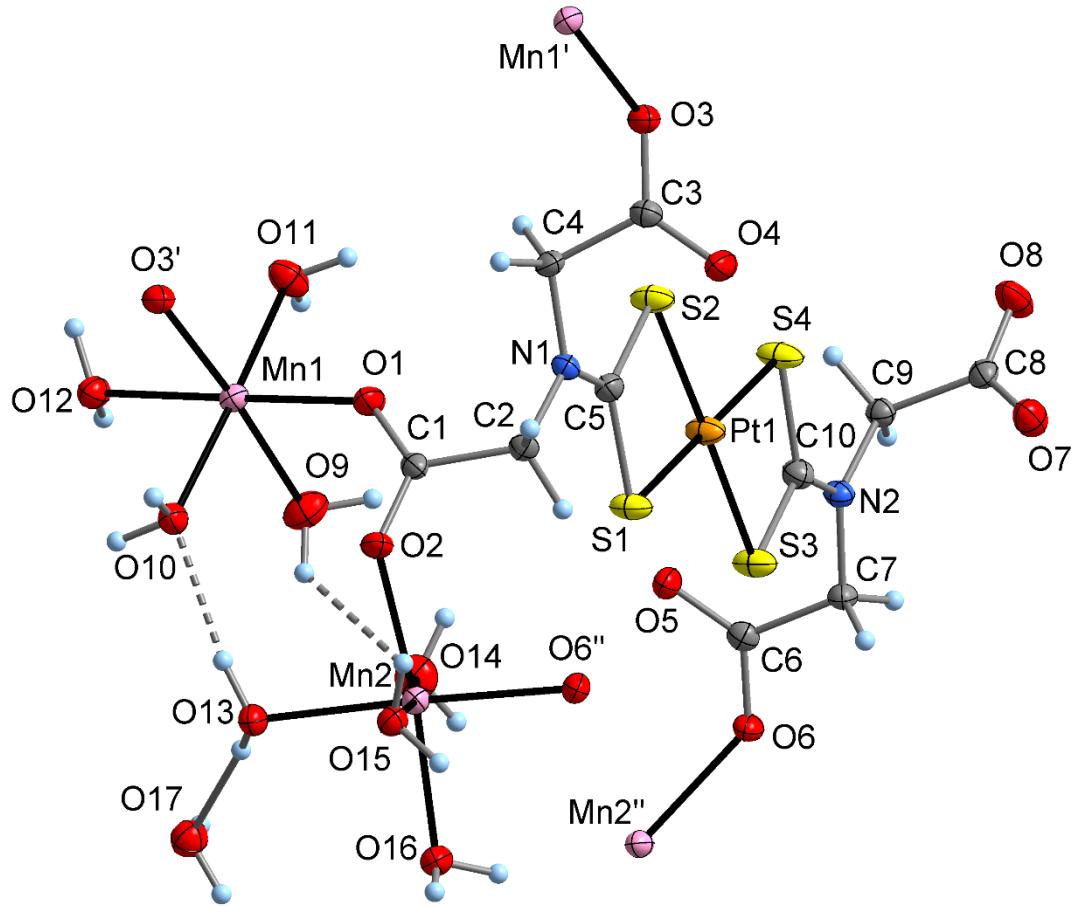


Figure S9. Molecular structure of hydrated $\text{Mn}_2[\text{Pt}(\text{L})_2]$ (**2-Mn**) in the crystal, showing the atom numbering scheme. Displacement ellipsoids drawn at the 50% probability level. Selected intermolecular distances (pm) and angles ($^\circ$): Pt1-S1 231.2(1), Pt1-S2 231.6(1), Pt1-S3 231.9(1), Pt1-S4 231.6(1), Mn1-O1 211.6(3), Mn1-O3' 215.1(3), Mn1-O9 224.9(3), Mn1-O10 214.8(3), Mn1-O11 217.1(3), Mn1-O12 222.7(3), Mn2-O2 214.7(2), Mn2-O6'' 217.1(2), Mn2-O13 220.1(2), Mn2-O14 216.1(3), Mn2-O15 216.5(3), Mn2-O16 217.2(3), C5-S1 172.2(4), C5-S2 172.2(4), C10-S3 172.5(4), C10-S4 172.5(4), C5-N1 131.1(5), C10-N2 130.9(5), S1-Pt1-S2 75.45(3), S1-Pt1-S3 104.47(3), S1-Pt1-S4 179.79(4), S2-Pt1-S3 178.73(4), S2-Pt1-S4 104.64(3), S3-Pt1-S4 75.44(3), O1-Mn1-O3' 94.7(1), O1-Mn1-O9 86.3(1), O1-Mn1-O10 91.4(1), O1-Mn1-O11 92.1(1), O1-Mn1-O12 178.4(1), O3'-Mn1-O9 175.8(1), O3'-Mn1-O10 86.6(1), O3'-Mn1-O11 94.7(1), O3'-Mn1-O12 86.2(1), O2-Mn2-O6'' 98.5(1), O2-Mn2-O13 83.6(1), O2-Mn2-O14 87.2(1), O2-Mn2-O15 89.8(1), O2-Mn2-O16 173.2(1), O6''-Mn2-O13 O6''-Mn2-O14 97.8(1), O6''-Mn2-O15 90.0(1), 177.5(1), O6''-Mn2-O16 88.2(1), S1-C5-S2 110.7(2), S3-C10-S4 110.5(2).

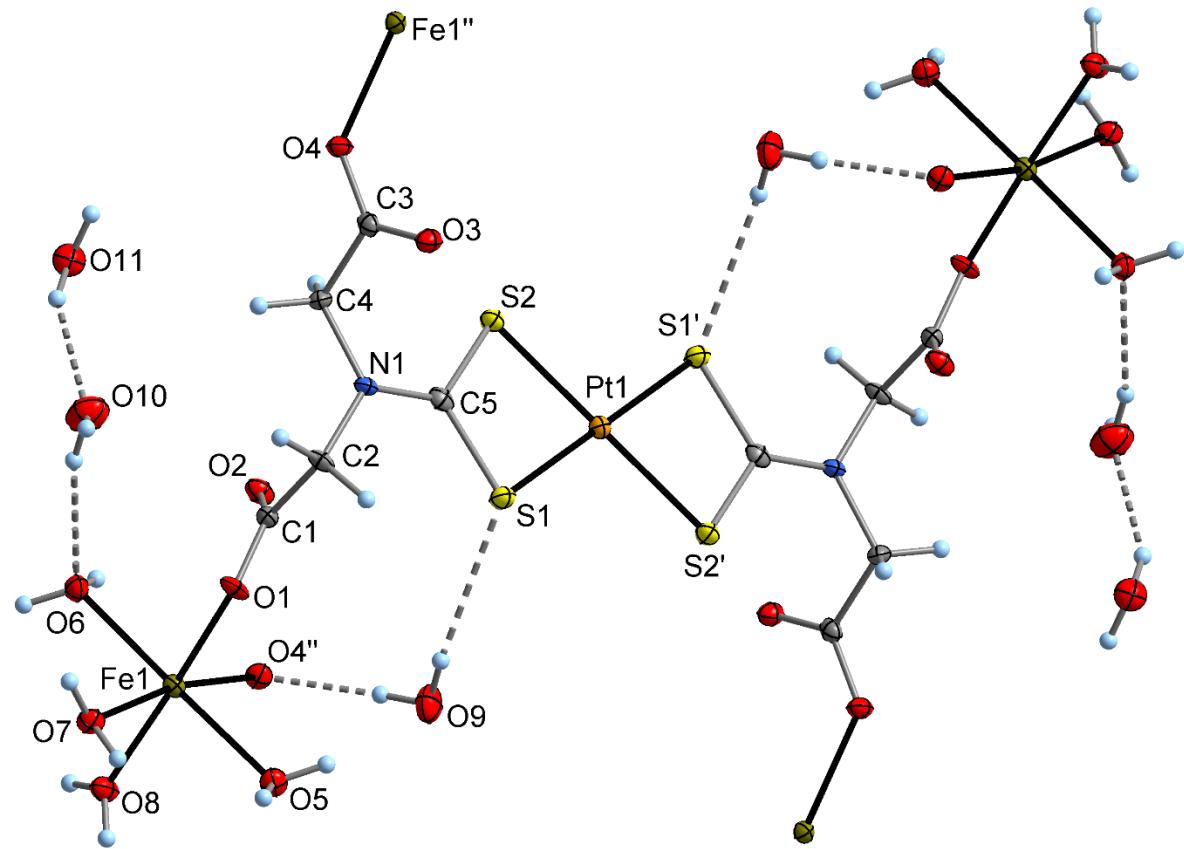


Figure S10. Molecular structure of $\text{Fe}_2[\text{Pt}(\text{L})_2]$ (**2-Fe**) · $14\text{H}_2\text{O}$ in the crystal, showing the atom numbering scheme. Displacement ellipsoids drawn at the 50% probability level. The Pt atom is situated on a crystallographic centre of inversion. Selected intermolecular distances (pm) and angles (°): Pt1-S1 231.9(1), Pt1-S2 230.8(1), Fe1-O1 205.7(3), Fe1-O4' 212.3(3), Fe1-O5 220.2(3), Fe1-O6 217.5(3), Fe1-O7 216.0(3), Fe1-O8 210.0(3), C5-S1 172.7(4), C5-S2 171.4(4), C5-N1 131.8(5), S1-Pt1-S2 75.36(3), S1-Pt1-S2' 104.64(3), O1-Fe1-O4' 97.6(1), O1-Fe1-O5 88.8(1), O1-Fe1-O6 89.7(1), O1-Fe1-O7 89.6(1), O1-Fe1-O8 173.8(1), O4'-Fe1-O5 85.2(1), O4'-Fe1-O6 95.5(1), O4'-Fe1-O7 169.8(1), O4'-Fe1-O8 88.5(1), S1-C5-S2 110.6(2).

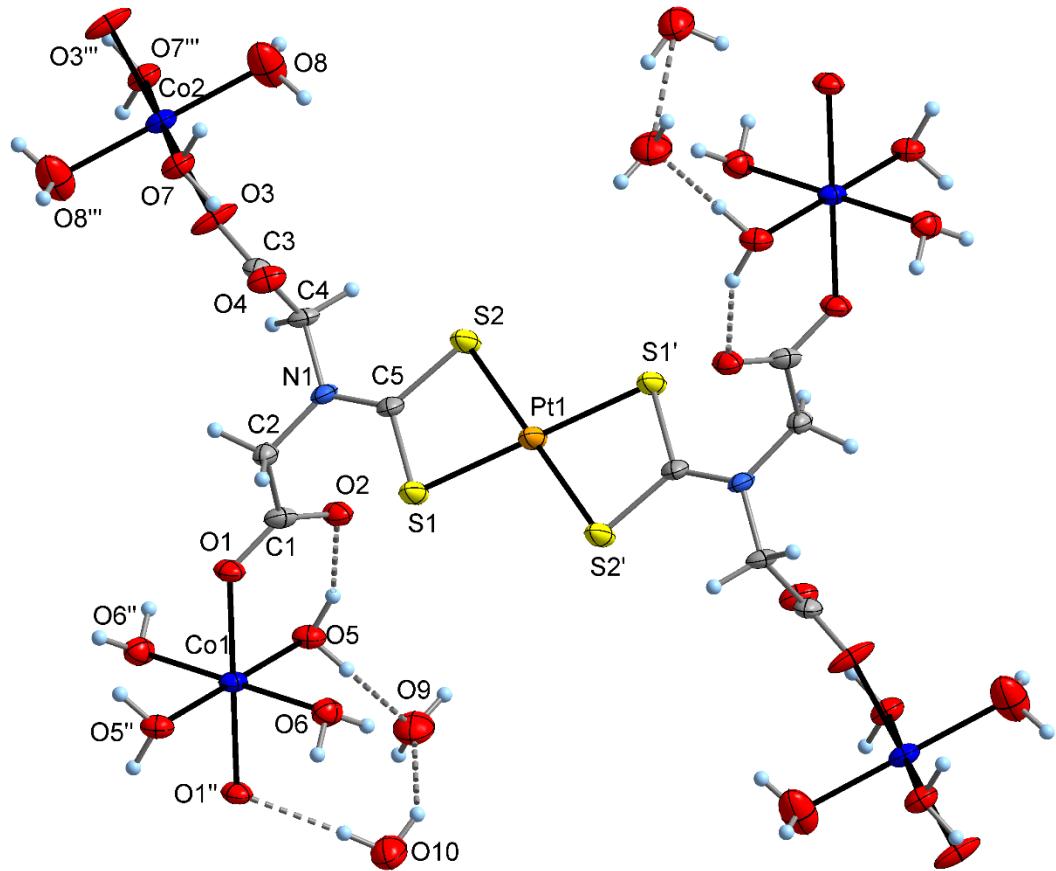


Figure S11. Molecular structure of hydrated $\text{Co}_2[\text{Pt}(\text{L})_2]$ (**2-Co**) in the crystal, showing the atom numbering scheme. Displacement ellipsoids drawn at the 50% probability level. The Co and Pt atoms are situated on crystallographic centres of inversion. Selected intermolecular distances (pm) and angles ($^\circ$): Pt1-S1 230.8(2), Pt1-S2 232.4(1), Co1-O1 209.3(4), Co1-O5 213.2(4), Co1-O6 206.8(4), Co2-O3 207.5(4), Co2-O7 210.9(4), Co2-O8 207.4(5), C5-S1 172.9(6), C5-S2 172.2(6), C5-N1 130.1(7), S1-Pt1-S2 75.60(5), S1-Pt1-S2' 104.40(5), O1-Co1-O5 88.1(2), O1-Co1-O5'' 91.9(2), O1-Co1-O6 91.7(2), O1-Co1-O6'' 88.3(2), O3-Co2-O7 89.9(2), O3-Co2-O7''' 90.1(2), O3-Co2-O8 90.9(2), O3-Co2-O8''' 89.1(2), S1-C5-S2 110.7(3).

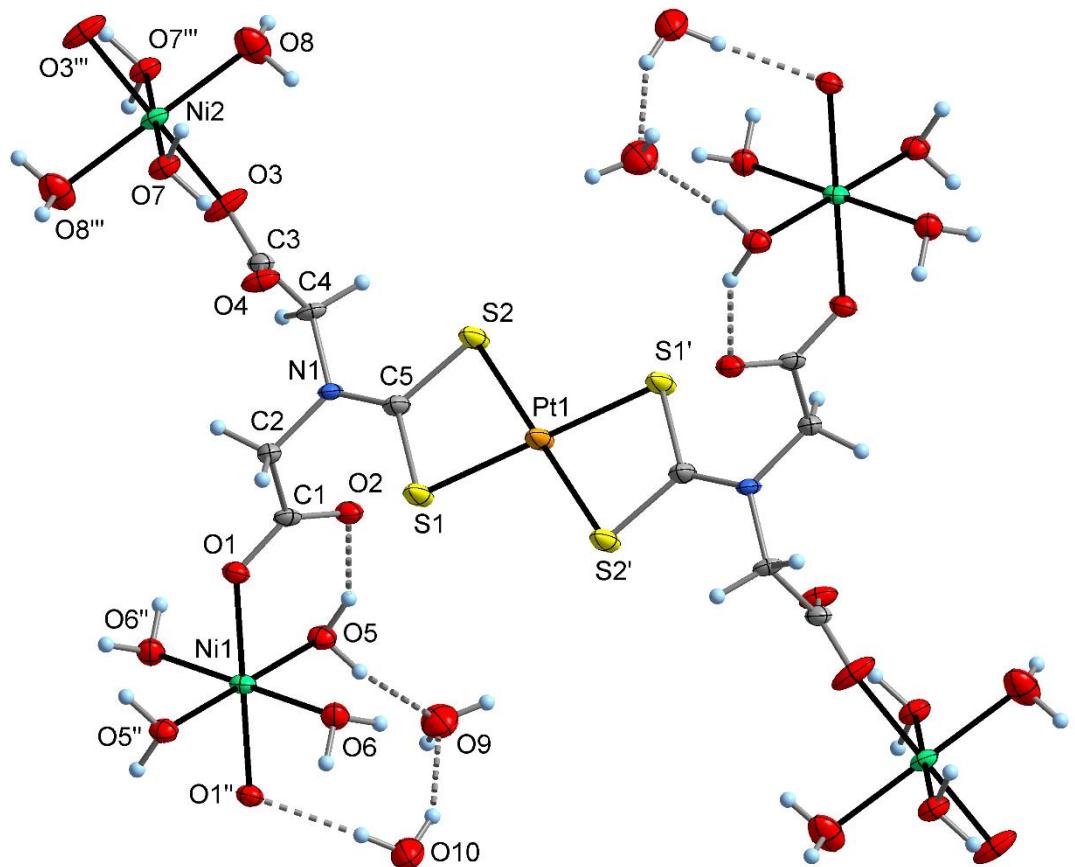


Figure S12. Molecular structure of $\text{Ni}_2[\text{Pt}(\text{L})_2]$ (**2-Ni**) · 12H₂O in the crystal, showing the atom numbering scheme. Displacement ellipsoids drawn at the 50% probability level. The Ni and Pt atoms are situated on crystallographic centres of inversion. Selected intermolecular distances (pm) and angles (°): Pt1-S1 230.99(9), Pt1-S2 232.03(8), Ni1-O1 206.6(2), Ni1-O5 206.6(2), Ni1-O6 205.3(2), Ni2-O3 203.0(2), Ni2-O7 204.9(2), Ni2-O8 207.3(3), C5-S1 172.1(3), C5-S2 173.0(3), C5-N1 130.6(4), S1-Pt1-S2 75.55(3), S1-Pt1-S2' 104.45(3), O1-Ni1-O5 89.0(1), O1-Ni1-O5'' 91.0(1), O1-Ni1-O6 91.0(1), O1-Ni1-O6'' 89.0(1), O3-Ni2-O7 91.5(1), O3-Ni1-O7''' 88.5(1), O3-Ni2-O8 91.6(1), O3-Ni2-O8''' 88.4(1), S1-C5-S2 110.6(2).

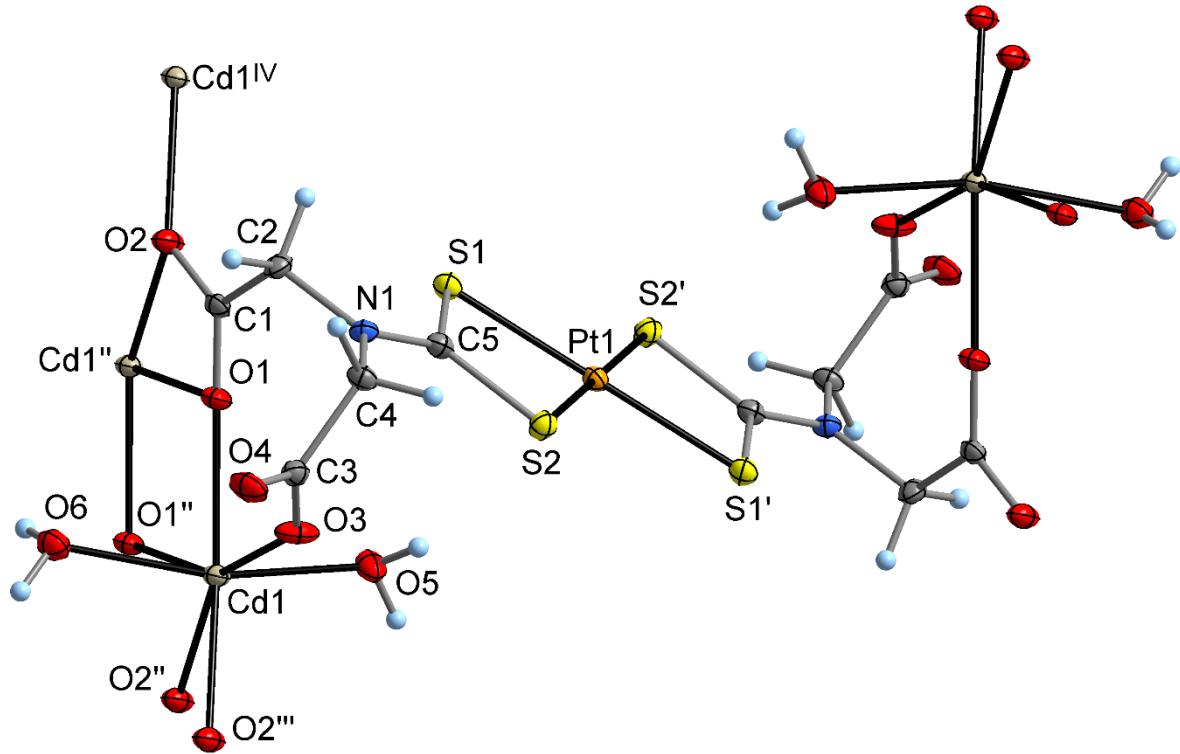


Figure S13. Molecular structure of $\text{Cd}_2[\text{Pt}(\text{L})_2]$ (**2-Cd**) · $4\text{H}_2\text{O}$ in the crystal, showing the atom numbering scheme. Displacement ellipsoids drawn at the 50% probability level. The Pt atom is situated on a crystallographic centre of inversion. Selected intermolecular distances (pm) and angles (°): Pt1-S1 231.41(6), Pt1-S2 232.18(6), Cd1-O1 236.1(2), Cd1-O1'' 248.0(2), Cd1-O2'' 246.5(2), Cd1-O2''' 231.1(2), Cd1-O3 222.8(2), Cd1-O5 227.1(2), Cd1-O6 227.1(2), C5-S1 172.1(2), C5-S2 172.7(2), C5-N1 131.5(3), S1-Pt1-S2 75.34(2), S1-Pt1-S2' 104.66(2), O1-Cd1-O1'' 71.54(7), O1-Cd1-O2'' 121.95(6), O1-Cd1-O2''' 168.41(7), O1-Cd1-O3 83.87(7), O1-Cd1-O5 82.38(7), O1-Cd1-O6 82.93(7), O1''-Cd1-O2'' 52.45(6), O1''-Cd1-O2''' 117.01(6), O1''-Cd1-O3 155.40(7), O1''-Cd1-O5 90.71(7), O1''-Cd1-O6 78.31(7), O2''-Cd1-O2''' 68.60(8), O2''-Cd1-O3 150.84(6), O2''-Cd1-O5 84.16(7), O2''-Cd1-O6 98.05(7), O2'''-Cd1-O3 87.27(7), O2'''-Cd1-O5 104.56(7), O2'''-Cd2-O6 91.05(7), O3-Cd1-O5 86.52(8), O3-Cd1-O6 98.52(8), S1-C5-S2 110.5(1).