Hydrogen bond nets in dithionate metal salt crystals

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Seven dithionate aqua complexes of the transition metal ions Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+} and Cd^{2+} were synthesized and their crystal structures determined, giving three coordination polymers – *catena*-poly-[*trans*-tetraaquamanganese-μ-dithionato-κ^2O,O'], $[Mn(H_2O)_4(S_2O_6)]$ **1**, *catena*-poly-[*trans*-tetraaquacopper-μ-dithionato-κ^2O,O'], $[Cu(H_2O)_4(S_2O_6)]$, **5** and *catena*-poly-[*trans*-tetraaquacadmium-μ-dithionato-κ^2O,O'], $[Cd(H_2O)_4(S_2O_6)]$ **7** – and four complex salts – hexaaquairon(2+) dithionate hydrate, $[Fe(H_2O)_6](S_2O_6)\cdot H_2O$ **2**, hexaaquacobalt(2+) dithionate, $[Co(H_2O)_6](S_2O_6)$ **3**, hexaaquanickel(2+) dithionate, $[Ni(H_2O)_6](S_2O_6)$ **4** and hexaaquazinc(2+) dithionate, $[Zn(H_2O)_6](S_2O_6)$ **6**, Figure 1. All crystallized in the triclinic space group $P\bar{1}$. Hirshfeld surface fingerprint plots[1–3] were used to map the interactions within the crystal structures. The structures were analyzed by Quantum Theory of Atoms in Molecules[4,5] to determine the bond critical points and to estimate the energy of the hydrogen bonds. The structural differences were rationalized using Pauling packing rules.[6]

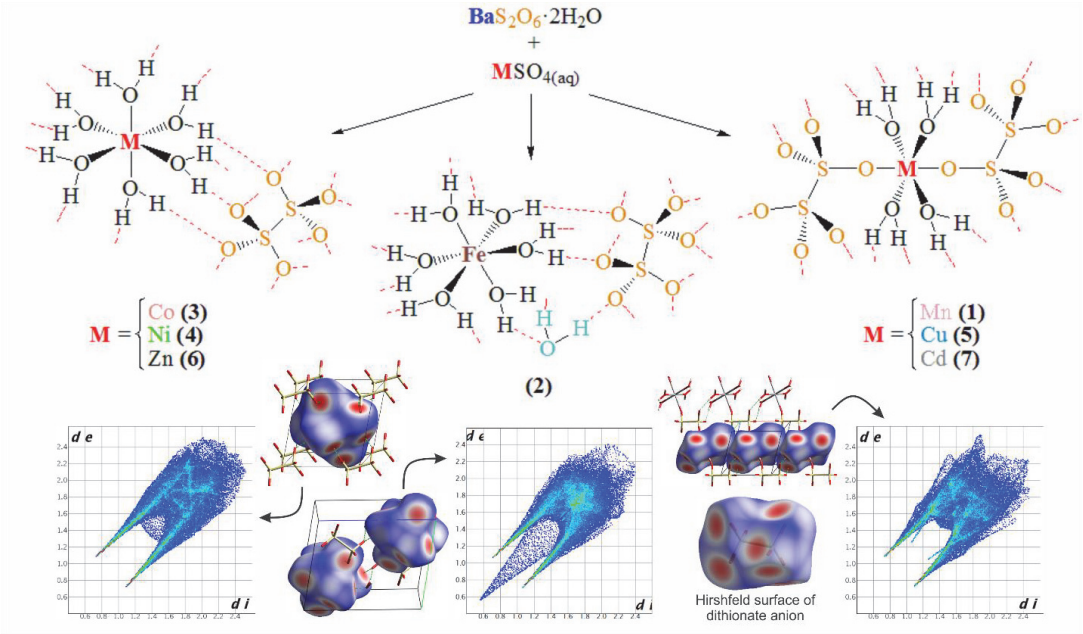

Figure 1. Synthetic scheme, Hirshfeld surfaces and fingerprint plots of complex salts and coordination polymers with the anion dithionate.

References

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