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Crystal Structures of $[M(H_2O)_6](BF_4)_2$, M = Mg, Mn, Fe, Co, Ni, and Zn. James A. Kaduk, Innovene USA LLC, P.O. Box 3011 MC F-9, Naperville IL 60566.

Although hexagonal lattice parameters have been reported for these compounds [1], their crystal structures have never been reported. The structure of a plausible analog, $Mg(ClO_4)_2(H_2O)_6$, has been reported in $Pmn2_1$ [2]. Isolation of the Fe species in a plant deposit prompted laboratory synthesis of the other compounds. The crystal structures of these hygroscopic compounds (which melt near room temperature) were refined using the Rietveld method.

The Fe compound was identified by indexing the powder pattern and using lattice matching techniques. The orthorhombic $[Mg(H_2O)_6](ClO_4)_2$ model yielded a successful refinement, but the displacement coefficients of one of the two independent tetrafluoroborate anions were larger than seemed reasonable, given the strong O-H≅≅≅F hydrogen bonds. This Afeature@ persisted in the refinements of the Mg, and Co structures, while the Mn and Zn structures seemed more chemically-reasonable. In the Ni structure, a second Ni site seemed to be populated. Grinding generated profile broadening characteristic of stacking faults in this compound. In an attempt to decide whether the true symmetry was orthorhombic or hexagonal, single crystals of the Mg and Ni compounds were grown. The Mg compound is orthorhombic, but the Ni compounds seems to be truly hexagonal. Quantum chemical calculations have been used to derive accurate hydrogen positions and to quantify the strengths of the hydrogen bonds.

[1] K. C. Moss, D. R. Russell, and D. W. A. Sharp, *Acta Cryst.*, 14, 330-330 (1961).
[2] C. D. West, *Zeit. Krist.*, 88, 480-493 (1935).