

## Poster Presentation

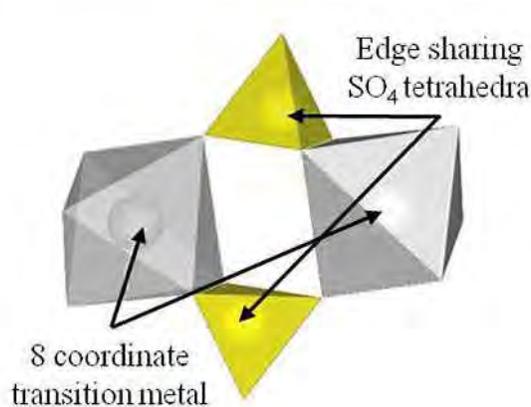
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Structures of 2 new sulfates,  $\text{Na}_2\text{M}(\text{SO}_4)_2$  ( $M=\text{Co}, \text{Ni}$ ), with rare  $\text{SO}_4^{2-}$  coordination

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In this study the structures of two new sulfates,  $\text{Na}_2\text{M}(\text{SO}_4)_2$  ( $M=\text{Co}, \text{Ni}$ ), were determined via both single crystal diffraction and neutron and laboratory X-ray diffraction data. The structural analysis was initiated with single crystal diffraction of the cobalt analogue and while this elucidated the cation positions the oxygen positions were still elusive. Therefore, combined Rietveld refinements of laboratory and neutron powder diffraction data was performed employing both hard constraints and soft restraints. The 5 K neutron data of both compounds are isostructural with the room temperature data as shown by Rietveld refinements. Refinements show that the transition metal ions are in a pseudo octahedral coordination that is better represented by a trigonal bipyramid, where one of the ligands is an edge of a  $\text{SO}_4^{2-}$  tetrahedra. This rare coordination of sulfate tetrahedra was corroborated by spectroscopic techniques: UV-vis, Raman, and infrared. Additionally these compounds adopt large unit cells within the space group  $C2/c$ :  $\text{Na}_2\text{Co}(\text{SO}_4)_2$  vol=4137.17(1) $\text{\AA}^3$  and  $\text{Na}_2\text{Ni}(\text{SO}_4)_2$  vol=4080.17(5)  $\text{\AA}^3$ .



**Keywords:** Sulfate, Structure solution, Powder diffraction