

Charge density study of K₂SO₄ diffraction data from ChemMatCARS, APS

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ABSTRACT

Single crystal synchrotron diffraction data on K₂SO₄ have been collected at the ChemMatCARS beamline (15-ID-B) at the Advanced Photon Source at Argonne National Laboratory. Preliminary studies show that the quality of the data is very high with an internal R-value of 4.52 % and an overall completeness of 99.4 % with $\sin\theta/\lambda$ from 0.46 to 1.25 Å⁻¹ and only two missing reflections in the low order data. Using a high energy, high intensity and very monochromatic beam from a synchrotron source makes it possible to carry out very accurate diffraction experiments on micron sized crystals (~30 μm) with absorption and extinction practically eliminated. Thus, K₂SO₄ diffraction data are used to illustrate that high quality single crystal diffraction data suitable for charge density studies can be obtained at the ChemMatCARS beamline. Here we present the charge density of K₂SO₄ modeled by the multipole formalism^[1] using the program package XD^[2].

[1] Hansen N. K.; Coppens, P.; Acta Cryst. A, 1978, 34, 909-921.

[2] Program XD2006; Volkov, A.; Macchi, P.; Farrugia, L. J.; Gatti, C.; Mallinson, P.; Richter, T.; Koritsanszky, T. (2006)

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