The copper sulfate hydration cycle. Crystal structures of $CuSO_4$ (Chalcocyanite), $CuSO_4 \cdot H_2O$ (Poitevinite), $CuSO_4 \cdot 3H_2O$ (Bonattite) and $CuSO_4 \cdot 5H_2O$ (Chalcanthite) at low temperature using non-spherical atomic scattering factors†

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Electronic Crystal Structure Models

Contents

Eight Mercury CSD .mrxy (binary format) electronic structure model files are provided, corresponding to the models presented in Figs. 1-5 of the paper. *Aspects of the appearance will depend on the current settings of your Mercury software, such as the Atom radii and Bond thickness, Atom colours and Label size. Whether or not H atoms are shown as displacement ellipsoids will depend on the Ellipsoid Settings… within the Display/Styles menu.*

Mercury CSD is available free of charge to the educational and research communities by the Cambridge Crystallographic Data Centre and can be downloaded from https://www.ccdc.cam.ac.uk/support-and-resources/downloads/. Mercury is of course able to read the CIF files directly, but for inorganic solids such as the copper(II) sulfates it takes some effort and advanced knowledge of the software to build the kinds of models displayed in our paper. These binary .mryx files preserve the models as built up by the authors. *This data is provided free, but explicitly without warranty or liability. Users of our provided models are responsible to learn the basics of the Mercury CSD software, which is well supported on the CCDC websites.*

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