Poster

Solving ambiguities: redetermining the crystal structures of rare Ag(II) compound using 3DED

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Typically for crystals of small size (<1000 μm^3), powdered X-ray diffraction (PXRD) is a useful alternative to the single-crystal X-ray diffraction (SCXRD) technique. Nevertheless, single-crystal diffraction experiments remain preferable for obtaining highly detailed and accurate crystal structures. Over the past two decades, rapid progress has been made in 3D electron diffraction (3DED) and it has become a viable tool for single-crystal measurements of submicron-size crystals, which are not large enough for SCXRD [1]. In this presentation, we will reexamine the crystal structures of two rare examples of silver(II) compounds: $AgSO_4$ and $KAgF_3$. These Ag(II) compounds have exciting potential in the development of next-generation electronics due to their strong antiferromagnetic 1D interactions making them direct analogs of the 1D Cu2+ systems. Growing sizeable crystals of both of these compounds is a challenge, thus, in the literature, their crystal structures were experimentally determined only via PXRD, although, the results present some uncertainty. $AgSO_4$ was first determined to be a *P*-1 space group based on PXRD data [2], which was later revised to *C*2/*c* [3], while DFT calculations predicted $I4_1/a$ space group [4]. $KAgF_3$, on the other hand, was reported to crystallize in the *Pnma* space group below 230 K transitioning to *Pcma* above this temperature [5]. However, our recent synchrotron PXRD results contradict the literature, hinting at a potentially higher transition temperature. With the help of 3DED characterization, we set out to conclusively address these ambiguities and accurately redetermine their crystal structures.

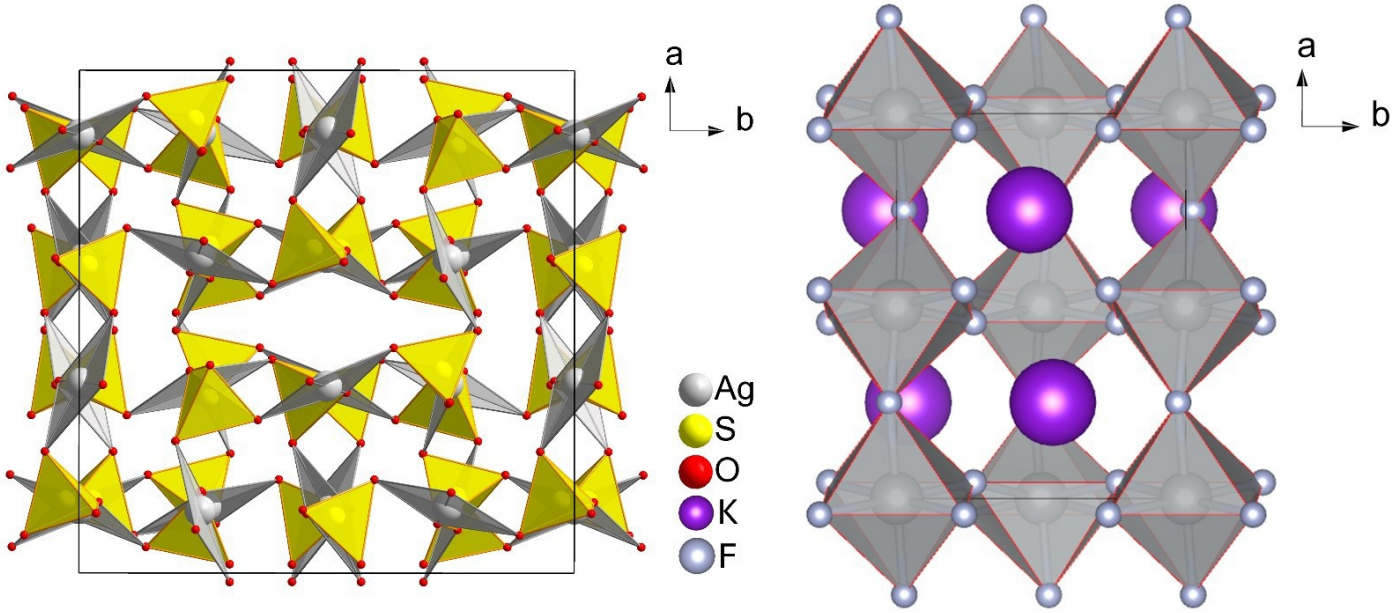

Figure 1. Crystal structure of α-$AgSO_4$ (left) and *Pnma* $KAgF_3$ (right) determined by 3DED

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