

Keywords: copper stereochemistry, copper topology, bond valence

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The response of frameworks to *P* and *T*: Of tilts and tetrahedra in feldspars. Ross Angel^a, Lindsay Sochalski-Kolbus^a, Mario Tribaudino^b, Fabrizio Nestola^c, Andrew Walker^d. ^a*Crystallography Lab, Virginia Tech, Blacksburg, USA.* ^b*Scienze della Terra, Università di Parma, Italy.* ^c*Geosciences, University of Padua, Italy.* ^d*Earth Sciences, University College London, UK.*

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The complex and often non-linear structural response of framework structures to changes in pressure, temperature, and especially composition (e.g. the plateau effect), is due to the delicate balance of forces between the framework components of strongly-bonded polyhedra and the interactions between the framework and extra-framework species. For example, we have previously shown [1] that whether the tilts of the octahedra in perovskites increase or decrease with increasing pressure depends on the relative strength of the bonding between the framework and the extra-framework cation compared to the strength of the cation-oxygen bonds within the octahedra.

Feldspars are far more structurally complex than perovskites and have previously resisted the challenge of quantifying their behaviour in this way. However, Megaw (1974) showed [2] that the rigid-unit deformations of the tetrahedral framework of feldspars can be decomposed in to four tilts of the four tetrahedra that comprise the 4-rings that lie parallel to (010). Of these four tilts Megaw showed that only two, an outward tilt of the T2 tetrahedra and a wrinkle of the 4-ring, change significantly between different alkali feldspars. Analysis of the high-pressure and high-temperature data now available, from both experiment and DFT calculations, confirms that these are the dominant tilt mechanisms. In particular, we have found that changes in the wrinkle tilt are responsible for changes in the length of the feldspar crankshaft, and are thus responsible for 70% of the volume change of alkali feldspars with *P*, *T*, or composition.

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Keywords: high-pressure mineralogy, feldspars, high-pressure structures

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A Whole New Family of Perovskite Based Structures. Joke Hadermann^a, Artem Abakumov^{a,b}, G. Van Tendeloo^a, E.V. Antipov^b. ^a*Electron Microscopy for Materials Science, University of Antwerp, Belgium.* ^b*Inorganic Chemistry Department, Moscow State University, Russia.*

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A family of new complex oxides has been discovered, with structures that are perovskite based, but unlike any known perovskite based structure. [1 - 6] The family is created by

introducing periodic crystallographic shear planes, which was previously considered as impossible in perovskites because of the presence of the A cations (in contrast to ReO₃ type structures with vacant A positions). However, when using A cations with a lone electron pair, crystallographic shear planes can effectively be established, slicing the perovskite structure into blocks separated by a periodic interfaces. Along these interfaces the corner-sharing of the metal-oxygen polyhedra is replaced by edge-sharing and tunnels are created, where the A cations and their lone pairs reside. The structures demonstrate enormous flexibility with respect to variations of the cation and oxygen content due to the controllable variable orientation of the shear planes. The common structural characteristics, variety of the chemical compositions and underlying driving forces will be explained.

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Mineralogical Adventures of a Powder

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Since the saga surrounding jadarite/kryptonite a few years ago [1], a number of weird, wonderful and often very rare minerals have found their way onto our newest powder diffractometer at NRC. Advances in both instrumentation and software for laboratory diffractometers make some older fine-grained minerals worth another look as well as new ones. Our CuK α capillary setup with a focussing primary mirror and PSD detector isn't suited to all mineral compositions but there are many that are amenable to this particular configuration. Three of the samples were from the Francon Quarry in Montreal, Quebec; strontiodresserite [2], montroyalite and a fluorine-modified gibbsite. Data have also been collected from some Australian minerals, including angastonite [3], stichtite [4], woodallite, and widgiemoolthalite. Although stichtite and woodallite were available in significant quantities, many of these minerals were only available in very small samples and are still very challenging even for capillary geometry. Data were successfully collected from all of the samples, and analyses attempted to extract any new structural information. In one case this was a full *ab-initio* crystal

structure solution as seen in Figure 1 using charge-flipping and simulated annealing, with post-refinement DFT analysis to locate hydrogen atoms. For some samples unit cell parameters were all that could be extracted. These examples show that many long-ignored fine-grained minerals may be worth another look with a combination of modern diffractometer optics, detectors and software. A full crystal structure solution will not be possible in all cases but new information can often be found to add to the sum of mineralogical knowledge.

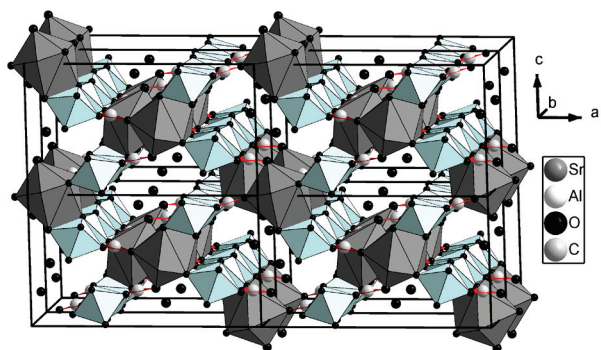


Figure 1. Crystal structure of strontiodresserite

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Keywords: minerals characterization, powder indexing, structure from powder diffraction