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Structural investigation of the disordered $\text{Cu}_{3-x}\text{SbO}_{5.5+y}$ ternary oxide

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Many different electrolytes with perovskite and fluorite-type structures have been extensively explored and characterised. Minimal focus has been given to potential Bixbyite-type electrolytes. A ternary copper antimony oxide previously referred to as $\text{Cu}_9\text{Sb}_4\text{O}_{19}$ with an unresolved crystal structure looked like a promising candidate to study. This was synthesised using classic solid state techniques under high temperature and oxygen pressure. Refinement of lab X-ray diffraction data strongly indicated that this material was isostructural with Cu_3TeO_6 with a curiously large degree of oxygen vacancies. Refinement of neutron diffraction patterns revealed the system was much more complicated than first anticipated, confirming the under occupancy of oxygen and revealing the mixed occupation of $\text{Cu}^{2+}/\text{Sb}^{5+}$ sites in the cationic sub-lattice. The final composition can be refined to $\text{Cu}_{3-x}\text{SbO}_{5.5+3x/2}$. X-ray absorption experiments confirmed the local coordination significantly differs from Cu_3TeO_6 complementing the diffraction data. This is an interesting material in a good position for many potential applications like; oxygen membranes, sensors or as a cathode/electrolyte material warranting further investigation.

Topic

Chemistry

Primary authors: SPASOVSKI, Martin (University of Auckland); SÖHNEL, Tilo (The University of Auckland)

Presenter: SPASOVSKI, Martin (University of Auckland)

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