The Pan African Conference on Crystallography (PCCR2)
and
The African Light Source Conference (AfLS2)

Contribution ID: **198** Type: **Oral Presentations**

Crystal structure of a silver-, cobalt- and iron-based phosphate with an alluaudite-like structure: Ag 1.655 Co 1.64 Fe 1.36 (PO 4) 3

Thursday, 31 January 2019 11:15 (15 minutes)

The new silver-, cobalt- and iron-based phosphate, silver cobalt iron tris(orthophosphate), Ag 1.655 Co 1.64 Fe 1.36 (PO 4) 3 , was synthesized by solid-state reactions. Its structure is isotypic to that of Na 2 Co 2 Fe(PO 4) 3 , and belongs to the alluaudite family, with a partial cationic disorder, the Ag I atoms being located on an inversion centre and twofold rotation axis sites (Wyckoff positions 4a and 4e), with partial occupancies of 0.885 (2) and 0.7688 (19), respectively. One of the two P atoms in the asymmetric unit completely fills one 4e site while the Co and Fe atoms fill another 4e site, with partial occupancies of 0.86 (5) and 0.14 (5), respectively. The remaining Co 2+ and Fe 3+ cations are distributed on a general position, 8f, in a 0.39 (4):0.61 (4) ratio. All O atoms and the other P atoms are in general positions. The structure is built up from zigzag chains of edge-sharing [MO6] (M = Fe/Co) octahedra stacked parallel to [101]. These chains are linked together through PO 4 tetrahedra, forming polyhedral sheets perpendicular to [010]. The resulting framework displays two types of channels running along [001], in which the Ag I atoms (coordination number eight) are located as in show figure 1.

Primary author: BOURAIMA, Adam (Mohammed V University, Chemistry department, Rabat, Morocco)

Presenter: BOURAIMA, Adam (Mohammed V University, Chemistry department, Rabat, Morocco)

Session Classification: PCCr2

Track Classification: PCCr2