MS14-P37 | Crystal structure of $CaBaFe_4O_7$

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Magnetic materials that transport information via magnetic excitations are promising candidates for spintronics applications. Such materials are often chemically complex and difficult to synthesise. Such materials should be ferro- or ferri-magnetic with a high Curie temperature and have a large charge gap to minimize particle-hole excitations along with long magnon lifetimes and mean-free paths. Swedenborgite, CaBaFe4O7 has been identified as a possible new candidate being a ferrimagnet with a polar space group. It displays two magnetic transitions at 210K and 275K and a structural phase transition at around 350K to a hitherto unknown phase. The resulting crystal structure in the high-temperature phase has now been solved from X-ray and neutron single crystal diffraction at 400K and verified against high-resolution neutron powder diffraction data. Similar to the room-temperature phase in that it consists of alternating layers of triangular and Kagome Fe-O tetrahedra. The compound is found to retain its polar character in the high-temperature phase and shows a rather complex modulation of the Fe-O tetrahedra. A bond-valence analysis indicates mixed Fe+2/Fe+3 [1].

[1] R. S. Perry, H. Kurebayashi, A. Gibbs, and M. J. Gutmann, Phys. Rev. Materials 2, 054403 (2018).