Veblenite: a new Ti-silicate related to Hoh structures
Fernando Camara, Elena Sokolova, Frank C. Hawthorne, Ralph Rowe, Joel Grice, and Kim Tait
E-mail: fernando.camaraaartigas@unito.it

Veblenite, ideally KNaFe2TiO8[Mn,Mo]8(Si,Al)4O22(OH)6, triclinic, P 1, a 5.376(3), b 27.506(2), c 18.697(2) Å, α 140.301(3), β 93.033(3), γ 95.664(3). V 1720.96(14) Å3, has no natural or synthetic analogues. It is a new mineral occurring at Ten Mile Lake, Seal Lake area, Labrador, Newfoundland, Canada, as red brown single laths and fibres included in feldspar. In the crystal structure of veblenite, M octahedra share common edges to form a wavy octahedral sheet parallel to (001). SiO4 tetrahedra share corners to form SiO4 groups and SiO22− and TiO86− groups. This is the first occurrence of an eight-membered Si-O ribbon in a mineral crystal structure. The Nb-dominant D octahedra, SiO4 groups and SiO22− and TiO86− groups share common vertices to form a heteropolyhedral (H) sheet. Two H sheets and an O sheet constitute an HOH block. Along [001], HOH blocks connect via common vertices of D octahedra and cations at the A(1).2 and B interstitial sites. In the intermediate space between two adjacent HOH blocks, two [100] channels of different size can be identified. A narrow channel of the width of an SiO4 group contains the A(1) site mainly occupied by K. A large channel has the width of four SiO4 groups (SiO22− and TiO86− groups) and contains A(2) sites partly occupied by K and H2O groups.

The crystal structure of veblenite is related to several HOH structures where the O sheet is ideally composed of Fe2+ oxahedra, such as jinsanjhangeite [1], niobophyllite [2] (astrophyllite group) and nafertitiite [3]. Veblenite differs from those structures in the topology and chemistry of the H sheet. In jinsanjhangeite, the H sheet consists of (Si,Al)4O8 groups and Ti-dominant octahedra. In niobophyllite, the H sheet is composed of (Si,Al)4O8 astrophyllite ribbons [a double ribbon of (Si,Al)4O8 groups] and Nb-dominant octahedra. In nafertitiite, the H sheet is composed of (Si,Al)4O8 ribbons [a triple ribbon of (Si,Al)4O8 groups] and Ti-dominant octahedra. In veblenite, the H sheet is composed of (Si,Al)4O8 groups (as in jinsanjhangeite), (Si,Al)4O8 ribbons [a new type of a quadruple ribbon of (Si,Al)4O8 groups which can be built of two astrophyllite ribbons] and Nb-dominant octahedra. The above reported setting is obtained from the reduced cell a 5.376(3), b 17.7419(10), c 18.6972(11) Å, α 97.991(1), β 93.033(2), γ 95.664(3). V 1720.96(14) Å3.

Keywords: layered, polyanion, surfactant

Intercalated transition-metal dichalcogenides at different temperatures
SK Imran Ali, Sander van Smaalen, Steffen Zoebisch, Bernd Harbrecht
Department of Crystallography, University of Bayreuth (Germany).
Department of Chemistry, Philips University, Marburg (Germany).
E-mail: sk.imran@uni-bayreuth.de

Transition metal dichalcogenides (MX2, M=transition metal and X=chalcogen) are of considerable interest due to layer-type structural properties. The transition metal has trigonal prismatic or octahedral coordination by six chalcogen atoms which is further connected to neighbouring coordination spheres to form a layered structure. Interaction between atoms within a slab are mainly covalent. Slab to slab interaction are weak, and in general are of the type of van der Waals interaction. Due to this weak interlayer interaction several different slab stacking sequences (crystal polytype) are possible. Intercalation compounds of transition metal dichalcogenides can be formed with a wide range of guest atoms or molecules including alkali metals and transition metals. The intercalated guest atom may be incorporated on octahedral or tetrahedral sites surrounded by chalcogen atoms in the van der Waals gaps. Intercalation of Cu atom in 6R-CuM,S2 shows...