The crystal structure of blödite under extreme conditions and its implications to planetary mineralogy

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An exceptionally large and pure crystal of blödite, $Na_2Mg(SO_4)_2(H_2O)_4$, with a high degree of perfection from the mineral collection of the Natural History Museum in Copenhagen gave us possibility to study the crystal structure of this mineral under various pressures and temperatures. The measurements were performed on the laboratory diffractometers as well as at the ESRF synchrotron facility and ILL neutron diffraction instrument in Grenoble.

Blödite is monoclinic, $P2_1/a$, Z = 2, $a = 11.115(9)$, $b = 8.242(2)$, $c = 5.538(1)$ Å, $\beta = 100.82(4)^\circ$ (at room conditions).

At high pressure up to 11 GPa no phase transition is observed. The density increases by 20%. The compressibility is anisotropic with $\beta_a : \beta_b : \beta_c = 0.72{:}0.94{:}1$. Na coordination polyhedron is the most compressible, whereas the SO_4 coordination tetrahedron remains practically incompressible in this pressure range. The increased strength of H-$O_{acceptor}$ bonding with pressure with concomitant strengthening of the Metal-O_{water} bonding is observed.

Neutron diffraction down to 20 K shows accurate positions of the hydrogens, and the two water molecules with different strengths of hydrogen bonds.

Blödite shows an isotropic expansion with temperature with volume increase of only 1% up to the point of dehydration. It dehydrates in two steps, at 110° C and 225° C. During the first dehydration it transforms to löweite ($Na_{12}Mg_7(SO_4)_{13}(H_2O)_{15}$). At the second dehydration step, löweite disintegrates to α-$Na_2Mg_2(SO_4)_3$ with still unknown crystal structure and vanthoffite ($Na_6Mg(SO_4)_4$). α-$Na_2Mg_2(SO_4)_3$ transforms at 590° C to β-$Na_2Mg_2(SO_4)_3$ with the crystal structure of the langbeinite type.

Blödite is an important mineral phase on the surfaces of water saturated planets. On the Earth it is found in evaporites from sulphate lakes. On surfaces of Jupiter moons Ganymede and Europa it is expected to be constituent of the icy surface material, and due to its increased stability under pressure it is expected also to play an important role in the under-surface composition of these planets. Our investigation defines its relations to the other hydrous and anhydrous Na-Mg sulphates and helps understanding the genetic cycles of complex sulphates from the volcanic to the lacustrine environments.