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# The high-pressure behavior of bloedite: A synchrotron single-crystal X-ray diffraction study

**Paola Comodi[1,*], Sabrina Nazzareni[1], Tonci Balić-Žunić [2], Azzurra Zucchini[1] and Michael Hanfland[3]**

[1]Dipartimento di Scienze della Terra, Piazza Università, 06100 Perugia, Italy
[2]Natural History Museum, University of Copenhagen, Øster Voldgade 5-7, 1350 Copenhagen K, Denmark
[3]ESRF, 6 Rue Jules Horowitz, 38000 Grenoble, France

## Abstract

High-pressure single-crystal synchrotron X-ray diffraction was carried out on a single crystal of bloedite [$Na_2Mg(SO_4)_24H_2O$] compressed in a diamond-anvil cell. The volume-pressure data, collected up to 11.2 GPa, were fitted by a second- and a third-order Birch-Murnaghan equation of state (EOS), yielding $V_0$ = 495.6(7) Å$^3$ with $K_0$ = 39.9(6) GPa, and $V_0$ = 496.9(7) Å$^3$, with $K_0$ = 36(1) GPa and $K'$ = 5.1 (4) GPa$^{-1}$, respectively. The axial moduli were calculated using a Birch-Murnaghan EOS truncated at the second order, fixing $K'$ equal to 4, for *a* and *b* axes and a third-order Birch-Murnaghan EOS for *c* axis. The results were $a_0$ = 11.08(1) and $K_0$ = 56(3) GPa, $b_0$ = 8.20(2) and $K_0$ = 43(3) GPa, and $c_0$ = 5.528(5), $K_0$ = 40(2) GPa, $K'$ = 1.7(3) GPa$^{-1}$. The values of the compressibility for *a*, *b*, and *c* axes are $\beta_a$ = 0.0060(3) GPa$^{-1}$, $\beta_b$ = 0.0078(5) GPa$^{-1}$, $\beta_c$ = 0.0083(4) GPa$^{-1}$ with an anisotropic ratio of $\beta_a$:$\beta_b$:$\beta_c$ = 0.72:0.94:1. The evolution of crystal lattice and geometrical parameters indicates no phase transition up to 11 GPa. Sulfate polyhedra are incompressible, whereas the Mg polyhedral bulk modulus is 95 GPa. The sodium polyhedron is the softest part of the whole structure with a bulk modulus of 41 GPa. Pressure decreases significantly the distortion of Na coordination. Up to 10 GPa, the donor-acceptor oxygen distances decrease significantly and the difference between the two water molecules decreases with an increase in the strengths of hydrogen bonds. At the same time, the bond lengths from Na and Mg to O atoms of the water molecules decrease faster than other bonds to these cations suggesting that there is a coupling between the Na-Ow and Mg-Ow bond strengths and the "hydrogen transfer" to acceptor O atoms.

**Keywords:** Bloedite, high pressure, single-crystal X-ray diffraction, equation of state