ON THE TRUE SPACE-GROUP SYMMETRY OF NORSETHITE, BaMg(CO$_3$)$_2$

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The crystal structure of norsethite was solved by LIPPMANN (1968) (X-ray powder data, synthetic material) in space group $R32$. EFFENBERGER & ZEMANN (1985) discussed three structure models based on single-crystal two-circle diffractometer data: ordered models in space group (1) $R\overline{3}m$ (most appropriate), and (2) $R32$; (3) split oxygen position model in $R\overline{3}m$.

A re-investigation (NONIUS four-circle diffractometer, CCD detector) was performed at 100, 150, 200, 250 and 273 K. The crystal structure is characterized by layers parallel to (001) of alternating Ba$^{[12]}$O$_{12}$ and Mg$^{[6]}$O$_6$ polyhedra with the CO$_3$ groups in between. With decreasing temperature the cell parameters a and c as well as their ratio c/a decrease. At low temperature the structure refinements according model (1) exhibit minor shortenings of the Ba–O and Ca–O bond lengths (C–O varies insignificantly only) going along with reduced displacements of the Ba, Mg and C atoms; the decrease of the anisotropy is significant for the Ba and Mg atoms only. More complex is the situation for the O atom: at room temperature a strong anisotropic displacement of the O atom with the maximal elongation in the [010] direction occurs. Whereas the equivalent isotropic displacement is proportional to the temperature, its anisotropy is inversely proportional. Successive refinements according to model (2) and (3) were performed.

Images taken with a STOE StadiVari diffractometer (Pilatus 300 K pixel-detector, Mo microfocus X-ray source) revealed a doubling of the lattice parameter c, however the number of detectable reflections did not allow a structure refinement.

EFFENBERGER, H., ZEMANN, J. (1985): Z. Kristallogr., 171, 275-280.
LIPPMANN, F. (1968): Tschermaks Min. Petr. Mitt., 12, 299-318.