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Structure and properties of diaspore, AlO(OH), up to 50 GPa from experiment and theory

A. Friedrich (1), E. Haussühl (1), D.J. Wilson (1), R. Boehler (2), W. Morgenroth (3), B. Winkler (1), E.A. Juarez-Arellano (1), K. Refson (4), V. Milman (5)

(1) Institut für Geowissenschaften, J.W. Goethe-Universität Frankfurt, Frankfurt am Main, Germany, (2) Max-Planck-Institut für Chemie, Mainz, Germany, (3) Department of Chemistry, Aarhus University, Denmark, (4) Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, U.K., (5) Accelrys Inc., Cambridge, U.K.

(friedrich@kristall.uni-frankfurt.de / Phone: +49-69-79822103)

High-pressure studies of minerals with hydrogen bonds of intermediate strength, like diaspore, are important for a deeper understanding of the potential of high pressure to induce or strengthen hydrogen bonds, and of the resultant change of the physical properties of these materials.

Single-crystal structure refinements showed that diaspore retains its structure up to at least 50 GPa at ambient temperature. The experimental results on the compression of diaspore are in excellent agreement with complementary DFT calculations. The structural compression is mainly due to the pressure-induced shortening of the hydrogen bond. The DFT calculations provide accurate information on the response of the hydrogen bond geometry and O-H stretching modes to compression. From the present results we infer that the hydrogen bond becomes significantly more symmetric with pressure up to 50 GPa. The stretching frequencies of the O-H bond decrease approximately linearly with increasing pressure, and therefore also with increasing O-H bond length and decreasing hydrogen bond length.

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