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High-pressure X-ray diffraction, Raman, and computational studies of $MgCl_2$ up to 1 Mbar: Extensive pressure stability of the β-$MgCl_2$ layered structure.[1] ELISSAIOS STAVROU, JOSEPH ZAUG, SORIN BASTEA, I-FENG KUO, JONATHAN CROWHURST, Lawrence Livermore National Laboratory, BORA KALKAN, MARTIN KUNZ, Advanced Light Source, Lawrence Berkeley Laboratory, ZUZANA KONOPKOVA, Deutsches Elektronen-Synchrotron (HASYLAB) — Magnesium chloride with the rhombohedral layered $CdCl_2$-type structure (α-$MgCl_2$) has been studied using x-ray diffraction and Raman spectroscopy up to 1 Mbar. The results reveal a second-order phase transition to a hexagonal layered CdI_2-type structure at 0.7 GPa. This phase transition affects the stacking of the Cl anions, resulting to a shorter *c*-axis. An anisotropic compression along *c*-axis was observed during initial compression; altered above 10 GPa due to the repulsion between adjacent Cl-layers. According to previous theoretical studies, a series of phase transitions towards, initially, the 3D rutile (6-fold Mg cations) at 17 GPa and to fluorite structure (8-fold Mg cations) at 70 GPa are proposed. According to our experimental study $MgCl_2$ remains in a 2D layered structure up to 1Mbar keeping the 6-fold coordination of Mg cations. This observation contradicts with the general structural behavior of compressed AB_2 compounds; we conducted *ab-initio* calculations to elucidate the mechanisms that extend the remarkable structural stability of $MgCl_2$.

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