High-pressure X-ray diffraction, Raman, and computational studies of MgCl$_2$ up to 1 Mbar: Extensive pressure stability of the $\beta$-MgCl$_2$ layered structure.\textsuperscript{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 ($\alpha$-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 \textit{ab-initio} calculations to elucidate the mechanisms that extend the remarkable structural stability of MgCl$_2$.

\textsuperscript{1}This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

Elissaios Stavrou
Lawrence Livermore National Laboratory

Date submitted: 30 Oct 2015

Electronic form version 1.4