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High-pressure and high-temperature polymorphism in the CaCO3 at pressures to 30 GPa

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We determined phase transitions in $CaCO_3$ at pressures up to 30 GPa and high-temperatures using *in situ* X-ray diffraction and synchrotron radiation. In additional to geological importance this investigation has crystal-chemical and fundamental aspect as in this region enigmatic phase transitions from aragonite to disordered calcite or other phases takes place. The degree of orientational disorder in calcite drastically grow in the narrow temperature range of 1200-1230 K (at 1 bar) producing fully disordered phase (by orientation of CO_3 triangles) (Ishizawa et al., 2013). Despite of such apparent significance, there is just a few works where this phase transition was investigated by X-ray diffraction at high pressures (Suito et al., 2001). The results are not unequivocal, because disordered calcite was determined by only common similarity of diffraction patterns, whereas unit cell parameters were not determined. By the same reason the compressibility of disordered calcite is also unknown. The lack of the experimental results is explained by grain growth and disordering phase transitions in $CaCO_3$ at temperatures close to the melting point and as a result difficulties in getting relatively high quality diffraction patterns with amount of peaks enough for unit cell parameters determination. In present experiments we observed transition of aragonite to presumably disordered calcite phase at 1 and 3 GPa and 1273-1473 K, however at 5 and 8 GPa and higher temperature we observed transition to new phase, which we tentatively named disordered aragonite. At 14 GPa we did not observe transition of aragonite in the experiment to 1900 K, however at 20 GPa and at 31 GPa transition from aragonite to new phase(s) was observed at 1773 and 1373 K, respectively. The structures of the new phases will be refined based on diffraction data and subsequent *ab initio* computations.

Keywords: high pressure, calcium carbonate, phase transition, aragonite, X-ray diffraction