Abstract Submitted
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Tetrahedrally bonded carbonates and aqueous carbonate anions under extreme conditions[1] DING PAN, GIULIA GALLI, Institute for Molecular Engineering, the University of Chicago, DEEP CARBON OBSERVATORY COLLABORATION — The carbonate ion, CO_3^{2-}, has a trigonal planar structure composed of carbon bonded with three oxygen atoms. The existence of tetrahedrally bonded carbonate units, CO_4, analogous to SiO_4 in silicates, has long been under debate. Using a combination of first-principles calculations and in situ infrared spectroscopy measurements [1], we provided definitive evidence that in magnesite, at pressures above 80 GPa, sp^2 bonded CO_3 trigonal groups transforms into sp^3 bonded CO_4 tetrahedral units. These units were found to be asymmetric, with two longer and two shorter C-O bonds. In addition, using first principles molecular dynamics we investigated carbonate anions in water at high temperature and pressure, corresponding to Earth's upper mantle conditions. We found significant quantities of bicarbonate ions dissolved in the liquid. The relevance of our simulation results for geophysical models of hydrous carbonates in the Earth will be discussed.

[1] Our work, Nat. Comm. 2014 (submitted).

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