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Experiments of CO_2 adsorption in zeolites and structural stability of carbonate phases at high-pressure and temperature conditions using synchrotron X-ray diffraction

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High-pressure and high-temperature techniques are used to strongly modify the atomic interactions of matter while in situ synchrotron X-ray diffraction characterizes the samples. This has enabled reliable experimental studies in a wide range of P-T conditions, like those presented here. Firstly, I will present the results of two CO_2-loaded pure-silica zeolites where the content of adsorbed CO_2 molecules and the location of these guest molecules in the porous frameworks were accurately determined. Subsequently, I will show experimental results that, combined with DFT calculations, accurately constrain the P-T phase diagrams of several naturally-occurring carbonate minerals in the 0-20 GPa pressure and 300-1000 K temperature ranges. In particular, the compressibility, thermal expansivity, the anisotropy and the evolution of the atomic environments was determined. Novel dense carbonate phases were found and fully characterized. These results offer new insights into the high-pressure high-temperature chemistry of carbon dioxide and carbonates, with implications in geophysics (deep carbon cycle) and the potential design of efficient CO_2 capture strategies.

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