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Formation and Manipulation of Water Nanostructures inside Zeolites. Yongjae Lee,^{*} Joseph A. Hriljac,[†] John B. Parise,[‡] Thomas Vogt,^{*} ^{*}Physics and Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, [†]Chemical Sciences, Univ. of Birmingham, Birmingham, B15 2TT, UK, [‡]Geosciences, State Univ. of New York, Stony Brook, NY 111794.

We have identified a nascent field of chemical crystallography, which merits a concentrated effort: the pressure and simultaneous temperature dependent chemistry of guest molecules in zeolitic nanochannels. Nanochannels occurring in zeolites have been recognized early on as miniature reactors, which drive chemical reactions due to their shape and site selectivity. Their built-in flexibility allows altering the chemical environment within the channels in response to applied hydrostatic pressure and temperature. In natrolite channels ($\text{Na}_{16}\text{Al}_{16}\text{Si}_{24}\text{O}_{80}\cdot 16\text{H}_2\text{O}$), two distinctively overhydrated states (“pressure-induced hydration”) are observed under pressure (24H₂O near 1GPa and 32H₂O above 1.2GPa), accompanied by anomalous volume swelling of the host zeolitic scaffolding (“pressure-induced expansion”). The resulting water nanostructures evolve with pressure and temperature. This high-pressure chemistry of zeolites demonstrates pressure is a unique method to synthesize, stabilize and manipulate certain zeolitic guest structures and also opens the way to a possible tuning of the nanochannel selectivity.