Supporting information for: Systematic Study of the Thermal Properties of Zeolitic Frameworks

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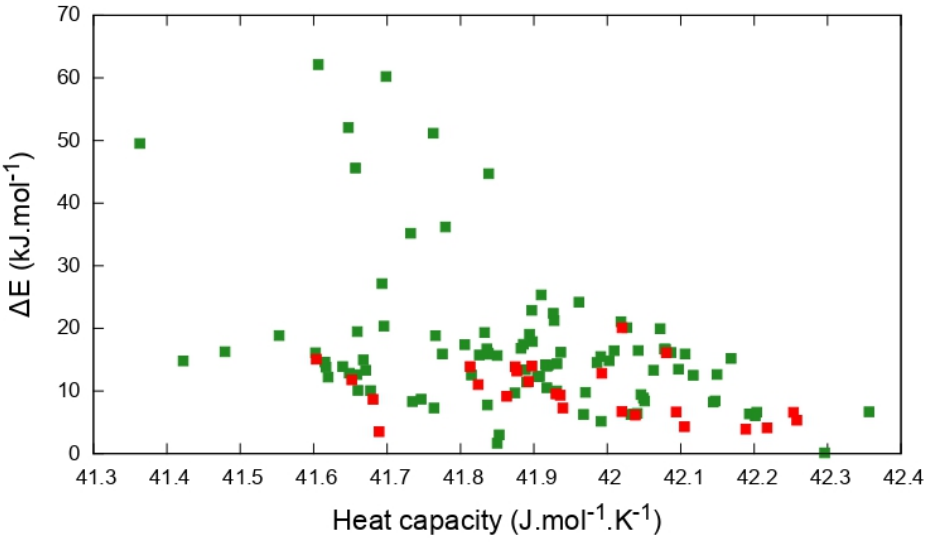

Figure S1: Relative energy with respect to α-quartz (ΔE per SiO_2 unit) plotted against the heat capacity, also normalised per SiO_2 unit. Heat capacity values are given at 300 K. Green squares correspond to theoretical structures and red ones correspond to experimentally synthesized structures.

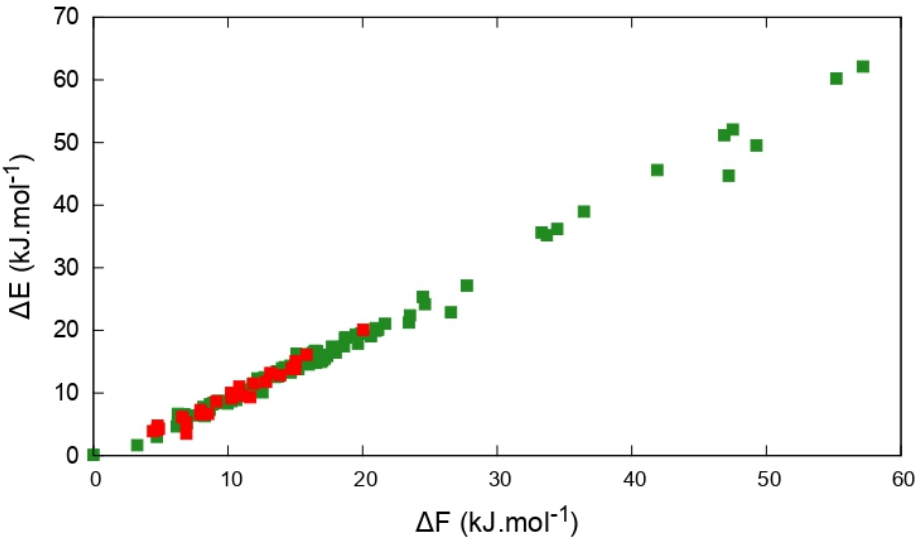

Figure S2: Relative energy with respect to α-quartz (ΔE per SiO_2 unit) plotted against the free energy, also normalised per SiO_2 unit. Free energy is given at 300 K. Green squares correspond to theoretical structures and red ones correspond to experimentally synthesized structures.

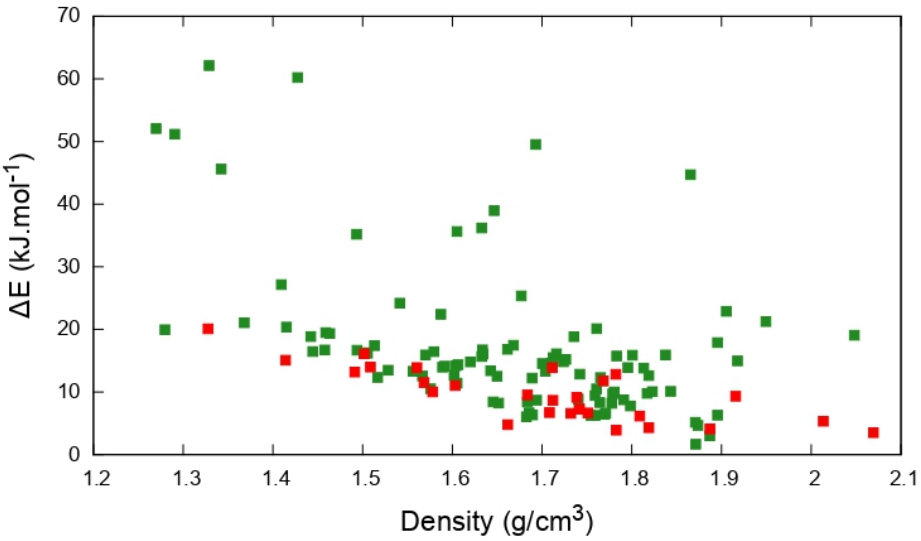

Figure S3: Relative energy with respect to α-quartz (ΔE per SiO_2 unit) plotted against the density. Green squares correspond to theoretical structures and red ones correspond to experimentally synthesized structures

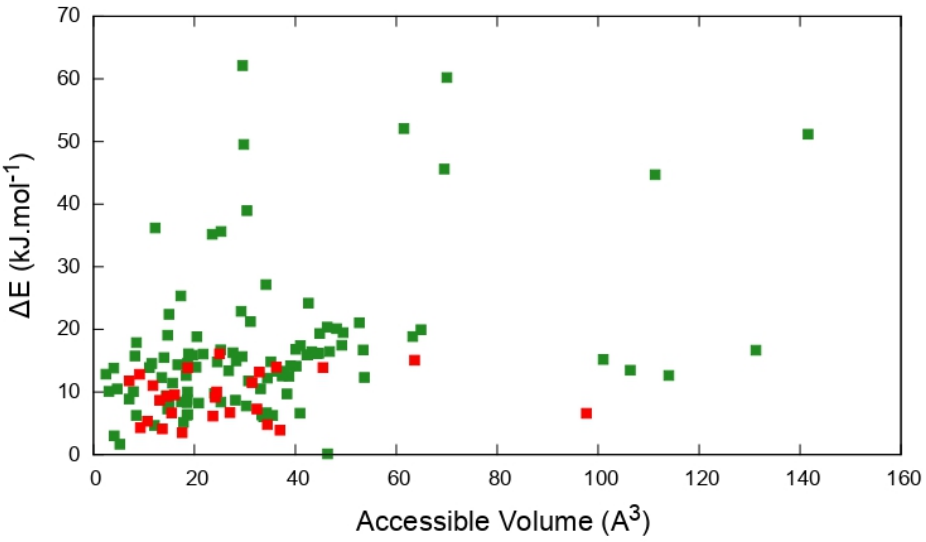

Figure S4: Relative energy with respect to α-quartz (ΔE per SiO_2 unit) plotted against the accessible volume, also normalised per SiO_2 unit. Green squares correspond to theoretical structures and red ones correspond to synthesized structures

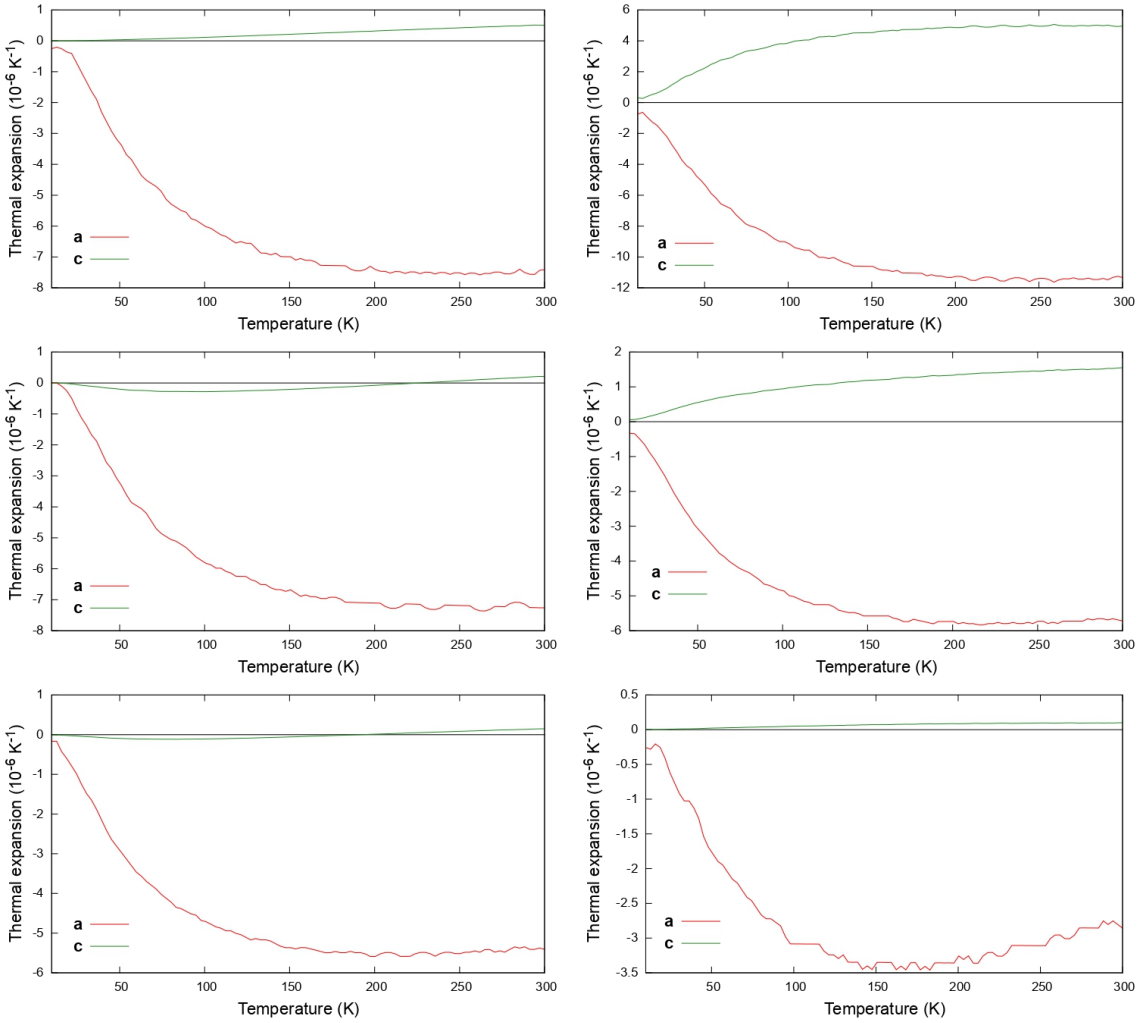

Figure S5: Evolution of the individual lattice parameters thermal expansion coefficients with respect to the temperature for respectively the AFV, AVL and SIV frameworks on the left side and the APC, PHI and UOZ frameworks on the right side.

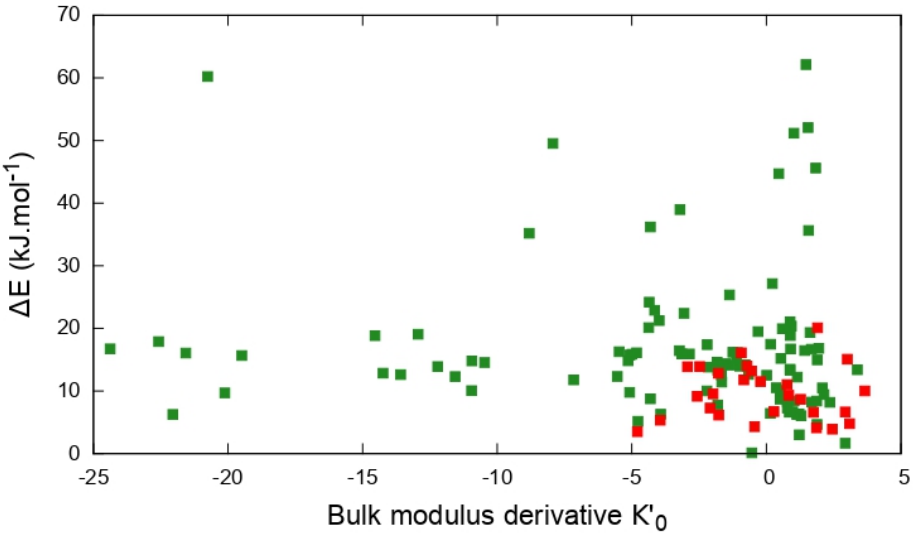

Figure S6: Energy relative to α-quartz (ΔE per SiO_2 unit) plotted against the pressure-derivative of the bulk modulus K_0' obtained through the Birch-Murnaghan EOS. Green squares correspond to theoretical structures and red ones correspond to synthesized structures.

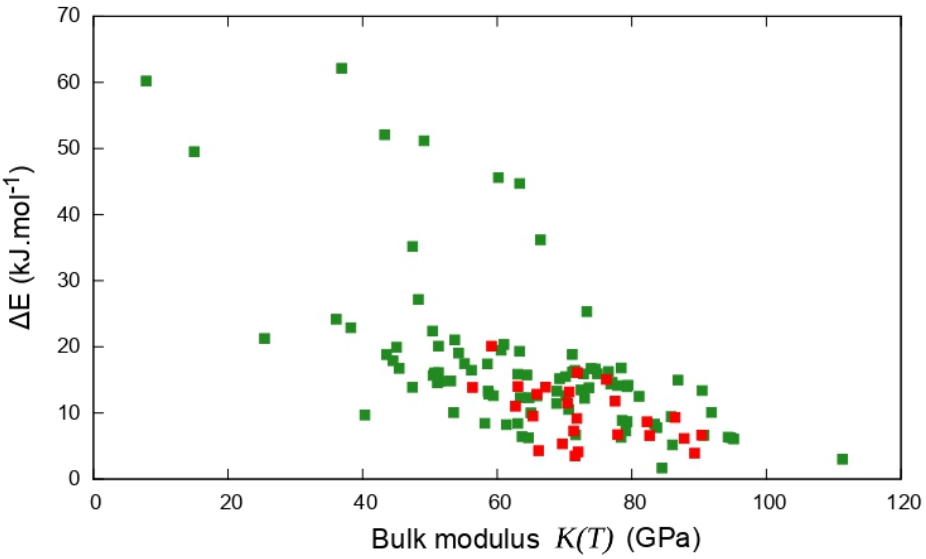

Figure S7: ΔE of SiO_2 unit with the α-quartz as reference compared to the temperature-dependent bulk modulus $K(T = 300\ \mathrm{K})$. Green squares correspond to theoretical structures and red ones correspond to synthesized structures.

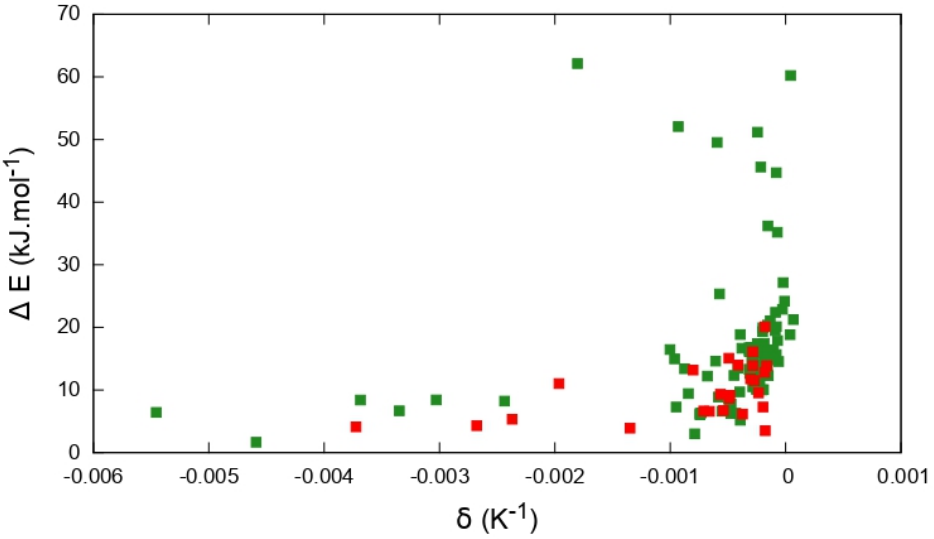

Figure S8: ΔE of SiO_2 unit with the α-quartz as reference compared to the temperature coefficient of elastic stiffness δ. Green squares correspond to theoretical structures and red ones correspond to synthesized structures.

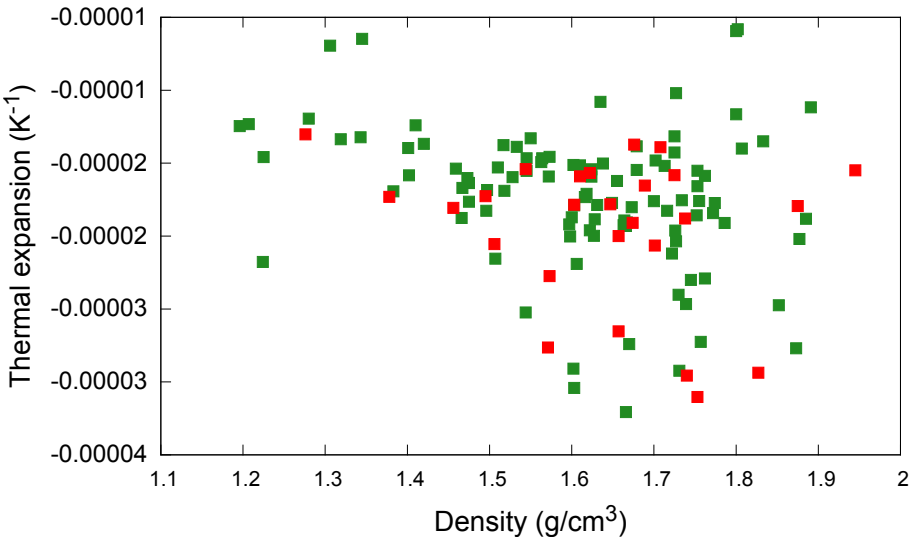

Figure S9: Thermal expansion coefficient plotted against the zeolitic framework density. Green squares correspond to theoretical structures and red ones correspond to synthesized structures.