Electronic Supplementary Material (ESI) for RSC Advances.

Reprobing the mechanism of negative thermal expansion in siliceous faujasite

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Supporting Information:

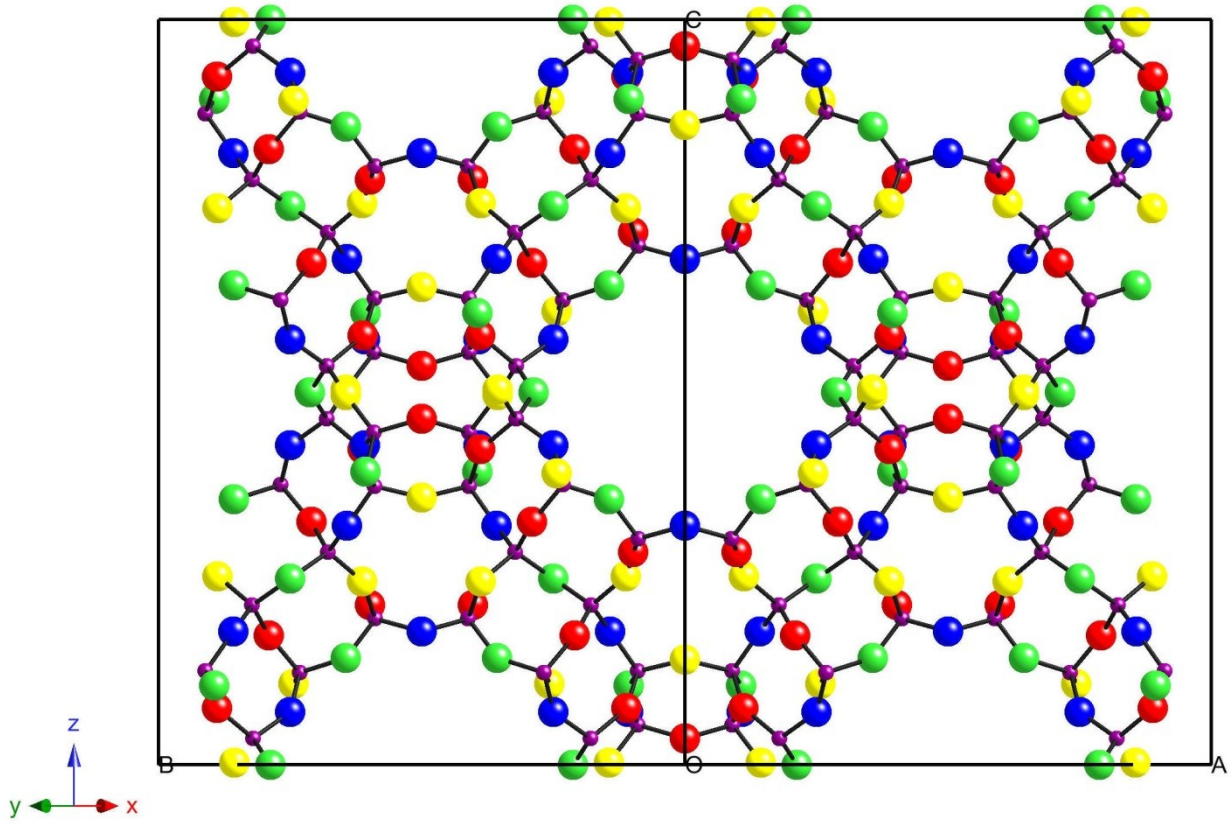
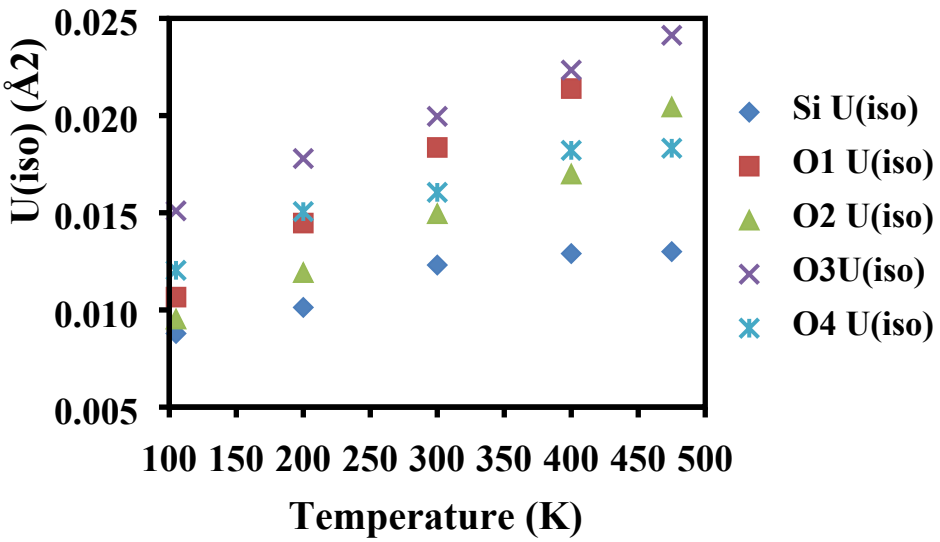


Fig. S1 The crystallographic structure of siliceous faujasite viewed along the <110> direction. Si, O1, O2, O3 and O4 atoms are coloured purple, green, yellow, red and blue respectively.

(a)



(b)

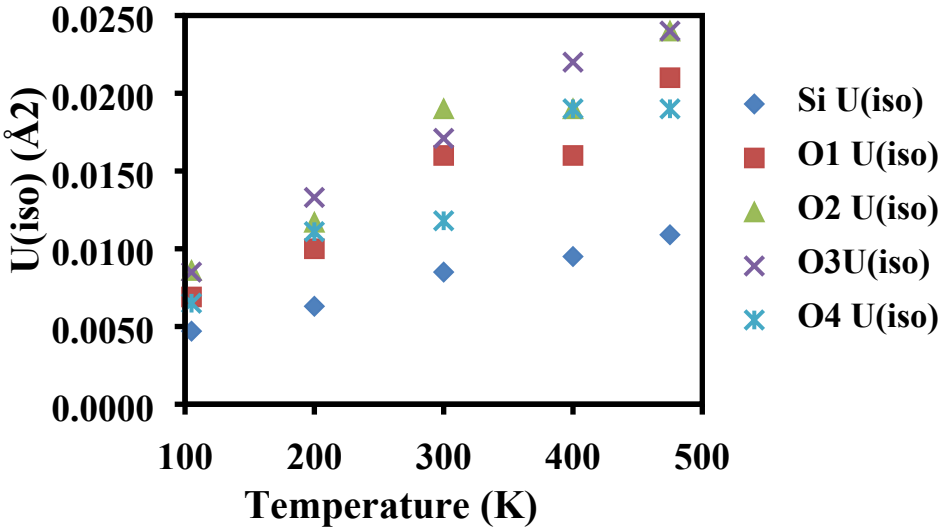


Fig. S2 The isotropic thermal displacement parameters for the constituent atoms of siliceous faujasite derived from the (a) real-space refinements and (b) Rietveld refinements as a function of temperature. The estimated standard deviations lie in the ranges 0.002 – 0.009 Å^2 and 0.0004 – 0.001 Å^2, for the data points in (a) and (b) respectively.

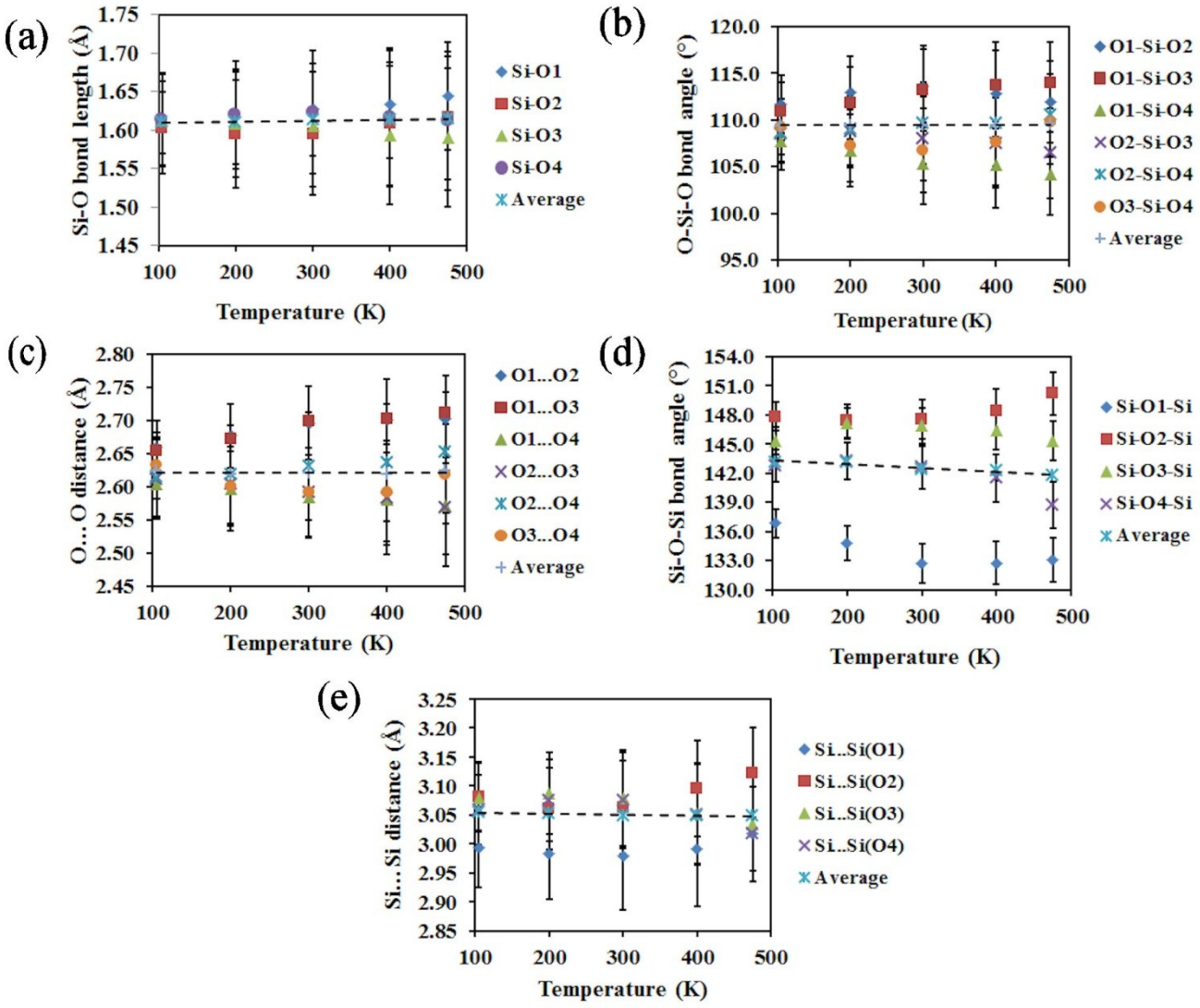


Fig. S3 The variation of various geometric parameters derived from the real-space refinements as a function of temperature for siliceous faujasite. Dashed lines indicate linear fits to the average parameters. The estimated uncertainties, calculated assuming unity uncertainties in G(r), lie in the ranges 0.04 – 0.09 Å, 3.0 – 4.8 °, 0.04 – 0.09 Å, 1.4 – 2.4 °, 0.06 – 0.09 Å for the data points in (a), (b), (c), (d) and (e) respectively.