Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supporting Information for

Assessing negative thermal expansion in mesoporous metal-organic frameworks by molecular simulation

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Table S1 Comparison of simulated lattice parameters to experimentally reported data

	a,b,c / Å	α,β,γ / °	Reference
DUT-6	30.245 (30.3)	90.0 (91.7)	[S1]
DUT-60	42.650 (42.3)	90.0 (87.6)	[S2]
MOF-210†	71.1, 50.9 (72.4, 52.3)	60, 110.9 (60.0, 111.2)	[S3]
DUT-49	46.588 (46.5)	90.0 (90.0)	[S4]
MOF-399	68.3112 (67.5)	90.0 (90.0)	[S5]
PCN-68	59.153 (60.2)	90.0 (90.0)	[S6]
NU-110	68.706 (70.4)	90.0 (90.0)	[S7]

†This cell was transformed from the primitive cell using the box flip routine in lammps

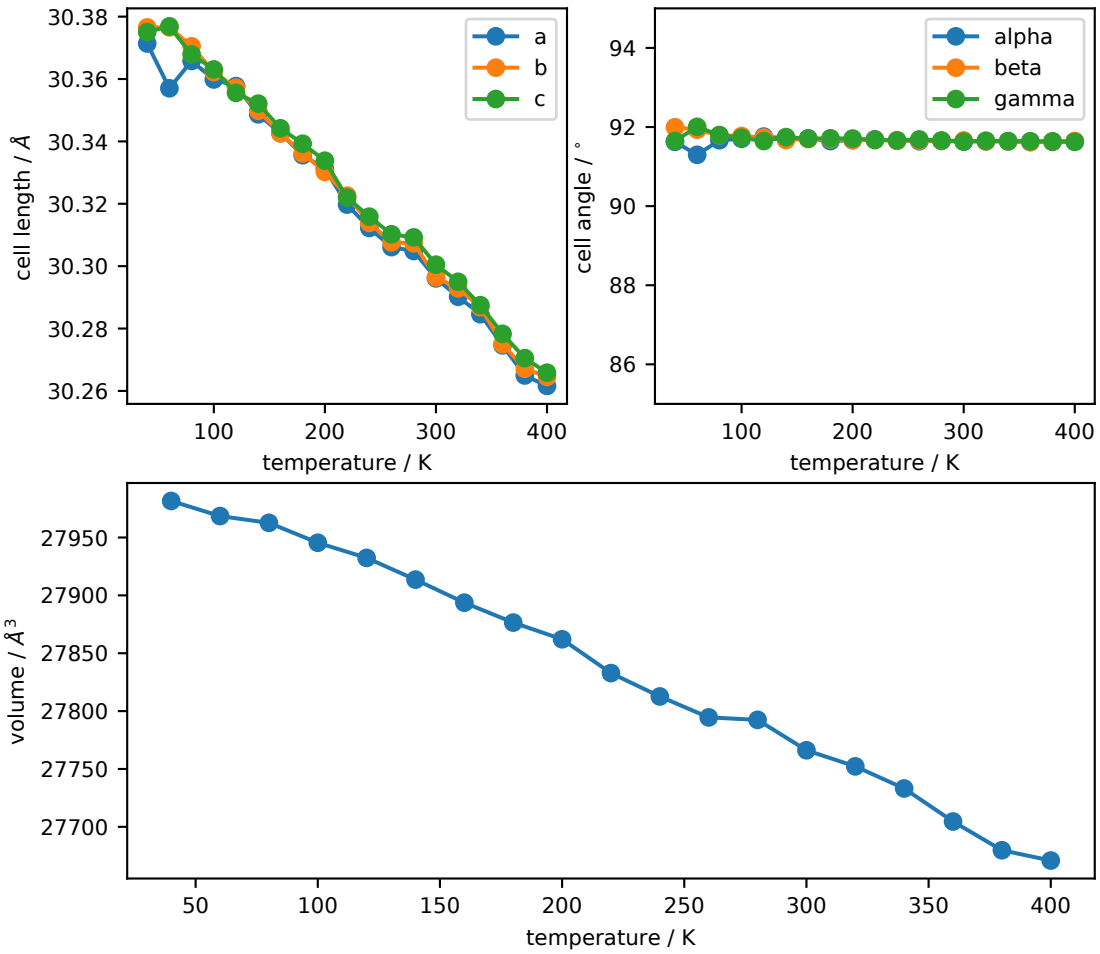

Fig. S1 Average cell parameters and volume of DUT-6 in response to increasing temperature.

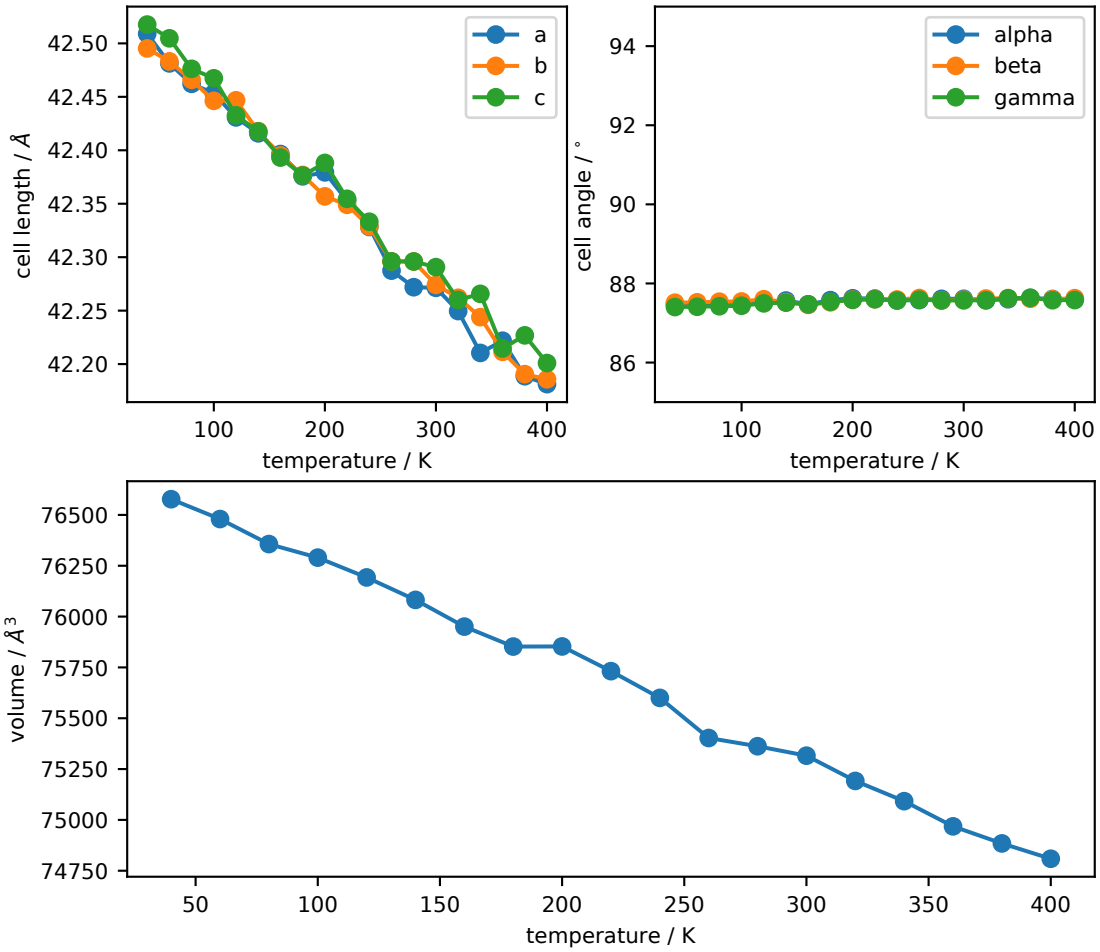

Fig. S2 Average cell parameters and volume of DUT-60 in response to increasing temperature.

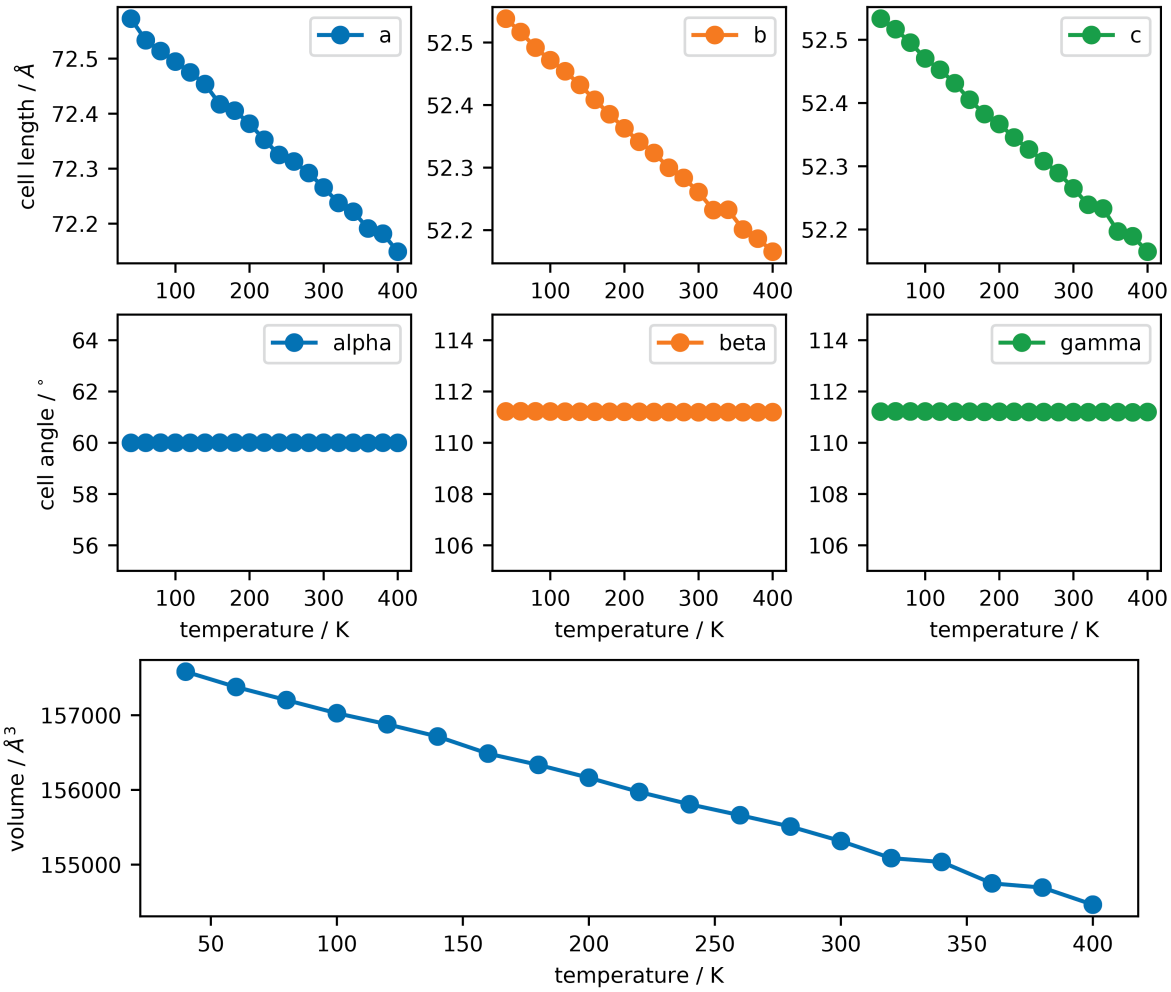

Fig. S3 Average cell parameters and volume of MOF-210 in response to increasing temperature.

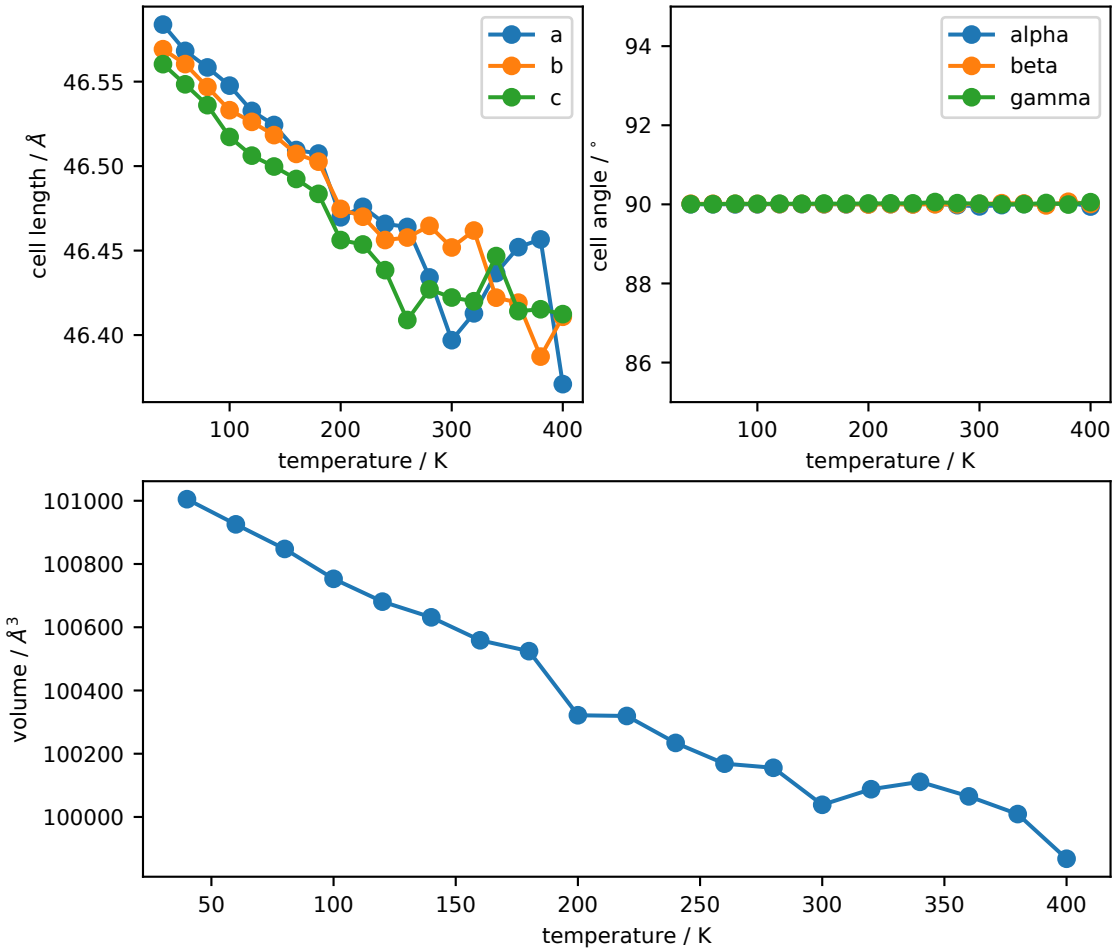

Fig. S4 Average cell parameters and volume of DUT-49 in response to increasing temperature.

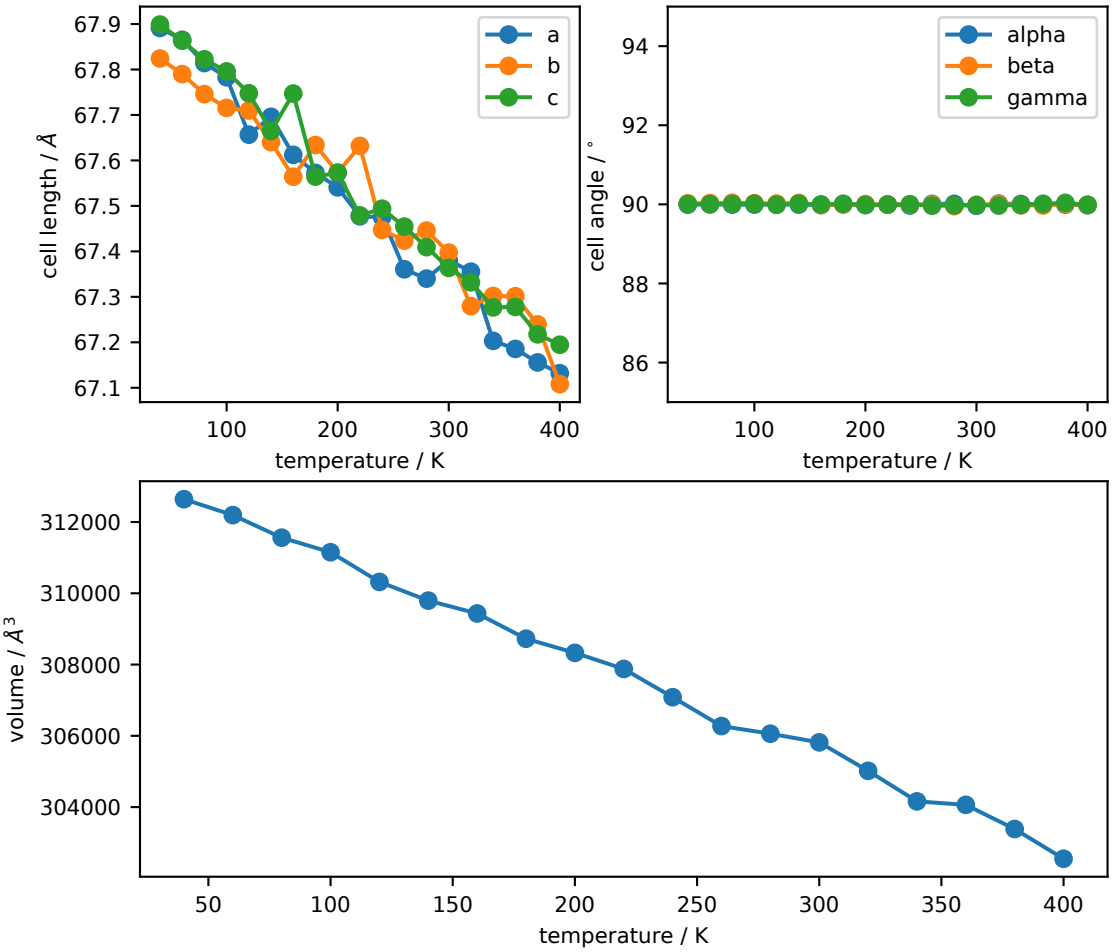

Fig. S5 Average cell parameters and volume of MOF-399 in response to increasing temperature.

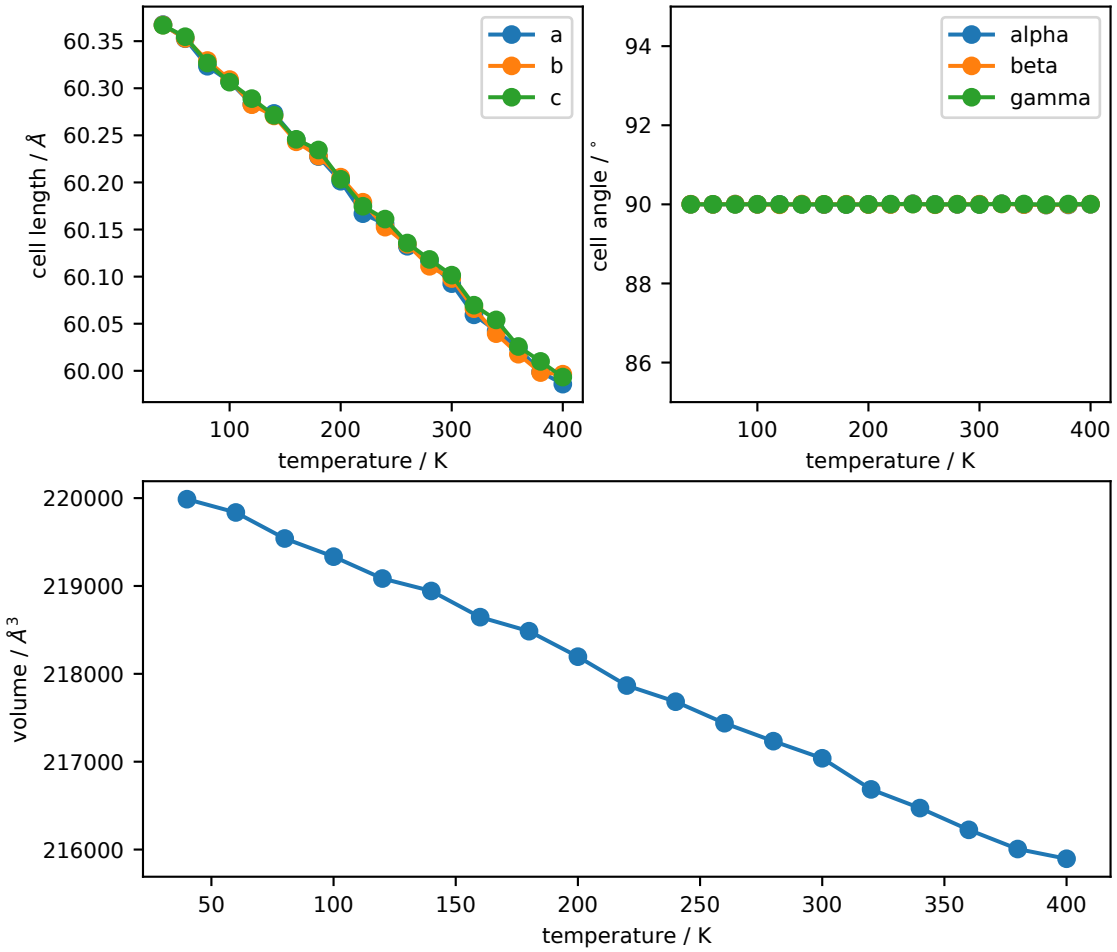

Fig. S6 Average cell parameters and volume of PCN-68 in response to increasing temperature.

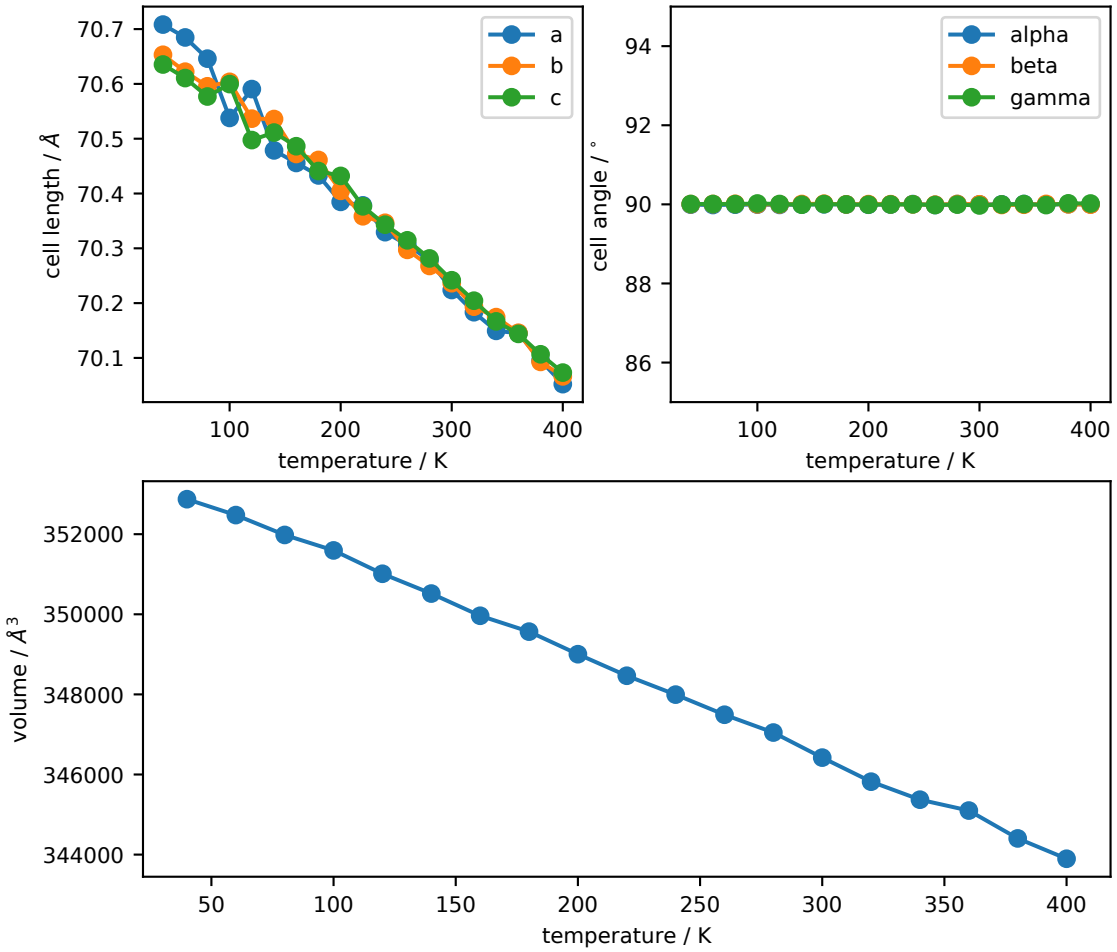

Fig. S7 Average cell parameters and volume of NU-110 in response to increasing temperature.

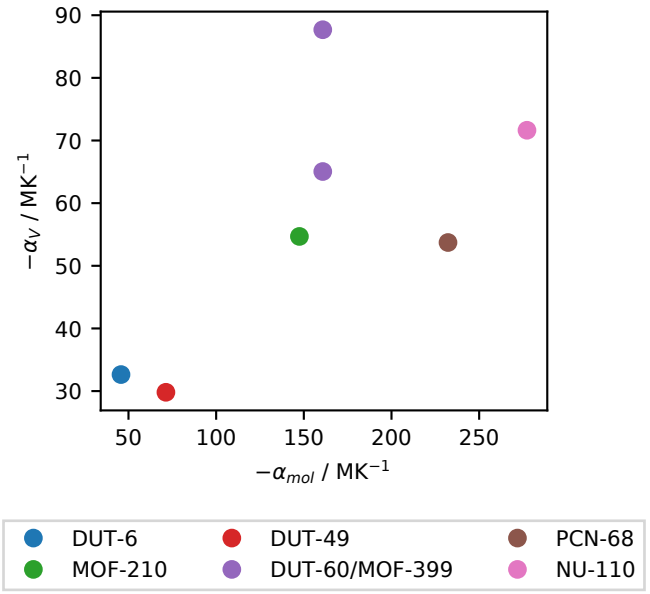

Fig. S8 Correlation between molecular coefficient of expansion, α_{mol}, and volumetric coefficient of expansion, α_V.

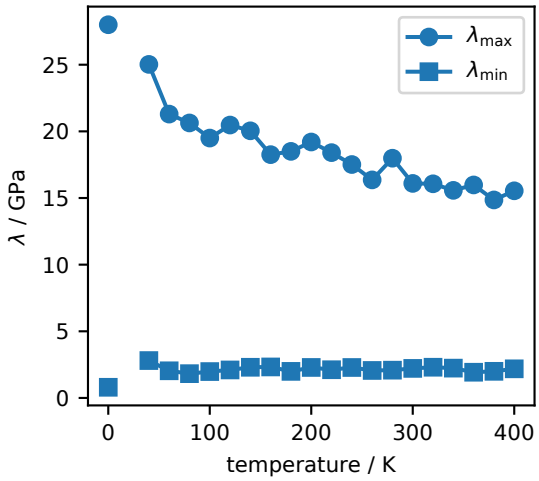

Fig. S9 Maximum and minimum (λ_{max} and λ_{min}) eigenvalues of the stiffness matrix for DUT-6 over the studied temperature range. Values at 0 K correspond to DFT simulation reported previously.[S2]

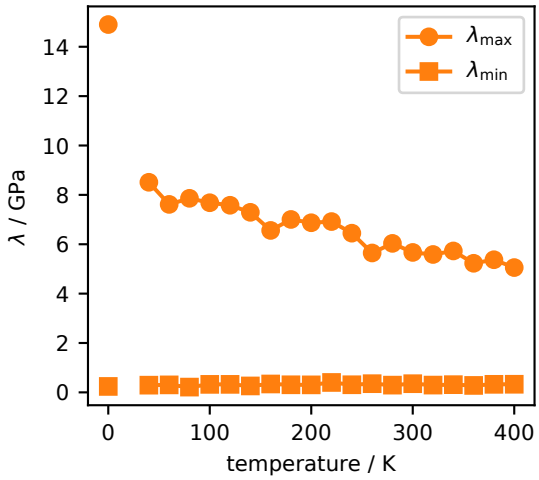

Fig. S10 Maximum and minimum (λ_{max} and λ_{min}) eigenvalues of the stiffness matrix for DUT-60 over the studied temperature range. Values at 0 K correspond to DFT simulation reported previously.[S2]

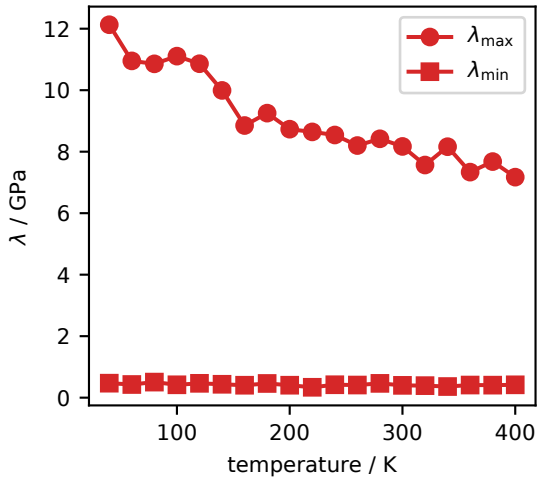

Fig. S11 Maximum and minimum (λ_{max} and λ_{min}) eigenvalues of the stiffness matrix for MOF-210 over the studied temperature range.

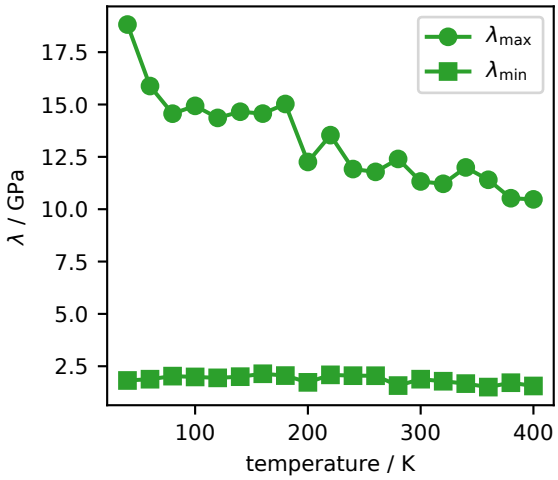

Fig. S12 Maximum and minimum (λ_{max} and λ_{min}) eigenvalues of the stiffness matrix for DUT-49 over the studied temperature range.

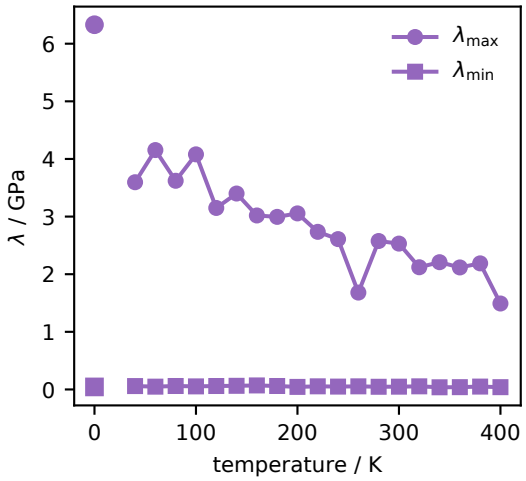

Fig. S13 Maximum and minimum (λ_{max} and λ_{min}) eigenvalues of the stiffness matrix for MOF-399 over the studied temperature range. Values at 0 K correspond to DFT simulation reported previously.[S2]

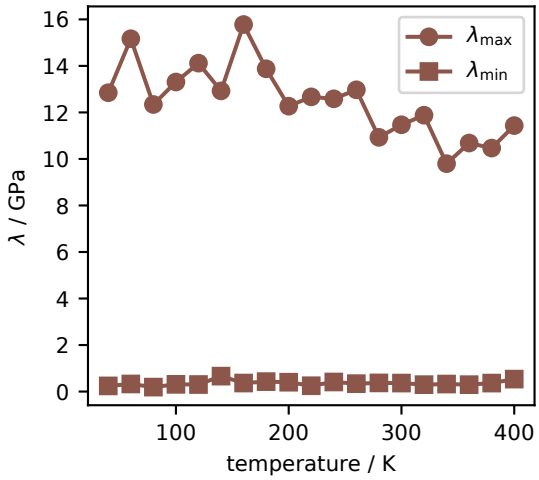

Fig. S14 Maximum and minimum (λ_{max} and λ_{min}) eigenvalues of the stiffness matrix for PCN-68 over the studied temperature range.

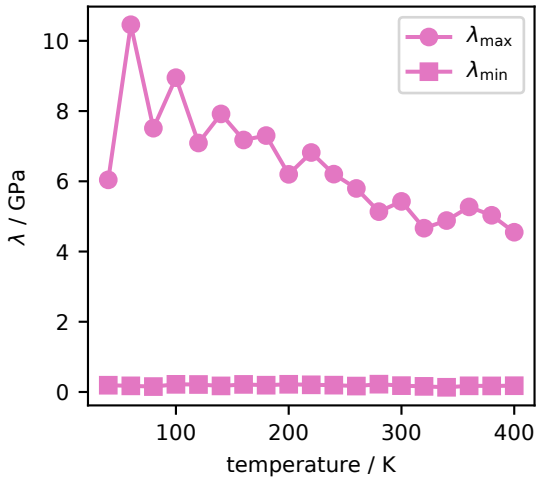

Fig. S15 Maximum and minimum (λ_{max} and λ_{min}) eigenvalues of the stiffness matrix for NU-110 over the studied temperature range.

References

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