

Electronic supporting information (ESI) for article: Various Approaches to Studying the Phase Transition in an Octamethylcyclotetrasiloxane Crystal: from X-Ray Structural Analysis to Metadynamics

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Table S1. Crystallographic data of octamethylcyclotetrasiloxane at different temperatures.

Temperature/K	100	150	200	210	221	230	240	250	270
Crystal system	tetragonal	tetragonal	tetragonal	tetragonal	tetragonal	tetragonal	tetragonal	tetragonal	tetragonal
Space group	P4 ₂ /n	P4 ₂ /n	P4 ₂ /n	P4 ₂ /n	P4 ₂ /n	P4 ₂ /n	I4 ₁ /a	I4 ₁ /a	I4 ₁ /a
a/Å	15.9596(16)	15.9938(15)	16.0373(19)	16.051(2)	16.0690(19)	16.083(3)	16.0850(16)	16.0850(16)	16.250(7)
b/Å	15.9596(16)	15.9938(15)	16.0373(19)	16.051(2)	16.0690(19)	16.083(3)	16.0850(16)	16.0850(16)	16.250(7)
c/Å	6.3737(15)	6.4099(14)	6.4481(17)	6.4589(18)	6.4719(17)	6.517(3)	6.8911(9)	6.8911(9)	6.943(4)
α /°	90	90	90	90	90	90	90	90	90
β /°	90	90	90	90	90	90	90	90	90
γ /°	90	90	90	90	90	90	90	90	90
Volume/Å ³	1623.4(5)	1639.7(5)	1658.4(6)	1664.0(6)	1671.1(6)	1685.7(10)	1782.9(4)	1782.9(4)	1833.3(19)
Z	4	4	4	4	4	4	4	4	4
$\rho_{\text{calc}}/\text{cm}^{-3}$	1.214	1.202	1.188	1.184	1.179	1.169	1.105	1.105	1.075
μ/mm^{-1}	0.364	0.360	0.356	0.355	0.354	0.350	0.331	0.331	0.322
2 Θ range for data collection/°	3.61 to 61.564	3.602 to 61.25	3.592 to 61.196	3.588 to 61.288	3.584 to 61.316	3.582 to 61.18	5.064 to 61.428	5.064 to 61.536	5.014 to 51.988
Reflections collected	5755	10212	10231	10350	10524	9559	6271	6282	2110
R _{int}	0.0313	0.0444	0.0522	0.0548	0.0520	0.0734	0.0398	0.0382	0.0471
Data/restraints/parameters	2160/0/77	2511/0/77	2530/0/77	2557/0/77	2572/0/77	2557/0/77	1376/0/39	1381/0/39	886/0/39
Goodness-of-fit on F ²	1.072	1.034	1.032	1.042	1.001	1.066	1.090	1.087	1.043
R ₁ [I > 2 σ (I)]	0.0477	0.0472	0.0572	0.0611	0.0598	0.0883	0.0545	0.0560	0.0907
wR ₂ [all data]	0.1220	0.1295	0.1553	0.1596	0.1599	0.2423	0.1724	0.1906	0.2999
Largest diff. peak/hole / e Å ⁻³	0.43/-0.26	0.36/-0.24	0.44/-0.22	0.42/-0.26	0.42/-0.25	0.51/-0.34	0.39/-0.28	0.45/-0.30	0.72/-0.41

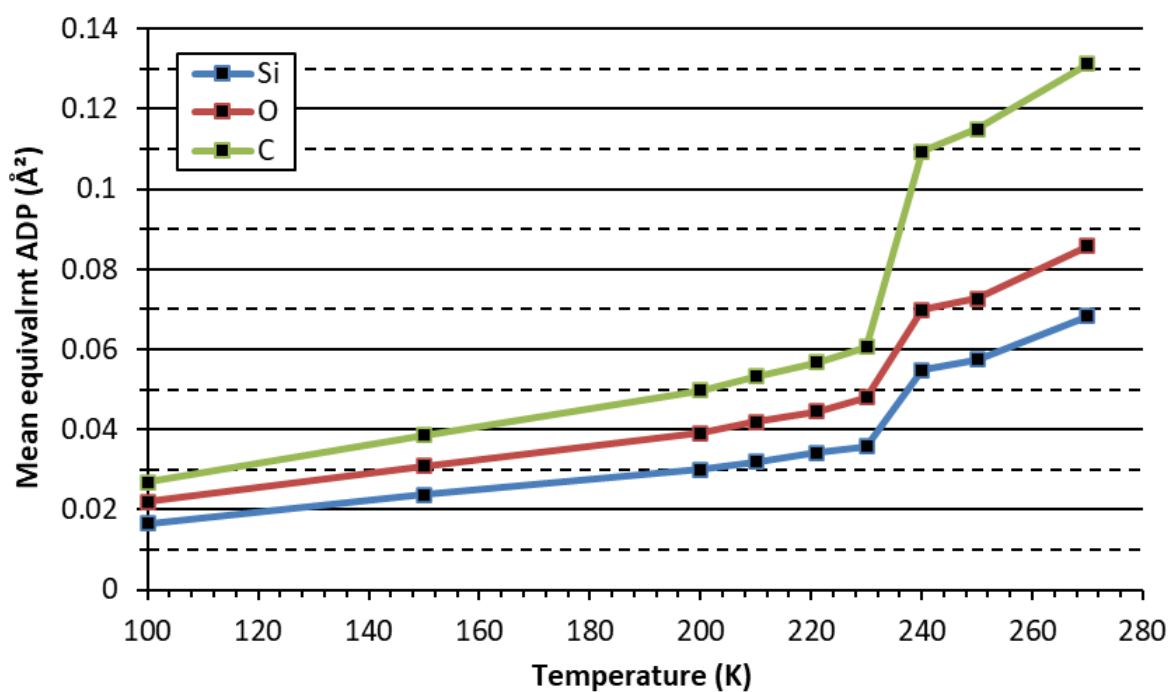


Figure S1. Isotropic atom displacement parameters (U_{eq}) averaged by atom type.