High-Pressure Phase Transition, Pore Collapse and Amorphisation in the Siliceous 1D Zeolite, TON.

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Table S1. Atomic positions, atomic displacement parameters and occupation factors of TON at ambient pressure (orthorhombic, space group *Cmc2₁*). The carbon atoms account for the residue in the pores (decomposition products of the organic template, adsorbed species etc.).

*Cmc*2$_1$	*x*	*y*	*z*	B_{iso} (Å²)	Occ.
O1	0.094(2)	0.428(2)	0.70(2)	2.7(7)	1.0
O2	0.091(2)	0.216(3)	0.22(2)	2.7(7)	1.0
O3	0.276(3)	0.380(2)	0.69(3)	2.7(7)	1.0
O4	0.227(3)	0.495(4)	-0.01(1)	2.7(7)	1.0
O5	0.266(4)	0.265(3)	0.380(8)	2.7(7)	1.0
O6	0	0.301(3)	0.560(8)	2.7(7)	1.0
O7	0	0.347(3)	0.068(7)	2.7(7)	1.0
Si1	0.295(2)	0.049(1)	0.225(6)	3.1(4)	1.0
Si2	0.207(1)	0.210(1)	0.181(6)	3.1(4)	1.0
Si3	0	0.273(2)	0.25	3.1(4)	1.0
Si4	0	0.373(2)	0.761(6)	3.1(4)	1.0
C1	0.5	0.446(5)	0.1171	1.0(9)	0.42(3)
C2	0.5	0.446(5)	0.3671	1.0(9)	0.42(3)

Table S2. Atomic positions, atomic displacement parameters and occupation factors of TON at 1.56(2)6 GPa (orthorhombic, space group *Pbn*2_1). The carbon atoms account for the residue in the pores (decomposition products of the organic template, adsorbed species etc.).

Pbn2_1	*x*	*y*	*z*	B_{iso} (Å²)	Occ.
O1	0.074(2)	0.566(2)	0.18(1)	2.7(6)	1.0
O1_2	0.612(2)	0.079(2)	0.21(1)	2.7(6)	1.0
O2	0.060(2)	0.797(2)	0.75(1)	2.7(6)	1.0
O2_2	0.617(2)	0.267(3)	0.69(1)	2.7(6)	1.0
O3	0.238(3)	0.644(2)	0.17(1)	2.7(6)	1.0
O3_2	0.798(3)	0.104(2)	0.18(1)	2.7(6)	1.0
O4	0.233(3)	0.493(2)	0.339(7)	2.7(6)	1.0
O4_2	0.727(3)	0.971(2)	0.356(7)	2.7(6)	1.0
O5	0.202(3)	0.793(2)	0.081(6)	2.7(6)	1.0
O5_2	0.751(3)	0.244(2)	0.066(6)	2.7(6)	1.0
O6	0.483(4)	0.805(2)	0.567(6)	2.7(6)	1.0
O7	0.503(4)	0.846(2)	0.046(6)	2.7(6)	1.0
Si1	0.283(2)	0.967(2)	0.662(8)	4.5(4)	1.0
Si1_2	0.807(2)	0.445(2)	0.690(9)	4.5(4)	1.0
Si2	0.175(2)	0.802(2)	0.720(9)	4.5(4)	1.0
Si2_2	0.734(2)	0.268(2)	0.746(9)	4.5(4)	1.0
Si3	0.487(2)	0.777(2)	0.217(8)	4.5(4)	1.0
Si4	0.492(2)	0.876(2)	0.75	4.5(4)	1.0
C1	0.050(4)	0.050(4)	0.1171	2(1)	0.204
C2	0.050(4)	0.050(4)	0.3671	2(1)	0.204
C3	-0.055(4)	-0.055(4)	0.1171	2(1)	0.204
C4	-0.055(4)	-0.055(4)	0.3671	2(1)	0.204

Table S3. Si-O-Si bridging angles (°) in TON at ambient pressure and 0.42(2) GPa (orthorhombic, space group *Cmc2*$_1$).

Angle	0.1 MPa	0.42(2) GPa
Si1 O1 Si4	153(3)	153(2)
Si2 O2 Si3	145(2)	144.7(18)
Si1 O3 Si2	150(3)	151(3)
Si1 O4 Si1	157(5)	153(4)
Si2 O5 Si2	149(4)	139(3)
Si3 O6 Si4	146(3)	135(2)
Si3 O7 Si4	142(4)	129(3)

Table S4. Si-O-Si bridging angles (°) in TON at 1.56(2) GPa (orthorhombic, space group *Pbn*2$_1$).

Angle	1.56(2) GPa
Si1_2 O1 Si4	143(3)
Si1 O1_2 Si4	177(3)
Si2 O2 Si3	130(3)
Si2_2 O2_2 Si3	149(3)
Si1_2 O3 Si2_2	163(4)
Si1 O3_2 Si2	150(3)
Si1 O4 Si1_2	131(5)
Si1 O4_2 Si1_2	142(5)
Si2 O5 Si2_2	132(4)
Si2 O5_2 Si2_2	136(5)
Si3 O6 Si4	141(3)
Si3 O7 Si4	143(4)

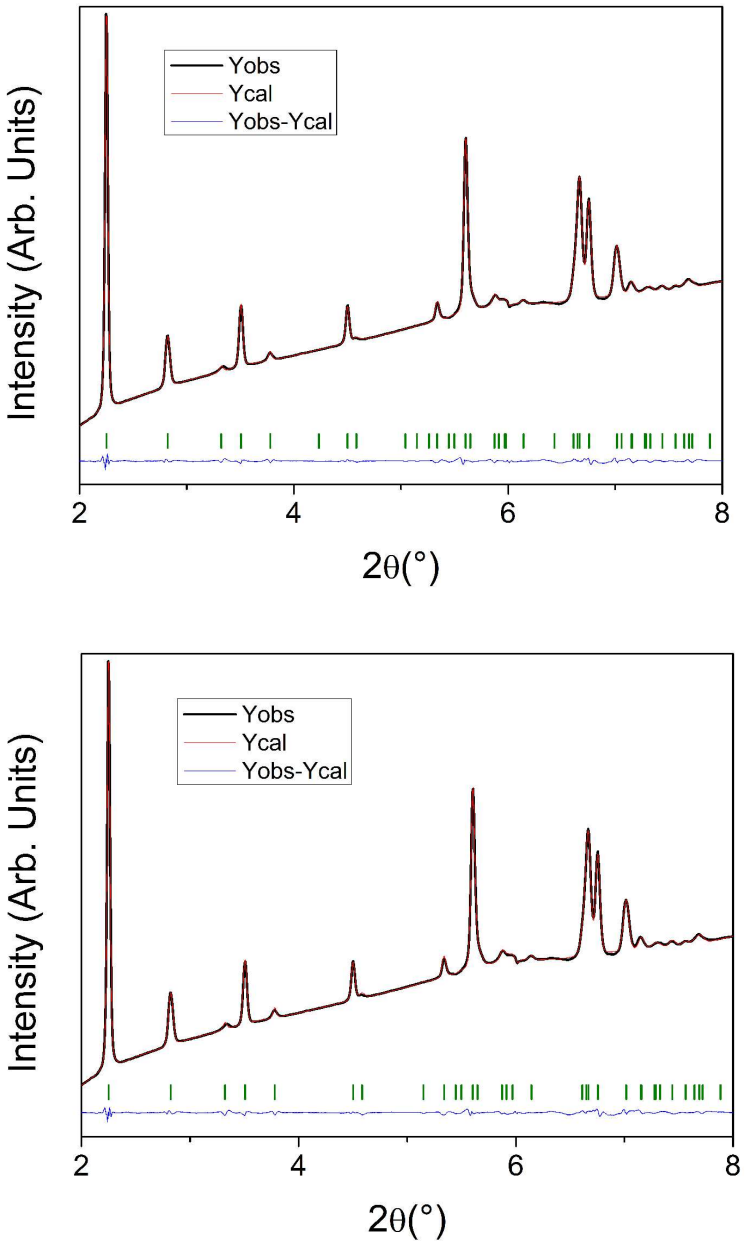

Figure S1. Low-angle region (2°-8°) of the experimental (black), calculated (red) and difference (blue) profiles obtained from the Rietveld refinement of the $P2_1$ structure (R_p=11.8%, R_{wp}=4.4%, R_{Bragg}=6.2%) (top) and the $Pbn2_1$ structure (R_p=12.2%, R_{wp}=4.6%, R_{Bragg}=6.0%) of TON at 1.56(2) GPa (bottom). Vertical bars indicate the calculated positions of the Bragg reflections.