Supporting Information

Sequence of phase transitions in $(NH_4)_3SiF_7$

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Table 1S. Fractional atomic coordinates and isotropic displacement parameters (Å^2) of $(NH_4)_3SiF_7$

	x	*y*	*z*	B_{iso}
*P*4/*mbm* (G_1 phase) at T = 303 K				
Si1	0	0.5	0	3.4 (3)
F1	0	0	0.5	8.0 (3)
F2	0.3578 (4)	0.8578 (4)	0	8.0 (3)
F3	0.0998 (2)	0.5998 (2)	0.2050 (5)	8.0 (3)
N1	0	0	0	3.8 (3)
N2	0.2980 (4)	0.7980 (4)	0.5	3.8 (3)
Pbam (G_2 phase) at T = 213 K				
Si1	0	0.5	0	3.5 (4)
Si2	0	0	0	2.5 (4)
F1	0.7618 (7)	0.7550 (9)	0.5	4.9 (3)
F2	-0.031 (1)	0.1404 (8)	0	4.9 (3)
F3	0.1451 (8)	0.4615 (8)	0	4.9 (3)
F4	-0.0288 (6)	0.4077 (4)	0.205 (1)	4.9 (3)
F5	0.3935 (5)	0.5186 (5)	0.802 (1)	4.9 (3)
N1	0.750 (1)	0.759 (1)	0	2.6 (3)
N2	-0.015 (1)	0.199 (1)	0.5	2.6 (3)
N3	0.203 (1)	0.490 (1)	0.5	2.6 (3)
P-1 (G_4 phase) at T = 183 K				
Si1	0	0	0	1.6 (5)
Si2	0	0.5	0.5	1.0 (5)
Si3	0	0	0.5	3.0 (6)
Si4	0	0.5	0	3.0 (6)
F1	0.503 (5)	0.260 (2)	0.258 (2)	3.2 (2)
F2	0.506 (5)	0.760 (1)	0.229 (1)	3.2 (2)
F3	-0.001 (4)	0.146 (1)	0.010 (1)	3.2 (2)
F4	0.012 (4)	0.639 (2)	0.476 (1)	3.2 (2)
F5	-0.008 (4)	0.557 (1)	0.146 (2)	3.2 (2)
F6	0.037 (4)	0.048 (1)	0.360 (2)	3.2 (2)
F7	0.172 (3)	0.389 (2)	0.039 (2)	3.2 (2)
F8	0.818 (4)	0.887 (2)	0.471 (2)	3.2 (2)
F9	0.173 (4)	-0.006 (2)	0.887 (2)	3.2 (2)
F10	0.784 (3)	0.538 (2)	0.606 (2)	3.2 (2)

F11	0.233 (4)	0.584 (2)	-0.032 (2)	3.2 (2)
F12	0.778 (4)	0.086 (2)	0.526 (2)	3.2 (2)
F13	0.257 (3)	-0.014 (2)	0.075 (2)	3.2 (2)
F14	0.793 (4)	0.484 (2)	0.409 (2)	3.2 (2)
N1	0.004 (7)	0.270 (2)	0.257 (2)	2.0 (3)
N2	0.014 (7)	0.772 (2)	0.254 (2)	2.0 (3)
N3	0.484 (5)	0.210 (2)	0.003 (2)	2.0 (3)
N4	0.518 (5)	0.705 (2)	0.501 (2)	2.0 (3)
N5	0.487 (6)	-0.006 (2)	0.300 (2)	2.0 (3)
N6	0.503 (6)	0.520 (2)	0.212 (2)	2.0 (3)
$P2_1/c$ (G_5 phase) at T = 133 K				
Si1	0	0	0.5	1.8 (2)
Si2	0.5	0	0.5	1.8 (2)
Si3	0	0	0	1.8 (2)
Si4	0.5	0	0	1.8 (2)
F1	0.257 (1)	0.763 (1)	0.240 (2)	2.3 (2)
F2	0.743 (1)	0.770 (1)	0.249 (2)	2.3 (2)
F3	0.007 (1)	0.140 (1)	0.031 (1)	2.3 (2)
F4	0.499 (1)	0.133 (1)	-0.034 (1)	2.3 (2)
F5	-0.006 (1)	0.441 (1)	0.863 (1)	2.3 (2)
F6	0.493 (1)	0.480 (1)	0.854 (1)	2.3 (2)
F7	0.087 (1)	0.391 (1)	0.039 (1)	2.3 (2)
F8	0.632 (1)	0.414 (1)	0.025 (1)	2.3 (2)
F9	0.877 (1)	0.079 (1)	0.538 (1)	2.3 (2)
F10	0.418 (1)	0.122 (1)	0.522 (1)	2.3 (2)
F11	0.924 (1)	0.537 (1)	0.616 (1)	2.3 (2)
F12	0.403 (1)	0.468 (1)	0.602 (1)	2.3 (2)
F13	0.115 (1)	-0.001 (1)	0.077 (1)	2.3 (2)
F14	0.623 (1)	0.023 (1)	0.093 (1)	2.3 (2)
N1	0.007 (2)	0.775 (1)	0.260 (2)	1.0 (2)
N2	0.494 (2)	0.759 (1)	0.258 (2)	1.0 (2)
N3	0.255 (2)	0.203 (1)	-0.011 (2)	1.0 (2)
N4	0.746 (2)	0.210 (1)	-0.003 (2)	1.0 (2)
N5	0.253 (2)	0.465 (1)	0.791 (2)	1.0 (2)
N6	0.742 (2)	0.508 (1)	0.799 (2)	1.0 (2)

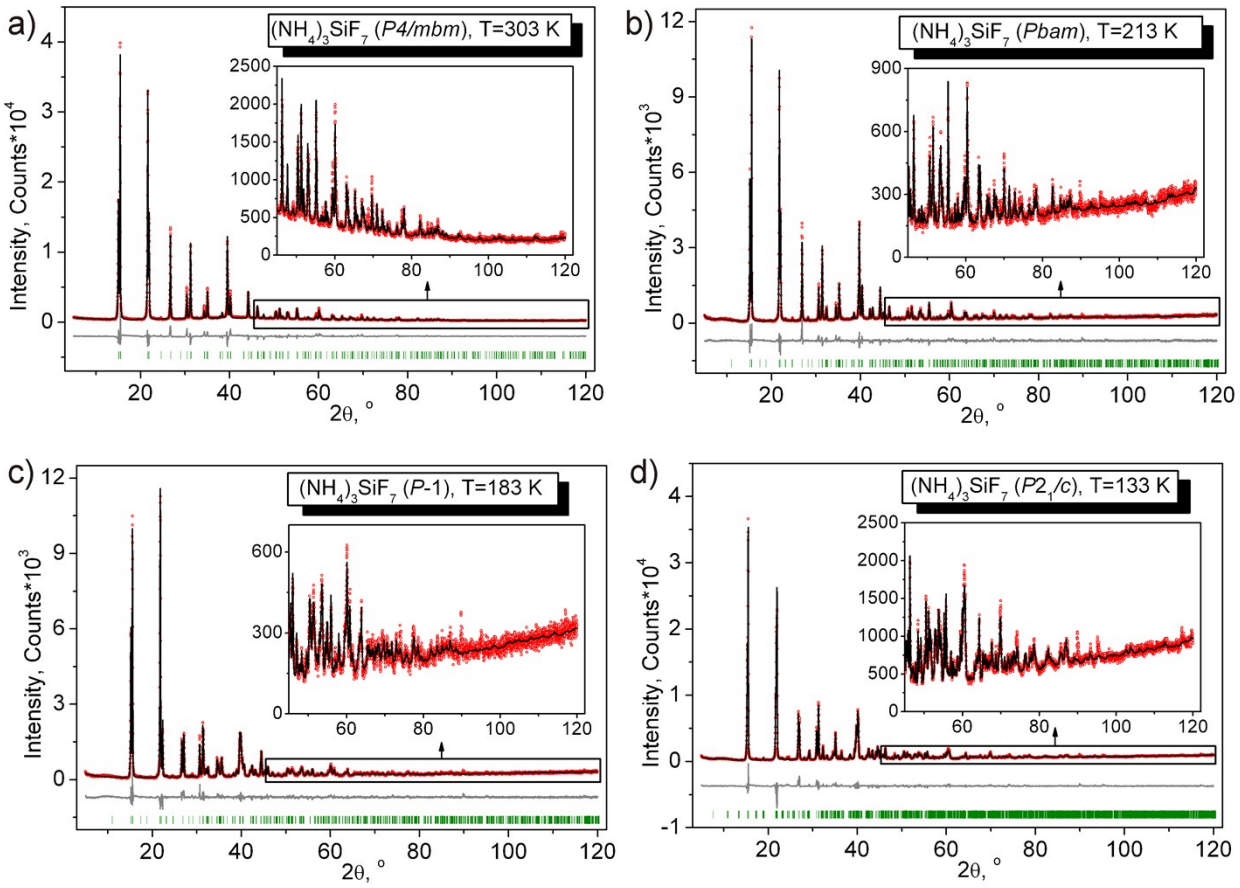

Figure 1S. Difference Rietveld plot of $(NH_4)_3SiF_7$ at: a) T = 303 K in G_1 phase (*P4/mbm*); b) T = 213 K in G_2 phase (*Pbam*); c) T = 183 K in G_4 phase (*P*-1); d) T = 133 K in G_5 phase ($P2_1/c$).

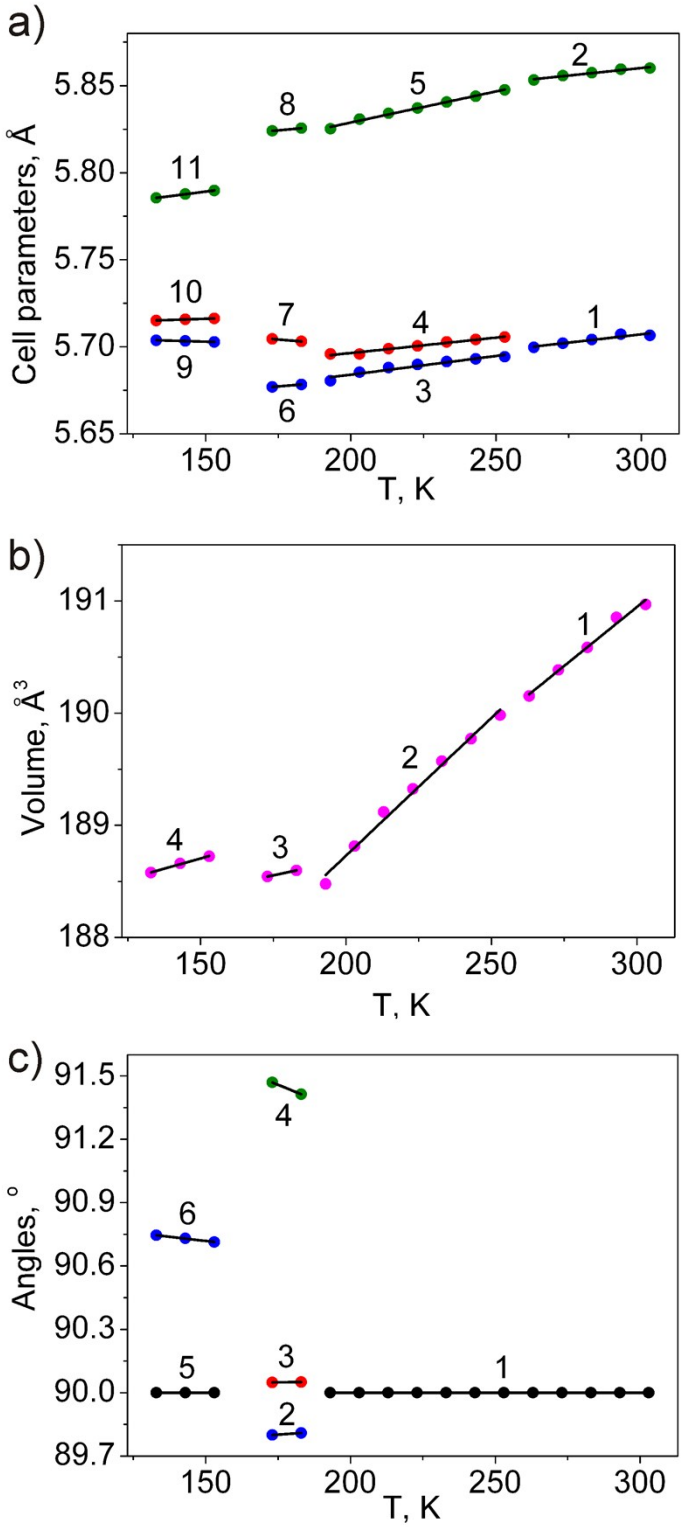

Figure 2S. Temperature dependence of: a) the cell parameters $a/2^{1/2}$ (1) and c (2) in G_1 phase, $b/2$ (3), $a/2$ (4) and c (5) in G_2 phase, $b/2$ (6), $c/2$ (7) and a (8) in G_4 phase, $b/2$ (9), $c/2$ (10) and $a/2$ (11) in G_5 phase; b) the cell volume of formula unit $V/2$ (1) in G_1 phase, $V/4$ (2) in G_2 phase, $V/4$ (3) in G_4 phase, $V/8$ (4) in G_5 phase; c) α, β, γ (1) in G_1 and G_2 phases, β (2), α (3), γ (4) in G_4 phase, α, γ (5) and β (6) in G_5 phase.