Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary materials

Table 1SM. Unit cell parameters and thermal expansion coefficients of the low-temperature modification of $(NH_4)_3Sc(SO_4)_3$ upon temperature

T, °C	*a*, Å	b, Å	*c*, Å	β, °	*V*, Å^3	*V/Z*, Å^3	α_a, ×10^{-6} Å	α_b, ×10^{-6} Å^{-1}	α_c, ×10^{-6} Å^{-1}	α_V, ×10^{-6} Å^{-3}
25	9.0524(	15.4622(	9.2165(	108.43(	1223.9(	305.97(2)				
40	9.0608(	15.4628(	9.2198(	108.41(	1225.6(	306.41(2)	61.7	2.58	23.9	94.0
50	9.0683(	15.4643(	9.2208(	108.42(	1226.8(	306.71(2)	82.7	9.69	10.8	98.7
60	9.0748(	15.4662(	9.2226(	108.41(	1228.1(	307.04(2)	71.6	12.3	19.5	10.7
70	9.0814(	15.4664(	9.2238(	108.41(	1229.3(	307.31(2)	72.6	1.29	13.0	89.9
80	9.0878(	15.4685(	9.2248(	108.41(	1230.4(	307.60(2)	70.4	13.6	10.8	91.8
90	9.0918(	15.4663(	9.2268(	108.41(	1231.0(	307.75(2)	44.0	-14.2	21.7	51.1
100	9.0922(	15.4643(	9.2284(	108.41(	1231.2(	307.79(2)	4.71	-12.9	17.5	11.6
Mea							**58.2**	**1.75**	**16.8**	**77.7**

$\alpha_a = \frac{1}{a}\left(\frac{\partial L}{\partial R}\right)$, $\alpha_b = \frac{1}{b}\left(\frac{\partial L}{\partial R}\right)$, $\alpha_c = \frac{1}{c}\left(\frac{\partial L}{\partial R}\right)$, $\alpha_V = \frac{1}{V}\left(\frac{\partial L}{\partial R}\right)$

Table 2SM. Unit cell parameters and thermal expansion coefficients of the high-temperature modification of $(NH_4)_3Sc(SO_4)_3$ upon temperature

T, °C	*a*, Å	*c*, Å	*V*, Å^3	*V/Z*, Å^3	α_a, ×10^{-6} Å^{-1}	α_c, ×10^{-6} Å^{-1}	α_V, ×10^{-6} Å^{-3}
80	15.4278(4)	9.2190(2)	1900.3(1)	316.72(2)			
90	15.4309(4)	9.2203(2)	1901.3(1)	316.89(2)	20.1	14.1	53.6
100	15.4329(4)	9.2228(2)	1902.4(1)	317.06(2)	13.0	27.1	53.6
110	15.4350(4)	9.2251(2)	1903.3(1)	317.22(2)	13.6	24.9	52.0
120	15.4391(4)	9.2262(2)	1904.6(1)	317.43(2)	26.6	11.9	65.2
140	15.4435(3)	9.2305(2)	1906.6(1)	317.76(2)	14.2	23.3	51.9
150	15.4457(4)	9.2327(2)	1907.5(1)	317.92(2)	14.2	23.8	51.4
160	15.4495(4)	9.2342(2)	1908.8(1)	318.13(2)	24.6	16.2	65.5
180	15.4552(4)	9.2382(2)	1911.0(1)	318.50(2)	18.4	21.6	58.3
200	15.4618(4)	9.2410(2)	1913.3(1)	318.88(2)	21.3	15.1	58.3
220	15.4672(4)	9.2441(2)	1915.2(1)	319.20(2)	17.5	16.8	51.4
240	15.4743(4)	9.2469(2)	1917.6(1)	319.59(2)	22.9	15.1	61.0
260	15.4801(4)	9.2491(2)	1919.5(1)	319.91(2)	18.7	11.9	49.2
280	15.4873(4)	9.2525(2)	1921.9(1)	320.32(2)	23.2	18.4	64.8
Mean					**19.1**	**18.5**	**56.6**

$\alpha_a = \frac{1}{a}\left(\frac{\partial L}{\partial R}\right)$, $\alpha_b = \frac{1}{b}\left(\frac{\partial L}{\partial R}\right)$, $\alpha_c = \frac{1}{c}\left(\frac{\partial L}{\partial R}\right)$, $\alpha_V = \frac{1}{V}\left(\frac{\partial L}{\partial R}\right)$

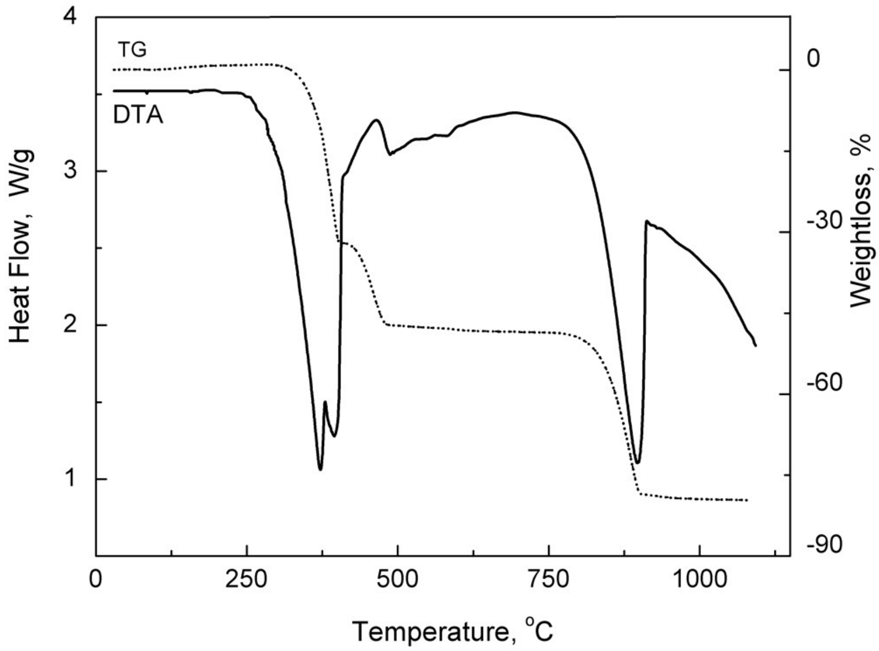

Fig. 1SM. TG and DTA curves of $(NH_4)_3Sc(SO_4)_3$ at a heating rate of 10 °/min in air

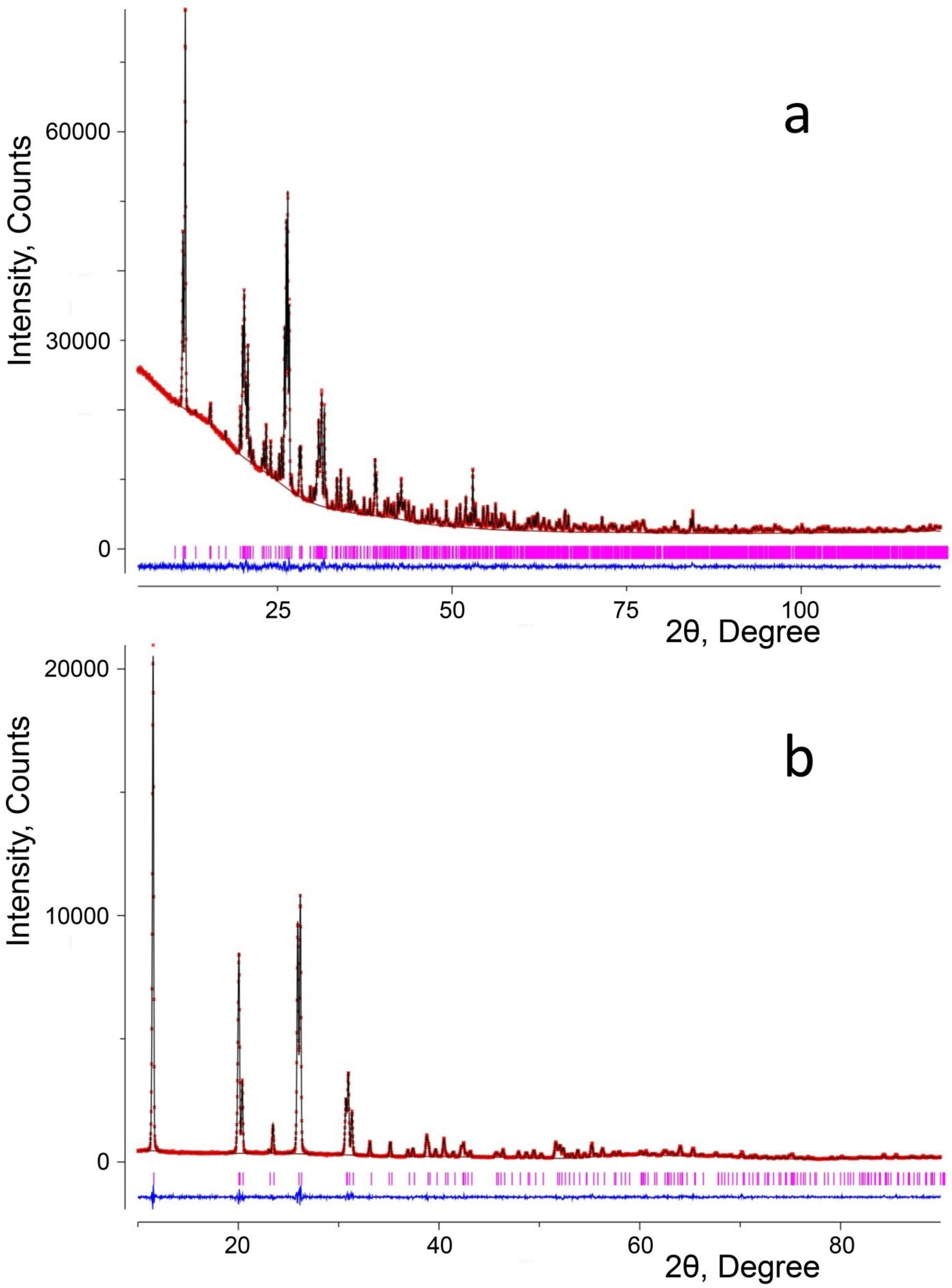

Fig. 4 Experimental (crosses), calculated (solid line), and difference (bottom line) XRPD patterns of the low-temperature (a) and high-temperature modifications (b) of $(NH_4)_3Sc(SO_4)_3$. Series of tick marks correspond to the Bragg reflection.