Structural phase transitions in the double salts $(NH_4)_2PO_3F \cdot NH_4NO_3$ and $(NH_4)_2XO_4 \cdot 3NH_4NO_3$ (X = Se, Cr)

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Supplementary materials
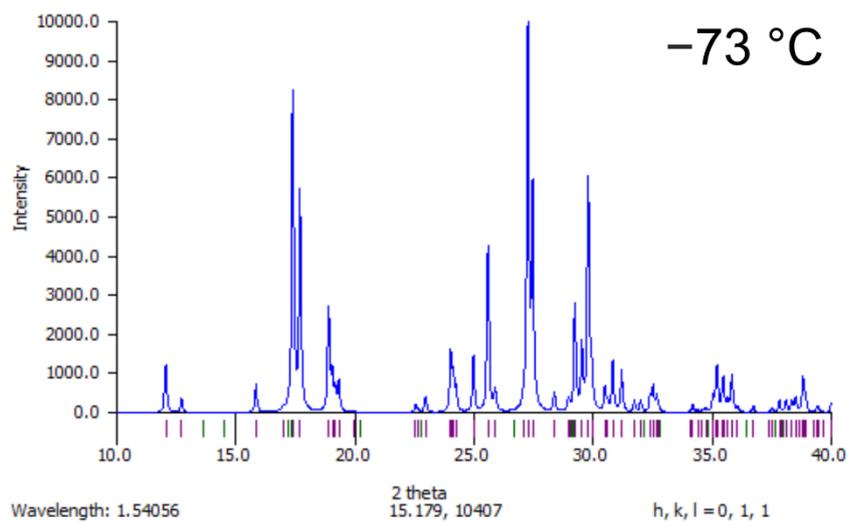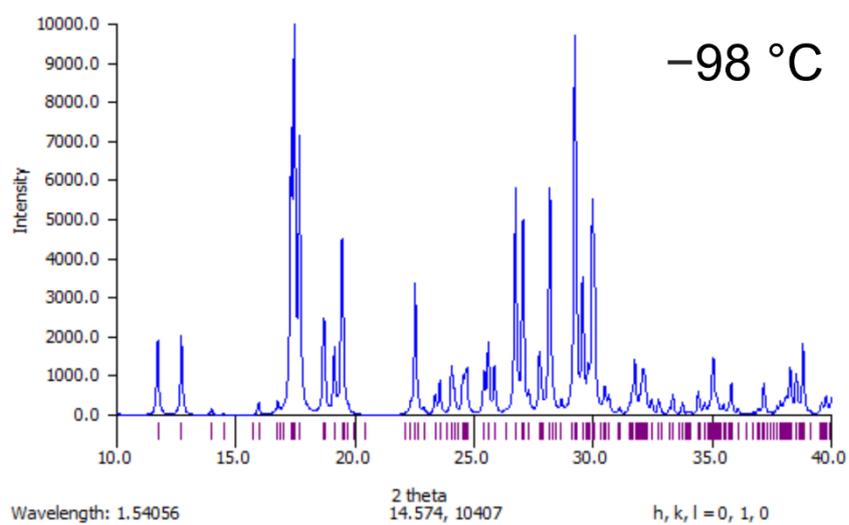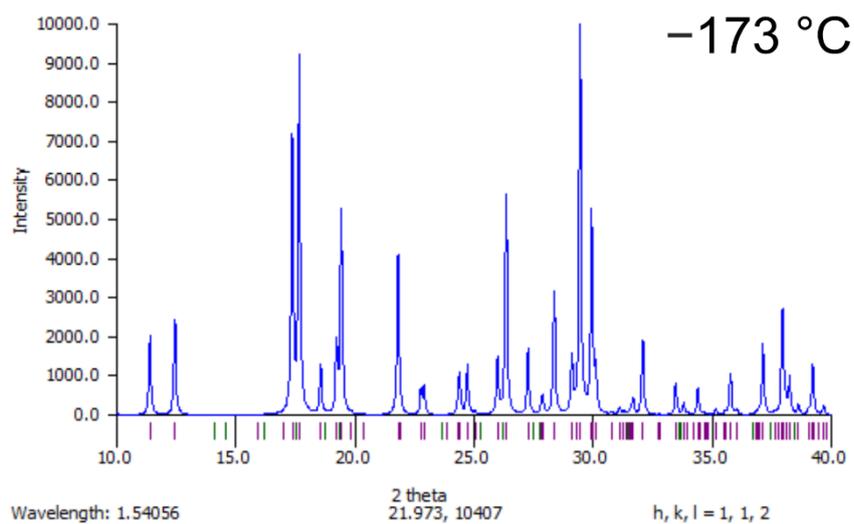
Figure S1. PXRD simulations based on single-crystal data for the different (NH₄)₂PO₃F·NH₄NO₃ polymorphs.
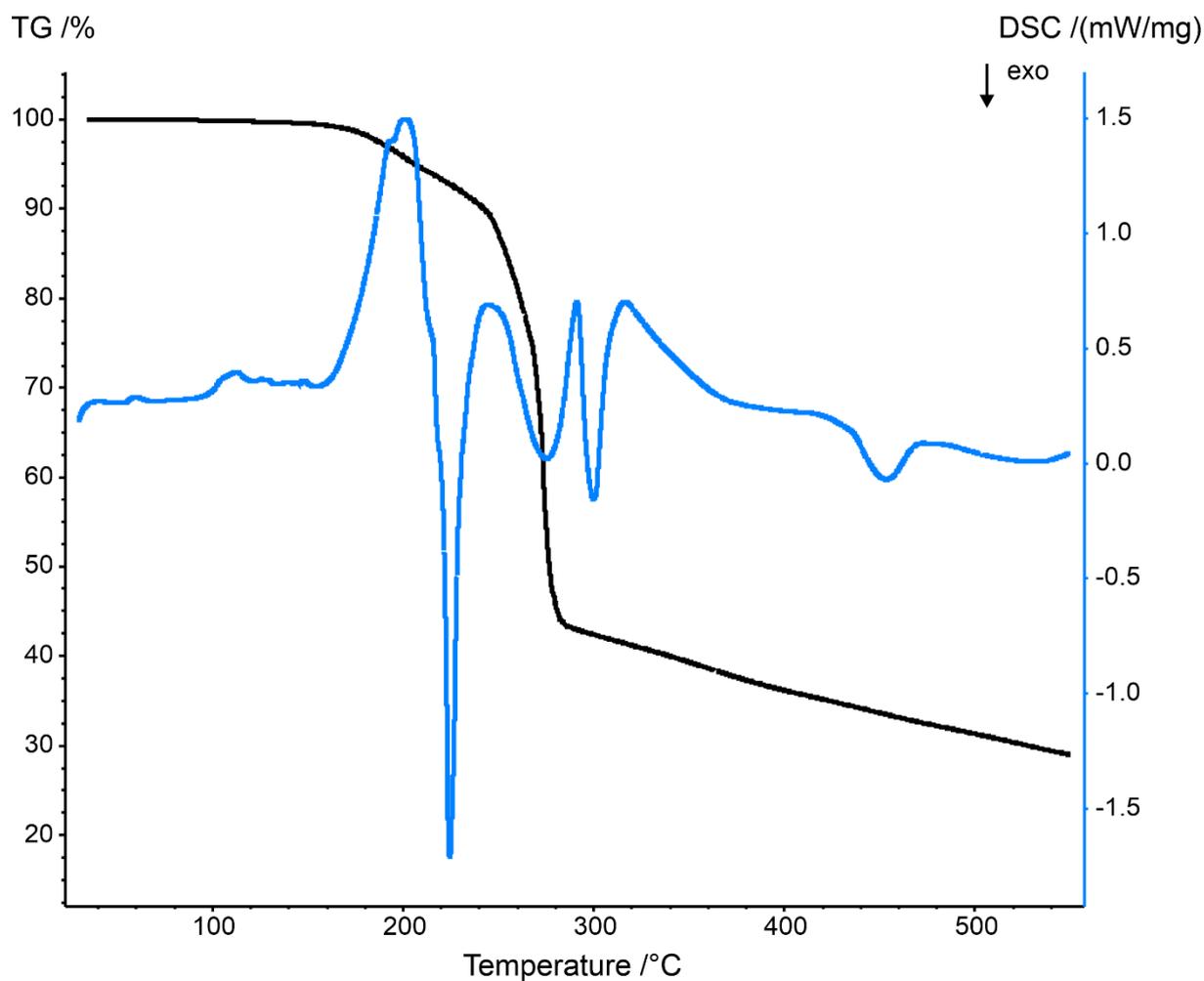
Figure S2. TG curve (black) and DSC curve (blue) of $(NH_4)_2PO_3F \cdot NH_4NO_3$-(I) in the temperature range 30-550 °C.
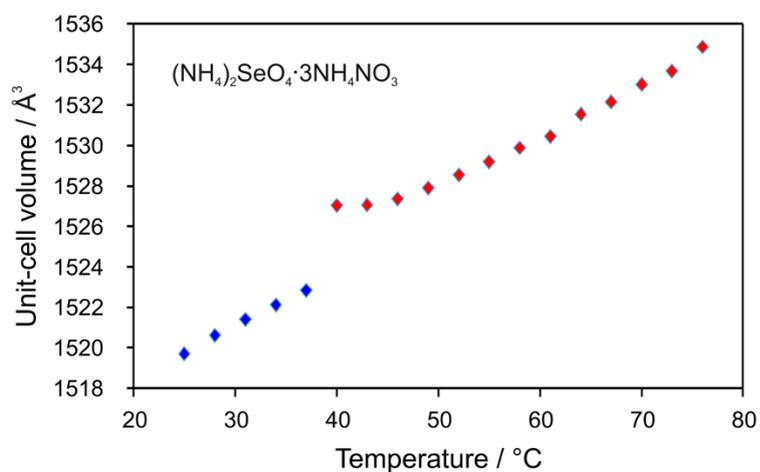
Figure S3. Evolution of the refined unit cell volume (Rietveld method) of $(NH_4)_2SeO_4 \cdot 3NH_4NO_3$ across the phase transition between 37 °C and 40 °C. Blue symbols represent polymorph-(I), red symbols polymorph-(II). For better comparison, the unit cell volume of polymorph-(II) was doubled.

Table S1. Data collection and refinement details of $(NH_4)_2PO_3F \cdot NH_4NO_3$-(I) at 22 °C.

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M_r	214.11
Space group, No	$P2_1/n$, 14
Z	4
Crystal form, color	plate, colourless
Crystal dimension / mm^3	$0.55 \times 0.45 \times 0.10$
a / Å	10.2455(13)
b / Å	6.0600(9)
c / Å	14.590(2)
α / °	90
β / °	104.077(4)
γ / °	90
V / $Å^3$	878.7(2)
X-ray density /$g \cdot cm^{-3}$	1.619
Radiation type	Mo $K\alpha$
μ / mm^{-1}	0.338
T_{min}, T_{max}	0.674, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	42981, 3131, 2562
R_{int}	0.0398
$(\sin \theta/\lambda)_{max}$ / $Å^{-1}$	0.818
No. of reflections	3131
No. of parameters	147
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.1023, 1.05
$\Delta \varrho_{max}$, $\Delta \varrho_{min}$ ($e^- \cdot Å^{-3}$)	0.40, −0.36
CSD-code	2294150

Table S2. Data collection and refinement details of $(NH_4)_2SeO_4 \cdot 3NH_4NO_3$-(II) at different temperatures.

	−23 °C	−73 °C	−123 °C
M_r	419.20	419.20	419.20
Space group, No	$P2_1/c$, 14	$P2_1/c$, 14	$P2_1/c$, 14
Z	4	4	4
Crystal form, color	plate, colourless	plate, colourless	plate, colourless
Crystal dimension / mm^3	0.30 × 0.20 × 0.05	0.30 × 0.20 × 0.05	0.08 × 0.08 × 0.05
a / Å	10.0678(5)	10.0580(13)	10.0493(7)
b / Å	6.0089(3)	6.0210(9)	6.0481(5)
c / Å	24.9034(13)	24.743(4)	24.4978(19)
α / °	90	90	90
β / °	92.745(2)	92.858(4)	93.058(2)
γ / °	90	90	90
V / Å^3	1504.84(13)	1496.5(4)	1486.8(2)
X-ray density /g·cm^{-3}	1.850	1.861	1.873
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ / mm^{-1}	2.579	2.593	2.610
T_{min}, T_{max}	0.691, 0.765	0.689, 0.786	0.818, 0.974
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	74830, 6661, 5149	80351, 6636, 5348	73401, 6558, 5654
R_{int}	0.0442	0.0480	0.0400
$(\sin \theta/\lambda)_{max}$ / Å^{-1}	0.819	0.819	0.818
No. of reflections	6661	6636	6558
No. of parameters	316	260	260
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.070, 1.08	0.039, 0.096, 1.04	0.028, 0.065, 1.06
$\Delta\varrho_{max}$, $\Delta\varrho_{min}$ (e$^-$·Å^{-3})	0.57, −0.40	1.67, −1.55	1.28, −0.80
CSD-code	2294153	2294154	2294156

Table S3. Data collection and refinement details of $(NH_4)_2CrO_4 \cdot 3NH_4NO_3$-(II) at different temperatures.

	−23 °C	−73 °C	−123 °C
M_r	392.24	392.24	392.24
Space group, No	$P2_1/c$, 14	$P2_1/c$, 14	$P2_1/c$, 14
Z	4	4	4
Crystal form, color	plate, yellow	plate, yellow	plate, yellow
Crystal dimension / mm^3	0.08 × 0.08 × 0.01	0.30 × 0.20 × 0.05	0.08 × 0.08 × 0.01
a / Å	10.0139(17)	10.0009(7)	9.9715(11)
b / Å	5.9360(10)	5.9349(4)	5.9252(7)
c / Å	25.033(4)	24.9469(18)	24.870(3)
α / °	90	90	90
β / °	92.431(4)	92.480(2)	92.528(2)
γ / °	90	90	90
V / Å^3	1486.7(4)	1479.32(18)	1468.0(3)
X-ray density /g·cm^{-3}	1.752	1.761	1.775
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Mo $K\alpha$
μ / mm^{-1}	0.853	0.858	0.864
T_{min}, T_{max}	0.653, 0.772	0.656, 0.755	0.647, 0.767
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	44963, 4335, 2852	59486, 6413, 4028	44438, 4273, 3346
R_{int}	0.0686	0.0780	0.0558
$(\sin \theta/\lambda)_{max}$ / Å^{-1}	0.703	0.805	0.703
No. of reflections	4335	6413	4273
No. of parameters	288	288	288
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.126, 1.04	0.043, 0.122, 1.01	0.035, 0.098, 1.04
Δ_{Qmax}, Δ_{Qmin} (e$^-$·Å^{-3})	0.62, −0.45	0.73, −0.63	0.96, −0.44
CSD-code	2294158	2294160	2294152

Table S4. Selected bond lengths and interactions /Å of (NH₄)₂PO₃F·NH₄NO₃-(II) at 22 °C and of (NH₄)₂XO₄·3NH₄NO₃-(II) at different temperatures.

(NH₄)₂PO₃F·NH₄NO₃-(II) at 22 °C

P1—O2	1.4952(9)	N1—O5	1.241(2)
P1—O3	1.5035(9)	N1—O4	1.2443(19)
P1—O1	1.5067(9)	N1—O6	1.2442(19)
P1—F1	1.5946(9)		

(NH₄)₂SeO₄·3NH₄NO₃ at −23 °C

Se1—O3	1.6316(10)	N2—O8	1.2522(16)
Se1—O4	1.6200(13)	N2—O9	1.2540(16)
Se1—O1	1.6282(11)	N2—O10	1.2498(16)
Se1—O2	1.6411(10)	N3—O12A	1.189(3)
N1—O5A	1.253(4)	N3—O11A	1.263(3)
N1—O6A	1.312(7)	N3—O13A	1.244(4)
N1—O7A	1.300(7)	N3—O12B	1.355(10)
N1—O5B	1.286(7)	N3—O11B	1.127(9)
N1—O6B	1.119(11)	N3—O13B	1.192(13)
N1—O7B	1.123(11)		

(NH₄)₂SeO₄·3NH₄NO₃ at −73 °C

Se1—O3	1.6279(17)	N2—O8	1.255(2)
Se1—O4	1.6326(14)	N2—O9	1.258(2)
Se1—O1	1.6331(15)	N2—O10	1.253(2)
Se1—O2	1.6467(14)	N3—O12	1.210(3)
N1—O5	1.225(3)	N3—O11	1.242(3)
N1—O6	1.233(3)	N3—O13	1.253(2)
N1—O7	1.257(3)		

(NH₄)₂CrO₄·3NH₄NO₃ at −23 °C

Se1—O3	1.6392(16)	N2—O8	1.253(2)
Se1—O4	1.631(2)	N2—O9	1.255(2)
Se1—O1	1.6377(18)	N2—O10	1.253(2)
Se1—O2	1.6530(16)	N3—O12	1.201(3)
N1—O5A	1.162(18)	N3—O11	1.243(3)
N1—O6A	1.344(11)	N3—O13	1.250(3)
N1—O7A	1.246(9)		
N1—O5B	1.31(2)		
N1—O6B	1.056(19)		
N1—O7B	1.281(10)		

(NH₄)₂CreO₄·3NH₄NO₃ at −73 °C

Cr1—O4	1.6337(15)	N2—O8	1.2556(19)
Cr1—O3	1.6410(12)	N2—O9	1.2561(19)
Cr1—O1	1.6418(13)	N2—O10	1.2524(19)
Cr1—O2	1.6602(12)	N3—O12	1.215(2)
N1—O5A	1.133(9)	N3—O11	1.246(2)
N1—O6A	1.313(9)	N3—O13	1.252(2)
N1—O7A	1.253(5)		
N1—O5B	1.370(10)		
N1—O6B	1.106(16)		

N1—O7B 1.284(7)

(NH₄)₂CrO₄·3NH₄NO₃ at −123 °C

Cr1—O4	1.6357(15)	N2—O8	1.2575(19)
Cr1—O3	1.6391(13)	N2—O9	1.2539(19)
Cr1—O1	1.6441(13)	N2—O10	1.2545(19)
Cr1—O2	1.6629(12)	N3—O12	1.220(2)
N1—O5A	1.135(8)	N3—O11	1.247(2)
N1—O6A	1.339(8)	N3—O13	1.259(2)
N1—O7A	1.274(4)		
N1—O5B	1.375(9)		
N1—O6B	1.099(12)		
N1—O7B	1.287(5)		

Table S5. $(NH_4)_2PO_3F \cdot NH_4NO_3$-(I). Numerical details of hydrogen-bonding interactions at 22 °C and at −73 °C.

$D—H \cdots A$	$D—H$	$H \cdots A$	$D \cdots A$	$D—H \cdots A$
22 °C				
N2—H1⋯O3[i]	0.90 (1)	1.93 (1)	2.8254 (15)	176 (2)
N2—H2⋯O1[ii]	0.90 (1)	1.98 (1)	2.8354 (14)	158 (2)
N2—H3⋯O6[iii]	0.90 (1)	2.18 (1)	2.9896 (18)	149 (2)
N2—H4⋯O1	0.90 (1)	1.91 (1)	2.8052 (14)	174 (2)
N3—H5⋯O1	0.90 (1)	1.94 (1)	2.8335 (15)	173 (2)
N3—H6⋯O3[iv]	0.90 (1)	1.96 (1)	2.8431 (15)	167 (2)
N3—H7⋯O4[v]	0.90 (1)	2.24 (2)	2.8407 (17)	124 (2)
N3—H8⋯O2[iii]	0.90 (1)	1.96 (1)	2.8277 (15)	162 (2)
N4—H9⋯O4[vi]	0.90 (1)	2.22 (1)	3.049 (3)	152 (2)
N4—H10⋯O5[vii]	0.90 (1)	2.20 (1)	3.065 (3)	162 (2)
N4—H11⋯O3[viii]	0.90 (1)	1.93 (1)	2.8157 (19)	168 (2)
N4—H12⋯O2	0.90 (1)	1.89 (1)	2.7779 (19)	168 (2)
−73 °C				
N2—H1⋯O3[i]	0.90 (1)	1.93 (1)	2.8243 (10)	173 (1)
N2—H2⋯O1[ii]	0.90 (1)	1.94 (1)	2.8099 (9)	161 (1)
N2—H3⋯O6[iii]	0.90 (1)	2.19 (1)	2.9755 (11)	146 (1)
N2—H4⋯O1	0.90 (1)	1.90 (1)	2.7965 (9)	172 (1)
N3—H5⋯O1	0.90 (1)	1.93 (1)	2.8266 (10)	171 (1)
N3—H6⋯O3[iv]	0.90 (1)	1.95 (1)	2.8311 (10)	168 (1)
N3—H7⋯O4[v]	0.90 (1)	2.17 (1)	2.8509 (10)	132 (1)
N3—H8⋯O2[iii]	0.90 (1)	1.92 (1)	2.7890 (10)	163 (1)
N4—H9⋯O4[vi]	0.90 (1)	2.18 (1)	3.0200 (14)	156 (1)
N4—H10⋯O5[vii]	0.90 (1)	2.16 (1)	3.0104 (15)	158 (1)
N4—H11⋯O3[viii]	0.90 (1)	1.92 (1)	2.8048 (11)	166 (1)
N4—H12⋯O2	0.90 (1)	1.87 (1)	2.7624 (11)	169 (1)

Symmetry codes: (i) x, $y+1$, z; (ii) $−x+3/2$, $y+1/2$, $−z+3/2$; (iii) $−x+1$, $−y+1$, $−z+1$; (iv) $−x+1$, $−y$, $−z+1$; (v) $x+1$, y, z; (vi) $−x$, $−y$, $−z+1$; (vii) $−x$, $−y+1$, $−z+1$; (viii) $−x+1/2$, $y+1/2$, $−z+3/2$.

Table S6. $(NH_4)_2PO_3F \cdot NH_4NO_3$-(II). Numerical details of hydrogen-bonding interactions at −98 °C.

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N2A—H1$A\cdots$O1A^i	0.90 (1)	1.92 (1)	2.8071 (8)	170 (1)
N2A—H2$A\cdots$O1B^{ii}	0.90 (1)	1.98 (1)	2.8714 (8)	173 (1)
N2A—H3$A\cdots$O5A^{iii}	0.90 (1)	1.97 (1)	2.8514 (9)	166 (1)
N2A—H4$A\cdots$O2A	0.90 (1)	1.97 (1)	2.8622 (8)	172 (1)
N3A—H5$A\cdots$O1A	0.90 (1)	1.99 (1)	2.8878 (8)	178 (1)
N3A—H6$A\cdots$O3A^{iv}	0.90 (1)	1.93 (1)	2.8119 (8)	168 (1)
N3A—H7$A\cdots$O6A^v	0.90 (1)	1.94 (1)	2.8169 (8)	165 (1)
N3A—H8$A\cdots$O2A^{iii}	0.90 (1)	2.02 (1)	2.8694 (8)	156 (1)
N4A—H9$A\cdots$O3B^{iv}	0.90 (1)	1.93 (1)	2.8056 (8)	163 (1)
N4A—H10$A\cdots$O6A	0.90 (1)	1.97 (1)	2.8649 (9)	175 (1)
N4A—H11$A\cdots$O2B^{iii}	0.90 (1)	2.02 (1)	2.8891 (8)	163 (1)
N4A—H12$A\cdots$O3A	0.90 (1)	1.93 (1)	2.8164 (8)	170 (1)
N2B—H1$B\cdots$O3B^i	0.90 (1)	1.94 (1)	2.8288 (8)	170 (1)
N2B—H2$B\cdots$O1A^{ii}	0.90 (1)	1.92 (1)	2.7890 (8)	163 (1)
N2B—H3$B\cdots$O4B^{ii}	0.90 (1)	2.14 (1)	2.9414 (9)	149 (1)
N2B—H4$B\cdots$O1B	0.90 (1)	1.89 (1)	2.7845 (8)	173 (1)
N3B—H5$B\cdots$O1B^{vi}	0.90 (1)	1.96 (1)	2.8589 (8)	174 (1)
N3B—H6$B\cdots$O3B^i	0.90 (1)	1.94 (1)	2.8190 (8)	167 (1)
N3B—H7$B\cdots$O5B	0.90 (1)	2.14 (1)	2.8467 (8)	134 (1)
N3B—H7$B\cdots$O4B^{vii}	0.90 (1)	2.33 (1)	2.9010 (8)	122 (1)
N3B—H8$B\cdots$O2B	0.90 (1)	1.98 (1)	2.8422 (8)	161 (1)
N4B—H9$B\cdots$O5B^{viii}	0.90 (1)	2.22 (1)	3.0515 (11)	154 (1)
N4B—H10$B\cdots$O6B^{iii}	0.90 (1)	2.16 (1)	2.9738 (12)	150 (1)
N4B—H11$B\cdots$O2A^{iii}	0.90 (1)	1.90 (1)	2.7802 (10)	166 (1)
N4B—H12$B\cdots$O2B	0.90 (1)	1.91 (1)	2.8012 (9)	169 (1)

Symmetry codes: (i) x, y+1, z; (ii) −x+2, −y+1, −z+1; (iii) −x+1, −y+1, −z+1; (iv) −x+1, −y, −z+1; (v) x+1, y, z; (vi) −x+2, −y+1, −z; (vii) x, y+1, z−1; (viii) x, y−1, z.

Table S7. $(NH_4)_2PO_3F \cdot NH_4NO_3$-(III). Numerical details of hydrogen-bonding interactions at −173 °C.

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N2—H1$\cdots$O3^i	0.90 (1)	1.97 (1)	2.8611 (10)	173 (1)
N2—H2$\cdots$O1^{ii}	0.90 (1)	1.98 (1)	2.8720 (9)	174 (1)
N2—H3$\cdots$O5^{iii}	0.90 (1)	1.96 (1)	2.8505 (10)	170 (1)
N2—H4$\cdots$O1	0.90 (1)	1.89 (1)	2.7811 (10)	173 (1)
N3—H5$\cdots$O1	0.90 (1)	2.05 (1)	2.9446 (9)	177 (1)
N3—H6$\cdots$O3^{iv}	0.90 (1)	1.99 (1)	2.8551 (9)	161 (1)
N3—H7$\cdots$O6^v	0.90 (1)	1.90 (1)	2.7800 (10)	165 (1)
N3—H8$\cdots$O2^{iii}	0.90 (1)	1.96 (1)	2.8347 (9)	163 (1)
N4—H9$\cdots$O2^{vi}	0.90 (1)	1.96 (1)	2.8328 (9)	164 (1)
N4—H10$\cdots$O6	0.90 (1)	1.93 (1)	2.8250 (10)	178 (1)
N4—H11$\cdots$O3^{vii}	0.90 (1)	1.91 (1)	2.7841 (9)	163 (1)
N4—H12$\cdots$O2	0.90 (1)	1.97 (1)	2.8508 (10)	168 (1)

Symmetry codes: (i) x, y+1, z; (ii) −x+3/2, y+1/2, −z+3/2; (iii) −x+1, −y+1, −z+1; (iv) −x+1, −y, −z+1; (v) x+1, y, z; (vi) −x+1/2, y−1/2, −z+3/2; (vii) −x+1/2, y+1/2, −z+3/2.

Table S8. Complexity parameters calculated with the crystIT program

	atoms per unit cell	atoms per reduced unit cell	positions per reduced unit cell	unique species	Coordinatorial degrees of freedom (arity sum)	I_comb in bit/position	I_comb_max in bit/position
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(I)	96	96	96	24	72	4.584963	4.584963
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(II)	96	96	96	48	144	5.584963	5.584963
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(III)	96	96	96	24	72	4.584963	4.584963
$(NH_4)_2SeO_4 \cdot 3NH_4NO_3$-(I)	84	84	90	51	135	5.600861	5.672425
$(NH_4)_2SeO_4 \cdot 3NH_4NO_3$-(II)	168	168	168	42	126	5.392317	5.392317
$(NH_4)_2CrO_4 \cdot 3NH_4NO_3$-(I)	84	84	90	51	135	5.610320	5.672425
$(NH_4)_2CrO_4 \cdot 3NH_4NO_3$-(II)	168	168	180	51	135	5.624767	5.672425

	I_comb_norm	I_comb_tot in bit/reduced unit cell	I_comb_density in bit/Å³	I_coor in bit/freedom	I_coor_max in bit/freedom	I_coor_norm
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(I)	1.000000	440.156400	0.502589	4.584963	4.584963	1.000000
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(II)	1.000000	536.156400	0.610669	5.584963	5.584963	1.000000
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(III)	1.000000	440.156400	0.495406	4.584963	4.584963	1.000000
$(NH_4)_2SeO_4 \cdot 3NH_4NO_3$-(I)	0.987384	504.077458	0.661946	5.491853	5.491853	1.000000
$(NH_4)_2SeO_4 \cdot 3NH_4NO_3$-(II)	1.000000	905.909327	0.612742	5.392317	5.392317	1.000000
$(NH_4)_2CrO_4 \cdot 3NH_4NO_3$-(I)	0.989051	504.928803	0.671452	5.491853	5.491853	1.000000
$(NH_4)_2CrO_4 \cdot 3NH_4NO_3$-(II)	0.991598	1012.458090	0.694099	5.491853	5.491853	1.000000

	I_coor_tot in bit/reduced unit cell	I_coor_density in bit/Å³	I_conf in bit/(position + freedom)	I_conf_max in bit/(position + freedom)	I_conf_norm	I_conf_tot in bit/ reduced unit cell	I_conf_density in bit/Å³
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(I)	330.1173	0.376942	5.570191	5.584963	0.997355	935.792027	1.068527
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(II)	804.2346	0.916003	6.555913	6.584963	0.995589	1573.419143	1.792084
$(NH_4)_2PO_3F \cdot NH_4NO_3$-(III)	330.1173	0.371554	5.570191	5.584963	0.997355	935.792027	1.053255
$(NH_4)_2SeO_4 \cdot 3NH_4NO_3$-(I)	741.4002	0.973595	6.506407	6.584963	0.988070	1463.941510	1.922424
$(NH_4)_2SeO_4 \cdot 3NH_4NO_3$-(II)	679.4320	0.459557	6.377546	6.392317	0.997689	1874.998394	1.268218
$(NH_4)_2CrO_4 \cdot 3NH_4NO_3$-(I)	741.4002	0.985911	6.510190	6.584963	0.988645	1464.792855	1.947875
$(NH_4)_2CrO_4 \cdot 3NH_4NO_3$-(II)	741.4002	0.508273	6.553032	6.584963	0.995151	2064.205121	1.415133

Definitions of parameters given in Kaußler, C.; Kieslich, G. *crystIT*: complexity and configurational entropy of crystal structures via information theory. *J. Appl. Crystallogr.* **2021**, *54*, 306-316.

Table S9. Absolute atomic displacements ($|u|$ /Å) of the pair $(NH_4)_2PO_3F \cdot NH_4NO_3$-(I) and -(III), and of $(NH_4)_2XO_4 \cdot 3NH_4NO_3$ crystal structures in space group $P2_1$ (reference structure $(NH_4)_2SO_4 \cdot 3NH_4NO_3$), as well as their lattice distortion (S), arithmetic mean distance d_{av} /Å and measure of similarity (δ). For all calculations, H atoms in the crystal structures were not considered for comparison; for the disordered nitrate group in the $(NH_4)_2XO_4 \cdot 3NH_4NO_3$ structures, only atoms of the major orientation were taken into account.

$(NH_4)_2PO_3F \cdot NH_4NO_3$-(I) and -(III)		$(NH_4)_2XO_4 \cdot 3NH_4NO_3$		
Atom pair	$|u|$	Atom pair	$|u|$ /Å for X = Se	$|u|$ /Å for X = Cr
O3	0.1290	O13	0.0126	0.0445
O1	0.1352	O11	0.0280	0.1368
P1	0.1361	O10	0.0270	0.1476
O2	0.1629	X1	0.0308	0.1026
N3	0.1746	O9	0.0361	0.1007
N2	0.2866	N2	0.0374	0.0425
F1	0.2967	N1	0.0407	0.0915
N4	0.5936	N8	0.0429	0.0247
N1	0.8871	O8	0.0473	0.1173
O4	1.0942	N3	0.0544	0.1467
O5	1.3640	O12	0.0516	0.2149
O6	2.3975	O7	0.0559	0.1561
		N4	0.0711	0.0703
		N6	0.0709	0.0442
		N7	0.0760	0.0726
		O6	0.0845	0.1435
		N5	0.1039	0.2391
		O1	0.1182	0.2207
		O5	0.1353	0.2547
		O3	0.1526	0.1871
		O2	0.1530	0.1720
		O4	0.1704	0.3629
S	0.0238		0.0074	0.0056
$d_{av.}$ (Å)	0.6381		0.0728	0.1406
δ	0.280		0.014	0.092

Table S10. (NH$_4$)$_2$SeO$_4$·3NH$_4$NO$_3$-(I). Numerical details of hydrogen-bonding interactions at 50 °C.

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O2[i]	0.95	1.91	2.840 (4)	167
N4—H4B···O13A	0.87	2.37	3.190 (7)	156
N4—H4B···O13B	0.87	2.16	2.92 (2)	146
N4—H4C···O7	0.98	2.39	3.083 (5)	128
N4—H4C···O8[ii]	0.98	2.18	3.007 (5)	141
N4—H4D···O12B[i]	0.82	2.47	3.096 (18)	134
N5—H5A···O4[i]	0.95	1.79	2.721 (4)	165
N5—H5B···O6[ii]	0.98	2.27	2.994 (6)	130
N5—H5C···O7[i]	0.92	2.18	2.965 (6)	144
N5—H5D···O13A	0.95	2.03	2.973 (6)	173
N6—H6A···O4	0.96	2.10	3.027 (6)	162
N6—H6B···O1[iii]	0.98	1.93	2.891 (5)	165
N6—H6C···O6[iv]	0.93	2.20	3.017 (6)	145
N6—H6D···O5	0.78	2.46	3.159 (5)	150
N6—H6D···O11A	0.78	2.48	3.006 (5)	126
N7—H7A···O2[vi]	0.98	2.01	2.916 (3)	154
N7—H7B···O1[iii]	1.03	2.26	3.193 (6)	150
N7—H7B···O2[iii]	1.03	2.16	2.997 (8)	137
N7—H7C···O3	0.85	2.18	2.957 (6)	151
N7—H7D···O8	0.87	2.27	2.973 (5)	137
N7—H7D···O9	0.87	2.33	2.996 (5)	134
N8—H8A···O3[vi]	0.91	2.14	2.925 (4)	144
N8—H8B···O1[vii]	0.94	2.09	3.001 (5)	161
N8—H8C···O10[iii]	0.92	2.16	3.069 (5)	167
N8—H8D···O8	0.96	2.11	3.008 (5)	154

Symmetry codes: (i) −x+2, y−1/2, −z+1; (ii) −x+2, y+1/2, −z+1; (iii) x, y−1, z; (iv) −x+1, y+1/2, −z+1; (v) x−1, y, z; (vi) −x+2, y−1/2, −z+2; (vii) x+1, y−1, z.

Table S11. (NH$_4$)$_2$SeO$_4$·3NH$_4$NO$_3$-(II). Numerical details of hydrogen-bonding interactions at −173 °C.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N4—H4A⋯O13[i]	0.88 (1)	2.12 (1)	2.9373 (12)	155 (2)
N4—H4B⋯O12[ii]	0.88 (1)	2.37 (1)	3.0097 (13)	131 (1)
N4—H4B⋯O13[iii]	0.88 (1)	2.29 (1)	3.0332 (12)	143 (1)
N4—H4C⋯O7	0.88 (1)	2.12 (1)	2.9133 (12)	149 (2)
N4—H4D⋯O2[ii]	0.89 (1)	1.92 (1)	2.8052 (11)	172 (2)
N5—H5A⋯O6[iv]	0.89 (1)	2.10 (1)	2.8903 (12)	149 (1)
N5—H5B⋯O4[v]	0.88 (1)	1.90 (1)	2.7654 (11)	168 (2)
N5—H5C⋯O13[vi]	0.89 (1)	2.02 (1)	2.8969 (12)	168 (2)
N5—H5D⋯O7[v]	0.88 (1)	2.05 (1)	2.9116 (12)	166 (2)
N6—H6A⋯O4	0.88 (1)	2.02 (1)	2.8977 (11)	172 (2)
N6—H6B⋯O1[iii]	0.88 (1)	1.95 (1)	2.8122 (11)	167 (2)
N6—H6C⋯O6[iv]	0.89 (1)	2.35 (2)	2.9186 (12)	122 (1)
N6—H6C⋯O10	0.89 (1)	2.26 (1)	3.0504 (11)	148 (2)
N6—H6D⋯O5	0.88 (1)	2.39 (1)	3.1036 (12)	139 (1)
N6—H6D⋯O5[v]	0.88 (1)	2.44 (1)	3.0939 (12)	132 (1)
N7—H7A⋯O2[iii]	0.88 (1)	1.99 (1)	2.8663 (11)	171 (2)
N7—H7B⋯O9[vii]	0.89 (1)	2.14 (1)	2.9551 (12)	152 (2)
N7—H7C⋯O3	0.89 (1)	1.93 (1)	2.8202 (11)	173 (2)
N7—H7D⋯O2[viii]	0.90 (1)	2.00 (1)	2.8718 (11)	166 (2)
N8—H8A⋯O10	0.89 (1)	2.15 (1)	2.9772 (12)	154 (2)
N8—H8B⋯O3[ix]	0.89 (1)	2.33 (2)	2.9699 (11)	129 (1)
N8—H8B⋯O10[ix]	0.89 (1)	2.46 (2)	3.1260 (12)	132 (1)
N8—H8C⋯O8[x]	0.90 (1)	1.97 (1)	2.8643 (12)	174 (2)
N8—H8D⋯O1	0.89 (1)	1.98 (1)	2.8650 (12)	172 (2)

Symmetry codes: (i) −x+2, y−3/2, −z+3/2; (ii) −x+2, y−1/2, −z+3/2; (iii) x, y−1, z; (iv) −x+1, y+1/2, −z+3/2; (v) −x+1, y−1/2, −z+3/2; (vi) x−1, y−1, z; (vii) x+1, y, z; (viii) −x+2, −y+1, −z+2; (ix) −x+1, −y+1, −z+2; (x) x, y+1, z.

Table S12. (NH$_4$)$_2$CrO$_4$·3NH$_4$NO$_3$-(I). Numerical details of hydrogen-bonding interactions at 60 °C.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N4—H4A···O2^i	0.95	1.88	2.804 (5)	166
N4—H4B···O13A	0.87	2.47	3.286 (13)	157
N4—H4B···O13B	0.87	2.23	3.03 (3)	153
N4—H4C···O7	0.97	2.39	3.098 (9)	129
N4—H4C···O8^{ii}	0.97	2.16	2.974 (10)	141
N4—H4D···O9^i	0.82	2.48	3.072 (10)	131
N5—H5A···O4^i	0.95	1.79	2.735 (6)	174
N5—H5B···O6^{ii}	0.97	2.25	2.983 (12)	131
N5—H5C···O7^i	0.91	2.16	2.920 (11)	141
N5—H5C···O11A^i	0.91	2.43	3.074 (19)	128
N5—H5D···O13A	0.94	2.02	2.965 (13)	179
N5—H5D···O13B	0.94	2.34	3.28 (3)	173
N6—H6A···O3	0.95	2.25	2.877 (10)	123
N6—H6A···O4	0.95	2.44	3.345 (15)	158
N6—H6B···O1^{iv}	0.97	1.91	2.853 (10)	162
N6—H6C···O6^v	0.93	2.17	2.990 (12)	146
N6—H6D···O5	0.78	2.61	3.292 (8)	148
N6—H6D···O11A	0.78	2.46	3.019 (9)	130
N7—H7A···O2^{vii}	0.98	1.95	2.855 (5)	153
N7—H7B···O1^{iv}	1.03	2.12	3.047 (10)	150
N7—H7B···O2^{iv}	1.03	2.22	3.032 (15)	135
N7—H7C···O2	0.85	2.45	3.100 (16)	134
N7—H7C···O3	0.85	2.23	2.988 (10)	149
N7—H7D···O8	0.87	2.35	3.019 (9)	134
N7—H7D···O9	0.87	2.28	2.974 (8)	137
N8—H8A···O3^{vii}	0.91	2.17	2.958 (8)	145
N8—H8B···O1^{ix}	0.94	2.13	3.027 (8)	159
N8—H8C···O10^{iv}	0.92	2.26	3.164 (14)	168
N8—H8D···O8	0.96	2.09	2.971 (10)	152

Symmetry codes: (i) −x+2, y−1/2, −z+1; (ii) −x+2, y+1/2, −z+1; (iii) x+1, y, z; (iv) x, y−1, z; (v) −x+1, y+1/2, −z+1; (vi) x−1, y, z; (vii) −x+2, y−1/2, −z+2; (viii) −x+2, y−3/2, −z+2; (ix) x+1, y−1, z.

Table S13. (NH$_4$)$_2$CrO$_4$·3NH$_4$NO$_3$-(II). Numerical details of hydrogen-bonding interactions at −173 °C

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O12[i]	0.88 (1)	2.21 (2)	2.999 (2)	148 (3)
N4—H4B···O2[i]	0.89 (1)	1.88 (1)	2.774 (2)	173 (3)
N4—H4C···O6A	0.88 (1)	2.19 (2)	2.923 (6)	140 (3)
N4—H4C···O5B	0.88 (1)	2.18 (2)	2.951 (6)	145 (3)
N4—H4D···O13[iii]	0.89 (1)	2.05 (1)	2.927 (2)	171 (3)
N5—H5A···O5A[iv]	0.89 (1)	2.09 (2)	2.848 (7)	143 (3)
N5—H5A···O7B[iv]	0.89 (1)	2.23 (1)	3.113 (4)	171 (3)
N5—H5B···O6A[v]	0.89 (1)	2.09 (2)	2.937 (6)	158 (3)
N5—H5B···O6B[v]	0.89 (1)	1.99 (2)	2.851 (5)	162 (3)
N5—H5C···O4[v]	0.90 (1)	1.85 (1)	2.741 (2)	172 (3)
N5—H5D···O13[vi]	0.89 (1)	2.06 (1)	2.942 (2)	169 (3)
N6—H6A···O4	0.89 (1)	2.06 (1)	2.941 (2)	177 (3)
N6—H6B···O5A[iv]	0.89 (1)	2.13 (2)	2.833 (7)	136 (3)
N6—H6B···O5B[iv]	0.89 (1)	2.26 (2)	3.051 (6)	148 (3)
N6—H6C···O7B	0.88 (1)	2.32 (2)	3.154 (3)	159 (3)
N6—H6D···O1[ii]	0.89 (1)	1.95 (1)	2.836 (2)	178 (3)
N7—H7A···O2[vii]	0.90 (1)	1.98 (2)	2.834 (2)	159 (3)
N7—H7B···O9[viii]	0.90 (1)	2.11 (2)	2.911 (2)	148 (3)
N7—H7C···O2[ii]	0.89 (1)	2.02 (1)	2.881 (2)	163 (3)
N7—H7D···O3	0.90 (1)	1.99 (1)	2.871 (2)	167 (3)
N8—H8A···O1	0.90 (1)	1.98 (1)	2.874 (2)	171 (3)
N8—H8B···O8[ix]	0.90 (1)	1.99 (1)	2.885 (2)	171 (3)
N8—H8C···O3[xi]	0.90 (1)	2.28 (2)	2.964 (2)	133 (2)
N8—H8C···O10[xi]	0.90 (1)	2.56 (3)	3.114 (2)	121 (2)
N8—H8D···O10	0.90 (1)	2.07 (1)	2.935 (2)	160 (3)

Symmetry codes: (i) −x+2, y−1/2, −z+3/2; (ii) x, y−1, z; (iii) −x+2, y−3/2, −z+3/2; (iv) −x+1, y+1/2, −z+3/2; (v) −x+1, y−1/2, −z+3/2; (vi) x−1, y−1, z; (vii) −x+2, −y+1, −z+2; (viii) x+1, y, z; (ix) x, y+1, z; (x) −x+1, −y+2, −z+2; (xi) −x+1, −y+1, −z+2.