Supporting Information

Monoammonium trimetaphosphimate $(NH_4)H_2(PO_2NH)_3$

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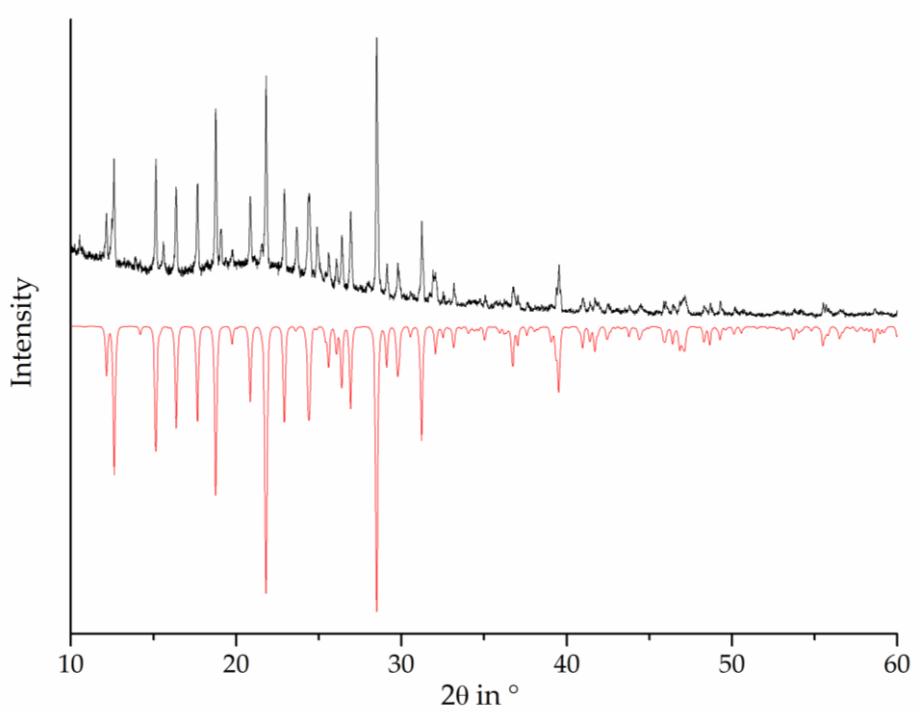


Figure S1: Comparison of measured (black) and calculated (red, based on the single-crystal data) PXRD pattern of $(NH_4)H_2(PO_2NH)_3$.

Table S1: Atomic coordinates and Wyckoff positions from single-crystal data of $(NH_4)H_2(PO_2NH)_3$

	Wyckoff	x	y	z	s.o.f.	U_{eq}/U_{iso}
P1	4*e*	0.22067(3)	0.40213(2)	0.57771(2)	1	0.01610(10)
P2	4*e*	0.21941(3)	0.19791(2)	0.53761(2)	1	0.01505(9)
P3	4*e*	0.07432(3)	0.32215(2)	0.36152(2)	1	0.01523(9)
O1	4*e*	0.32018(9)	0.11981(7)	0.55770(8)	1	0.02307(19)
O2	4*e*	0.08092(9)	0.16515(7)	0.55722(8)	1	0.02198(19)
HO2	4*e*	0.0902(18)	0.1544(14)	0.6260(12)	1	0.033
O3	4*e*	0.32661(9)	0.45497(7)	0.53699(8)	1	0.0253(2)
O4	4*e*	0.12235(10)	0.37712(7)	0.26971(7)	1	0.0243(2)
O5	4*e*	-0.06252(9)	0.28118(7)	0.33082(7)	1	0.0229(2)
O6	4*e*	0.17275(10)	0.44816(8)	0.67998(8)	1	0.0282(2)
HO6	4*e*	0.2324(16)	0.4830(13)	0.7274(14)	1	0.042
N1	4*e*	0.08299(10)	0.38613(8)	0.48082(8)	1	0.0172(2)
HN1	4*e*	0.0106(15)	0.3790(13)	0.5119(14)	1	0.026
N2	4*e*	0.18632(10)	0.23440(8)	0.40340(8)	1	0.0180(2)
HN2	4*e*	0.2546(15)	0.2347(13)	0.3689(15)	1	0.027
N3	4*e*	0.26952(11)	0.29131(8)	0.61756(9)	1	0.0224(2)
HN3	4*e*	0.3383(16)	0.2832(13)	0.6794(14)	1	0.034
P11	4*e*	0.30618(3)	0.90489(2)	0.41159(2)	1	0.01678(10)
P12	4*e*	0.26143(3)	0.70359(2)	0.44876(2)	1	0.01585(9)
P13	4*e*	0.42080(3)	0.81738(2)	0.63251(2)	1	0.01500(9)
O11	4*e*	0.14349(9)	0.64093(7)	0.42120(8)	1	0.0254(2)
O12	4*e*	0.39386(9)	0.66084(7)	0.42755(8)	1	0.02244(19)
HO12	4*e*	0.3837(18)	0.6522(14)	0.3594(13)	1	0.034
O13	4*e*	0.55228(9)	0.77015(7)	0.67486(7)	1	0.0221(2)
O14	4*e*	0.36701(10)	0.87916(7)	0.71569(7)	1	0.02338(19)
O15	4*e*	0.20566(9)	0.96253(7)	0.46835(9)	1	0.0264(2)
HO15	4*e*	0.2427(18)	1.0104(12)	0.5062(15)	1	0.040
O16	4*e*	0.34693(10)	0.95701(8)	0.31611(8)	1	0.0295(2)
N11	4*e*	0.43298(10)	0.87834(8)	0.51436(8)	1	0.0171(2)
HN11	4*e*	0.5070(15)	0.8751(13)	0.4921(15)	1	0.026
N12	4*e*	0.23209(11)	0.80355(8)	0.37274(9)	1	0.0217(2)
HN12	4*e*	0.1694(17)	0.7994(13)	0.3099(13)	1	0.033
N13	4*e*	0.30117(10)	0.73697(8)	0.58363(8)	1	0.0181(2)
HN13	4*e*	0.2357(16)	0.7350(13)	0.6211(15)	1	0.027
N21	4*e*	0.54842(12)	0.56220(9)	0.65633(11)	1	0.0254(2)
H21A	4*e*	0.6044(18)	0.5572(14)	0.6126(15)	1	0.038
H21B	4*e*	0.5398(19)	0.6207(11)	0.6597(16)	1	0.038
H21C	4*e*	0.4745(16)	0.5403(14)	0.6254(15)	1	0.038
H21D	4*e*	0.5851(19)	0.5356(14)	0.7230(14)	1	0.038
N22	4*e*	0.07235(15)	0.57064(10)	0.19386(13)	1	0.0348(3)
H22A	4*e*	0.017(2)	0.5886(15)	0.1361(16)	1	0.052
H22B	4*e*	0.076(2)	0.5983(15)	0.2581(15)	1	0.052
H22C	4*e*	0.087(2)	0.5144(12)	0.2213(19)	1	0.052
H22D	4*e*	0.1467(18)	0.5780(16)	0.1721(19)	1	0.052

Table S2: Anisotropic displacement parameters (U_{ij} in Å²) with standard deviations in parentheses.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	0.01559(15)	0.01791(16)	0.01378(15)	-0.00367(10)	0.00056(11)	-0.00264(10)
P2	0.01485(15)	0.01667(16)	0.01287(15)	0.00057(10)	0.00099(10)	0.00008(10)
P3	0.01634(16)	0.01881(17)	0.00944(15)	-0.00072(10)	-0.00004(11)	-0.00040(10)
O1	0.0203(4)	0.0217(4)	0.0264(4)	0.0034(3)	0.0029(3)	0.0042(3)
O2	0.0195(4)	0.0272(5)	0.0197(4)	0.0008(3)	0.0051(3)	-0.0037(3)
O3	0.0207(4)	0.0259(5)	0.0294(5)	-0.0010(4)	0.0053(3)	-0.0063(4)
O4	0.0341(5)	0.0245(5)	0.0153(4)	0.0031(3)	0.0074(3)	-0.0002(4)
O5	0.0179(4)	0.0315(5)	0.0165(4)	-0.0037(3)	-0.0034(3)	-0.0034(3)
O6	0.0251(5)	0.0379(6)	0.0216(4)	-0.0155(4)	0.0049(4)	-0.0055(4)
N1	0.0153(4)	0.0218(5)	0.0138(4)	-0.0045(4)	0.0008(3)	0.0003(4)
N2	0.0201(5)	0.0224(5)	0.0118(4)	0.0010(4)	0.0037(3)	0.0040(4)
N3	0.0250(5)	0.0199(5)	0.0172(5)	-0.0008(4)	-0.0078(4)	-0.0021(4)
P11	0.01571(16)	0.01884(16)	0.01420(15)	0.00429(10)	-0.00071(11)	0.00153(10)
P12	0.01530(15)	0.01889(17)	0.01255(15)	-0.00171(10)	0.00088(11)	-0.00124(10)
P13	0.01630(16)	0.01829(16)	0.00923(15)	0.00056(10)	-0.00021(11)	-0.00042(10)
O11	0.0225(4)	0.0299(5)	0.0230(4)	-0.0066(4)	0.0029(3)	-0.0083(4)
O12	0.0213(4)	0.0284(5)	0.0180(4)	-0.0012(4)	0.0050(3)	0.0048(3)
O13	0.0194(4)	0.0261(5)	0.0174(4)	0.0031(3)	-0.0042(3)	0.0009(3)
O14	0.0317(5)	0.0240(5)	0.0152(4)	-0.0032(3)	0.0066(3)	-0.0003(4)
O15	0.0194(4)	0.0233(5)	0.0360(5)	-0.0039(4)	0.0046(4)	0.0028(3)
O16	0.0260(5)	0.0387(6)	0.0222(4)	0.0159(4)	0.0015(4)	0.0004(4)
N11	0.0142(4)	0.0224(5)	0.0137(4)	0.0040(4)	0.0007(3)	-0.0016(4)
N12	0.0237(5)	0.0208(5)	0.0159(5)	0.0006(4)	-0.0075(4)	0.0000(4)
N13	0.0185(4)	0.0246(5)	0.0112(4)	-0.0023(4)	0.0031(3)	-0.0043(4)
N21	0.0243(5)	0.0229(6)	0.0287(6)	0.0010(4)	0.0050(4)	-0.0026(4)
N22	0.0425(7)	0.0255(6)	0.0341(7)	-0.0040(5)	0.0020(6)	-0.0005(6)

Table S3: Hydrogen bonding in $(NH_4)H_2(PO_2NH)_3$: distances between donors, H atoms and acceptors, O-H and N-H distances with soft restraints to 0.85(2) Å and 0.89(2) Å, respectively.

donor atom	H atom	donor-H distance in Å	acceptor atom	H-acceptor distance in Å	donor-acceptor distance in Å	angle donor-H-acceptor in °
O2	HO2	0.822(14)	O4	1.738(14)	2.5567(13)	174(2)
O6	HO6	0.891(15)	O16	1.645(15)	2.5352(15)	177.4(19)
N1	HN1	0.900(14)	O11	1.929(14)	2.8282(14)	178.0(18)
N2	HN2	0.881(14)	O13	2.148(14)	3.0114(14)	166.3(16)
N3	HN3	0.920(14)	O13	1.880(14)	2.7828(13)	166.8(17)
O12	HO12	0.808(14)	O14	1.746(15)	2.5515(13)	174(2)
O15	HO15	0.854(14)	O1	1.778(15)	2.6214(14)	168.6(18)
N11	HN11	0.854(14)	O1	1.980(14)	2.8323(13)	174.8(18)
N12	HN12	0.886(14)	O5	1.830(14)	2.7065(13)	170.0(18)
N13	HN13	0.879(14)	O5	1.986(14)	2.8464(14)	165.8(17)
N21	H21A	0.853(15)	O3	2.057(15)	2.8674(16)	158.5(18)
N21	H21B	0.827(15)	O13	2.104(15)	2.9228(16)	170.6(19)
N21	H21C	0.832(15)	O3	2.049(15)	2.8555(15)	163.2(19)
N21	H21D	0.891(15)	O14	2.332(18)	3.0226(16)	134.3(16)
N22	H22A	0.840(16)	O2	2.560(17)	3.3637(17)	161(2)
N22	H22B	0.854(15)	O11	2.022(16)	2.8417(17)	161(2)
N22	H22C	0.855(16)	O4	2.021(16)	2.8729(17)	174(2)
N22	H22D	0.860(16)	O14	2.293(18)	3.0610(18)	149(2)

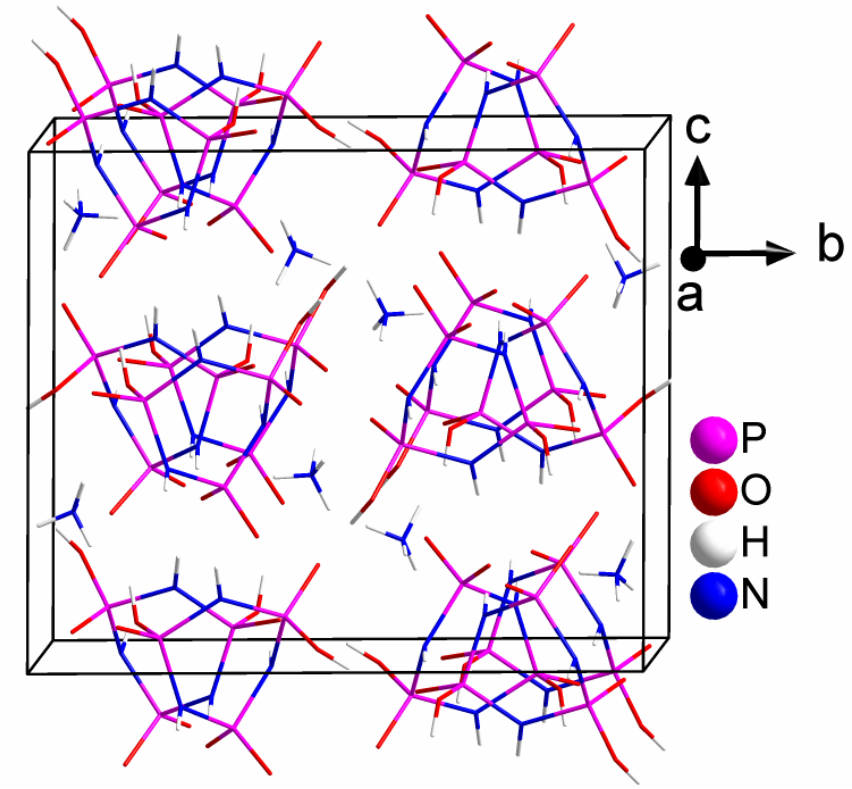


Figure S2: Unit-cell content of $(NH_4)H_2(PO_2NH)_3$.

Table S4: Torsion angles and puckering parameters of both P_3N_3 rings in $(NH_4)H_2(PO_2NH)_3$.

	ring 1	ring 2
torsion angle 1	-57.77(9)°	-54.28(9)°
torsion angle 2	34.05(9)°	36.74(9)°
torsion angle 3	28.30(8)	22.12(9)°
torsion angle 4	-57.25(8)°	-52.60(9)°
torsion angle 5	27.72(10)°	30.76(10)°
torsion angle 6	20.75(9)°	14.21(9)°
q_2	0.7079(9) Å	0.6611(9) Å
q_3	0.0053(9) Å	0.0061(2) Å
Θ	89.57(7)°	89.47(8)°
Φ	147.83(7)°	140.44(7)°

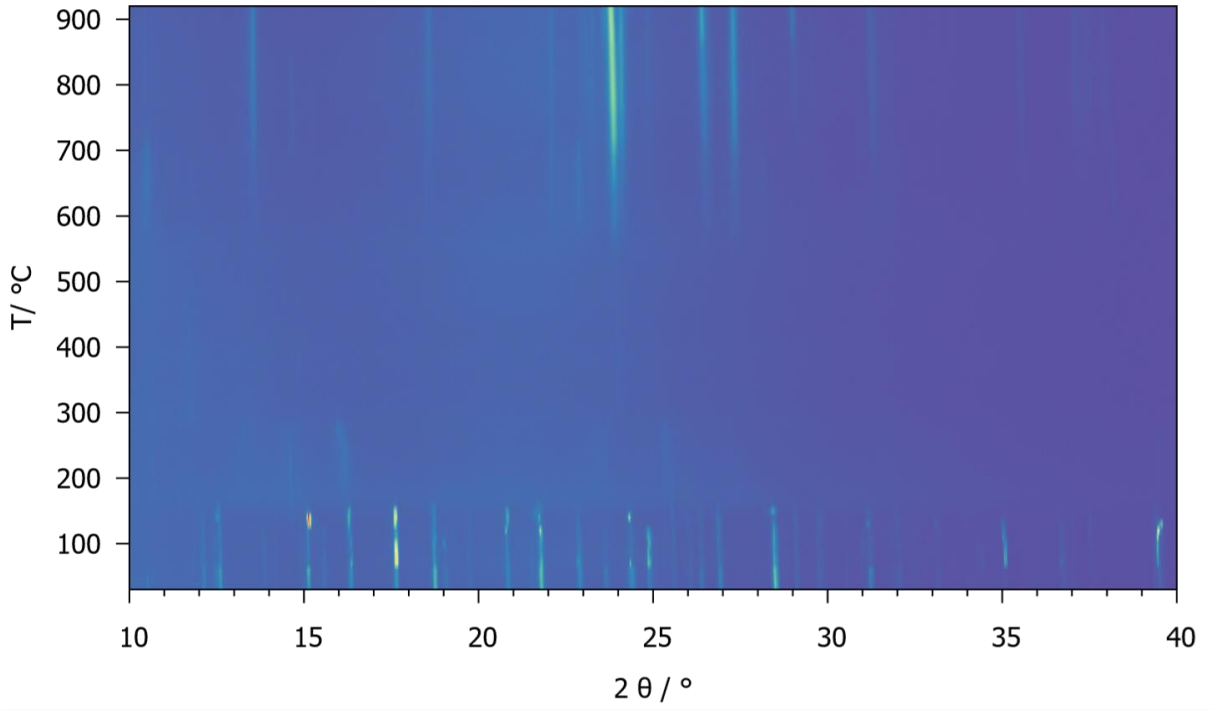


Figure S3: Temperature-dependent PXRD of $(NH_4)H_2(PO_2NH)_3$.