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Supporting information for article:

Migrating hydrogen in 2,4,6-triaminopyrimidinium(1+)*x* hydrogen trioxofluorophosphate(–)*x* monohydrate/2,4,6-triamino-pyrimidinium(2+)(1–*x*) trioxofluorophosphate(2–)(1–*x*) monohydrate (0.0 > *x* < 0.73) with changing temperature

Irena Matulková, Jan Fábry, Ivan Němec, Ivana Císařová and Přemysl Vaněk

Supporting Information

2,4,6-triaminopyrimidinium(1+)$_x$ hydrogen trioxofluorophosphate(1-)$_x$ monohydrate / 2,4,6-triaminopyrimidinium(2+)$_{(1-x)}$ trioxofluorophosphate(2-)$_{(1-x)}$ monohydrate, x∈ <0.0, 0.73>, with changing temperature

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FIGURES

Figure S1: The constituting molecules at measured temperatures. The displacement parameters are shown at the 50% probability level.

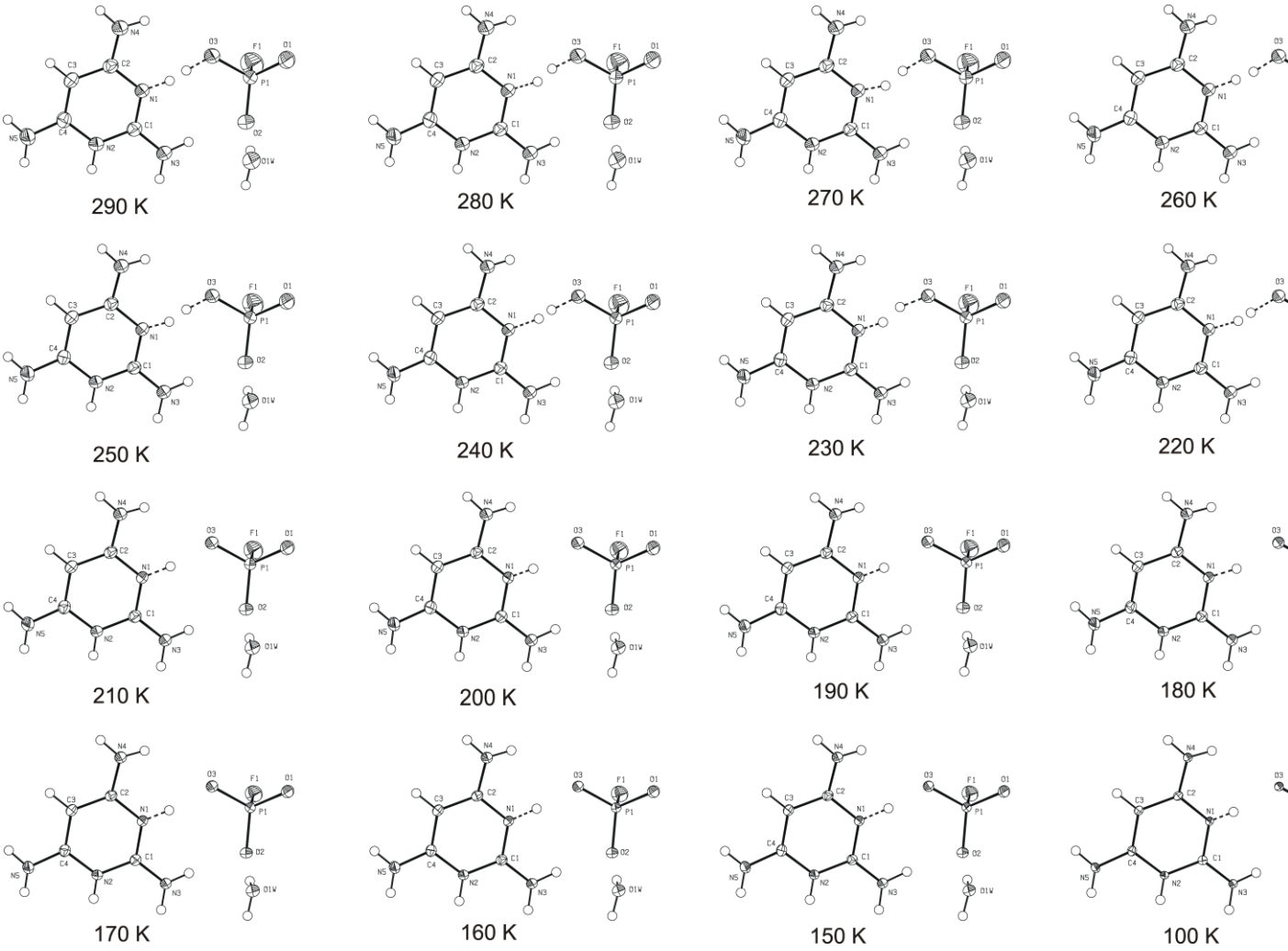
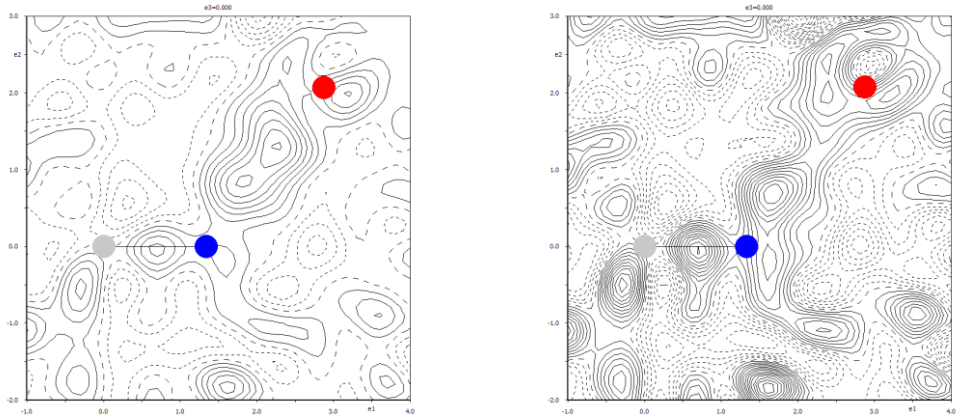


Figure S2: Difference and residual electron density maps in the vicinity of N1...O3 hydrogen bond for the temperatures 290 - 150 K and 100 K.

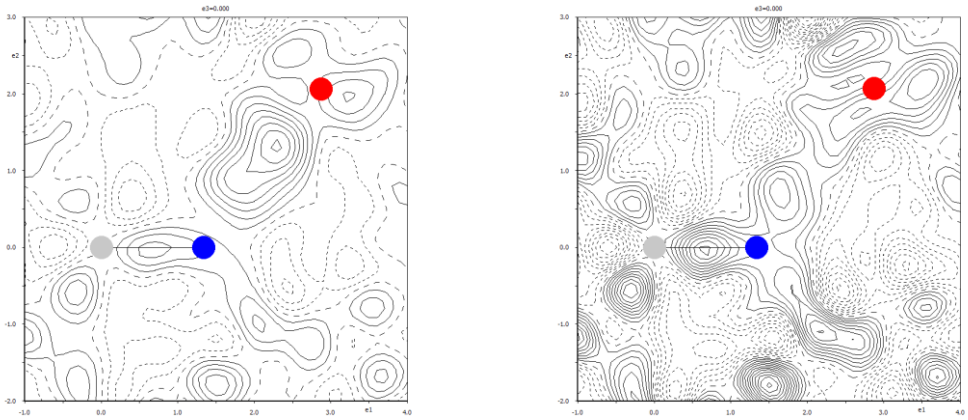
290 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and das hed lines, respec tively.

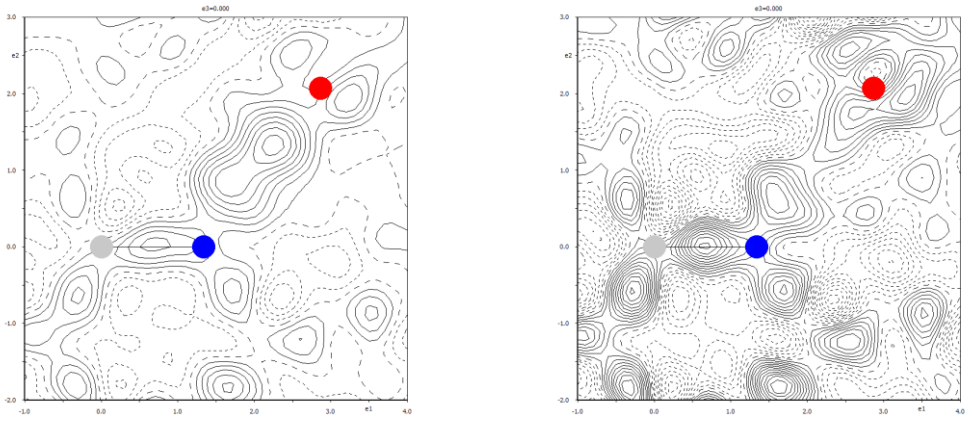
280 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

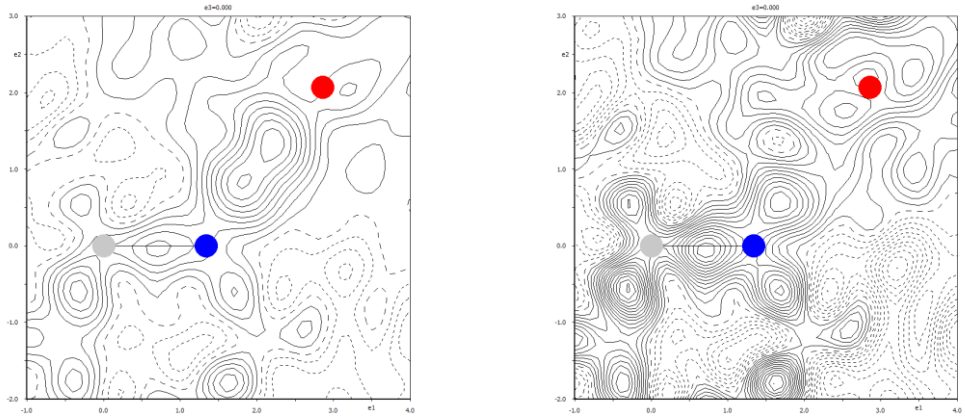
270 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

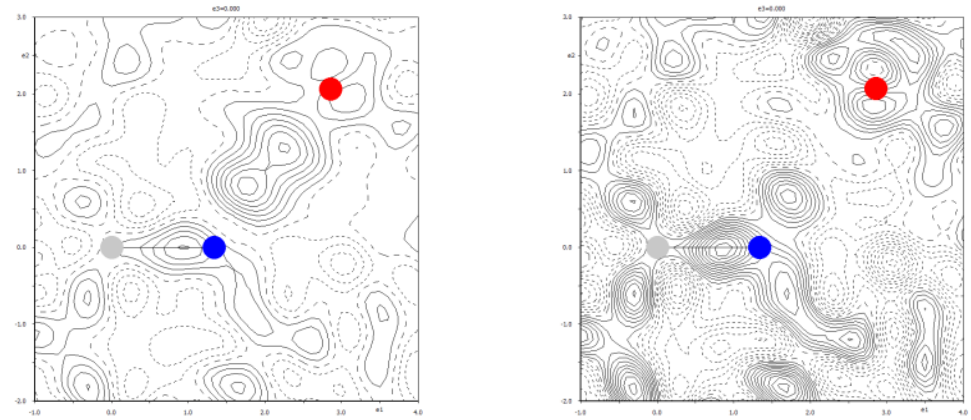
Right: Residual electron density between N1 (green) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

260 K



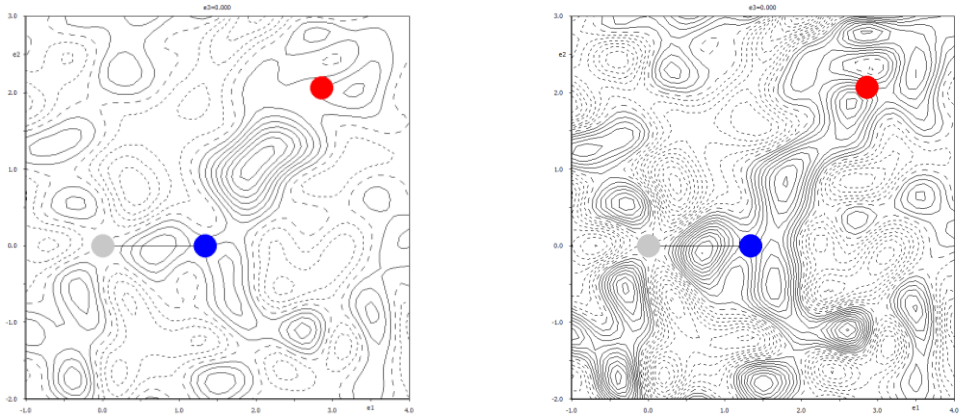
Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

250 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

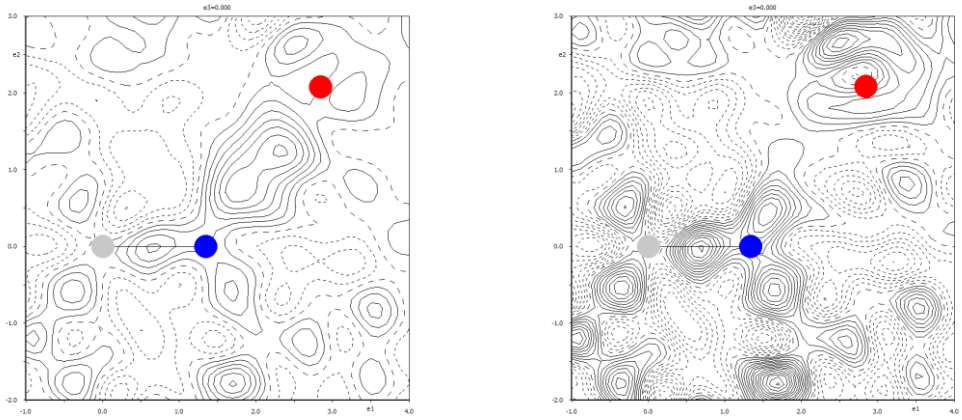
240 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

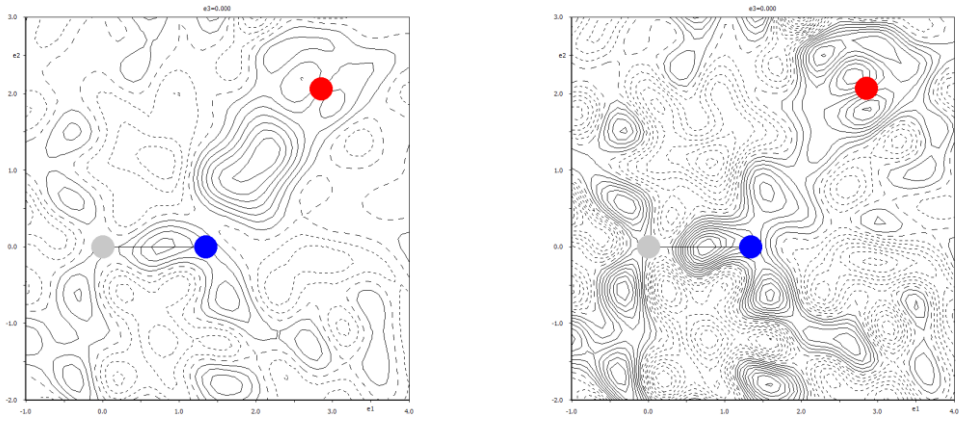
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

230 K



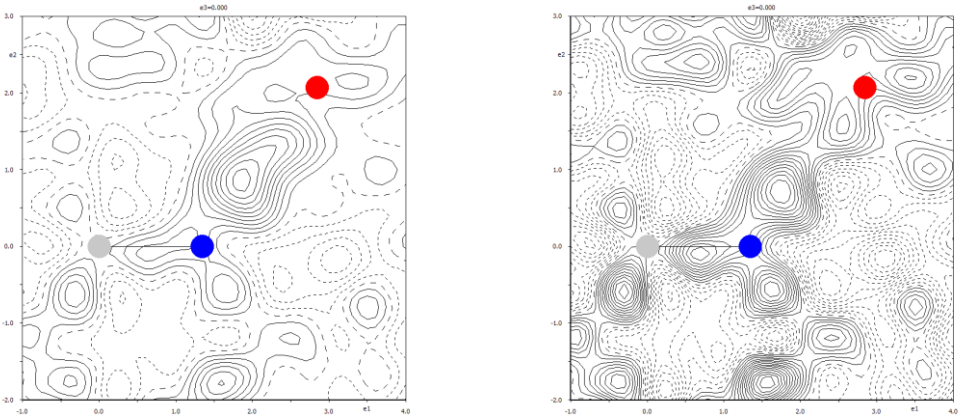
Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

220 K



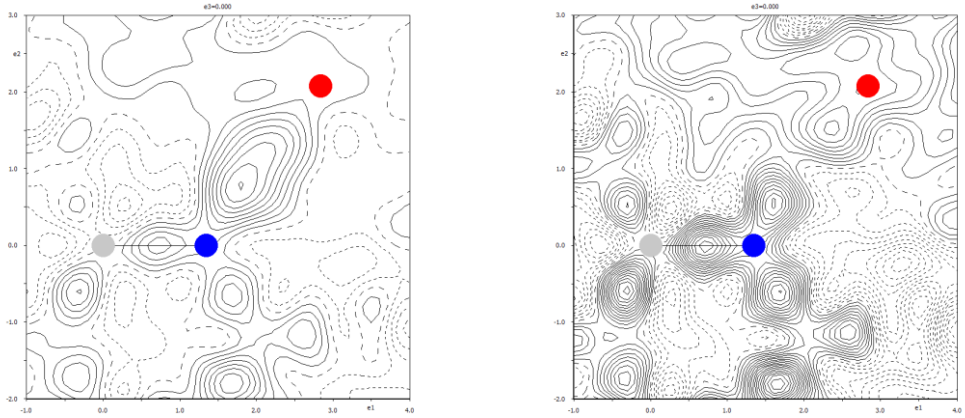
Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

210 K



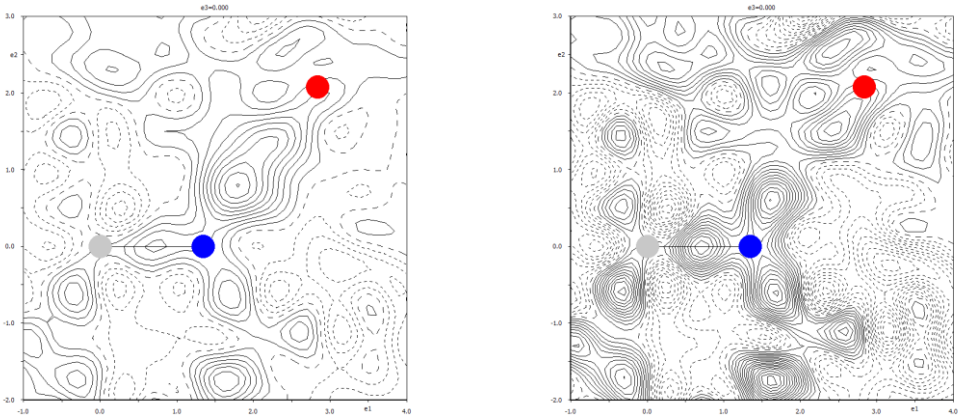
Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

200 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

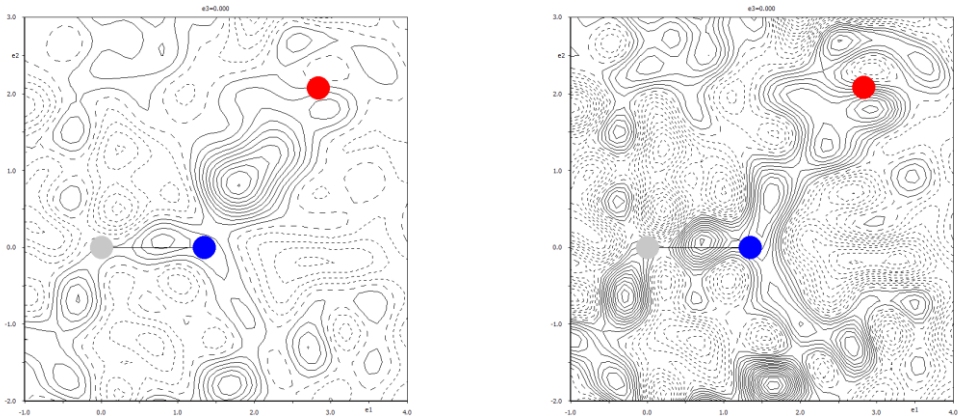
190 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

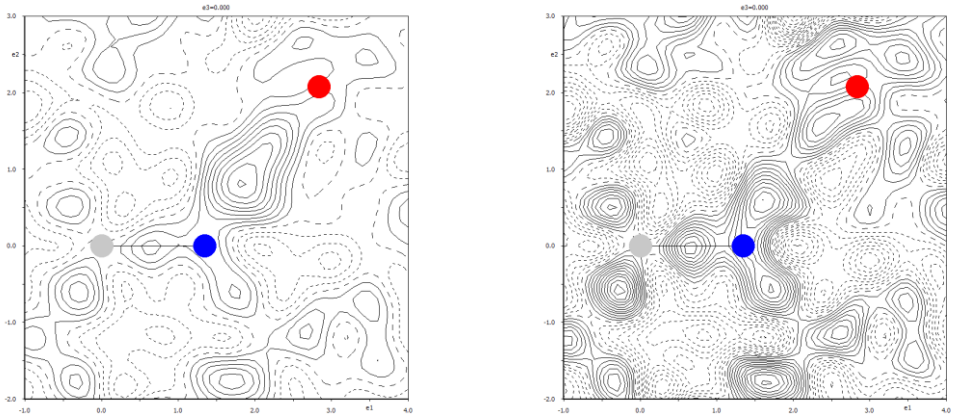
180 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

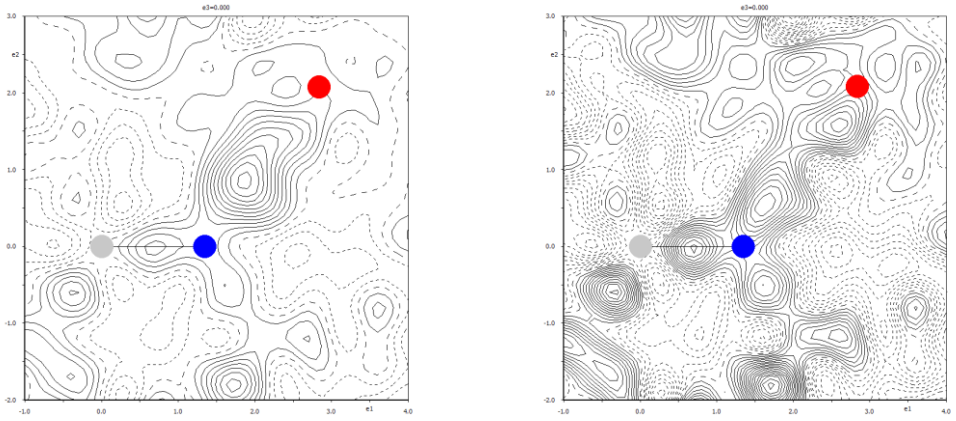
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

170 K



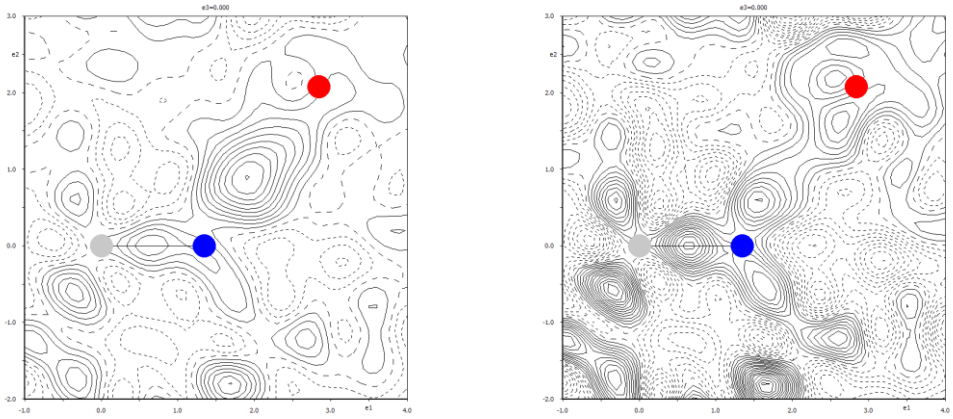
Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

160 K



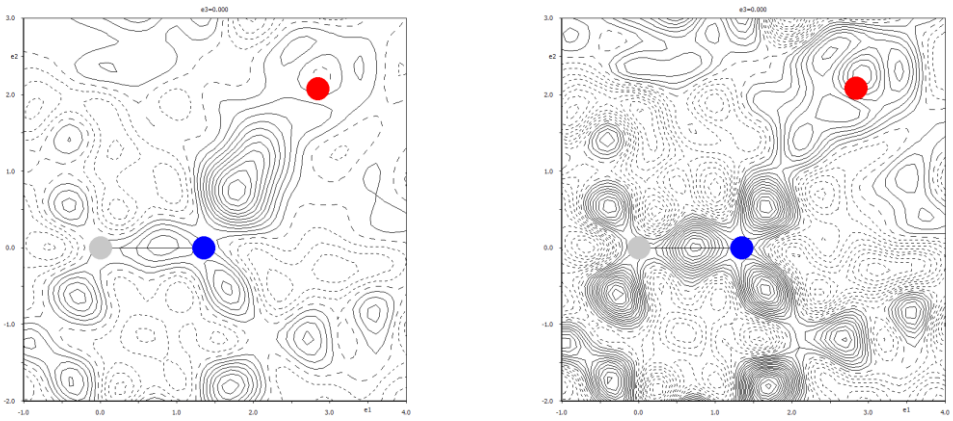
Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

150 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

100 K



Left: Difference electron density between N1 (blue) and O3 (red). H1n1 and H1o3 excluded from the model. The contours are in 0.05 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.
Right: Residual electron density between N1 (blue) and O3 (red). H1n1 and H1o3 included into the model. The contours are in 0.02 eÅ^{-3} increments; positive and negative electron densities are indicated by continuous and dotted lines, respectively.

Figure S3: The dependence of the lattice parameters *a* [Å] on temperature (Uncertainties on all observations are smaller than the symbols.)

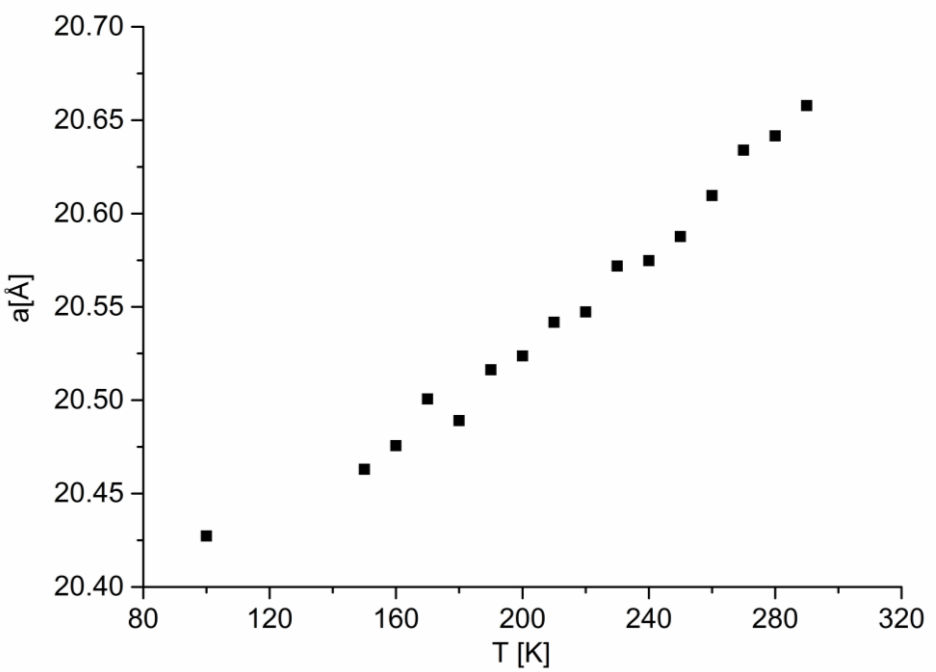


Figure S4: The dependence of the lattice parameters β [°] on temperature (Uncertainties on all observations are smaller than the symbols.)

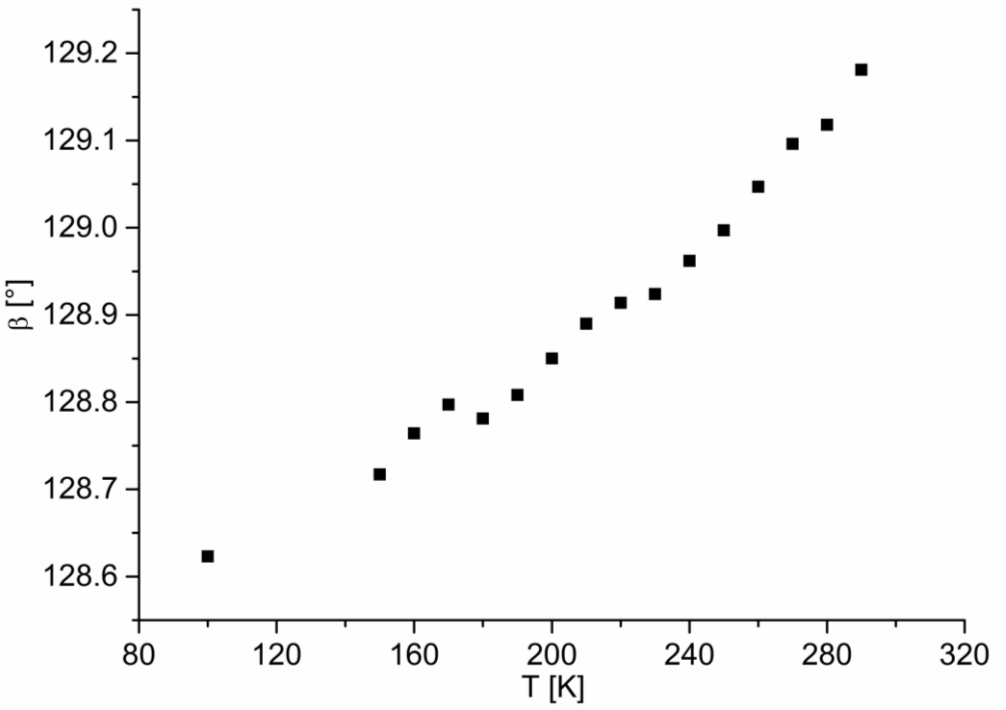


Figure S5: The dependence of the unit cell volume *V* [Å^3] on temperature (Uncertainties on all observations are smaller than the symbols.)

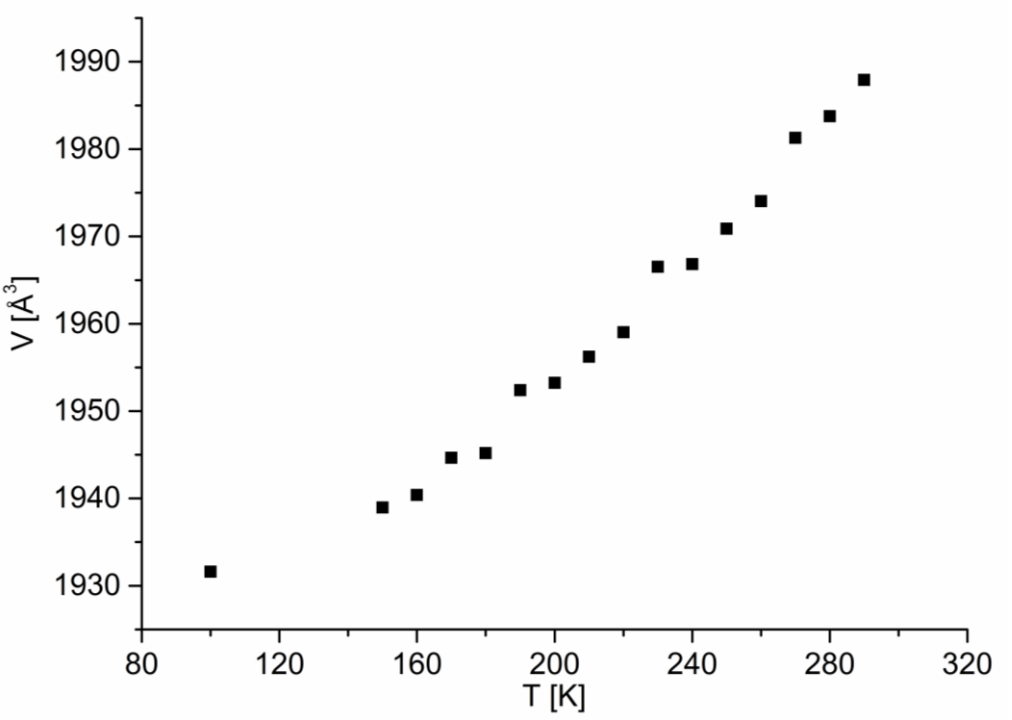
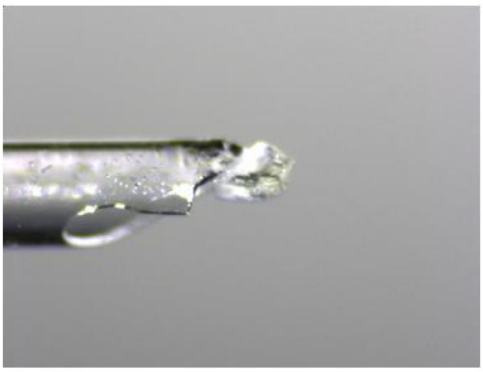
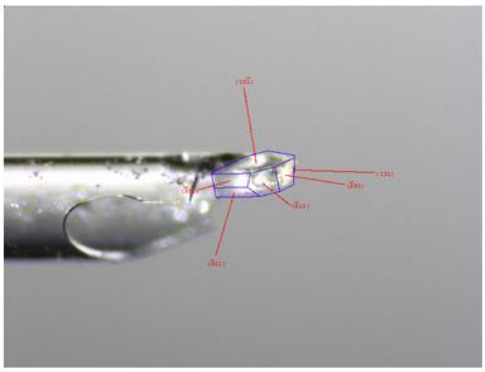


Figure S6: The measured title crystal. Left : without the Miller indices; right with the Miller indices.





TABLES

Table S1: Information about crystal data, details of the data collection and the refinement of the title structures

Crystal data	
Chemical formula	$C_4\ H_{11}\ F\ N_5\ O_4\ P$
	$(C_4N_5H_8)_{0.73}\ (FO_3HP)_{0.73}.(C_4\ N_5\ H_9)_{0.27}\ (FO_3P)_{0.27}\ (H_2O)$ (290 K) $(C_4N_5H_8)_{0.70}\ (FO_3HP)_{0.70}.(C_4\ N_5\ H_9)_{0.30}(FO_3P)_{0.30}\ (H_2O)$ (280 K) $(C_4N_5H_8)_{0.67}\ (FO_3HP)_{0.67}.(C_4\ N_5\ H_9)_{0.33}\ (FO_3P)_{0.33}\ (H_2O)$ (270 K) $(C_4N_5H_8)_{0.61}\ (FO_3HP)_{0.61}.(C_4\ N_5\ H_9)_{0.39}\ (F\ O_3P)_{0.39}\ (H_2O)$ (260 K) $(C_4N_5H_8)_{0.60}\ (FO_3HP)_{0.60}.(C_4\ N_5\ H_9)_{0.40}\ (FO_3P)_{0.40}\ (H_2O)$ (250 K) $(C_4N_5H_8)_{0.64}\ (FO_3HP)_{0.64}.(C_4\ N_5\ H_9)_{0.36}\ (FO_3P)_{0.36}\ (H_2O)$ (240 K) $(C_4N_5H_8)_{0.59}\ (FO_3HP)_{0.59}.(C_4\ N_5\ H_9)_{0.41}\ (FO_3P)_{0.41}\ (H_2O)$ (230 K) $(C_4N_5H_8)_{0.56}\ (FO_3HP)_{0.56}.(C_4\ N_5\ H_9)_{0.44}\ (FO_3P)_{0.44}\ (H_2O)$ (220 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (210 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (200 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (190 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (180 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (170 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (160 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (150 K) $(C_4N_5H_9)\ (FO_3HP)\ (H_2O)$ (100 K)
M_r	243.1
Crystal system, Space group	Monoclinic, C2/c
T (K)	290-150 in 10-K intervals, 100 K
a, *b*, *c* (Å), *β* (°), *V* (Å^3), *T* (K)	20.6578 (6), 8.9220 (2), 13.9144 (5), 129.181 (1), 1987.92 (11) (290K) 20.6416 (7), 8.9068 (2), 13.9075 (5), 129.118 (1), 1983.77 (11) (280 K) 20.6339 (7), 8.8975 (2), 13.9054 (4), 129.096 (1), 1981.28 (10) (270 K) 20.6096 (7), 8.8814 (3), 13.8865 (4), 129.047 (1), 1974.05 (11) (260 K) 20.5877 (6), 8.8673 (2), 13.8912 (4), 128.997 (1), 1970.88 (10) (250 K) 20.5748 (7), 8.8530 (3), 13.8869 (9), 128.962 (1), 1966.83 (16) (240 K) 20.5719 (6), 8.8396 (2), 13.9003 (4), 128.924 (1), 1966.53 (10) (230 K) 20.5473 (7), 8.8249 (2), 13.8851 (5), 128.914 (1), 1959.04 (11) (220 K) 20.5418 (7), 8.8120 (2), 13.8845 (9), 128.890 (1), 1956.23 (15), (210 K) 20.5237 (6), 8.8033 (2), 13.8813 (4), 128.850 (1), 1953.22 (10), (200 K)

	20.5134 (6), 8.7963 (2), 13.8768 (4), 128.806 (1), 1951.27 (10), (190 K) 20.4891 (6), 8.7848 (2), 13.8632 (4), 128.781 (1), 1945.18 (10), (180 K) 20.5006 (7), 8.7803 (2), 13.8618 (5), 128.797 (1), 1944.64 (11), (170 K) 20.4756 (7), 8.7798 (3), 13.8428 (5), 128.764 (1), 1940.40 (12), (160 K) 20.4630 (6), 8.7767 (2), 13.8368 (5), 128.717 (1), 1938.95 (10), (150 K) 20.4273 (6), 8.7714 (2), 13.7988 (7), 128.623 (1), 1931.62 (12), (100 K)	
Z	8	
Radiation type	Mo Kα	
μ (mm^{-1})	0.30 (290 K) 0.30 (280 K) 0.30 (270 K) 0.30 (260 K) 0.30 (250 K) 0.30 (240 K) 0.30 (230 K) 0.30 (220 K)	0.30 (210 K) 0.30 (200 K) 0.30 (190 K) 0.31 (180 K) 0.31 (170 K) 0.31 (160 K) 0.31 (150 K) 0.31 (100 K)
Crystal size	Plate 0.31 × 0.21 × 0.11 mm	
Crystal colour	Light yellow	
Data collection		
Diffractometer	Bruker D8 VENTURE Kappa Duo PHOTON 100 CMOS	
Absorption correction	Multi-scan	
T_{min}, T_{max}	0.913, 0.961 (290 K) 0.918, 0.959 (280 K) 0.918, 0.961 (270 K) 0.919, 0.964 (260 K) 0.915, 0.964 (250 K) 0.918, 0.968 (240 K) 0.910, 0.961 (230 K) 0.914, 0.962 (220 K)	0.921, 0.966 (210 K) 0.910, 0.962 (200 K) 0.915, 0.965 (190 K) 0.912, 0.972 (180 K) 0.914, 0.971 (170 K) 0.910, 0.974 (160 K) 0.910, 0.967 (150 K) 0.909, 0.967 (100 K)
No. of measured, independent and observed [I > 3σ(I)] reflections	8056, 2822, 2091 (290 K) 8158, 2784, 2095 (280 K) 11996, 2881, 2283 (270 K) 12441, 2889, 2444 (260 K) 11320, 2864, 2284 (250 K) 8371, 2850, 2155 (240 K) 8167, 2844, 2313 (230 K)	8452, 2806, 2311 (210 K) 19206, 2834, 2541 (200 K) 8385, 2818, 2355 (190 K) 7156, 2796, 2316 (180 K) 7611, 2744, 2310 (170 K) 8199, 2793, 2288 (160 K) 8948, 2756, 2325 (150 K)

	9737, 2845, 2272 (220 K)	10111, 2789, 2477 (100 K)
R_{int}	0.028 (290 K) 0.026 (280 K) 0.027 (270 K) 0.022 (260 K) 0.027 (250 K) 0.026 (240 K) 0.022 (230 K) 0.025 (220 K)	0.022 (210 K) 0.022 (200 K) 0.021 (190 K) 0.020 (180 K) 0.020 (170 K) 0.022 (160 K) 0.023 (150 K) 0.020 (100 K)
$(\sin \Theta/\lambda)_{max}$ (Å^{-1})	0.704 (290 K) 0.704 (280 K) 0.703 (270 K) 0.704 (260 K) 0.704 (250 K) 0.704 (240 K) 0.703 (230 K) 0.704 (220 K)	0.703 (210 K) 0.703 (200 K) 0.703 (190 K) 0.704 (180 K) 0.703 (170 K) 0.704 (160 K) 0.703 (150 K) 0.703 (100 K)
Refinement		
$R[F > 3\sigma(F)]$, $wR(I)$, S	0.0377, 0.0861, 1.83 (290 K) 0.0356, 0.0866, 1.93 (280 K) 0.0345, 0.0824, 2.02 (270 K) 0.0333, 0.0837, 2.33 (260 K) 0.0344, 0.0788, 1.91 (250 K) 0.0352, 0.0816, 1.80 (240 K) 0.0339, 0.0823, 2.00 (230 K) 0.0337, 0.0790, 1.93 (220 K)	0.0329, 0.0796, 2.02 (210 K) 0.0289, 0.0768, 2.45 (200 K) 0.0323, 0.0808, 2.04 (190 K) 0.0339, 0.0798, 1.97 (180 K) 0.0310, 0.0763, 2.00 (170 K) 0.0315, 0.0795, 1.95 (160 K) 0.0305, 0.0802, 2.07 (150 K) 0.0279, 0.0744, 2.16 (100 K)
No. of reflections	2822 (290 K) 2784 (280 K) 2881 (270 K) 2889 (260 K) 2864 (250 K) 2850 (240 K) 2844 (230 K) 2845 (220 K)	2807 (210 K) 2834 (200 K) 2818 (190 K) 2796 (180 K) 2744 (170 K) 2793 (160 K) 2756 (150 K) 2789 (100 K)
No. of parameters	166 (290 K) 166 (280 K)	165 (210 K) 165 (200 K)

	166 (270 K) 166 (260 K) 166 (250 K) 166 (240 K) 166 (230 K) 166 (220 K)	165 (190 K) 165 (180 K) 165 (170 K) 165 (160 K) 165 (150 K) 165 (100 K)
No. of restraints	2	
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	
Extinction correction	12600(1800) (290 K) 13000(2000) (280 K) 13100(1900) (270 K) 4200(1500) (260 K) 9700(1700) (250 K) 12400(1700) (240 K) 12800(1900) (230 K) 8400(1600) (220 K)	10700(1300) (210 K) 12400(1600) (200 K) 10400(1300) (190 K) 6300(900) (180 K) 7000(2000) (170 K) 6600(1000) (160 K) 6600(1400) (150 K) 6300(1000) (100 K)
$\Delta\rho_{max}$ (e Å^{-3}), $\Delta\rho_{min}$ (e Å^{-3}) (*T* K)	0.31, −0.32 (290 K) 0.30, −0.28 (280 K) 0.30, −0.32 (270 K) 0.32,−0.31 (260 K) 0.28, −0.31 (250 K) 0.26, −0.36 (240 K) 0.31, −0.32 (230 K) 0.29, −0.32 (220 K)	0.34, −0.35 (210 K) 0.40, −0.28 (200 K) 0.38, −0.33 (190 K) 0.39, −0.38 (180 K) 0.32, −0.32 (170 K) 0.36, −0.33 (160 K) 0.35, −0.32 (150 K) 0.41, −0.32 (100 K)

Table S2: Hydrogen bonds in the title structures

Temperature [K]	*D*—H···*A*	*D*—H [Å]	H···*A* [Å]	*D*···*A* [Å]	*D*—H···*A* [◦]
290 K	O3—H1o3···N1	0.9784 (11)	1.6064 (12)	2.5822 (16)	174.75 (6)
290 K	N1—H1n1···O3	0.9670 (12)	1.6255 (11)	2.5822 (16)	169.43 (6)
280 K	O3—H1o3···N1	0.9511 (11)	1.6275 (12)	2.5770 (16)	175.84 (12)
280 K	N1—H1n1···O3	1.0207 (11)	1.5802 (11)	2.5770 (16)	164.05 (6)
270 K	O3—H1o3···N1	0.9629 (10)	1.6167 (10)	2.5750 (14)	172.90 (6)
270 K	N1—H1n1···O3	0.9226 (10)	1.7092 (10)	2.5750 (14)	154.99 (6)
260 K	O3—H1o3···N1	0.9753 (9)	1.6052 (9)	2.5695 (13)	169.05 (6)
260 K	N1—H1n1···O3	0.9611 (9)	1.6191 (9)	2.5695 (13)	169.18 (8)
250 K	O3—H1o3···N1	0.9727 (10)	1.5993 (10)	2.5684 (14)	173.71 (9)
250 K	N1—H1n1···O3	0.9267 (10)	1.6636 (10)	2.5684 (14)	164.41 (6)
240 K	O3—H1o3···N1	0.9898 (10)	1.5790 (11)	2.5684 (15)	177.78 (6)
240 K	N1—H1n1···O3	1.0731 (11)	1.5047 (10)	2.5684 (15)	170.07 (6)
230 K	O3—H1o3···N1	0.9942 (9)	1.5797 (10)	2.5677 (14)	171.83 (6)
230 K	N1—H1n1···O3	0.8580 (10)	1.7222 (9)	2.5677 (14)	168.05 (6)
220 K	O3—H1o3···N1	1.0722 (10)	1.4991 (10)	2.5629 (14)	170.59 (6)
220 K	N1—H1n1···O3	1.0152 (10)	1.5718 (10)	2.5629 (14)	163.96 (6)
210 K	N1—H1n1···O3	1.0003 (10)	1.5678 (9)	2.5615 (13)	171.62 (6)
200 K	N1—H1n1···O3	0.8778 (8)	1.6920 (7)	2.5605 (11)	169.71 (5)
190 K	N1—H1n1···O3	0.9013 (10)	1.6719 (9)	2.5628 (13)	169.24 (8)
180 K	N1—H1n1···O3	0.9633 (10)	1.6218 (9)	2.5637 (13)	164.77 (6)
170 K	N1—H1n1···O3	0.9438 (9)	1.6219 (8)	2.5605 (12)	172.43 (5)
160 K	N1—H1n1···O3	1.0101 (10)	1.5546 (9)	2.5622 (14)	174.75 (8)
150 K	N1—H1n1···O3	1.0493 (10)	1.5149 (9)	2.5604 (13)	173.65 (6)
100 K	N1—H1n1···O3	0.8488 (8)	1.7207 (8)	2.5640 (11)	172.04 (5)
290 K	N2—H1n2···O1^{i}	0.866 (16)	1.885 (17)	2.7405 (16)	169.3 (15)
280 K		0.863 (16)	1.882 (16)	2.7363 (16)	170.3 (14)
270 K		0.849 (15)	1.890 (15)	2.7274 (14)	168.3 (15)
260 K		0.846 (14)	1.883 (14)	2.7177 (13)	168.9 (13)
250 K		0.866 (14)	1.857 (15)	2.7150 (14)	170.6 (13)
240 K		0.898 (15)	1.824 (16)	2.7101(15)	168.6 (15)
230 K		0.855 (15)	1.862 (15)	2.7040 (14)	167.9 (15)
220 K		0.878 (14)	1.826 (15)	2.6964 (14)	171.2 (13)
210 K		0.831 (15)	1.872 (15)	2.6922 (14)	168.5 (16)
200 K		0.861 (13)	1.835 (13)	2.6843 (11)	168.6 (12)
190 K		0.842 (15)	1.852 (15)	2.6836 (13)	169.2 (15)
180 K		0.825 (15)	1.860 (15)	2.6784 (14)	171.1 (18)
170 K		0.823 (14)	1.861 (14)	2.6765 (13)	170.9 (14)
160 K		0.908 (15)	1.772 (15)	2.6732 (14)	171.2 (13)
150 K		0.881 (14)	1.798 (14)	2.6735 (13)	171.8 (15)
100 K		0.858 (13)	1.815 (13)	2.6676 (12)	172.2 (12)
290 K	N3—H1n3···O2	0.910 (19)	1.993 (18)	2.8984 (17)	173.1 (16)
280 K		0.910 (18)	1.985 (18)	2.8919 (17)	174.1 (14)
270 K		0.853 (17)	2.038 (17)	2.8890 (15)	174 (2)
260 K		0.872 (17)	2.012 (16)	2.8809 (14)	174.7 (17)
250 K		0.875 (17)	2.002 (17)	2.8744 (15)	174.1 (17)
240 K		0.903 (17)	1.971 (17)	2.8717 (16)	175.0 (19)
230 K		0.878 (16)	1.994 (16)	2.8672(15)	172.8 (19)

220 K		0.879 (17)	1.980 (16)	2.8578 (15)	175.7 (19)
210 K		0.828 (17)	2.031 (16)	2.8553 (14)	173 (2)
200 K		0.873 (15)	1.980 (14)	2.8492(11)	173.7 (14)
190 K		0.820 (17)	2.034 (16)	2.8480 (14)	172 (2)
180 K		0.827 (17)	2.020 (16)	2.8427 (14)	173 (2)
170 K		0.805 (16)	2.046 (15)	2.8433 (13)	171 (2)
160 K		0.891 (16)	1.955(16)	2.8396 (14)	171.7 (18)
150 K		0.894 (16)	1.951 (16)	2.8381 (14)	171.3 (18)
100 K		0.818 (15)	2.026 (14)	2.8334 (12)	169 (2)
290 K	N3—H2n3···O1w^{ii}	0.881 (16)	1.976 (16)	2.8448 (17)	169 (3)
280 K		0.909 (16)	1.945 (15)	2.8407 (16)	168 (2)
270 K		0.900 (15)	1.953 (14)	2.8355 (14)	166 (2)
260 K		0.908 (14)	1.944 (14)	2.8325 (13)	166 (2)
250 K		0.927 (14)	1.918 (14)	2.8299 (14)	167 (2)
240 K		0.905 (15)	1.931 (15)	2.8265 (15)	170 (2)
230 K		0.877 (15)	1.964 (14)	2.8254 (14)	167 (3)
220 K		0.906 (14)	1.929 (14)	2.8194 (14)	167 (2)
210 K		0.894 (12)	1.936 (14)	2.8160 (14)	168 (2)
200 K		0.907 (13)	1.920 (12)	2.8151 (11)	168 (2)
190 K		0.876 (14)	1.952 (14)	2.8121 (13)	167 (2)
180 K		0.861 (15)	1.962 (15)	2.8099 (14)	168 (3)
170 K		0.901 (14)	1.929 (13)	2.8061 (13)	164 (2)
160 K		0.893 (14)	1.920 (14)	2.8038 (14)	170 (2)
150 K		0.895 (14)	1.919 (14)	2.8033 (13)	169 (2)
100 K		0.882 (13)	1.931 (13)	2.7985 (12)	168 (2)
290 K	N4—H1n4···O2^{iii}	0.919 (18)	2.01 (2)	2.9257 (17)	172 (2)
280 K		0.907 (18)	2.02 (2)	2.9247 (17)	172 (2)
270 K		0.893 (17)	2.037 (19)	2.9238 (16)	172 (2)
260 K		0.876 (16)	2.051 (18)	2.9192 (14)	171 (2)
250 K		0.881 (16)	2.041 (17)	2.9174 (14)	173 (2)
240 K		0.905 (17)	2.018 (18)	2.9155 (16)	171 (2)
230 K		0.918 (16)	2.002 (19)	2.9112 (15)	170 (2)
220 K		0.910(15)	2.005 (17)	2.9080 (15)	171(2)
210 K		0.917 (16)	1.997 (19)	2.9023 (16)	169 (2)
200 K		0.857 (13)	2.063 (13)	2.9026 (12)	166 (2)
190 K		0.897 (16)	2.010 (18)	2.8992 (15)	171 (2)
180 K		0.881 (17)	2.021 (19)	2.8950 (16)	171 (3)
170 K		0.891 (16)	2.012 (18)	2.8924 (15)	169 (2)
160 K		0.901 (15)	2.001 (17)	2.8921 (14)	170 (2)
150 K		0.897 (15)	2.001 (17)	2.8898 (14)	171 (2)
100 K		0.887 (14)	2.006 (16)	2.8834 (13)	170 (2)
290 K	N4—H2n4···F1^{iv}	0.82 (2)	2.472 (18)	2.9438 (18)	117.6 (12)
280 K		0.83 (2)	2.460 (17)	2.9384 (17)	117.5 (11)
270 K		0.823 (18)	2.464 (17)	2.9365 (16)	117.5 (11)
260 K		0.800 (18)	2.455 (16)	2.9294 (15)	119.2(10)
250 K		0.789 (18)	2.462 (17)	2.9285 (16)	119.1 (11)
240 K		0.782 (19)	2.447 (17)	2.9258 (17)	120.8 (12)
230 K		0.794 (18)	2.463 (17)	2.9252 (16)	118.5 (12)
220 K		0.793 (18)	2.447 (17)	2.9192 (16)	119.3 (11)
210 K		0.787 (18)	2.464 (16)	2.9176 (15)	118.0 (11)

200 K		0.809 (16)	2.434 (14)	2.9098 (12)	118.6 (9)
190 K		0.770 (18)	2.471 (16)	2.9135 (15)	118.1 (12)
180 K		0.798 (18)	2.462 (17)	2.9109 (15)	116.9 (12)
170 K		0.789 (17)	2.448 (15)	2.9068 (14)	118.3 (11)
160 K		0.818 (18)	2.423 (16)	2.9029 (15)	118.4(11)
150 K		0.789 (18)	2.432 (16)	2.9002 (15)	119.2 (11)
100 K		0.798 (16)	2.424 (14)	2.8879 (12)	118.2 (10)
290 K	N5—H1n5···O1w^{v}	0.93 (2)	2.03 (2)	2.919 (2)	159 (2)
280 K		0.92 (2)	2.04 (3)	2.917 (2)	158 (2)
270 K		0.904 (18)	2.05 (2)	2.9160 (19)	159 (2)
260 K		0.900 (18)	2.05 (2)	2.9121 (17)	160(2)
250 K		0.895 (17)	2.05 (2)	2.9098 (18)	160 (2)
240 K		0.896 (19)	2.05 (2)	2.9090 (19)	159 (2)
230 K		0.880 (19)	2.07 (2)	2.9084 (19)	160 (2)
220 K		0.879 (17)	2.07 (2)	2.9045 (18)	158 (2)
210 K		0.891 (18)	2.05 (2)	2.9010 (19)	160 (2)
200 K		0.876 (15)	2.07 (2)	2.8990 (14)	157 (2)
190 K		0.905 (18)	2.03 (2)	2.8981 (18)	161(2)
180 K		0.898 (19)	2.02 (2)	2.8939 (19)	163 (2)
170 K		0.879 (17)	2.06 (2)	2.8952 (18)	158 (2)
160 K		0.898 (18)	2.04 (2)	2.8916 (17)	159 (2)
150 K		0.893 (17)	2.05 (2)	2.8931 (16)	158 (2)
100 K		0.896 (16)	2.03 (2)	2.8884 (15)	159.1 (19)
290 K	N5—H2n5···O3^{i}	0.887 (18)	2.22 (2)	3.0545 (19)	157.5 (17)
280 K		0.890 (18)	2.19 (2)	3.0496 (18)	161.3 (16)
270 K		0.883 (17)	2.194 (19)	3.0424 (17)	161.1 (14)
260 K		0.877 (17)	2.190 (18)	3.0348 (15)	161.4 (14)
250 K		0.898 (16)	2.165 (18)	3.0285 (16)	161.3 (15)
240 K		0.881 (17)	2.175 (19)	3.0191 (17)	160.1 (16)
230 K		0.881 (17)	2.161 (18)	3.0132 (16)	162.5 (14)
220 K		0.912 (16)	2.127 (18)	3.0035 (16)	160.9 (16)
210 K		0.874 (17)	2.151 (18)	2.9981 (16)	163.2 (14)
200 K		0.852 (14)	2.178 (16)	2.9906 (12)	159.4 (14)
190 K		0.882 (16)	2.133 (18)	2.8975 (15)	163.0 (14)
180 K		0.903 (17)	2.106 (18)	2.9774 (16)	162.1 (15)
170 K		0.861 (16)	2.136 (17)	2.9758 (15)	164.9(13)
160 K		0.882 (16)	2.122 (18)	2.9737 (16)	162.0 (16)
150 K		0.918 (16)	2.073 (18)	2.9705 (15)	165.5 (14)
100 K		0.895 (13)	2.087 (16)	2.9611 (13)	165.3 (11)
290 K	O1w—H1ow···O2	0.83 (3)	1.94 (2)	2.759 (2)	175 (2)
280 K		0.84 (3)	1.92 (2)	2.757 (2)	175 (2)
270 K		0.81 (2)	1.95 (2)	2.757 (2)	174.0 (19)
260 K		0.79 (2)	1.96 (2)	2.7509 (17)	171.6 (18)
250 K		0.83 (2)	1.92 (2)	2.7494 (19)	174.5 (18)
240 K		0.84 (2)	1.91 (2)	2.746 (2)	176.6 (19)
230 K		0.83 (2)	1.92 (2)	2.746 (2)	175.6(18)
220 K		0.85 (2)	1.90 (2)	2.7408 (19)	174.4 (17)
210 K		0.82 (2)	1.92 (2)	2.740 (2)	173.1 (17)
200 K		0.84 (2)	1.90 (2)	2.7385 (16)	173.8 (14)
190 K		0.83 (2)	1.91 (2)	2.7378 (19)	173.3 (17)

180 K		0.85 (2)	1.89 (2)	2.733 (2)	174.4 (18)
170 K		0.84 (2)	1.90 (2)	2.7329 (18)	172.4 (16)
160 K		0.83 (2)	1.90 (2)	2.7302 (19)	176.4 (18)
150 K		0.85 (2)	1.88 (2)	2.7281 (19)	175.7 (17)
100 K		0.85 (2)	1.88 (2)	2.7268 (16)	174.7 (14)
290 K	O1w—H2ow···O1^{ii}	0.837 (16)	1.866 (16)	2.6873 (15)	166.8 (17)
280 K		0.847 (16)	1.854 (15)	2.6853 (14)	166.7 (16)
270 K		0.834 (15)	1.860 (14)	2.6804 (13)	167.5(15)
260 K		0.850 (14)	1.843 (14)	2.6757 (12)	165.9 (14)
250 K		0.858 (15)	1.841 (14)	2.6758 (13)	163.9 (14)
240 K		0.855 (15)	1.836 (14)	2.6738 (14)	166.2 (15)
230 K		0.840 (15)	1.850 (14)	2.6737 (13)	166.7 (14)
220 K		0.864 (14)	1.829 (14)	2.6694 (13)	163.6 (14)
210 K		0.853 (14)	1.829 (14)	2.6647 (13)	165.8 (14)
200 K		0.847 (13)	1.832 (12)	2.6611 (10)	165.6 (13)
190 K		0.865 (14)	1.817 (13)	2.6623 (12)	164.9 (13)
180 K		0.858 (14)	1.820 (14)	2.6609 (12)	166.3 (14)
170 K		0.843 (13)	1.829 (13)	2.6596 (11)	168.1 (13)
160 K		0.861 (14)	1.819 (13)	2.6591 (12)	164.7 (13)
150 K		0.870 (14)	1.809 (13)	2.6592 (12)	165.1 (13)
100 K		0.852 (12)	1.823 (12)	2.6567 (10)	165.3 (12)

Symmetry codes:
i: *x*, *y*-1, *z*;
ii: -*x* + 1/2, *y* - 1/2, -*z* + 1/2;
iii: *x* + 1/2, -*y* + 3/2, *z* + 1/2;
iv: -*x* + 1, *y*, -*z* + 3/2;
v: -*x* + 1, -*y* + 1, -*z* + 1.

Table S3: The overview of the structure determinations with $[PO_3F]^{2-}$ and $[HPO_3F]^{-}$

Refcodes/collection codes refer to the hits in the Cambridge Crystal Structure Database, version 5.37 (November 2015) with addenda up to February 2016 (Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst*. B**72**, 171-179) as well as to the hits in the Inorganic Crystal Structure Database (2016), version 2016-1 (Fachinformationszentrum Karlsruhe, Germany, and the U.S. Department of Commerce on the behalf of the United States.)

Compound	P-F (Å)	P-O (Å)	P-O (Å)	P-O (Å)	Reference	Refcode/ collection code	R-factor	Temp.
$[PO_3F]^{2-}$ (The structures contain hydrogen bonds)								
$LiK(PO_3F)(H_2O)$	1.594	1.527	1.511	1.509	Galigne J.L., Durand J. & le Cot L. (1974). Acta Cryst., B30, 697- 701.	2044	0.056	RT
$Cu_2K(OH)(PO_3F)_2(H_2O)$	1.569	1.497	1.502	1.502	Moewius F., Ziemer B., Reck G., Meisel M., Grunze H. (1987) Z. Anorg. Allg. Chem. 547, 75-82.	62646	0.0251	RT
$CaPO_3F.2H_2O$	1.583	1.515	1.506	1.503	Perloff A. (1972) Acta Cryst., B28, 2183-2191.	2802	0.02	RT
$Li(NH_4)(PO_3F)$	1.592	1.513	1.507	1.506	Durand J., le Cot L., Galigne J.L. (1978). Acta Cryst., B34, 388-391.	1439	0.047	RT
$(NH_4)Ag_3(PO_3F)_2$	1.588	1.523	1.505	1.493	Weil M. (2007). Acta Cryst., C63, i31- i33.	172980	0.0381	293 K
	1.592	1.522	1.508	1.489				
	1.596	1.515	1.498	1.485				
	1.585	1.532	1.520	1.492				
$(NH_4)(MnF_2PO_3F)$	1.570	1.518	1.517	1.503	Armstrong J.A., Williams E.R. & Weller M.T. (2011). J. Am. Chem. Soc., 133, 8252-8263.	261594	0.0294	Information not given in CIF
$(NH_4)Mn(PO_3F)F_2$	1.571	1.518	1.517	1.502	Armstrong J.A., Williams E.R. & Weller M.T. (2013). Dalton Trans., 42 2302-2308.	424945	0.0292	120 K

$(NH_4)_2Fe_2(PO_3F)_2FCl_2$	1.558	1.510	1.505	1.488	Keates A.C., Armstrong J.A., Weller M.T. (2013). Dalton Trans., 42, 10715-10724.	425627	0.0362	100 K
	1.560	1.511	1.507	1.491				
$Mn(PO_3F)(H_2O)_2$	1.577	1.518	1.507	1.500	Weil M., Baran E. J., Kremer R.K. & Libowitzky E. (2015). Z. Anorg. Allg. Chem., 641, 184-191.	428896	0.0322	296 K
bis(μ^3-Phosphorofluoridato)-hexakis(1-(pyridin-2-yl)ethanone oxime)-tri-nickel bis(hexafluorophosphate) methanol solvate sesquihydrate	1.573	1.541	1.523	1.523	Dermitzaki D., Raptopoulou C.P., Psycharis V., Escuer A., Perlepes S.P. & Stamatatos T.C. (2014). Dalton Trans., 43, 14520-14524.	VOGDIG	0.0796	183 K
	1.577	1.533	1.527	1.512				
tetrakis(acetonitrile)-copper tris(hydrogen) tetrakis((μ^6-fluorophosphato)-(μ^3-oxo))-hexakis(μ^2-oxo)-tetracosaoxo-dodeca-molybdenum trihydronium acetonitrile solvate dotriacontahydrate	1.553	1.508	1.508	1.505	Fielden J., Quasdorf K., Cronin L. & Kogerler P. (2012). Dalton Trans., 41, 9876-9878.	VEHXAJ	0.0671	193 K
	1.563	1.512	1.511	1.511				
catena((μ^2-4,4'-Bipyridyl)-bis(μ^3-fluorophosphato)-di-zinc)	1.556	1.507	1.502	1.500	Halasyamani S.P., Drewitt M.J. & O'Hare D. (1997). Chem. Comm., 867-868.	RUFLIN	0.03	150 K
	1.5641	1.506	1.504	1.501				
$(Co_2F_4O_6P_{22}^-)_n$, $n(C_2H_{10}N_{22}^+)$	1.574	1.509	1.506	1.502	Armstrong J.A., Williams E.R. & Weller M.T. (2012). Dalton Trans., 41, 14180-14187.	NUNWAW	0.0636	100 K
catena((μ^4-Fluorophosphato-O,O')-(μ^2-phenazine)-di-copper(i))	1.581	1.520	1.493	1.475	Kuroda-Sowa T., Munakata M., Matsuda H., Akiyama S. & Maekawa M. (1995). J. Chem. Soc., Dalton Trans., 2201-2208.	ZEBCUE	0.033	RT
catena-(4-aminocyclohexan aminium (μ -chloro)-tetrakis(μ -fluorophosphato)-tetra-copper(ii) hemihydrate)	1.565	1.570	1.517	1.517	Williams E.R., Marshall K. & Weller M.T. (2015). CrystEngComm, 17, 160-164.	ZOQFIW	0.0912	120 K
	1.543	1.534	1.524	1.524				
	1.576	1.557	1.509	1.506				

catena-(piperazinium (μ-chloro)-tetrakis(μ-fluorophosphato)-tetra-copper(ii))	1.549	1.559	1.514	1.514	Williams E.R., Marshall K. & Weller M.T. (2015). CrystEngComm, 17, 160-164.	ZOQFOC	0.0874	120 K
	1.563	1.551	1.528	1.528				
	1.543	1.559	1.541	1.521				
tris(2-carbamoylguanidinium) hydrogen fluorophosphonate fluorophosphonate monohydrate	1.573	1.512	1.495	1.479	Fábry J., Fridrichová M., Dušek M., Fejfarová K. & Krupková R. (2012). Acta Cryst., E68, o47-o48.	SAHKET	0.0303	RT
$(NH_4)_2(Cu(H_2O)_2(PO_3F)_2)$	1.577	1.505	1.505	1.496	Berraho M., Vegas A., Martinez-Ripoll M., Rafiq M. (1994). Acta Cryst., C50, 666-668.	74551	0.048	RT
$(NH_4)_3Fe(PO_3F)_2F_2$	1.565	1.511	1.484	1.484	Keates A.C., Armstrong J. A., Weller M. T. (2013). Dalton Trans., 42(30), 10715-10724.	425616	0.0556	Temperature not given in CIF
	1.498	1.562	1.485	1.485				
$(C_4H_8O_2)_n$,n$(H_4Cu_2F_2O_8P_2)$ catena((Aqua-(μ_2-fluorophosphato)-copper(ii)) 1,4-dioxane solvate)	1.568	1.5259	1.5027	1.5027	Meisel M., Zeibig M., Mowius Zak, Z., Blake A. J. (1992). Z. Anorg. Allg. Chem., 614, 53-59.	JOZSUM	0.022	RT
bis(μ 2-Phosphorofluoridato)-tetrakis(pyridine-2-carbaldehyde oxime-*N*,*N*')-di-zinc(ii)	1.5851	1.5165	1.5096	1.4952	Konidaris K.F., Polyzou C.D., Kostakis G.E., Tasiopoulos A.J., Roubeau O., Teat S.J., Manessi-Zoupa E., Powell A.K., Perlepes S.P. (2012). Dalton Trans,. 41, 2862-2865.	WAQDID	0.0218	100 K
tetrakis(*N*-hydroxy-1-(pyridin-2-yl)ethanimine)-bis(μ -phosphorofluoridato)-di-nickel dihydrate	1.5882	1.5183	1.5053	1.4880	Dermitzaki D., Raptopoulou C.P., Psycharis V., Escuer A., Perlepes S.P. & Stamatatos T.C. (2014). Dalton Trans., 43, 14520-14524.	VOGQOZ	0.035	160 K
bis(*N*-hydroxy-1-(pyridin-2-yl) ethanimine)-(1,2-difluorodiphosphato)-nickel acetonitrile solvate hydrate LONG H-BOND	1.541	1.687	1.525	1.472	Dermitzaki D., Raptopoulou C.P., Psycharis V., Escuer A., Perlepes S.P. & Stamatatos T.C. (2014). Dalton Trans., 43, 14520-14524.	VOGQUF	0.1065	RT
	1.541	1.632	1.482	1.460				

$Na_5(N(CH_3)_4)(PO_3F)_3(H_2O)_{18}$	1.579	1.512	1.510	1.507	Prescott H.A. (2001). Thesis, Humboldt Universitaet, Berlin.	151291	0.0306	180 K
$(NH_4)_2(PO_3F)(H_2O)$	1.586	1.508	1.506	1.501	Perloff A. (1972). Acta Cryst., B28, 2183-2191.	2803	0.036	RT
$(NH_4)_2(PO_3F)(H_2O)$	1.597	1.514	1.514	1.503	Berndt A.F. & Sylvester J.M. (1972). Acta Cryst., B28, 2191-2193.	2804	0.128	RT
$Na_2(PO_3F)(H_2O)_{10}$	1.608	1.513	1.507	1.505	Prescott H.A., Troyanov S.I. & Kemnitz E. (2001). J. Sol. State Chem., 156, 415-421.	51338	0.0276	160 K
$(NH_4)_2(Ni(H_2O)_6)(PO_3F)_2$ H-positions not determined.	1.597	1.510	1.508	1.505	Berraho M., R'Kha C., Vegas A. & Rafiq M. (1992). Acta Cryst., C48, 1350-1352.	71561	0.03	RT
$Na_5(N(CH_3)_4)(PO_3F)_3(H_2O)_{18}$	1.599	1.517	1.504	1.498	Prescott H.A. (2001). Thesis, Humboldt Universitaet, Berlin.	151291	0.0306	180 K
	1.579	1.518	1.508	1.505				
$(C(NH_2)_3)_2(PO_3F)$	1.575	1.509	1.509	1.505	Prescott H.A. (2001). Thesis, Humboldt Universitaet, Berlin.	151292	0.0306	180 K
$(H(CO(NH(CH_3))_2))(H(PO_3F))$	1.573	1.509	1.509	1.509	Prescott H.A., Troyanov S.I., Feist M., Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	163103	0.0424	180 K
	1.567	1.504	1.504	1.504				
$(NH_4)_2PO_3F.H_2O$	1.600	1.515	1.511	1.509	Durand J., Beys L., Hillaire P., Aleonard S., le Cot L. (1978). Spectrochim. Acta A34, 123-127.	200317	0.051	RT
$(C_2H_{10}N_2)^{2+}PO_3F^{2-}$ bis(2-Carbamoylguanidinium) fluorophosphonate dihydrate	1.5853	1.5096	1.5074	1.5045	Fábry J., Dušek M., Krupková R. & Vaněk P. CSD Communication (Private Communication), 2006, CCDC 606529	JEHFUY	0.0255	RT
$(C_2H_{10}N_2)^{2+}PO_3F^{2-}$ Ethylenediammonium fluorotrioxophosphate	1.5944	1.5188	1.5148	1.5108	Fábry J., Dušek M., Krupková R. & Vaněk P. (2006). Acta Cryst., E62, o3217-o3219.	JEHFUY01	0.0246	150 K
bis(2-Carbamoylguanidinium) fluorophosphonate dihydrate	1.5930	1.5113	1.5091	1.5091	Fábry J., Fridrichová M., Dušek M., Fejfarová K & Krupková R. (2012). Acta Cryst., C68, o71-o75.	XAQYEV	0.0335	120 K

bis(2-Carbamoylguanidinium) fluorophosphonate dihydrate	1.584	1.532	1.499	1.497	Fábry J., Fridrichová M., Dušek M., Fejfarová K & Krupková R. (2012). Acta Cryst., C68, o71-o75.	XAQYEV01	0.0698	120 K
$[(C_1H_6N_3)^{1+}]_2(PO_3F)^{2-}$	1.573	1.509	1.509	1.509	Prescott H. A., Troyanov S., Feist M. & Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	XOMQAR	0.0436	180 K
bis(2-aminopyrimidinium) fluorophosphate	1.584	1.5205	1.5046	1.5008	Unpublished by the present author			
$[HPO_3F]^-$	**(The structures contain hydrogen bonds)**							
β-Rb(HPO_3F)	1.540	1.539	1.513	1.485	Prescott H.A. (2001). Thesis, Humboldt Universitaet, Berlin.	151293	0.0352	180 K
$Na_2Mn(HPO_3F)F_3$ Unusual hydrogen-bond O-H...F	1.491	1.599	1.533	1.533	Armstrong J.A., Williams E.R. & Weller M.T. (2013). Dalton Trans., 42, 2302-2308.	424942	0.0502	120 K
K(HPO_3F)	1.565	1.555	1.488	1.483	Prescott H.A., Troyanov S. I. & Kemnitz E. (2003). Z. Kristallogr., 218, 604-611.	391178	0.0214	180 K
4 ligands of [PO3F] are bonded while they are not acceptors of the H-bonds	1.584	1.567	1.487	1.471				
P3-F3	1.574	1.557	1.504	1.480				
P4-F4...H1-O3	1.567	1.545	1.512	1.463				
Rb(HPO_3F)	1.570	1.556	1.500	1.477	Prescott H.A., Troyanov S. I. & Kemnitz E. (2003). Z. Kristallogr., 218, 604-611.	391180	0.0365	180 K
	1.586	1.556	1.494	1.479				
$Na(HPO_3F)(H_2O)_{2.5}$	1.565	1.563	1.508	1.484	Prescott H.A., Troyanov S. I. & Kemnitz E. (2001). J. Solid State Chem., 156, 415-421.	51337	0.0276	160 K
$C_{54}H_{82}F_2N_4O_8P_2Pt_2$	1.548	1.530	1.502	1.479	Au R.H.W., Fraser C.S.A. Eisler D.J., Jennings M.C. & Puddephatt R.J. (2009). Organometallics, 28, 1719-1729.	BOXHUS	0.047	200 K
	1.551	1.527	1.481	1.471				

$((CH_3)_2NH_2)(HPO_3F)$	1.650	1.551	1.487	1.474	Samuel R.C., Krawiec M., Neilson R.H. & Watson W.H. (2001). Private Communication.	XESVEW 110589	0.073	RT
$(C(NH_2)_3)(HPO_3F)$	1.543	1.531	1.480	1.479	Prescott H.A. (2001). Thesis, Humboldt Universitaet, Berlin.	151288	0.0449	180 K
$(N(CH_3)_4)(HPO_3F)(H_2O)$ disorder	1.563	1.500	1.500	1.500	Prescott H.A. (2001). Thesis, Humboldt Universitaet, Berlin.	151290	0.0194	180 K
	1.563	1.484	1.484	1.484				
$(C(NH_2)_3)(H(PO_3F))$	1.544	1.531	1.480	1.479	Prescott H. A., Troyanov S.I., Feist M., Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	163101	0.0449	180 K
$(H(CO(NH(CH_3))_2))(H(PO_3F))$ Bond O-H…O	1.554	1.542	1.498	1.492	Prescott H. A., Troyanov S.I., Feist M., Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	163102 XOMPUK	0.0383	180 K
$(C_2H_7N_4O)^{1+}(HPO_3F)^{1-}$	1.564	1.560	1.500	1.469	Fábry J., Fridrichová M., Dušek M., Fejfarová K. & Krupková R. (2012). Acta Cryst., C68, o76-o83.	XAQYOF	0.0491	120 K
$(C_2H_7N_4O)^{1+}(HPO_3F)^{1-}{}_{0.76}(H_2PO_3)^{1-}{}_{0.24}$ Occupational disorder	1.563	1.563	1.485	1.485	Fábry J., Fridrichová M., Dušek M., Fejfarová K. & Krupková R. (2012). Acta Cryst., C68, o76-o83.	XAQYUL	0.0503	120 K
$(C_2H_7N_4O)^{1+}(HPO_3F)^{1-}{}_{0.12}(H_2PO_3)^{1-}{}_{0.88}$ Occupational disorder	1.57	1.5767	1.5027	1.4930	Fábry J., Fridrichová M., Dušek M., Fejfarová K. & Krupková R. (2012). Acta Cryst., C68, o76-o83.	XAQZAS	0.0191	120 K
$(C_2H_7N_4O)^{1+}(HPO_3F)^{1-}{}_{0.12}(H_2PO_3)^{1-}{}_{0.88}$ Occupational disorder	1.563	1.5729	1.4988	1.4934	Fábry J., Fridrichová M., Dušek M., Fejfarová K. & Krupková R. (2012). Acta Cryst., C68, o76-o83.	XAQZAS01	0.0225	120 K
$(C_4H_{12}N_2)^{2+}(HPO_3F)^{1-}{}_2$	1.5643	1.5495	1.5045	1.4833	Prescott H. A., Troyanov S., Feist M. & Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	XOMPAQ	0.0251	180 K
$(C_4H_{12}N_1)^{1+}(HPO_3F)^{1-}$	1.5656	1.5445	1.4853	1.4763	Prescott H. A., Troyanov S., Feist M. & Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	XOMPEU	0.0288	180 K
Triethylammonium hydrogen monofluorophosphate H-atom disordered	1.5655	1.534	1.5107	1.4521	Prescott H. A., Troyanov S., Feist M. & Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	XOMPIY	0.0387	180 K

$C_1H_7F_1N_3O_3P_1$	1.544	1.531	1.480	1.479	Prescott H. A., Troyanov S., Feist M. & Kemnitz E. (2002). Z. Anorg. Allg. Chem., 628, 1749-1755.	XOMPOE	0.0449	180 K
	1.549	1.554	1.488	1.482	Idrissi A. K., Rafiq M., Gougeon P. & Guerin R. (1995). Acta Cryst., C51, 1359-1361.	YUYKUY	0.046	RT
The structure also contains $[PO_3F]^{2-}$ group.	1.5602	1.5476	1.4850	1.4752	Fábry J., Fridrichová M., Dušek M., Fejfarová K. & Krupková R. (2012). Acta Cryst., E68, o47-o48.	SAHKET	0.0303	RT
$[H…PO_3F]^-$								
$K_3(H(PO_3F)_2)$ symmetric hydrogen bond !!!	1.594	1.542	1.492	1.487	Prescott H.A., Troyanov S.I. & Kemnitz E. (2003). Z. Kristallogr., 218, 604-611.	391179	0.0581	180 K
$(NH_4)_{0.926}K_{2.074}(H(PO_3F)_2)$ symmetric hydrogen bond !!!	1.595	1.536	1.490	1.484	Fábry J., Krupková R. & Císařová I. (2003). Acta Cryst., E59, i14-i16.	281209	0.0214	293 K
Ethylenediammonium(2+) μ-hydrogen-(dihydrogen phosphate)-(fluorotrioxophosphate) symmetric hydrogen bond !!!	1.559	1.519	1.509	1.484	Fábry J., Krupková R., Císařová I. & Vaněk P. (2005).	Unpublished results	0.0413	291 K
Title structure / 290 K	1.567	1.5331	1.4865	1.4776	title structure		0.0334	290 K
Title structure / 150 K	1.5742	1.5228	1.5038	1.4945	title structure		0.0306	150 K
$[PO_3F]^{2-}$	**(The structures contain no hydrogen bonds and both F and O are involved in the bonding)**							
$Na_2(PO_3F)$	1.619	1.507	1.503	1.489	Durand J., le Cot L., Galigne J.L. (1974). Acta Cryst., B30, 1565-1569.	2100	0.052	RT
$Na_2(PO_3F)$	1.594	1.499	1.494	1.475				
K_2PO_3F	1.548	1.531	1.531	1.443	Robinson M. T. (1958). J. Phys. Chem., 62, 925-928.	15691	0.185	RT
Rb_2PO_3F	1.610	1.502	1.493	1.493	Fábry J., Dušek M., Fejfarová K., Krupková R., Vaněk P. & Císařová I. (2006). Acta Cryst., C62, i49-i52.	172343	0.0209	290 K

Rb_2PO_3F	1.625	1.511	1.499	1.499	Fábry J., Dušek M., Fejfarová K., Krupková R., Vaněk P. & Císařová I. (2006). Acta Cryst., C62, i49-i52.	172344	0.0223	130 K
Cs_2PO_3F	1.607	1.506	1.506	1.497	Fábry J., Dušek M., Fejfarová K., Krupková R., Vaněk P. & Císařová I. (2006). Acta Cryst., C62, i49-i52.	172345	0.0264	240 K
Cs_2PO_3F	1.637	1.514	1.514	1.514	Fábry J., Dušek M., Fejfarová K., Krupková R., Vaněk P. & Císařová I. (2006). Acta Cryst., C62, i49-i52.	172346	0.0191	100 K
K_2PO_3F	1.609	1.486	1.486	1.479	Payen J., Durand J., le Cot L., Galigne J.L. (1979). Can. J. Chem., 57, 886-889.	200441	0.065	RT
K_3NaPO_3F	1.630	1.495	1.495	1.495	Durand J., Granier W., le Cot L. & Galigne J.L. (1975). Acta Cryst., B31, 1533-1535.	1904	0.067	RT
$[PO_3F]^-$	**(The structures contain no hydrogen bonds and only O are involved in the bonding)**							
$Sn(PO_3F)$	1.575	1.505	1.481	1.400	Berndt A.F. (1974). Acta Cryst., B30, 529-530.	2039	Not given	RT
Hg_2PO_3F	1.569	1.519	1.519	1.507	Weil M., Puchberger M. & Baran E. J. (2004). Inorg. Chem., 43, 8330-8335.	414292	0.0406	251 K
Ag_2PO_3F	1.575	1.512	1.510	1.507	Weil M., Puchberger M., Fueglein E., Baran E.J., Vannahme J., Jakobsen H.J. & Skibsted J. (2007). Inorg. Chem., 46, 801-808.	416858	0.0289	Information not given in CIF