Al(2)	48(*f*)	3/8	3/8	0.01258 (8)	0.0121 (3)
Mg(1)	16(*d*)	0	1/2	0	0.0170 (3)
Mg(2)	8(*b*)	1/8	5/8	1/8	0.0208 (5)

Table 2. *Selected geometric parameters* (Å)

Distorted icosahedron			Distorted pentagonal prism		
Mn 16(*c*)—	6 Al 96(*g*)	2.797 (1)	Al 48(*f*)—	2 Al 96(*g*)	2.720 (1)
	6 Al 48(*f*)	2.573 (1)		4 Al 96(*g*)	2.830 (1)
	12			4 Al 48(*f*)	2.825 (2)
				2 Mn 16(*c*)	2.573 (1)
Distorted pentagonal prism				12	
Al 96(*g*)—	2 Al 96(*g*)	2.746 (2)			
	2 Al 96(*g*)	2.922 (1)	Approximate hexagonal prism		
	1 Al 96(*g*)	2.749 (2)	Mg 16(*d*)—	12 Al 96(*g*)	3.112 (1)
	2 Al 48(*f*)	2.830 (1)		2 Mg 8(*b*)	3.143 (1)
	1 Al 48(*f*)	2.720 (1)		14	
	1 Mn 16(*c*)	2.797 (1)			
	1 Mg 8(*b*)	3.222 (1)	Friauf polyhedron (Fig. 1)		
	2 Mg 16(*d*)	3.112 (1)	Mg 8(*b*)—	12 Al 96(*g*)	3.222 (1)
	12			4 Mg 16(*d*)	3.143 (1)
				16	

Lorentz-polarization corrections were applied. Structure solution in space group $Fd\bar{3}m$ using direct methods located all the atomic positions and species correctly. The position with point symmetry $\bar{3}m$ was used as the origin of the atomic coordinate system in this structure solution instead of the position with point symmetry $\bar{4}3m$ used by Samson (1958). It was found that all the atomic positions obtained from this solution were equivalent to those derived in Samson's solution of the *E* phase with the position of Cr corresponding to Mn in our solution of the *T* phase. Final refinement of the structure was carried out using a full-matrix least-squares method. All calculations were performed using the *SHELXTL/PC* software system (Sheldrick, 1990).

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Lists of structure factors and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71742 (3 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI1077]

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$Nd_2(OH)_2(CrO_4)_2$ and $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$

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Abstract

The structures of neodymium hydroxide chromate and pentaaquaterbium(III) chromate dihydrate have been determined. Two kinds of Nd atoms, with different environments, are present in the structure of $Nd_2(OH)_2(CrO_4)_2$. The coordination polyhedron of the eight O atoms around the Nd atoms is a square antiprism. In $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$, the Tb atoms are nine-coordinated and are located in two types of site. The coordination polyhedra consist of both a tricapped trigonal prism and a monocapped square antiprism. In the two title compounds the CrO_4 groups are nearly regular tetrahedra, having mean Cr—O distances of 1.651 (7) and 1.650 (7) Å for $Nd_2(OH)_2(CrO_4)_2$ and $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$, respectively.

Comment

This work is part of a series of structural studies of lanthanoid chromates (Leppä-aho & Valkonen, 1991, 1992; Leppä-aho, 1993). At the moment six structures are known for rare-earth chromates: $[Ln_2(CrO_4)_3(H_2O)_5].2H_2O$ [Ln = Nd, Eu (Leppä-aho & Valkonen, 1991), La (Habekost, Christensen & Hazell, 1991) and Sm (Bueno, Parada, Monge & Ruiz-Valero, 1991*a*)]; $Ln_2(OH)_2(CrO_4)_2$ [Ln = Yb Leppä-aho & Valkonen, 1992), Er (Bueno, Parada, Monge & Ruiz-Valero, 1991*b*), Gd and Tb (Leppä-aho, 1993)]; $[Yb_2(OH)_2(CrO_4)_2(H_2O)_{2.5}].0.5H_2O$ (Leppä-aho & Valkonen, 1992); $La(OH)(CrO_4)$ (Bueno, Parada, Garcia, Puebla, Monge & Ruiz-Valero, 1989); $Ce(CrO_4)_2.2H_2O$ (Lindgren, 1977); $Ln_3(OH)(CrO_4)_4.3.5H_2O$ [Ln = La (Habekost, Christensen & Hazell, 1991), Pr and Nd (Leppä-aho, 1993)]. In the two title compounds, $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$ and $Nd_2(OH)_2(CrO_4)_2$, Tb has the highest and Nd the lowest atomic number known for this type of lanthanoid compound.

In the synthesis of $Nd_2(OH)_2(CrO_4)_2$, 264 mg of Nd_2O_3 was mixed with 4 cm^3 of 0.6 mol dm^{-3} H_2CrO_4; $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$ was synthesized by mixing 220 mg of Tb_4O_7 with 6 cm^3 of 0.3 mol dm^{-3} H_2CrO_4. The mixtures were put in a

Teflon-lined steel autoclave and the temperature was raised to 423 K, then slowly decreased (5 K per day) to room temperature. The estimated maximum pressure in the autoclave was 4.8×10^5 Pa.

For $Nd_2(OH)_2(CrO_4)_2$ and $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$, final atomic coordinates are given in Tables 1 and 3, respectively, and interatomic distances and O—Cr—O angles are given in Tables 2 and 4, respectively. The mean Nd—O distance for $Nd_2(OH)_2(CrO_4)_2$ is 2.468 (9) Å. There is not much difference between this average value and the average Nd—O distance of 2.49 (2) Å for $Nd_2(CrO_4)_3.7H_2O$ (Leppä-aho & Valkonen, 1991). The average length of the six Nd—O(OH) bonds is 2.463 (8) Å. The hydroxyl O atoms, O(OH)1 and O(OH)2, each form a bridge between three Nd atoms. These three Nd atoms are in one side of a pyramid formed by hydroxyl O atoms with an H atom at the apex of the pyramid. The Nd—O(OH)1—Nd angles are 103.1 (3), 109.8 (3) and 105.7 (2)°, and the Nd—O(OH)2—Nd angles are 98.8 (2), 104.5 (4) and 135.7 (4)°. One Nd—O(OH)—Nd angle deviates from tetrahedral geometry, as in the case of $Yb_2(OH)_2(CrO_4)_2$ (Leppä-aho & Valkonen, 1992). A view of the structure of $Nd_2(OH)_2(CrO_4)_2$ can be seen in Fig. 1. To test for possible hydrogen bonding, O(OH)···O distances of less than 3.0 Å were determined. There are four and three distances of less than 3.0 Å for O(OH)1 and O(OH)2, respectively. The shortest distances are O(OH)1···O8 [2.75 (1) Å] and O(OH)2···O7 [2.76 (1) Å].

In $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$, the average Tb—O distance is 2.433 (7) Å and the average Tb—O(*W*) distance is 2.456 (8) Å. A correspondingly small difference between the Ln—O and Ln—O(*W*) distances is found for $Ln_2(CrO_4)_3.7H_2O$ [Ln = Nd, Eu (Leppä-aho & Valkonen, 1991)] and $La_2(CrO_4)_3.7H_2O$ (Habekost, Christensen & Hazell, 1991). Although the difference is not statistically significant, the average Ln—O distances are 0.02–0.03 Å shorter than the Ln—O(*W*) distances in all four compounds. Environments and coordination polyhedra of the Tb1 and Tb2 atoms are as Leppä-aho & Valkonen (1991) found for $Ln_2(CrO_4)_3.7H_2O$ (Ln = Nd, Eu). Fig. 2 shows how the lanthanoid polyhedra are connected to Cr tetrahedra in all dimensions. In a search for possible hydrogen bonds, from three to six O atoms were found at a distance of less than 3.0 Å around the water O atoms. The shortest O(*W*)···O distance for each water O atom is in the range 2.65 (1)–2.739 (9) Å.

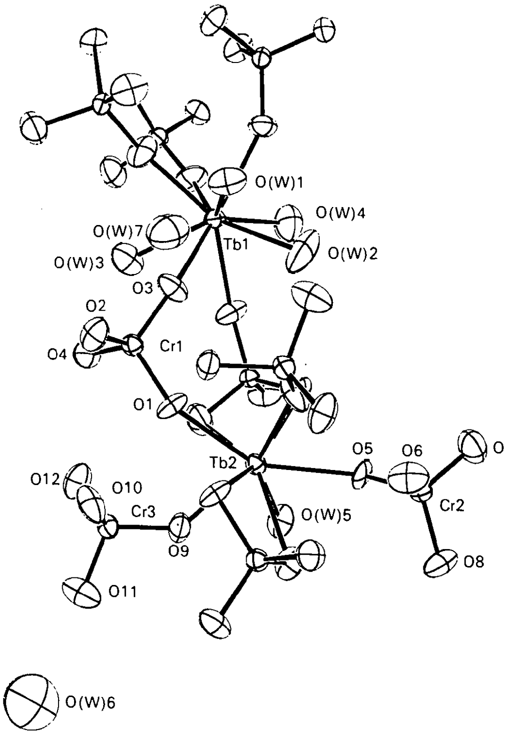

Fig. 2. *ORTEP*II (Johnson, 1976) plot showing the atomic numbering scheme for $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$. Atoms are drawn as displacement ellipsoids representing the 90% probability level.

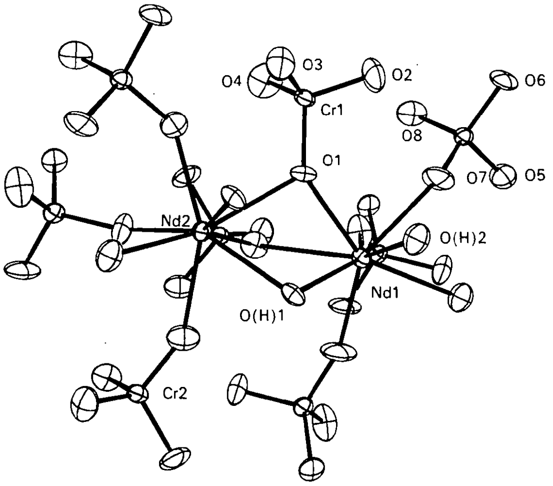

Fig. 1. *ORTEP*II (Johnson, 1976) plot showing the atomic numbering scheme for $Nd_2(OH)_2(CrO_4)_2$. Atoms are drawn as displacement ellipsoids representing the 90% probability level.

Experimental

$Nd_2(OH)_2(CrO_4)_2$

Crystal data

M_r = 554.48
Monoclinic
$P2_1/c$
a = 8.416 (2) Å
b = 11.425 (3) Å
c = 12.360 (2) Å
β = 136.61 (1)°
V = 816.5 (4) Å^3

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 7.52–17.55°
μ = 15.137 mm^{-1}
T = 296 K
Parallelepiped

$Z = 4$
$D_x = 4.51$ Mg m^{-3}
0.05 × 0.05 × 0.04 mm
Brown

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.85$, $T_{\max} = 1.22$
3734 measured reflections
3734 independent reflections
2139 observed reflections [$I > 3\sigma(I)$]
$\theta_{\max} = 35°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 18$
$l = -19 \rightarrow 19$
2 standard reflections frequency: 60 min intensity variation: none

Refinement

Refinement on F
$R = 0.041$
$wR = 0.048$
$S = 4.957$
2139 reflections
127 parameters
H-atom parameters not refined
Unit weights applied
$(\Delta/\sigma)_{\max} < 0.01$
$\Delta\rho_{\max} = 2.152$ e Å^{-3}
$\Delta\rho_{\min} = -2.094$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Tables 2.2A and 2.3.1)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* $Nd_2(OH)_2(CrO_4)_2$

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Nd1	0.52780 (6)	0.44536 (5)	0.15751 (4)	0.00177 (5)
Nd2	0.10262 (6)	0.42402 (5)	0.18301 (4)	0.00165 (5)
Cr1	0.1290 (2)	0.1783 (1)	−0.0051 (1)	0.0018 (2)
Cr2	0.6776 (2)	0.1886 (2)	0.0358 (1)	0.0018 (2)
O1	0.214 (1)	0.3171 (7)	0.0594 (7)	0.0030 (8)
O2	0.214 (1)	0.1358 (8)	−0.0824 (7)	0.0040 (8)
O3	−0.155 (1)	0.1763 (9)	−0.1456 (7)	0.004 (1)
O4	0.239 (1)	0.0914 (8)	0.1410 (8)	0.005 (1)
O5	0.930 (1)	0.2337 (8)	0.1147 (8)	0.004 (1)
O6	0.523 (1)	0.1196 (7)	−0.1371 (7)	0.0031 (9)
O7	0.533 (1)	0.3039 (8)	0.0057 (7)	0.004 (1)
O8	0.731 (1)	0.0998 (7)	0.1628 (7)	0.004 (1)
O(OH)1	0.2273 (9)	0.5561 (7)	0.0986 (6)	0.0022 (8)
O(OH)2	0.221 (1)	0.4886 (8)	−0.1305 (7)	0.0035 (9)

Table 2. *Selected geometric parameters* (Å,°) *for* $Nd_2(OH)_2(CrO_4)_2$

Nd1—O1	2.436 (8)	Nd2—O8	2.398 (8)
Nd1—O3	2.353 (7)	Nd2—O(OH)1	2.461 (9)
Nd1—O4	2.395 (8)	Nd2—O(OH)1	2.415 (5)
Nd1—O6	2.67 (1)	Nd2—O(OH)2	2.505 (9)
Nd1—O7	2.50 (1)	Cr1—O1	1.683 (8)
Nd1—O(OH)1	2.419 (8)	Cr1—O2	1.63 (1)
Nd1—O(OH)2	2.495 (6)	Cr1—O3	1.643 (6)
Nd1—O(OH)2	2.48 (1)	Cr1—O4	1.64 (1)
Nd2—O1	2.61 (1)	Cr2—O5	1.650 (9)
Nd2—O2	2.409 (9)	Cr2—O6	1.686 (7)
Nd2—O5	2.401 (9)	Cr2—O7	1.643 (9)
Nd2—O6	2.505 (7)	Cr2—O8	1.64 (1)
O1—Cr1—O2	109.9 (5)	O5—Cr2—O6	111.8 (5)
O1—Cr1—O3	107.8 (4)	O5—Cr2—O7	108.0 (5)
O1—Cr1—O4	110.1 (4)	O5—Cr2—O8	106.9 (4)
O2—Cr1—O3	107.4 (4)	O6—Cr2—O7	109.0 (3)
O2—Cr1—O4	109.3 (5)	O6—Cr2—O8	110.3 (4)
O3—Cr1—O4	112.3 (5)	O7—Cr2—O8	110.8 (5)

$[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$

Crystal data

$M_r = 791.94$
Monoclinic
$P2_1/c$
$a = 7.9218$ (9) Å
$b = 18.950$ (2) Å
$c = 13.142$ (2) Å
$\beta = 128.02$ (1)°
$V = 1554.3$ (4) Å^3
$Z = 4$
$D_x = 3.38$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 8.61$-$11.65°$
$\mu = 11.171$ mm^{-1}
$T = 296$ K
Needle
0.25 × 0.025 × 0.025 mm
Yellow

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.79$, $T_{\max} = 1.20$
6996 measured reflections
6996 independent reflections
4777 observed reflections [$I > 3\sigma(I)$]
$\theta_{\max} = 35°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 30$
$l = -21 \rightarrow 21$
2 standard reflections frequency: 60 min intensity variation: none

Refinement

Refinement on F
$R = 0.043$
$wR = 0.053$
$S = 5.374$
4777 reflections
217 parameters
H-atom parameters not refined
Unit weights applied
$(\Delta/\sigma)_{\max} < 0.01$
$\Delta\rho_{\max} = 3.147$ e Å^{-3}
$\Delta\rho_{\min} = -3.454$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Tables 2.2A and 2.3.1)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Tb1	0.05903 (5)	0.24369 (2)	0.74647 (3)	0.00238 (3)
Tb2	0.31728 (5)	0.50187 (2)	1.06392 (3)	0.00229 (3)
Cr1	−0.1122 (2)	0.35265 (7)	0.9293 (1)	0.0023 (1)
Cr2	0.4943 (2)	0.64587 (7)	0.9433 (1)	0.0021 (1)
Cr3	0.1725 (2)	0.45867 (7)	1.2735 (1)	0.0026 (1)
O1	0.0102 (9)	0.4301 (3)	0.9902 (5)	0.0039 (7)
O2	−0.3659 (8)	0.3730 (4)	0.8605 (5)	0.0042 (7)
O3	−0.0906 (9)	0.3223 (4)	0.8219 (5)	0.0041 (7)
O4	−0.0232 (9)	0.2924 (3)	1.0422 (5)	0.0039 (7)
O5	0.5268 (8)	0.5684 (3)	1.0151 (5)	0.0034 (6)
O6	0.2444 (9)	0.6714 (4)	0.8474 (6)	0.0049 (8)
O7	0.5802 (9)	0.6289 (4)	0.8599 (5)	0.0052 (8)
O8	0.641 (1)	0.7068 (4)	1.0515 (6)	0.0048 (8)
O9	0.3304 (8)	0.4931 (4)	1.2431 (5)	0.0038 (7)
O10	−0.0823 (8)	0.4813 (4)	1.1580 (5)	0.0048 (8)
O11	0.245 (1)	0.4893 (5)	1.4099 (6)	0.0063 (9)
O12	0.196 (1)	0.3718 (4)	1.2848 (6)	0.0051 (8)
O(*W*)1	−0.268 (1)	0.3067 (4)	0.5635 (6)	0.0055 (9)
O(*W*)2	0.138 (1)	0.3544 (4)	0.6943 (8)	0.008 (1)
O(*W*)3	0.080 (1)	0.1903 (4)	0.9240 (6)	0.0053 (8)
O(*W*)4	0.407 (1)	0.2348 (5)	0.7799 (6)	0.0071 (9)
O(*W*)5	0.6913 (8)	0.5051 (4)	1.2466 (5)	0.0044 (7)
O(*W*)6	0.168 (2)	0.5764 (6)	1.546 (1)	0.013 (2)
O(*W*)7	−0.542 (1)	0.3815 (5)	0.5885 (7)	0.007 (1)

Table 4. *Selected geometric parameters* (Å, °) *for* $[Tb_2(CrO_4)_3(H_2O)_5].2H_2O$

Tb1—O3	2.461 (8)	Tb2—O9	2.298 (7)
Tb1—O4	2.438 (7)	Tb2—O10	2.320 (5)
Tb1—O6	2.350 (7)	Tb2—O(*W*)5	2.405 (4)
Tb1—O8	2.410 (5)	Cr1—O1	1.668 (6)
Tb1—O12	2.356 (7)	Cr1—O2	1.664 (6)
Tb1—O(*W*)1	2.499 (6)	Cr1—O3	1.627 (8)
Tb1—O(*W*)2	2.407 (9)	Cr1—O4	1.648 (6)
Tb1—O(*W*)3	2.453 (8)	Cr2—O5	1.678 (6)
Tb1—O(*W*)4	2.518 (9)	Cr2—O6	1.634 (6)
Tb2—O1	2.408 (6)	Cr2—O7	1.638 (9)
Tb2—O1	2.574 (7)	Cr2—O8	1.634 (6)
Tb2—O2	2.507 (7)	Cr3—O9	1.663 (8)
Tb2—O5	2.463 (8)	Cr3—O10	1.670 (5)
Tb2—O5	2.441 (8)	Cr3—O11	1.617 (8)
Tb2—O7	2.608 (7)	Cr3—O12	1.653 (7)
O1—Cr1—O2	101.9 (3)	O6—Cr2—O7	110.3 (4)
O1—Cr1—O3	112.7 (4)	O6—Cr2—O8	109.6 (4)
O1—Cr1—O4	112.2 (3)	O7—Cr2—O8	110.9 (4)
O2—Cr1—O3	110.4 (3)	O9—Cr3—O10	110.4 (3)
O2—Cr1—O4	110.8 (4)	O9—Cr3—O11	108.8 (4)
O3—Cr1—O4	108.7 (4)	O9—Cr3—O12	110.5 (4)
O5—Cr2—O6	112.7 (4)	O10—Cr3—O11	108.6 (4)
O5—Cr2—O7	102.8 (4)	O10—Cr3—O12	110.2 (3)
O5—Cr2—O8	110.4 (3)	O11—Cr3—O12	108.4 (4)

Cell constants were obtained from a least-squares refinement. Lorentz and polarization corrections were applied to the data. Positions of lanthanoid and Cr atoms were established by direct methods and the remaining atoms were located in subsequent $\Delta\rho$ maps. H atoms were not located. All calculations were performed with a MicroVAX 3100 computer using the Enraf-Nonius structure determination package *SDP-Plus* (Frenz, 1978) which incorporates the direct-methods program *MULTAN*11/82 (Main *et al.*, 1982).

The author would like to thank Professor Jussi Valkonen for reviewing the manuscript.

Lists of structure factors, anisotropic displacement parameters and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71654 (64 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB1084]

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Acta Cryst. (1994). C**50**, 666–668

A Copper Monofluorophosphate, $Cu(H_2O)_2(NH_4)_2(PO_3F)_2$

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Abstract

The structure of diammonium diaquabis(monofluorophosphato)copper, $2[NH_4][Cu(PO_3F)_2(H_2O)_2]$, consists of CuO_6 octahedra and NH_4 and PO_3F tetrahedra held together by hydrogen bonds involving one H atom of the ammonium group and the H atoms of the water molecules. The Cu atoms are octahedrally coordinated by two water molecules at the apical positions and four O atoms belonging to four PO_3F groups.

Comment

This work forms part of a structural study of monofluorophosphates (Berraho, R'Kha, Vegas & Rafiq, 1992, and references therein). The structure of the title compound (Fig. 1) can be described on the basis of $Cu(H_2O)_2(PO_3F)_4^{2-}$ complex anions and NH_4^+ cations. The Cu atoms have octahedral coordination, which is somewhat deformed by the Jahn–Teller