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Diammonium tris[hexaaquacobalt(II)] tetrakis[hydrogenphosphate(III)], $(NH_4)_2[Co(H_2O)_6]_3(HPO_3)_4$

Rachid Ouarsal,[a] Brahim El Bali,[b] Mohammed Lachkar,[a] Michal Dusek[c]* and Karla Fejfarova[c]

[a]Département de Chimie, Laboratoire d'Ingénierie des Matériaux, Organométalliques et Moléculaires, 'LIMOM', Faculté des Sciences, Université Sidi Mohamed Ben Abdellah, BP 1796 Atlas, 30000 Fès, Morocco, [b]Department of Chemistry, Faculty of Sciences, University Mohammed 1st, PO Box 524, 60 000 Oujda, Morocco, and [c]Academy of Sciences of the Czech Republic, Institute of Physics, Na Slovance 2, 182 21 Praha 8, Czech Republic

Correspondence e-mail: dusek@fzu.cz

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$(NH_4)_2[Co(H_2O)_6]_3(HPO_3)_4$ is a member of the isotypic $(NH_4)_2[T(H_2O)_6]_3(HPO_3)_4$ family, where T = Co, Ni or Mg. The structure of $(NH_4)_2[Co(H_2O)_6]_3(HPO_3)_4$ is composed of the units $[Co(H_2O)_6]^{2+}$, $(HPO_3)^{2-}$ and NH_4^+, which interact *via* an intricate network of hydrogen bonds. One of the Co atoms is located at a site of $2/m$ symmetry, whereas the other central atoms, *viz*. the second Co, the two P and ammonium N atom, are located at sites of m symmetry.

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(P–O) = 0.001 Å
R factor = 0.021
wR factor = 0.073
Data-to-parameter ratio = 11.7

Comment

$(NH_4)_2[Co(H_2O)_6]_3(HPO_3)_4$ is a member of the $(NH_4)_2[T(H_2O)_6]_3(HPO_3)_4$ family that has currently three isotypic representatives with T = Co, Ni (Ouarsal *et al.*, 2005) and Mg (Messouri *et al.*, 2005). A detailed structure description of the $(NH_4)_2[T(H_2O)_6]_3(HPO_3)_4$ family has already been give for the Mg compound (Messouri *et al.*, 2005).

Fig. 1 shows the $[Co(H_2O)_6]^{2+}$, $(HPO_3)^{2-}$ and NH_4^+ coordination polyhedra. The packing of the main building units is shown in Figs. 2 and 3. No classical chemical bonds exist between the building units, which are connected solely by hydrogen bonds (Table 2).

The average P—O and P—H distances [1.527 (2) and 1.26 (3) Å, respectively] are virtually the same as the average distances in the isotypic Mg and Ni compounds of 1.527 (2)/1.25 (2) and 1.527 (2)/1.27 (3) Å, respectively.

The average Co—O distance in $(NH_4)_2[Co(H_2O)_6]_3(HPO_3)_4$ is 2.093 (2) Å, comparable to the average Co—O distances of 2.112 Å reported for $Co(HPO_3)\cdot H_2O$ (Sapina *et al.*, 1989), 2.143 Å for $Co_{11}(HPO_3)_8(OH)_6$ (Marcos *et al.*, 1993) or 2.101 Å for $NaCo(H_2PO_3)_3\cdot H_2O$ (Kratochvíl *et al.*, 1982).

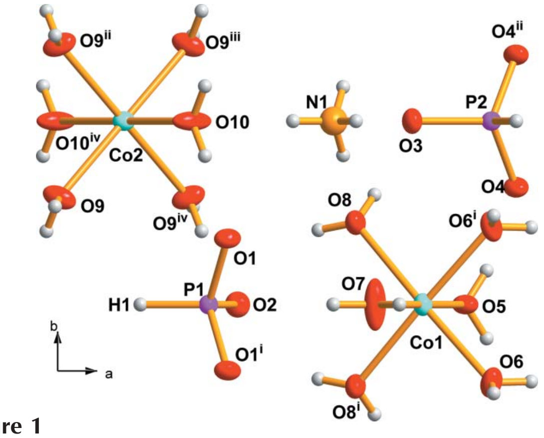

Figure 1
View of the $Co(H_2O)_6$, HPO_3 and NH_4 coordination polyhedra. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $x, -y, z$; (ii) $x, 1 - y, z$; (iii) $-x, 1 - y, -z$; (iv) $-x, y, -z$.]

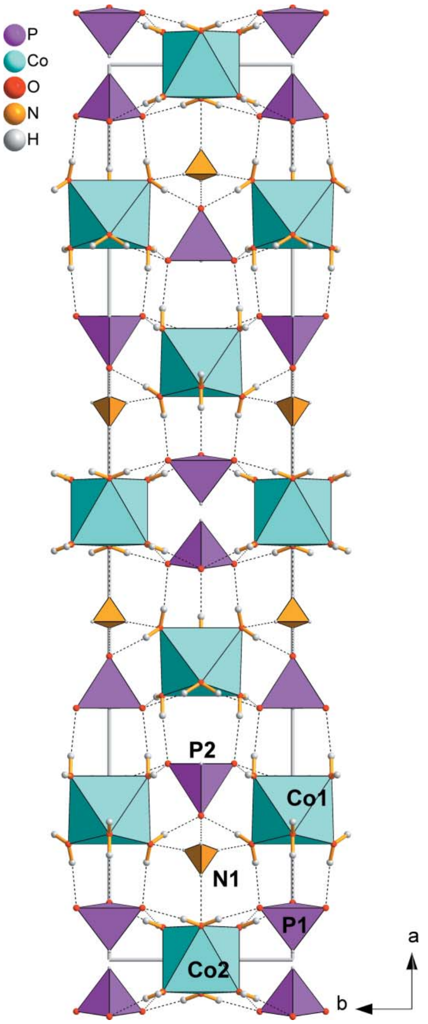

Figure 2
The packing of the title structure, viewed along the *c* axis.

The shortest Co···Co distance in the title compound, of 6.1873 (3) Å, is considerably longer than the values observed in the above-mentioned phosphites, *viz*. $Co(HPO_3)\cdot H_2O$ (3.015 Å), $Co_{11}(HPO_3)_8(OH)_6$ (2.757 Å) and $NaCo(H_2PO_3)_3\cdot H_2O$ (4.993 Å).

Experimental

In a solution of H_3PO_3 (10 ml), mixed with ammonia (0.4 *M*, 5 ml) to adjust the pH, $CoCl_2\cdot 6H_2O$ (10 mg) was dissolved. The mixture was heated to 300 K for 2 h and then left at room temperature for one week. Light-pink crystals deposited and were filtered off and washed with an 80:20 ethanol–water solution.

Crystal data

$(NH_4)_2[Co(H_2O)_6]_3(HPO_3)_4$
$M_r = 857.1$
Monoclinic, $C2/m$
$a = 34.3914$ (14) Å
$b = 7.0397$ (3) Å
$c = 6.1873$ (3) Å
$\beta = 91.638$ (3)°
$V = 1497.36$ (11) Å^3
$Z = 2$
$D_x = 1.900$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9315 reflections
$\theta = 3.3$–26.4°
$\mu = 1.97$ mm^{-1}
$T = 296$ K
Plate, pink
0.34 × 0.21 × 0.03 mm

Data collection

Oxford Diffraction Sapphire 2 CCD diffractometer
ω scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2004)
$T_{min} = 0.420$, $T_{max} = 0.795$
9315 measured reflections
1666 independent reflections
1546 reflections with $I > 3\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 26.4°$
$h = -42 \rightarrow 42$
$k = -8 \rightarrow 8$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.073$
$S = 1.53$
1666 reflections
143 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(I) + 0.0016I^2]$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

P1—O1	1.5250 (11)	Co1—O5	2.1297 (17)
P1—O2	1.5261 (16)	Co1—O6	2.0704 (13)
P1—H1	1.31 (2)	Co1—O7	2.1172 (19)
P2—O3	1.5351 (17)	Co1—O8	2.1132 (12)
P2—O4	1.5254 (12)	Co2—O9	2.0888 (13)
P2—H2	1.21 (3)	Co2—O10	2.072 (2)
O1—P1—O1^{i}	112.27 (7)	O8—Co1—O8^{i}	96.06 (5)
O1—P1—O2	112.41 (5)	O9—Co2—O9^{iii}	180
O1—P1—H1	106.3 (5)	O9—Co2—O9^{iv}	90.99 (5)
O2—P1—H1	106.7 (11)	O9—Co2—O9^{ii}	89.01 (5)
O3—P2—O4	111.75 (6)	O9—Co2—O10	93.64 (5)
O3—P2—H2	105.2 (12)	O9—Co2—O10^{iii}	86.36 (5)
O4—P2—O4^{ii}	112.75 (7)	O10—Co2—O10^{iii}	180
O4—P2—H2	107.5 (6)	H5—O5—H5^{i}	107.2 (17)
O5—Co1—O6	90.55 (5)	H61—O6—H62	107 (2)
O5—Co1—O7	176.84 (7)	H71—O7—H72	115 (3)
O5—Co1—O8	89.15 (5)	H81—O8—H82	102.7 (19)
O5—Co1—O8^{i}	89.15 (5)	H91—O9—H92	108 (2)
O6—Co1—O6^{i}	92.42 (5)	H100—O10—H100^{ii}	110.7 (19)
O6—Co1—O7	91.64 (5)	H110—N1—H112	115.6 (16)
O6—Co1—O8	178.15 (5)	H110—N1—H113	94 (3)
O6—Co1—O8^{i}	85.76 (5)	H112—N1—H112^{ii}	98.7 (17)
O7—Co1—O8	88.74 (5)	H112—N1—H113	117.4 (17)

Symmetry codes: (i) $x, -y, z$; (ii) $x, -y+1, z$; (iii) $-x, -y+1, -z$; (iv) $-x, y, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O4^{i}	0.81 (2)	1.89 (2)	2.6771 (15)	166 (1)
O6—H61···O4^{v}	0.81 (1)	1.92 (1)	2.7306 (16)	173 (2)
O6—H62···O4^{vi}	0.81 (1)	1.93 (1)	2.7279 (17)	170 (2)
O7—H71···O5^{vii}	0.81 (3)	2.08 (3)	2.887 (2)	178 (3)
O7—H72···O2^{vii}	0.82 (1)	1.87 (1)	2.682 (2)	180 (4)
O8—H81···O3	0.81 (2)	1.92 (2)	2.7249 (17)	173 (2)
O8—H82···O1	0.82 (2)	1.88 (1)	2.6890 (16)	171 (2)
O9—H91···O2^{iv}	0.82 (2)	1.90 (2)	2.7102 (16)	175 (1)
O9—H92···O1^{viii}	0.80 (1)	1.95 (1)	2.7319 (16)	165 (2)
O10—H100···O1	0.81 (2)	1.85 (2)	2.6624 (15)	175 (2)
N1—H110···O3	0.87 (2)	1.95 (2)	2.813 (3)	176 (3)
N1—H112···O8^{ix}	0.87 (2)	2.16 (2)	3.006 (2)	165 (2)
N1—H113···O10	0.87 (2)	2.32 (2)	3.182 (3)	173 (3)

Symmetry codes: (i) $x, -y, z$; (iv) $-x, y, -z$; (v) $-x+\frac{1}{2}, +y-\frac{1}{2}, -z+1$; (vi) $x, -y, z+1$; (vii) $x, y, z+1$; (viii) $-x, y, -z+1$; (ix) $x, -y+1, z-1$.

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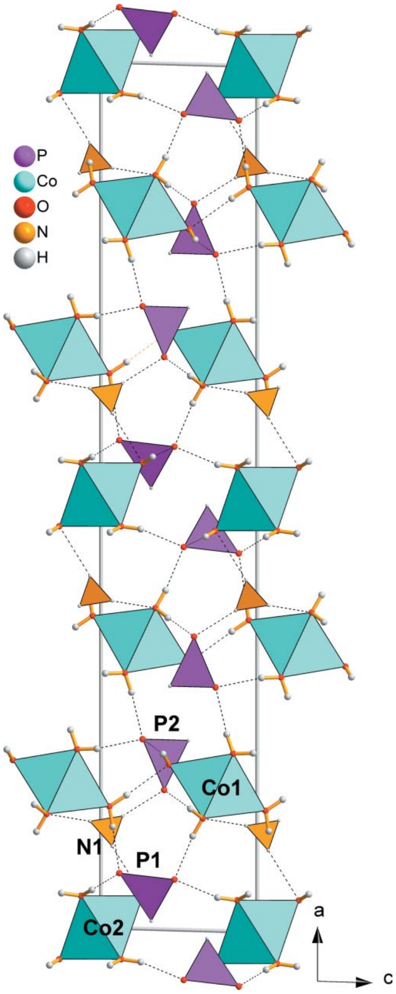

Figure 3
The packing of the title structure, viewed along the *b* axis.

The H atoms were located in a difference Fourier map. Their coordinates were refined independently. The O—H distances were restrained to 0.82 (1) Å and the N—H distances were restrained to 0.87 (1) Å. The H-atom isotropic displacement parameters were set at $1.2U_{\rm eq}$ of the parent atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2000* (Petricek *et al.*, 2000); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2000*.

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