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Disodium diaquabis(methylenediphosphonato-κ^2O,O')cobaltate(II) dihydrate

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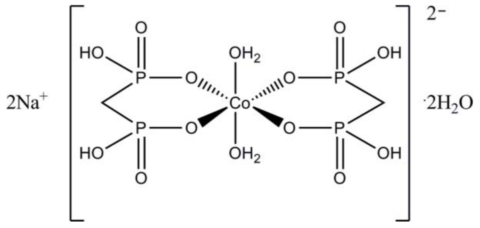
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(P–C) = 0.001 Å; R factor = 0.019; wR factor = 0.055; data-to-parameter ratio = 13.0.

In the title compound, $Na_2[Co(CH_4O_6P_2)_2(H_2O)_2]\cdot 2H_2O$, the asymmetric unit is composed of one methylenediphosphonate ligand and one water molecule, which both are coordinated to a Co^{II} atom, as well as a non-coordinated water molecule and a sodium cation. The Co^{II} atom occupies a special position on a crystallographic inversion centre. The slightly distorted Co^{II}O$_6$ octahedral coordination environment is composed of two bidentate methylenediphosphonate ligands and two coordinated water molecules in *trans* positions. The sodium ion is octahedrally coordinated to six O atoms with Na—O distances ranging from 2.3149 (12) to 2.6243 (12) Å. An extensive three-dimensional network of intermolecular as well as intramolecular O—H···O and C—H···O hydrogen bonding interacions is present.

Related literature

For general background to organic diphosphonic acids, see: Vega *et al.* (1996). For related structures, see: Bon *et al.* (2010); DeLaMatter *et al.* (1973); Harmony *et al.* (1984); Jurisson *et al.* (1983); Van der Merwe *et al.* (2010). For bond lengths and angles in related structures, see: Bao *et al.* (2003); Cao *et al.* (2007); Gong *et al.* (2006); Van der Merwe *et al.* (2009); Visser *et al.* (2010); Yin *et al.* (2003).



Experimental

Crystal data

$Na_2[Co(CH_4O_6P_2)_2(H_2O)_2]\cdot 2H_2O$
M_r = 524.94
Monoclinic, $P2_1/c$
a = 6.8694 (2) Å
b = 13.2860 (4) Å
c = 8.3541 (3) Å
β = 91.375 (1)°
V = 762.23 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.69 mm^{-1}
T = 100 K
0.52 × 0.24 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*, Bruker, 2007)
T_{min} = 0.474, T_{max} = 0.863
8742 measured reflections
1901 independent reflections
1838 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.055
S = 1.13
1901 reflections
146 parameters
7 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.0886 (10)	Co1—O2^i	2.1141 (10)
Co1—O7	2.0900 (10)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H6···O7	0.86 (1)	1.88 (1)	2.7154 (15)	164 (2)
C1—H4···O1^i	0.92 (2)	2.54 (2)	3.1449 (17)	123.9 (15)
C1—H3···O4^{ii}	0.92 (2)	2.53 (2)	3.4366 (17)	168.4 (17)
O3—H2···O2^{ii}	0.81 (3)	1.84 (3)	2.6394 (14)	176 (3)
O1—H1A···O6^{iii}	0.83 (2)	1.98 (2)	2.8008 (14)	173 (2)
O8—H7···O1^{iii}	0.83 (1)	2.57 (2)	3.2763 (15)	143 (2)
O1—H1B···O4^{iv}	0.83 (2)	1.84 (2)	2.6634 (15)	175 (2)
O5—H5···O6^v	0.82 (2)	1.81 (2)	2.6272 (14)	177 (3)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x, -y+1, -z+1$; (iv) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $-x, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2520).

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Acta Cryst. (2011). E**67**, m1468–m1469 Merwe *et al.* • $Na_2[Co(CH_4O_6P_2)_2(H_2O)_2]\cdot 2H_2O$ **m1469**

supplementary materials

Acta Cryst. (2011). E**67**, m1468-m1469   [**doi:10.1107/S1600536811038530**]

Disodium diaquabis(methylenediphosphonato-$\kappa^2 O,O'$)cobaltate(II) dihydrate

K. van der Merwe, H. G. Visser and J. A. Venter

Comment

The title compound forms part of an ongoing study involving methylene diphosphonate, and its coordination to various metal cores.

In the past 20 years numerous diphosphonate compounds have undergone intensive pharmacological studies primarily because of their possible use in treating bone diseases. This can be attributed to the fact that bisphosphonic acids are excellent anti-hypercalcemics and have a high affinity for bone tissue (Vega *et al.*, 1996).

In the title compound, $Na_2[Co(CH_4O_6P_2)_2(H_2O)_2]\cdot 2H_2O$, (Fig. 1, Table 1), the asymmetric unit is composed of one methylene diphosphonate ligand and one aqueous molecule which are coordinated to a Co(II) atom, as well as a non-coordinated aqueous solvent molecule and a sodium cation. The Co(II) atom occupies a special position on a crystallographic inversion centre. The sodium ion is octahedrally coordinated to six oxygen atoms with Na—O distances ranging from 2.3149 (12) to 2.6243 (12) Å. The octahedral geometry around the Co^{II} metal center is slightly distorted with O—Co—O angles ranging between 86.63 (4) ° and 93.14 (4) °. The Co—O bond lengths vary between 2.0886 (10) and 2.1141 (10) Å. These distances correspond to literature values (Bao *et al.* (2003); Cao *et al.* (2007); Gong *et al.* (2006); Yin *et al.* (2003); Van der Merwe *et al.* (2009); Visser *et al.* (2010).

A three-dimensional network is provided by numerous C—H–O and O—H–O hydrogen bonds (Figs. 2, 3 and Table 2).

Experimental

$CoCl_2\cdot 6H_2O$ (0,1696 g, 0,00071 mol) and methylene diphosphonate (0,3726 g, 0,00212 mol) were dissolved in distilled water (5 cm^3). Sodium hydroxide (3 cm^3, 1 *M*) was gradually added to the solution mixture which was heated for three days at 413 K. The final pH of the solution was adjusted to 1.23 with hydrochloric acid. Pink crystals, suitable for X-ray diffraction, were obtained. (Yield: 27.6%)

Refinement

All H atoms were located from difference Fourier maps and were refined isotropically without further restraints. The highest residual electron density was located 0.78 Å from C1.

Figures

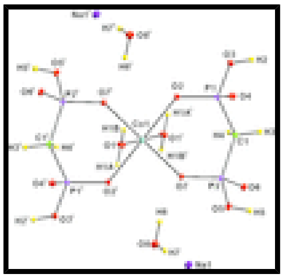


Fig. 1. Representation of the title compound, showing the numbering scheme and displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) 1-x, 1-y, -z].

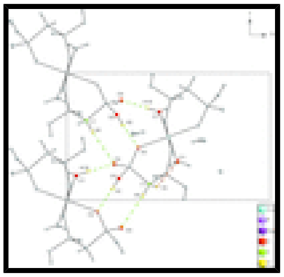


Fig. 2. The crystal packing of the title compound viewed along the *a* axis. Green dashed lines are employed to represent intermolecular hydrogen bonding and an orange dashed line was used to displace the intramolecular hydrogen bonding.

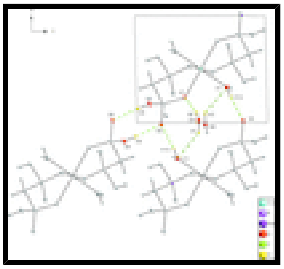


Fig. 3. The packing diagram of the title compound viewed along the *b* axis. Green dashed lines are utilized to display the extensive intermolecular hydrogen bonding.

Disodium diaquabis(methylenediphosphonato-κ^2*O,O*')cobaltate(II) dihydrate

Crystal data

$Na_2[Co(CH_4O_6P_2)_2(H_2O)_2]\cdot 2H_2O$

M_r = 524.94

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

a = 6.8694 (2) Å

b = 13.2860 (4) Å

c = 8.3541 (3) Å

β = 91.375 (1)°

V = 762.23 (4) Å^3

Z = 2

$F(000)$ = 530

D_x = 2.287 Mg m^{-3}

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 6202 reflections

θ = 2.9–28.4°

μ = 1.69 mm^{-1}

T = 100 K

Plate, pink

0.52 × 0.24 × 0.09 mm

Data collection

Bruker APEXII CCD diffractometer

phi and ω scans

1838 reflections with $I > 2\sigma(I)$

R_{int} = 0.022

Absorption correction: multi-scan (*SADABS*, Bruker, 2007)	θ_{max} = 28.4°, θ_{min} = 3.1°
T_{min} = 0.474, T_{max} = 0.863	$h = -8 \rightarrow 9$
8742 measured reflections	$k = -17 \rightarrow 16$
1901 independent reflections	$l = -11 \rightarrow 8$

Refinement

Refinement on F^2	7 restraints
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)] = 0.019$	$w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 0.4299P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.055$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.13$	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
1901 reflections	$\Delta\rho_{min}$ = −0.57 e Å^{-3}
146 parameters	

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.5	0.5	0.5	0.00488 (8)
P1	0.43774 (5)	0.30632 (3)	0.26142 (4)	0.00528 (9)
P2	0.17626 (5)	0.48657 (3)	0.20454 (4)	0.00578 (9)
Na1	0.06611 (8)	0.75775 (4)	0.22722 (7)	0.01006 (13)
O1	0.33424 (15)	0.45566 (8)	0.69412 (12)	0.0092 (2)
O2	0.52678 (14)	0.35119 (7)	0.41366 (11)	0.00758 (19)
O3	0.61219 (15)	0.25484 (8)	0.17312 (12)	0.0084 (2)
O4	0.27445 (14)	0.23364 (8)	0.28565 (12)	0.0087 (2)
O5	0.17550 (15)	0.58645 (8)	0.10142 (12)	0.0091 (2)
O6	−0.02026 (14)	0.43517 (8)	0.18700 (11)	0.00828 (19)
O7	0.23609 (15)	0.51625 (8)	0.37290 (12)	0.0081 (2)
O8	0.02069 (15)	0.67436 (8)	0.47388 (12)	0.0114 (2)
C1	0.3604 (2)	0.40539 (10)	0.12696 (15)	0.0072 (2)
H1A	0.241 (3)	0.4908 (15)	0.722 (3)	0.025 (6)*
H1B	0.321 (3)	0.3969 (13)	0.726 (3)	0.029 (6)*
H2	0.582 (4)	0.225 (2)	0.093 (3)	0.037 (7)*
H3	0.320 (3)	0.3732 (15)	0.035 (2)	0.015 (5)*
H4	0.469 (3)	0.4420 (15)	0.103 (2)	0.012 (4)*
H5	0.131 (4)	0.5780 (19)	0.011 (2)	0.038 (7)*
H6	0.092 (3)	0.6221 (13)	0.461 (3)	0.035 (5)*

H7	−0.091 (2)	0.6498 (18)	0.474 (3)	0.035 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.00514 (14)	0.00495 (14)	0.00451 (13)	−0.00021 (8)	−0.00063 (9)	−0.00021 (8)
P1	0.00519 (16)	0.00539 (17)	0.00524 (15)	0.00033 (12)	−0.00009 (11)	−0.00059 (11)
P2	0.00623 (17)	0.00582 (17)	0.00523 (17)	0.00061 (12)	−0.00118 (12)	−0.00022 (11)
Na1	0.0087 (3)	0.0113 (3)	0.0102 (3)	0.0003 (2)	−0.0008 (2)	0.0009 (2)
O1	0.0100 (5)	0.0072 (5)	0.0105 (4)	0.0011 (4)	0.0035 (4)	0.0019 (4)
O2	0.0107 (5)	0.0061 (5)	0.0059 (4)	0.0008 (4)	−0.0019 (3)	−0.0008 (3)
O3	0.0068 (5)	0.0104 (5)	0.0081 (4)	0.0017 (4)	−0.0002 (4)	−0.0032 (4)
O4	0.0072 (5)	0.0074 (5)	0.0116 (4)	−0.0008 (4)	0.0001 (3)	0.0000 (4)
O5	0.0121 (5)	0.0067 (5)	0.0084 (4)	0.0001 (4)	−0.0035 (4)	0.0013 (4)
O6	0.0071 (4)	0.0094 (5)	0.0083 (4)	−0.0004 (4)	−0.0013 (3)	−0.0002 (4)
O7	0.0080 (5)	0.0098 (5)	0.0064 (4)	0.0021 (4)	−0.0021 (3)	−0.0015 (3)
O8	0.0091 (5)	0.0141 (5)	0.0109 (5)	0.0018 (4)	0.0006 (4)	−0.0003 (4)
C1	0.0076 (6)	0.0077 (6)	0.0061 (6)	0.0001 (5)	0.0000 (5)	0.0000 (5)

Geometric parameters (Å, °)

Co1—O1	2.0886 (10)	Na1—O3^{iii}	2.3431 (12)
Co1—O1^{i}	2.0886 (10)	Na1—O4^{iv}	2.3612 (11)
Co1—O7	2.0900 (10)	Na1—O6^{iv}	2.4860 (12)
Co1—O7	2.0900 (10)	Na1—O5	2.6243 (12)
Co1—O7^{i}	2.0900 (10)	O1—H1A	0.831 (16)
Co1—O2	2.1141 (10)	O1—H1B	0.830 (16)
Co1—O2^{i}	2.1141 (10)	O3—Na1^{v}	2.3431 (12)
P1—O4	1.4975 (10)	O3—H2	0.81 (3)
P1—O2	1.5198 (10)	O4—Na1^{vi}	2.3612 (11)
P1—O3	1.5781 (10)	O5—H5	0.815 (16)
P1—C1	1.8021 (14)	O6—Na1^{vi}	2.4860 (12)
P2—O7	1.5083 (10)	O8—Na1^{vii}	2.3149 (12)
P2—O7	1.5083 (10)	O8—H6	0.856 (13)
P2—O6	1.5169 (10)	O8—H7	0.834 (13)
P2—O5	1.5820 (10)	C1—H3	0.92 (2)
P2—C1	1.7954 (14)	C1—H4	0.92 (2)
Na1—O8^{ii}	2.3149 (12)		

O1—Co1—O1^{i}	180	O5—P2—C1	107.49 (6)
O1—Co1—O7	86.63 (4)	O8^{ii}—Na1—O3^{iii}	115.88 (4)
O1^{i}—Co1—O7	93.37 (4)	O8^{ii}—Na1—O4^{iv}	84.24 (4)
O1—Co1—O7	86.63 (4)	O3^{iii}—Na1—O4^{iv}	159.88 (4)
O1^{i}—Co1—O7	93.37 (4)	O8^{ii}—Na1—O6^{iv}	83.04 (4)
O1—Co1—O7^{i}	93.37 (4)	O3^{iii}—Na1—O6^{iv}	92.19 (4)
O1^{i}—Co1—O7^{i}	86.63 (4)	O4^{iv}—Na1—O6^{iv}	90.55 (4)

O7—Co1—O7^{i}	180	O8^{ii}—Na1—O5	90.31 (4)
O7—Co1—O7^{i}	180	O3^{iii}—Na1—O5	81.45 (4)
O1—Co1—O2	93.14 (4)	O4^{iv}—Na1—O5	99.03 (4)
O1^{i}—Co1—O2	86.86 (4)	O6^{iv}—Na1—O5	167.75 (4)
O7—Co1—O2	90.28 (4)	Co1—O1—H1A	119.7 (16)
O7—Co1—O2	90.28 (4)	Co1—O1—H1B	125.4 (16)
O7^{i}—Co1—O2	89.73 (4)	H1A—O1—H1B	110 (2)
O1—Co1—O2^{i}	86.86 (4)	P1—O2—Co1	128.01 (6)
O1^{i}—Co1—O2^{i}	93.14 (4)	P1—O3—Na1^{v}	123.17 (6)
O7—Co1—O2^{i}	89.72 (4)	P1—O3—H2	114.8 (19)
O7—Co1—O2^{i}	89.72 (4)	Na1^{v}—O3—H2	122.0 (19)
O7^{i}—Co1—O2^{i}	90.27 (4)	P1—O4—Na1^{vi}	130.61 (6)
O2—Co1—O2^{i}	180.00 (5)	P2—O5—Na1	120.44 (5)
O4—P1—O2	115.31 (6)	P2—O5—H5	112.6 (18)
O4—P1—O3	111.31 (6)	Na1—O5—H5	112.6 (18)
O2—P1—O3	105.44 (6)	P2—O6—Na1^{vi}	121.18 (5)
O4—P1—C1	110.17 (6)	P2—O7—Co1	131.33 (6)
O2—P1—C1	109.98 (6)	Na1^{vii}—O8—H6	111.4 (16)
O3—P1—C1	103.94 (6)	Na1^{vii}—O8—H7	104.6 (17)
O7—P2—O6	115.45 (6)	H6—O8—H7	102 (2)
O7—P2—O6	115.45 (6)	P2—C1—P1	114.42 (7)
O7—P2—O5	106.61 (6)	P2—C1—H3	112.4 (12)
O7—P2—O5	106.61 (6)	P1—C1—H3	105.2 (12)
O6—P2—O5	109.49 (6)	P2—C1—H4	110.3 (12)
O7—P2—C1	108.36 (6)	P1—C1—H4	107.1 (12)
O7—P2—C1	108.36 (6)	H3—C1—H4	107.0 (17)
O6—P2—C1	109.14 (6)		

O4—P1—O2—Co1	−108.16 (8)	O6^{iv}—Na1—O5—P2	140.99 (16)
O3—P1—O2—Co1	128.63 (7)	Na1^{ii}—Na1—O5—P2	−161.48 (7)
C1—P1—O2—Co1	17.13 (9)	Na1^{vii}—Na1—O5—P2	16.59 (7)
O1—Co1—O2—P1	111.59 (7)	O7—P2—O6—Na1^{vi}	−74.24 (8)
O1^{i}—Co1—O2—P1	−68.41 (7)	O7—P2—O6—Na1^{vi}	−74.24 (8)
O7—Co1—O2—P1	24.95 (7)	O5—P2—O6—Na1^{vi}	165.48 (5)
O7—Co1—O2—P1	24.95 (7)	C1—P2—O6—Na1^{vi}	48.07 (7)
O7^{i}—Co1—O2—P1	−155.05 (7)	O6—P2—O7—Co1	134.82 (7)
O4—P1—O3—Na1^{v}	−126.78 (7)	O5—P2—O7—Co1	−103.34 (8)
O2—P1—O3—Na1^{v}	−1.06 (8)	C1—P2—O7—Co1	12.09 (10)
C1—P1—O3—Na1^{v}	114.66 (7)	O1—Co1—O7—P2	−136.95 (8)
O2—P1—O4—Na1^{vi}	97.12 (8)	O1^{i}—Co1—O7—P2	43.05 (8)
O3—P1—O4—Na1^{vi}	−142.84 (7)	O2—Co1—O7—P2	−43.82 (8)
C1—P1—O4—Na1^{vi}	−28.09 (9)	O2^{i}—Co1—O7—P2	136.18 (8)
O7—P2—O5—Na1	−35.73 (8)	O7—P2—C1—P1	46.92 (9)
O7—P2—O5—Na1	−35.73 (8)	O7—P2—C1—P1	46.92 (9)

O6—P2—O5—Na1	89.81 (7)	O6—P2—C1—P1	−79.55 (8)
C1—P2—O5—Na1	−151.75 (6)	O5—P2—C1—P1	161.78 (7)
O8^{ii}—Na1—O5—P2	−162.13 (6)	O4—P1—C1—P2	66.52 (9)
O3^{iii}—Na1—O5—P2	81.72 (6)	O2—P1—C1—P2	−61.67 (9)
O4^{iv}—Na1—O5—P2	−77.92 (7)	O3—P1—C1—P2	−174.14 (7)

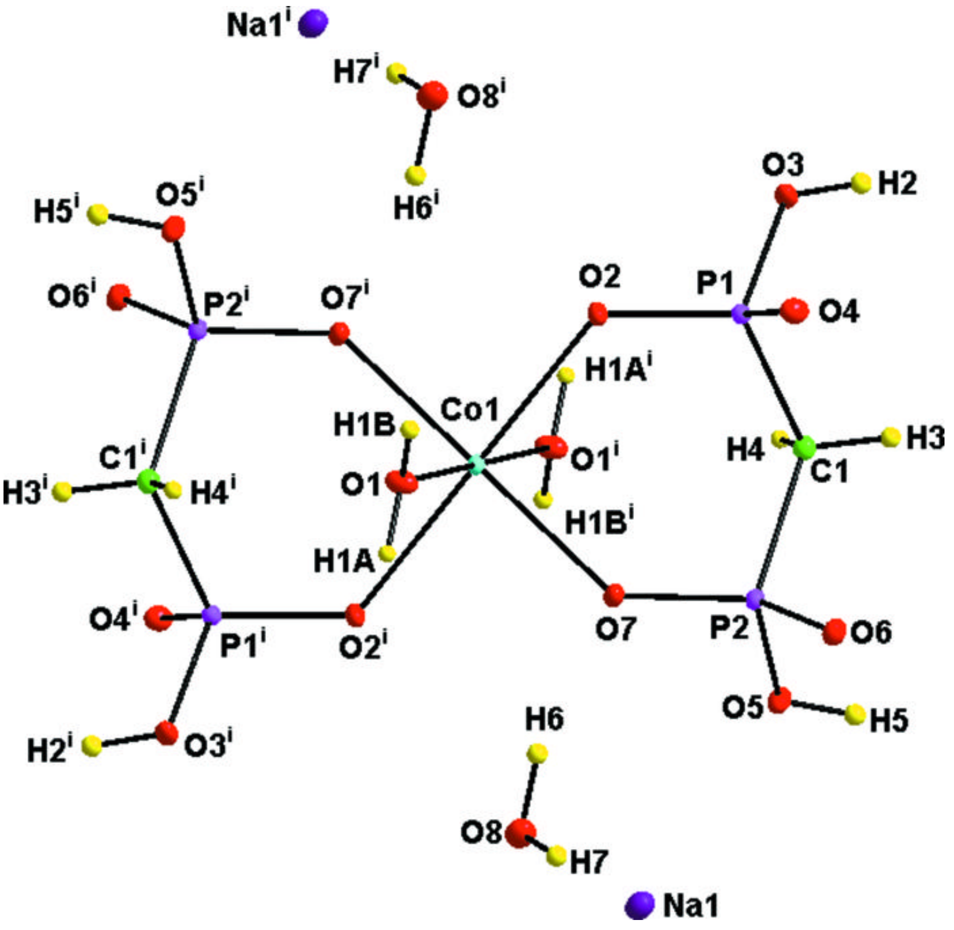
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) −*x*, *y*+1/2, −*z*+1/2; (v) −*x*+1, *y*−1/2, −*z*+1/2; (vi) −*x*, *y*−1/2, −*z*+1/2; (vii) *x*, −*y*+3/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H6···O7	0.86 (1)	1.88 (1)	2.7154 (15)	164 (2)
C1—H4···O1^{i}	0.92 (2)	2.54 (2)	3.1449 (17)	123.9 (15)
C1—H3···O4^{viii}	0.92 (2)	2.53 (2)	3.4366 (17)	168.4 (17)
O3—H2···O2^{viii}	0.81 (3)	1.84 (3)	2.6394 (14)	176 (3)
O1—H1A···O6^{ix}	0.83 (2)	1.98 (2)	2.8008 (14)	173 (2)
O8—H7···O1^{ix}	0.83 (1)	2.57 (2)	3.2763 (15)	143 (2)
O1—H1B···O4^{x}	0.83 (2)	1.84 (2)	2.6634 (15)	175 (2)
O5—H5···O6^{xi}	0.82 (2)	1.81 (2)	2.6272 (14)	177 (3)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (viii) *x*, −*y*+1/2, *z*−1/2; (ix) −*x*, −*y*+1, −*z*+1; (x) *x*, −*y*+1/2, *z*+1/2; (xi) −*x*, −*y*+1, −*z*.

Fig. 1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H6i
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O5i
O3
H2
O6i
P2i
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H1Ai
Co1
H1B
H4
H3
C1i
O1
O1i
C1
H3i
H4i
H1Bi
H1A
O4i
P1i
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P2
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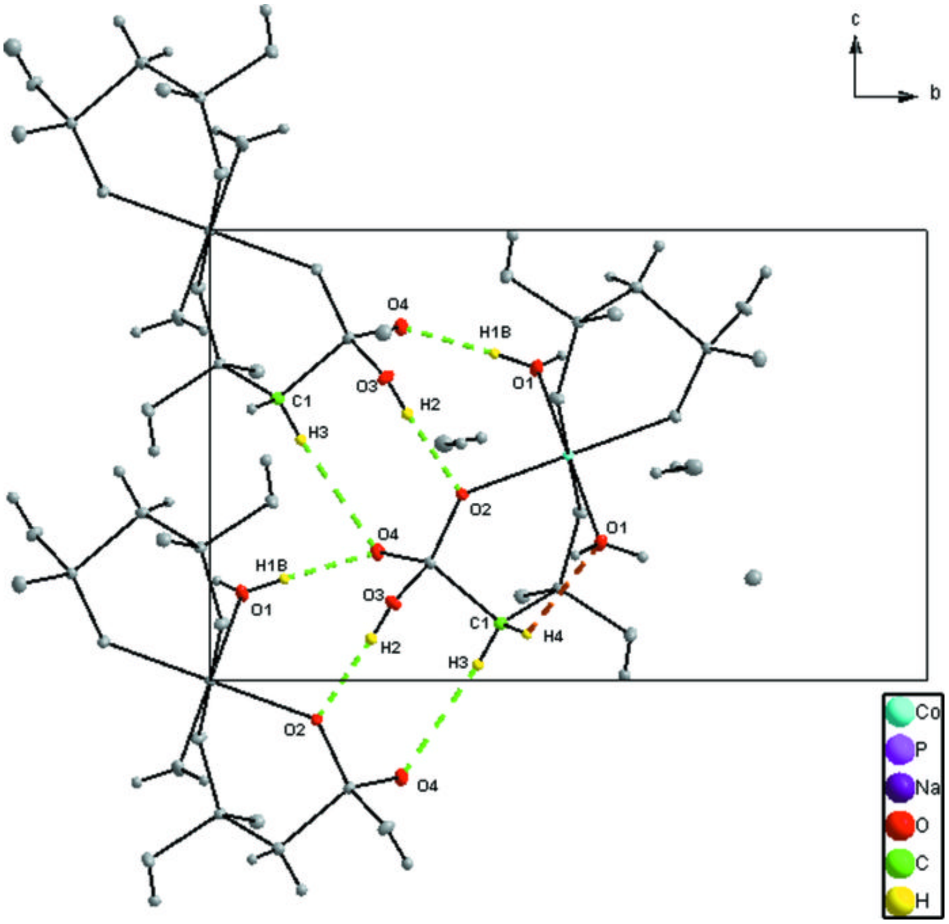
H5
H6
H2i
O3i
O8
H7
Na1

Fig. 2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O1
O3
C1
H2
H3
O2
O4
O1
H1B
O1
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C1
H2
H4
H3
O2
O4
Co
P
Na
O
C
H

Fig. 3