Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

$Ni_2Sr(PO_4)_2 \cdot 2H_2O$

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Received 19 October 2010; accepted 3 November 2010

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(P–O) = 0.003 Å; R factor = 0.019; wR factor = 0.052; data-to-parameter ratio = 9.3.

The title compound, dinickel(II) strontium bis[orthophosphate(V)] dihydrate, was obtained under hydrothermal conditions. The crystal structure consists of linear chains $_\infty^1[NiO_{2/2}(OH_2)_{2/2}O_{2/1}]$ of edge-sharing NiO_6 octahedra ($\overline{1}$ symmetry) running parallel to [010]. Adjacent chains are linked to each other through PO_4 tetrahedra (m symmetry) and arranged in such a way to build layers parallel to (001). The three-dimensional framework is accomplished by stacking of adjacent layers that are held together by SrO_8 polyhedra ($2/m$ symmetry). Two types of O—H⋯O hydrogen bonds involving the water molecule are present, *viz*. one very strong hydrogen bond perpendicular to the layers and weak trifurcated hydrogen bonds parallel to the layers.

Related literature

For catalytic properties of phosphates, see: Cheetham *et al.* (1999); Clearfield (1988). The crystal structure of anhydrous $Ni_2Sr(PO_4)_2$ has been reported by El Bali *et al.* (1993). For crystal structures of some hydrous orthophosphates of divalent cations, see: Assani *et al.* (2010); Effenberger (1999); Lee *et al.* (2008); Britvin *et al.* (2002); Stock (2002); Yakubovich *et al.* (2001). For bond-valence analysis, see: Brown & Altermatt (1985).

Experimental

Crystal data

$Ni_2Sr(PO_4)_2 \cdot 2H_2O$
M_r = 431.01
Monoclinic, $C2/m$
a = 8.8877 (3) Å
b = 6.0457 (3) Å
c = 7.3776 (3) Å
β = 114.173 (2)°
V = 361.66 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 12.99 mm^{-1}
T = 296 K
0.20 × 0.10 × 0.07 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.229, T_{max} = 0.403
2376 measured reflections
454 independent reflections
439 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.052
S = 1.12
454 reflections
49 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sr1—O1^{i}	2.626 (2)	Ni1—O3	2.0895 (18)
Sr1—O2	2.636 (3)	P1—O2	1.517 (3)
Sr1—O3	2.797 (3)	P1—O1	1.539 (2)
Ni1—O4	2.0285 (19)	P1—O3	1.564 (3)
Ni1—O1^{ii}	2.0499 (19)		

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, z$; (ii) $-x + 2, y, -z + 1$.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O4—H1⋯O4^{iii}	0.85 (6)	2.23 (7)	2.951 (4)	143 (7)
O4—H1⋯O1^{iv}	0.85 (6)	2.28 (4)	2.784 (3)	118 (4)
O4—H1⋯O1^{v}	0.85 (6)	2.28 (4)	2.784 (3)	118 (4)
O4—H2⋯O2^{vi}	0.85 (3)	1.67 (3)	2.511 (4)	169 (9)

Symmetry codes: (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x + \frac{3}{2}, -y + \frac{3}{2}, -z + 1$; (v) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + 1$; (vi) $x, y, z + 1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia,1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Unit of Support for Technical and Scientific Research (UATRS, CNRST) for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2418).

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supporting information

Acta Cryst. (2010). E**66**, i86–i87 [https://doi.org/10.1107/S1600536810045113]

$Ni_2Sr(PO_4)_2{\cdot}2H_2O$

Abderrazzak Assani, Mohamed Saadi, Mohammed Zriouil and Lahcen El Ammari

S1. Comment

Metal based phosphates continue to be interesting materials due to their remarkable variety of structures, associated with outstanding properties in widespread applications such as catalysis and ion-exchangers (Cheetham *et al.*, 1999; Clearfield, 1988).

Our focus of investigation is associated with mixed divalent orthophosphates with general formula $(M,M')_3(PO_4)_2.nH_2O$ (Assani *et al.*, 2010). This family of phosphates goes along with a diversity of structures, depending on the size difference of the (various) divalent cations (Effenberger, 1999) and on the degree of hydratation (Yakubovich *et al.*, 2001; Lee *et al.*, 2008), ranging from 0.5 H_2O in the manganese phosphate $Mn_3(PO_4)_2.0.5H_2O$ (Stock, 2002) to 22 H_2O in the case of $Mg_3(PO_4)_2.22H_2O$ (Britvin *et al.*, 2002). A topological comparison with their corresponding anhydrous phosphates clearly reveals substantial differences in their structural set-up.

By means of the hydrothermal method, we have synthesized a the hydrous strontium nickel phosphate, $Ni_2Sr(PO_4)_2.2H_2O$, representing a novel structure type. A partial three-dimensional plot of the crystal structure of the title compound is represented in Fig. 1, illustrating the connection of the metal-oxygen polyhedra. The network is built up from three different types of polyhedra more or less distorted, *viz*. SrO_8 polyhedra ($2/m$ symmetry) with distances ranging from 2.636 (2) Å to 2.797 (3) Å, NiO_6 octahedra ($\overline{1}$ symmetry) and PO_4 tetrahedra (m symmetry). Edge-sharing NiO_6 octahedra form an infinite chain ${}_{\infty}{}^{1}[NiO_{2/2}(OH_2)_{2/2}O_{2/1}]$ running parallel to [010], as shown in Fig. 2. Adjacent chains are connected by PO_4 tetrahedra and weak trifurcated hydrogen bonds (O4–H1···(O4,O1)) to build up layers parallel to (001). These layers are in turn linked by sheets of Sr^{2+} cations and by very strong hydrogen bond (O4–H2···O2) as shown in Fig. 2 and Table 2.

Bond valence sum calculations (Brown & Altermatt, 1985) for Ni^{2+}, Sr^{2+} and P^{5+} ions are as expected, *viz*. 2.03, 1.83 and 4.93 valence units, respectively. The values of the bond valence sums calculated for all oxygen atoms are: 1.83, 1.56 and 1.93 for O1, O2 and O3, respectively. The low bond valence sum of O2 indicates that it is considerably undersaturated and thus acts as an acceptor with a very short H-bond (Table 2).

It is particularly interesting to compare the crystal structures of this compound with that of its corresponding anhydrous phosphate (El Bali *et al.*, 1993). Indeed, both structures can be described by the stacking of two-dimensional layers connected to each other by Sr^{2+} ions. However, we can note the following important differences: The presence of NiO_5 polyhedra in the anhydrous phase and a different space group ($P\overline{1}$) and lattice parameters. Moreover, due to the lower symmetry, the polyhedra are more distorted in the anhydrous phase.

S2. Experimental

A typical hydrothermal synthesis has allowed to isolate the title compound from the reaction mixture of strontium carbonate ($SrCO_3$; 0.0738 g), metallic nickel (Ni; 0.0881 g) and 85 wt% phosphoric acid (H_3PO_4; 0,10 ml) and water (H_2O; 10 ml). The hydrothermal reaction was performed in a 23 ml Teflon-lined autoclave under autogeneous pressure at

468 K for two days. The product was filtered off, washed with deionized water and air dried. The resulting product consists of parallelepipedic turquoise crystals besides some gray powder.

S3. Refinement

All O-bound H atoms were initially located in a difference map and refined with O—H (0.85) distance restraints and a common U_{iso} for both H atoms for the water molecule.

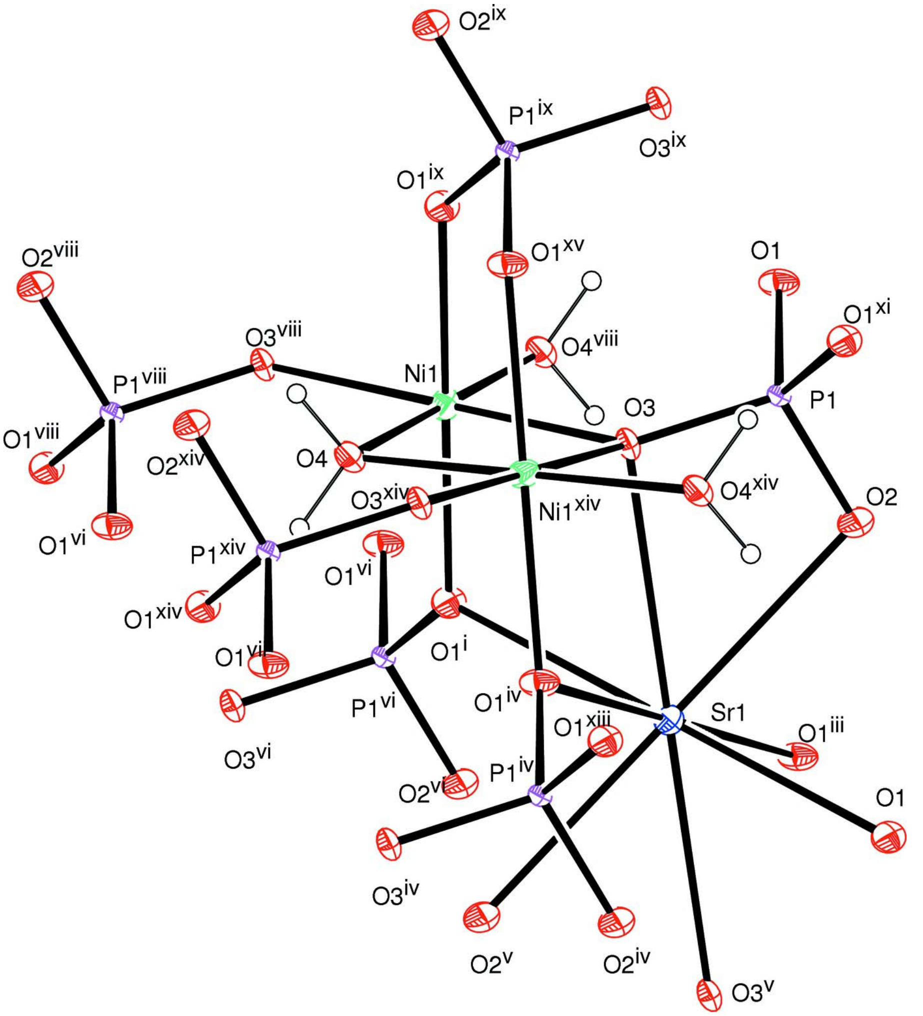

Figure 1

Partial plot of $Ni_2Sr(PO_4)_2,2H_2O$ crystal structure. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: (i) *x* - 1/2, -*y* + 3/2, *z*; (ii) -*x* + 3/2, *y* - 1/2, -*z*; (iii) -*x* + 3/2, -*y* + 3/2, -*z*; (iv) *x* - 1/2, *y* - 1/2, *z*; (v) -*x* + 1, -*y* + 1, -*z*; (vi) *x* - 1/2, *y* + 1/2, *z*; (vii) -*x* + 3/2, -*y* + 1/2, -*z*; (viii) -*x* + 3/2, -*y* + 3/2, -*z* + 1; (ix) -*x* + 2, *y*, -*z* + 1; (*x*) *x* + 1/2, *y* + 1/2, *z* + 1; (xi) *x*, -*y* + 1, *z*; (xii) *x* + 1/2, *y* - 1/2, *z*; (xiii) *x* + 1/2, *y* + 1/2, *z*; (xiv) -*x* + 3/2, *y* - 1/2, -*z* + 1; (xv) -*x* + 2, -*y* + 1, -*z* + 1.

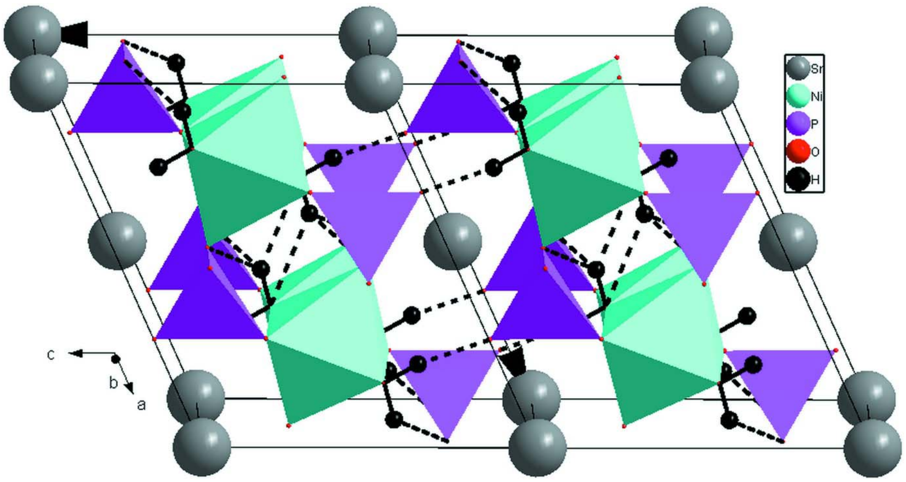

Figure 2

A three-dimensional polyhedral view of the crystal structure of the $Ni_2Sr(PO_4)_2.2H_2O$, showing the stacking of layers along the *c* axis and the hydrogen bonding scheme (dashed lines).

dinickel(II) strontium bis[orthophosphate(V)] dihydrate

Crystal data

$Ni_2Sr(PO_4)_2 \cdot 2H_2O$
$M_r = 431.01$
Monoclinic, $C2/m$
Hall symbol: -C 2y
$a = 8.8877$ (3) Å
$b = 6.0457$ (3) Å
$c = 7.3776$ (3) Å
$\beta = 114.173$ (2)°
$V = 361.66$ (3) Å^3
$Z = 2$

$F(000) = 416$
$D_x = 3.958$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 454 reflections
$\theta = 3.0$–27.4°
$\mu = 12.99$ mm^{-1}
$T = 296$ K
Parallelepiped, pale green
0.20 × 0.10 × 0.07 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.229$, $T_{max} = 0.403$

2376 measured reflections
454 independent reflections
439 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.0°$
$h = -11 \rightarrow 11$
$k = -7 \rightarrow 7$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.052$
$S = 1.12$
454 reflections
49 parameters
3 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0243P)^2 + 1.4658P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	$U_{iso}*/U_{eq}$
Sr1	0.5000	0.5000	0.0000	0.01385 (17)
Ni1	0.7500	0.7500	0.5000	0.00948 (17)
P1	0.91308 (11)	0.5000	0.22145 (14)	0.0053 (2)
O1	1.0211 (2)	0.7094 (3)	0.2739 (3)	0.0110 (4)
O2	0.7975 (3)	0.5000	0.0027 (4)	0.0143 (6)
O3	0.7992 (3)	0.5000	0.3363 (4)	0.0084 (5)
O4	0.6779 (3)	0.5000	0.6298 (4)	0.0128 (6)
H1	0.577 (4)	0.5000	0.610 (13)	0.15 (4)*
H2	0.730 (10)	0.5000	0.755 (4)	0.15 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0089 (3)	0.0253 (3)	0.0071 (3)	0.000	0.00297 (19)	0.000
Ni1	0.0100 (3)	0.0095 (3)	0.0083 (3)	0.00375 (18)	0.00307 (19)	0.00014 (19)
P1	0.0045 (4)	0.0055 (5)	0.0059 (5)	0.000	0.0020 (3)	0.000
O1	0.0090 (9)	0.0104 (10)	0.0116 (10)	−0.0040 (8)	0.0021 (7)	0.0013 (8)
O2	0.0100 (13)	0.0226 (17)	0.0080 (15)	0.000	0.0014 (11)	0.000
O3	0.0084 (12)	0.0086 (14)	0.0107 (13)	0.000	0.0066 (10)	0.000
O4	0.0076 (13)	0.0211 (17)	0.0107 (14)	0.000	0.0047 (11)	0.000

Geometric parameters (Å, º)

Sr1—O1^{i}	2.626 (2)	Ni1—O1^{i}	2.0499 (19)
Sr1—O1^{ii}	2.626 (2)	Ni1—O1^{vii}	2.0499 (19)
Sr1—O1^{iii}	2.626 (2)	Ni1—O3^{vi}	2.0895 (18)
Sr1—O1^{iv}	2.626 (2)	Ni1—O3	2.0895 (18)
Sr1—O2^{v}	2.636 (3)	P1—O2	1.517 (3)
Sr1—O2	2.636 (3)	P1—O1^{viii}	1.539 (2)
Sr1—O3	2.797 (3)	P1—O1	1.539 (2)
Sr1—O3^{v}	2.797 (3)	P1—O3	1.564 (3)
Ni1—O4^{vi}	2.0285 (19)	O4—H1	0.85 (5)

Ni1—O4	2.0285 (19)	O4—H2	0.85 (5)

O1^{i}—Sr1—O1^{ii}	180.0	O1^{i}—Ni1—O1^{vii}	180.0
O1^{i}—Sr1—O1^{iii}	96.00 (9)	O4^{vi}—Ni1—O3^{vi}	85.13 (8)
O1^{ii}—Sr1—O1^{iii}	84.00 (9)	O4—Ni1—O3^{vi}	94.87 (8)
O1^{i}—Sr1—O1^{iv}	84.00 (9)	O1^{i}—Ni1—O3^{vi}	90.62 (9)
O1^{ii}—Sr1—O1^{iv}	96.00 (9)	O1^{vii}—Ni1—O3^{vi}	89.38 (9)
O1^{iii}—Sr1—O1^{iv}	180.00 (7)	O4^{vi}—Ni1—O3	94.87 (8)
O1^{i}—Sr1—O2^{v}	76.18 (6)	O4—Ni1—O3	85.13 (8)
O1^{ii}—Sr1—O2^{v}	103.82 (6)	O1^{i}—Ni1—O3	89.38 (10)
O1^{iii}—Sr1—O2^{v}	103.82 (6)	O1^{vii}—Ni1—O3	90.62 (9)
O1^{iv}—Sr1—O2^{v}	76.18 (6)	O3^{vi}—Ni1—O3	180.0
O1^{i}—Sr1—O2	103.82 (6)	O2—P1—O1^{viii}	110.38 (10)
O1^{ii}—Sr1—O2	76.18 (6)	O2—P1—O1	110.38 (10)
O1^{iii}—Sr1—O2	76.18 (6)	O1^{viii}—P1—O1	110.64 (16)
O1^{iv}—Sr1—O2	103.82 (6)	O2—P1—O3	105.67 (16)
O2^{v}—Sr1—O2	180.0	O1^{viii}—P1—O3	109.83 (10)
O1^{i}—Sr1—O3	64.85 (6)	O1—P1—O3	109.83 (10)
O1^{ii}—Sr1—O3	115.15 (6)	P1—O1—Ni1^{vii}	127.73 (12)
O1^{iii}—Sr1—O3	115.15 (6)	P1—O1—Sr1^{ix}	121.08 (11)
O1^{iv}—Sr1—O3	64.85 (6)	Ni1^{vii}—O1—Sr1^{ix}	106.29 (8)
O2^{v}—Sr1—O3	126.37 (8)	P1—O2—Sr1	104.37 (14)
O2—Sr1—O3	53.63 (8)	P1—O3—Ni1	130.42 (7)
O1^{i}—Sr1—O3^{v}	115.15 (6)	P1—O3—Ni1^{x}	130.42 (7)
O1^{ii}—Sr1—O3^{v}	64.85 (6)	Ni1—O3—Ni1^{x}	92.66 (11)
O1^{iii}—Sr1—O3^{v}	64.85 (6)	P1—O3—Sr1	96.33 (13)
O1^{iv}—Sr1—O3^{v}	115.15 (6)	Ni1—O3—Sr1	99.48 (8)
O2^{v}—Sr1—O3^{v}	53.63 (8)	Ni1^{x}—O3—Sr1	99.48 (8)
O2—Sr1—O3^{v}	126.37 (8)	Ni1^{x}—O4—Ni1	96.34 (12)
O3—Sr1—O3^{v}	180.00 (9)	Ni1^{x}—O4—H1	116 (3)
O4^{vi}—Ni1—O4	180.0	Ni1—O4—H1	116 (3)
O4^{vi}—Ni1—O1^{i}	85.80 (10)	Ni1^{x}—O4—H2	112 (4)
O4—Ni1—O1^{i}	94.20 (10)	Ni1—O4—H2	112 (4)
O4^{vi}—Ni1—O1^{vii}	94.20 (10)	H1—O4—H2	105 (8)
O4—Ni1—O1^{vii}	85.80 (10)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H1···O4^{xi}	0.85 (6)	2.23 (7)	2.951 (4)	143 (7)
O4—H1···O1^{vi}	0.85 (6)	2.28 (4)	2.784 (3)	118 (4)
O4—H1···O1^{x}	0.85 (6)	2.28 (4)	2.784 (3)	118 (4)
O4—H2···O2^{xii}	0.85 (3)	1.67 (3)	2.511 (4)	169 (9)

Symmetry codes: (vi) −*x*+3/2, −*y*+3/2, −*z*+1; (x) −*x*+3/2, *y*−1/2, −*z*+1; (xi) −*x*+1, −*y*+1, −*z*+1; (xii) *x*, *y*, *z*+1.