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Poly[[hexaaqua(μ_2-fumarato-$\kappa^4O^1,O^{1'}:O^4,O^{4'}$)bis($\mu_3$-maleato-$\kappa^4O^1,O^{1'}:O^4:O^{4'}$)disamarium(III)] hexahydrate]

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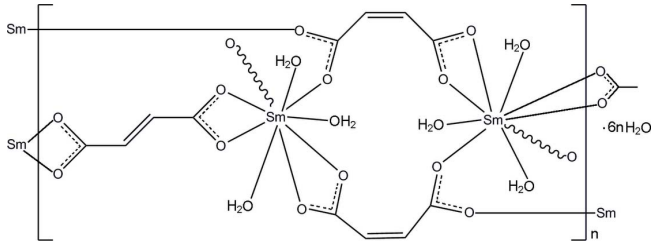
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.006 Å; R factor = 0.017; wR factor = 0.066; data-to-parameter ratio = 17.9.

In the title coordination polymer, $\{[Sm_2(C_4H_2O_4)_3(H_2O)_6]\cdot 6H_2O\}_n$, the Sm^{III} ion is nine-coordinated by four O atoms from three different maleate ligands, two O atoms from one fumarate ligand and three O atoms from three water molecules. The fumarate ligand lies on an inversion center. Adjacent Sm^{III} ions are bridged by the maleate and fumarate ligands, forming a layer parallel to (011). The layers are further linked by intermolecular O—H···O hydrogen bonds into a three-dimensional supramolecular network.

Related literature

For the structures of transition metal complexes with malonate ligands, see: Li *et al.* (2006); Ye *et al.* (2007); Zhu *et al.* (2007). For a related structure, see: Hansson & Thörnqwist (1975).



Experimental

Crystal data

$[Sm_2(C_4H_2O_4)_3(H_2O)_6]\cdot 6H_2O$
M_r = 859.08
Triclinic, $P\overline{1}$
a = 6.150 (3) Å
b = 10.679 (6) Å
c = 11.214 (6) Å
α = 69.99 (3)°
β = 79.64 (2)°
γ = 89.74 (2)°
V = 679.4 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 4.38 mm^{-1}
T = 290 K
0.08 × 0.07 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.732, T_{max} = 0.782
6707 measured reflections
3071 independent reflections
2950 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.066
S = 1.00
3071 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O6^{i}	0.85	1.88	2.680 (4)	156
O7—H7A···O11^{ii}	0.85	1.95	2.774 (5)	164
O8—H8A···O11^{iii}	0.85	1.94	2.770 (5)	164
O8—H8B···O10^{ii}	0.85	1.97	2.792 (5)	164
O9—H9A···O7^{iv}	0.85	2.10	2.893 (4)	155
O9—H9B···O3^{iv}	0.85	1.97	2.808 (4)	168
O10—H10A···O1^{v}	0.85	1.97	2.783 (4)	160
O10—H10B···O12	0.85	1.95	2.761 (5)	159
O11—H11B···O12	0.85	1.93	2.775 (5)	171
O11—H11A···O10^{iv}	0.85	1.95	2.755 (5)	157
O12—H12A···O4^{vi}	0.85	1.87	2.705 (5)	168
O12—H12B···O5^{ii}	0.89	1.98	2.744 (5)	142

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2363).

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Zhu, T., Li, B., Yang, G.-D. & Wu, L.-X. (2007). *Acta Cryst.* E**63**, m409–m410.

supporting information

Acta Cryst. (2010). E**66**, m1540 [https://doi.org/10.1107/S1600536810045204]

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Bao Li and Li-Xin Wu

S1. Comment

Diacids have been widely used to form metal–organic frameworks. Recently, we reported several compounds based on malonate ligand and different transition metal ions (Li *et al.*, 2006; Ye *et al.*, 2007; Zhu *et al.*, 2007). Hererin, we report the crystal structure of the title compound based on maleate ligand.

The structure of the title compound is shown in Fig. 1. The bond lengths and angles are normal and comparable with those reported for a similar structure (Hansson & Thörnqwist, 1975). The Sm^{III} ion is nine-coordinated by four O atoms from three maleate ligands, two O atoms from one fumarate ligand and three coordinated water molecules. The two carboxylate groups of the fumarate ligand and one of the carboxylate groups of the maleate ligand exhibit a chelating coordination mode, while the other carboxylate group of the maleate ligand binds Sm^{III} ions in a bidentate bridging mode. Adjacent Sm^{III} ions are bridged by the maleate and fumarate ligands, forming a layer parallel to (0 1 1) (Fig. 2). Additionly, abundant O—H···O hydrogen bonds stabilize the crystal structure of the title compound (Table 1).

S2. Experimental

Maleic acid and $Sm(NO_3)_3$ of analytical grade are used without further purification. $Sm(NO_3)_3$ (67.24 mg, 0.2 mmol) and maleic acid (69.64 mg, 0.6 mmol) were dissolved in water (10 ml), and the pH value was adjusted to about 3 using a dilute NaOH solution. The mixture was stirred for half an hour and then filtered. The filtrate was allowed to stand at room temperature for two weeks, giving colorless block-shaped crystals.

S3. Refinement

C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding atoms, with U_{iso}(H) = 1.2 U_{eq}(C). H atoms of the water molecules were initially located in a difference Fourier map, but were idealized and refined as riding atoms, with O—H = 0.85 Å and U_{iso}(H) = 1.5U_{eq}(O).

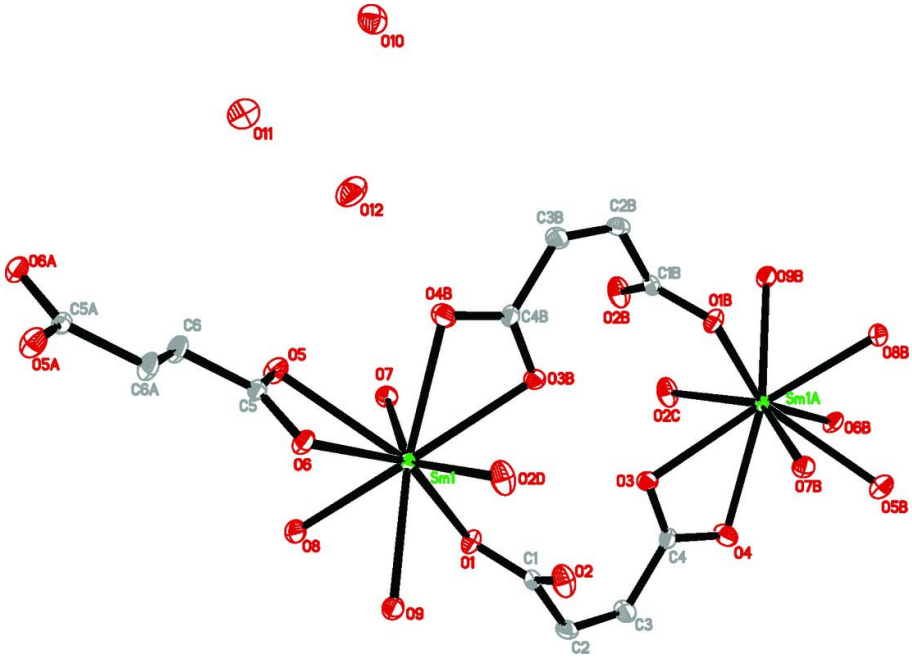

Figure 1

The asymmetric unit of the title compound, with the symmetry-related atoms to complete the Sm coordination. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) -*x*, 1-*y*, 1-*z*; (B) 2-*x*, 2-*y*, -*z*; (C) 1+*x*, *y*, *z*; (D) 1-*x*, 2-*y*, -*z*.]

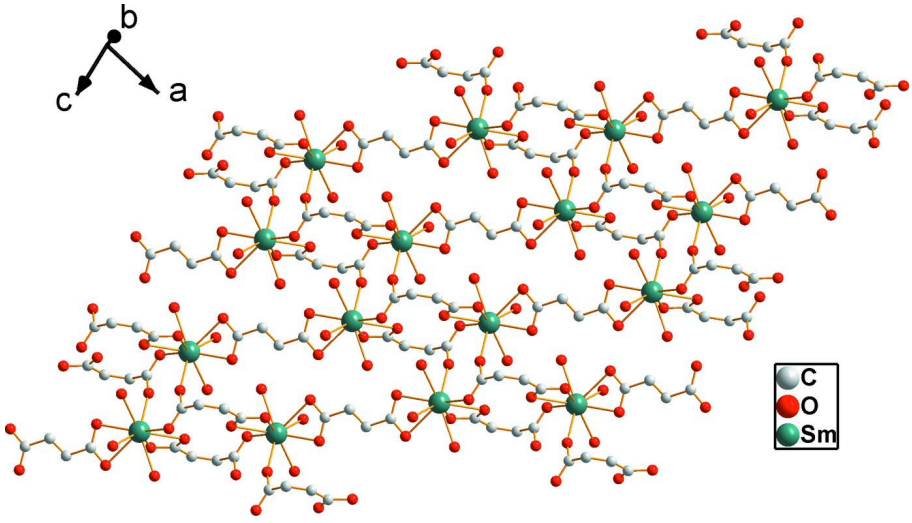

Figure 2

Crystal packing diagram of the title cmopound, showing the two-dimensional network.

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b = 10.679 (6) Å

c = 11.214 (6) Å
α = 69.99 (3)°
β = 79.64 (2)°
γ = 89.74 (2)°
V = 679.4 (6) Å^3
Z = 1
F(000) = 418
D_x = 2.100 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6497 reflections
θ = 3.3–27.5°
μ = 4.38 mm^{-1}
T = 290 K
Block, colorless
0.08 × 0.07 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotation anode
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.732, T_{max} = 0.782

6707 measured reflections
3071 independent reflections
2950 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 27.5°, θ_{min} = 3.3°
h = −7→7
k = −13→13
l = −14→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.066
S = 1.00
3071 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 3.0041P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.6917 (6)	1.1675 (4)	0.0453 (3)	0.0173 (7)
C2	0.7911 (7)	1.3067 (4)	0.0028 (4)	0.0256 (8)
H2	0.7026	1.3681	0.0269	0.031*
C3	0.9922 (7)	1.3525 (4)	−0.0657 (4)	0.0291 (9)
H3	1.0311	1.4423	−0.0853	0.035*
C4	1.1596 (6)	1.2717 (4)	−0.1134 (3)	0.0190 (7)
C5	0.2343 (6)	0.6379 (4)	0.4136 (3)	0.0176 (7)
C6	0.0980 (7)	0.5175 (4)	0.5083 (4)	0.0254 (8)
H6	0.1523	0.4658	0.5807	0.031*
O1	0.6917 (5)	1.0926 (3)	0.1584 (3)	0.0230 (6)
O2	0.6003 (5)	1.1329 (4)	−0.0303 (3)	0.0321 (7)
O3	1.1332 (4)	1.1467 (3)	−0.0770 (3)	0.0211 (5)
O4	1.3316 (5)	1.3327 (3)	−0.1921 (3)	0.0326 (7)
O5	0.4186 (5)	0.6652 (3)	0.4363 (3)	0.0253 (6)
O6	0.1671 (4)	0.7103 (3)	0.3142 (3)	0.0224 (5)
O7	0.8126 (4)	0.8515 (3)	0.3427 (3)	0.0223 (5)
H7B	0.8962	0.7909	0.3325	0.033*
H7A	0.8156	0.8534	0.4176	0.033*

O8	0.3684 (5)	0.9438 (3)	0.4042 (3)	0.0289 (6)
H8A	0.3148	1.0200	0.3882	0.043*
H8B	0.3346	0.9100	0.4861	0.043*
O9	0.1952 (4)	1.0193 (3)	0.1778 (3)	0.0236 (6)
H9A	0.0669	0.9933	0.2236	0.035*
H9B	0.1633	1.0477	0.1027	0.035*
O10	0.8053 (6)	0.1975 (3)	0.3360 (3)	0.0339 (7)
H10A	0.7981	0.1545	0.2853	0.051*
H10B	0.7485	0.2727	0.3128	0.051*
O11	0.2212 (5)	0.1916 (3)	0.3961 (3)	0.0322 (7)
H11B	0.3085	0.2599	0.3771	0.048*
H11A	0.1137	0.2035	0.3560	0.048*
O12	0.5308 (6)	0.4066 (3)	0.3112 (3)	0.0384 (8)
H12A	0.5696	0.4872	0.2639	0.058*
H12B	0.5062	0.4142	0.3894	0.058*
Sm1	0.50414 (3)	0.869449 (17)	0.223642 (16)	0.01447 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0152 (16)	0.0201 (17)	0.0163 (16)	0.0006 (13)	0.0001 (12)	−0.0074 (13)
C2	0.028 (2)	0.0164 (17)	0.029 (2)	0.0044 (15)	0.0018 (16)	−0.0079 (15)
C3	0.035 (2)	0.0138 (17)	0.033 (2)	−0.0033 (15)	0.0089 (17)	−0.0089 (16)
C4	0.0210 (17)	0.0184 (16)	0.0152 (16)	−0.0009 (14)	−0.0014 (13)	−0.0038 (13)
C5	0.0164 (16)	0.0167 (16)	0.0163 (16)	0.0012 (13)	−0.0015 (13)	−0.0023 (13)
C6	0.0252 (19)	0.0207 (18)	0.0224 (18)	−0.0066 (15)	0.0005 (15)	0.0002 (15)
O1	0.0281 (14)	0.0196 (13)	0.0172 (12)	−0.0039 (11)	−0.0035 (11)	−0.0013 (10)
O2	0.0257 (15)	0.051 (2)	0.0247 (15)	−0.0029 (14)	−0.0051 (12)	−0.0194 (14)
O3	0.0207 (13)	0.0153 (12)	0.0247 (13)	−0.0003 (10)	−0.0003 (10)	−0.0055 (10)
O4	0.0282 (15)	0.0187 (14)	0.0409 (18)	−0.0034 (12)	0.0135 (13)	−0.0076 (13)
O5	0.0186 (13)	0.0246 (14)	0.0274 (14)	−0.0048 (11)	−0.0072 (11)	−0.0006 (11)
O6	0.0169 (12)	0.0215 (13)	0.0219 (13)	−0.0008 (10)	−0.0043 (10)	0.0017 (10)
O7	0.0154 (12)	0.0271 (14)	0.0234 (13)	0.0044 (10)	−0.0063 (10)	−0.0062 (11)
O8	0.0423 (17)	0.0262 (15)	0.0168 (13)	0.0084 (13)	−0.0019 (12)	−0.0074 (11)
O9	0.0168 (12)	0.0270 (14)	0.0216 (13)	0.0030 (11)	−0.0029 (10)	−0.0021 (11)
O10	0.0396 (18)	0.0385 (18)	0.0292 (16)	0.0048 (14)	−0.0105 (13)	−0.0168 (14)
O11	0.0342 (17)	0.0299 (16)	0.0337 (16)	0.0009 (13)	−0.0113 (13)	−0.0101 (13)
O12	0.051 (2)	0.0229 (15)	0.0373 (18)	−0.0064 (14)	−0.0083 (15)	−0.0057 (13)
Sm1	0.01201 (10)	0.01535 (10)	0.01502 (10)	−0.00140 (6)	−0.00158 (6)	−0.00444 (7)

Geometric parameters (Å, º)

C1—O1	1.247 (5)	O9—H9A	0.8500
C1—O2	1.249 (5)	O9—H9B	0.8500
C1—C2	1.493 (5)	O10—H10A	0.8500
C2—C3	1.328 (6)	O10—H10B	0.8501
C2—H2	0.9300	O11—H11B	0.8500
C3—C4	1.484 (5)	O11—H11A	0.8500

C3—H3	0.9300	O12—H12A	0.8500
C4—O3	1.256 (5)	O12—H12B	0.8944
C4—O4	1.265 (5)	Sm1—O1	2.464 (3)
C5—O6	1.258 (5)	Sm1—O2^{ii}	2.377 (3)
C5—O5	1.262 (5)	Sm1—O3^{iii}	2.566 (3)
C5—C6	1.496 (5)	Sm1—O4^{iii}	2.486 (3)
C6—C6^{i}	1.327 (8)	Sm1—O5	2.593 (3)
C6—H6	0.9300	Sm1—O6	2.512 (3)
O7—H7B	0.8500	Sm1—O7	2.480 (3)
O7—H7A	0.8499	Sm1—O8	2.432 (3)
O8—H8A	0.8500	Sm1—O9	2.489 (3)
O8—H8B	0.8500		

O1—C1—O2	122.4 (4)	O2^{ii}—Sm1—O7	145.71 (10)
O1—C1—C2	118.2 (3)	O8—Sm1—O7	73.67 (10)
O2—C1—C2	119.2 (4)	O1—Sm1—O7	71.50 (10)
C3—C2—C1	127.1 (4)	O2^{ii}—Sm1—O4^{iii}	76.01 (12)
C3—C2—H2	116.4	O8—Sm1—O4^{iii}	137.15 (11)
C1—C2—H2	116.4	O1—Sm1—O4^{iii}	126.86 (10)
C2—C3—C4	125.2 (4)	O7—Sm1—O4^{iii}	80.70 (11)
C2—C3—H3	117.4	O2^{ii}—Sm1—O9	71.17 (11)
C4—C3—H3	117.4	O8—Sm1—O9	69.13 (10)
O3—C4—O4	120.7 (3)	O1—Sm1—O9	77.68 (10)
O3—C4—C3	121.5 (3)	O7—Sm1—O9	136.11 (10)
O4—C4—C3	117.7 (3)	O4^{iii}—Sm1—O9	143.16 (11)
O3—C4—Sm1^{iii}	62.2 (2)	O2^{ii}—Sm1—O6	79.19 (10)
O4—C4—Sm1^{iii}	58.6 (2)	O8—Sm1—O6	84.11 (11)
C3—C4—Sm1^{iii}	175.8 (3)	O1—Sm1—O6	152.27 (10)
O6—C5—O5	120.8 (3)	O7—Sm1—O6	121.53 (9)
O6—C5—C6	121.1 (3)	O4^{iii}—Sm1—O6	80.77 (10)
O5—C5—C6	118.1 (3)	O9—Sm1—O6	77.11 (10)
C6^{i}—C6—C5	121.8 (5)	O2^{ii}—Sm1—O3^{iii}	74.78 (10)
C6^{i}—C6—H6	119.1	O8—Sm1—O3^{iii}	140.72 (10)
C5—C6—H6	119.1	O1—Sm1—O3^{iii}	76.69 (9)
C1—O1—Sm1	115.9 (2)	O7—Sm1—O3^{iii}	71.03 (10)
C1—O2—Sm1^{ii}	161.0 (3)	O4^{iii}—Sm1—O3^{iii}	51.38 (9)
C4—O3—Sm1^{iii}	92.2 (2)	O9—Sm1—O3^{iii}	130.71 (9)
C4—O4—Sm1^{iii}	95.7 (2)	O6—Sm1—O3^{iii}	129.48 (9)
C5—O5—Sm1	92.2 (2)	O2^{ii}—Sm1—O5	121.78 (11)
C5—O6—Sm1	96.1 (2)	O8—Sm1—O5	70.25 (11)
Sm1—O7—H7B	110.4	O1—Sm1—O5	134.92 (9)
Sm1—O7—H7A	131.5	O7—Sm1—O5	70.75 (9)
H7B—O7—H7A	106.8	O4^{iii}—Sm1—O5	69.11 (11)
Sm1—O8—H8A	118.2	O9—Sm1—O5	115.51 (9)
Sm1—O8—H8B	137.9	O6—Sm1—O5	50.82 (9)
H8A—O8—H8B	102.8	O3^{iii}—Sm1—O5	112.47 (9)
Sm1—O9—H9A	118.7	O2^{ii}—Sm1—C4^{iii}	74.35 (11)
Sm1—O9—H9B	120.7	O8—Sm1—C4^{iii}	146.16 (11)

H9A—O9—H9B	100.2	O1—Sm1—C4^{iii}	101.68 (11)
H10A—O10—H10B	113.0	O7—Sm1—C4^{iii}	73.74 (10)
H11B—O11—H11A	115.2	O4^{iii}—Sm1—C4^{iii}	25.73 (10)
H12A—O12—H12B	100.4	O9—Sm1—C4^{iii}	144.26 (10)
O2^{ii}—Sm1—O8	139.41 (11)	O6—Sm1—C4^{iii}	105.51 (11)
O2^{ii}—Sm1—O1	103.29 (11)	O3^{iii}—Sm1—C4^{iii}	25.66 (9)
O8—Sm1—O1	76.25 (10)	O5—Sm1—C4^{iii}	90.53 (11)

Symmetry codes: (i) −*x*, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*; (iii) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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O9—H9*B*···O3^{vii}	0.85	1.97	2.808 (4)	168
O10—H10*A*···O1^{viii}	0.85	1.97	2.783 (4)	160
O10—H10*B*···O12	0.85	1.95	2.761 (5)	159
O11—H11*B*···O12	0.85	1.93	2.775 (5)	171
O11—H11*A*···O10^{vii}	0.85	1.95	2.755 (5)	157
O12—H12*A*···O4^{iii}	0.85	1.87	2.705 (5)	168
O12—H12*B*···O5^{v}	0.89	1.98	2.744 (5)	142

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