metal-organic compounds

Poly[[hexaaquabis(μ_3-*trans*-propene-1,2,3-tricarboxylato)trimanganese(II)] 0.2-hydrate]

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The title compound, $\{[Mn_3(C_6H_3O_6)_2(H_2O)_6] \cdot 0.2H_2O\}_n$, contains a three-dimensional open framework formed by each organic ligand μ_3-bridging three six-coordinated Mn^{II} atoms (one of which resides on a twofold crystallographic axis). Uncoordinated water molecules are located in the channels of the framework along the *c*-axis direction. The primary O—H···O intermolecular interactions have O···O distances ranging from 2.680 (4) to 3.020 (13) Å and O—H···O angles ranging from 125 (4) to 179 (4)°.

Related literature

For related literature, see: Dargay *et al.* (1972); Thomson *et al.* (1966); Villafranca & Mildvan (1972); Wang *et al.* (2004, 2005).
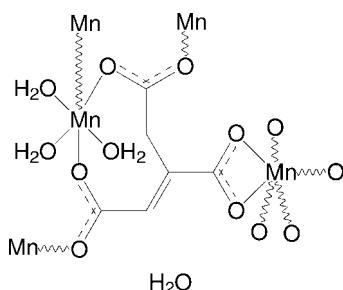
Experimental

Crystal data

[Mn$_3$(C$_6$H$_3$O$_6$)$_2$(H$_2$O)$_6$]·0.2H$_2$O
M_r = 618.69
a = 17.092 (7) Å
b = 9.602 (2) Å
c = 13.897 (5) Å
β = 116.367 (14)°
V = 2043.4 (12) Å^3
Z = 4

Monoclinic, $C2/c$
Mo $K\alpha$ radiation
μ = 1.92 mm^{-1}
T = 293 (2) K
0.4 × 0.26 × 0.25 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*SPHERE* in *CrystalClear*; Rigaku, 2002)

T_{min} = 0.868, T_{max} = 1.000 (expected range = 0.537–0.619)
6731 measured reflections
1896 independent reflections
1698 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.076
S = 1.25
1896 reflections
176 parameters
8 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1···O3[i]	0.919 (19)	2.05 (4)	2.687 (4)	125 (4)
O1W—H2···O2[ii]	0.93 (5)	1.75 (5)	2.680 (4)	176 (5)
O2W—H3···O1[iii]	0.92 (4)	2.18 (3)	2.843 (4)	129 (3)
O2W—H4···O5[iii]	0.915 (19)	2.011 (11)	2.921 (4)	173 (4)
O3W—H6···O4[iv]	0.92 (1)	1.838 (15)	2.735 (4)	163 (4)
O3W—H5···O5[v]	0.93 (4)	1.83 (3)	2.751 (4)	179 (4)
O4W—H7···O3W	0.92 (1)	2.12 (7)	3.020 (13)	162 (4)

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

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

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supplementary materials

Poly[[hexaaquabis(*μ3*-*trans*-propene-1,2,3-tricarboxylato)trimanganese(II)] 0.2-hydrate]

M.-S. Wang, G.-W. Zhou, G.-C. Guo and J.-S. Huang

Comment

trans-Propene-1,2,3-tricarboxylic acid (*trans*-aconitic acid, H_3L) is a weak competitive inhibitor of the action of aconitase in the famous Krebs cycle (Thomson *et al.*, 1966). Villagranca *et al.* detected an aconitase-manganous *trans*-aconitate complex by nuclear magnetic resonance (NMR) studies in 1972 (Villafranca & Mildvan, 1972), after which Dargay *et al.* reported the crystal structure of potassium dihydrogen *trans*-aconitate KH_2L and assumed that the active positions of L^{3-} ions in the aconitase-manganous *trans*-aconitate complex was the same as those in KH_2L (Dargay *et al.*, 1972). We deem that it is helpful to understand the active mechanism by the direct synthesis and structural characterization of a Mn(II) complex of the L^{3-} ligand. Herein, we report the synthesis and crystal structure of $Mn_3L_2(H_2O)_6 \cdot 0.2H_2O$ (I, Scheme 1).

As shown in Fig. 1, the crystallographically independent unit of (I) consists of one L^{3-} ligand, 1.5 Mn^{II} atoms as well as three coordinated water molecules. The Mn1 and Mn2 atoms are in special and general positions, respectively. The coordination geometry of Mn1 atom is characteristic of a triangular prism, in which O1, O2 and O5 atoms comprise the base planes. The Mn2 atom locates in a slightly distorted octahedral environment, in which three water molecules are arranged in a *mer*- fashion. The mean Mn2—O bond distance of 2.178 (3) Å is 0.080 (3) Å shorter than that of Mn1—O bonds. The L^{3-} ligand is four coordinated by two Mn1 and two Mn2 atoms. The three carboxylate groups of L^{3-} ligand show two kinds of coordination modes: one is μ2-*syn,trans*- for carboxylate groups with C4 and C5 atoms and the other μ2-*syn,syn*- for the third carboxylate group. Additionally, the 1- and 3-carboxylate groups of L^{3-} ligand form an 8-membered ring. In our previous work, we have found 8 kinds of coordination modes for L^{3-} ligand (Wang *et al.*, 2004; Wang *et al.*, 2005). The coordination modes of L^{3-} ligand in present example differs from those previously found by our group, and represents a new type. The C1—C2 vinyl bond has a bond distance of 1.313 (5) Å, which is similar to the reported values by our group.

Fig. 2a depicts the 3-D metal-organic framework of (I) viewed along the *b* axis direction. This framework can be simplified as a (3,4)-connect network by treating the C2, C4 and C5 atoms in L^{3-} ligand as well as Mn2 atoms as 3-connected nodes while Mn1 atoms as 4-connected nodes. The resulting (3,4)-connected network has a short vertex symbol of $(4.6.8)_2(4.10.12)_2(6^2.10^2.14^2)$. Fig. 2 b shows a perspective view of the crystal structure of 1 along the c direction, which reveals an open metal-organic framework with channels hosting lattice water molecules. The O—H···O hydrogen bonds presented in the crystal structure are listed (Table 1). The O—H···O hydrogen bonds in the framework have O···O distances falling in the range of 2.680 (4)–2.921 (4) Å, which are shorter than those of host–guest hydrogen bonds (O4W—H···O3w, 3.02 (1) Å).

Experimental

A mixture of H_3L (174 mg, 1 mmol) and Na_2CO_3 (159 mg, 1.5 mmol) was added into 8 ml water and reacted until no air bubbles appeared, after which $MnCl_2 \cdot 4H_2O$ (297 mg, 1.5 mmol) and pyridine (0.08 ml, 1 mmol) were added and let them

supplementary materials

react for further several minutes. Pale-yellow prismatic crystals of (I) suitable for single-crystal X-ray diffraction analysis were obtained by evaporation of the final solution under ambient environment.

Refinement

Water H atoms were located in a difference Fourier map and refined as riding in their located positions, with $U_{iso}(H) = 1.5U_{eq}(O)$. The *DFIX* commands were used to restrain the O—H bond distances of water molecules (Table 1). Other H atoms were allowed to ride on their respective parent atoms with C—H distances of 0.93 and 0.97 Å for methyne and methylene groups, respectively, and were included in the refinement with isotropic displacement parameters $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures
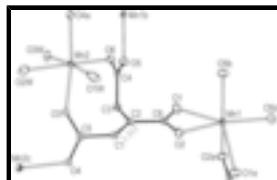
Fig. 1. *ORTEP* drawing with 30% probability displacement ellipsoids of the coordination environment of metal centers. Hydrogen atoms are omitted for clarity.
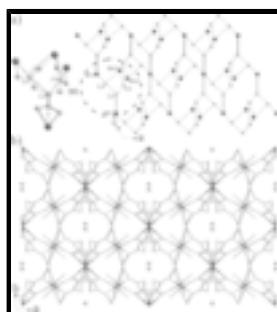
Fig. 2. 3-D packing diagram viewed along the (*a*) *b* axis and (*b*) *c* axis directions. Hydrogen atoms are omitted for clarity.

Poly[[hexaaquabis(µ3-*trans*-propene-1,2,3-tricarboxylato)trimanganese(II)] 0.2-hydrate]

Crystal data

$[Mn_3(C_6H_3O_6)_2(H_2O)_6]\cdot0.2H_2O$	$F_{000} = 1244$
$M_r = 618.69$	$D_x = 2.011$ Mg m^{-3}
Monoclinic, $C2/c$	Melting point: not measured K
Hall symbol: -C 2yc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 17.092$ (7) Å	Cell parameters from 3076 reflections
$b = 9.602$ (2) Å	$\theta = 3.2–27.5°$
$c = 13.897$ (5) Å	$\mu = 1.92$ mm^{-1}
$\beta = 116.367$ (14)°	$T = 293$ (2) K
$V = 2043.4$ (12) Å^3	Prism, pale yellow
$Z = 4$	$0.4 \times 0.26 \times 0.25$ mm

Data collection

Rigaku Mercury CCD	1896 independent reflections

diffractometer

Radiation source: rotating-anode generator	1698 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
$T = 293(2)$ K	$\theta_{max} = 25.5°$
ω scans	$\theta_{min} = 3.2°$
Absorption correction: multi-scan (SPHERE in CrystalClear; Rigaku, 2002)	$h = -15 \rightarrow 20$
$T_{min} = 0.868$, $T_{max} = 1.000$	$k = -11 \rightarrow 11$
6731 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.076$	$w = 1/[\sigma^2(F_o^2) + (0.008P)^2 + 2.8742P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.25$	$(\Delta/\sigma)_{max} < 0.001$
1896 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
176 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
8 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	$U_{iso}*/U_{eq}$	Occ. (<1)
Mn1	0.5000	0.49519 (8)	0.7500	0.0217 (2)	
Mn2	0.26523 (4)	0.24539 (6)	0.20029 (4)	0.01995 (18)	
O1	0.50955 (18)	0.3760 (3)	0.6094 (2)	0.0342 (7)	
O2	0.39711 (18)	0.3454 (3)	0.6427 (2)	0.0308 (7)	
O3	0.2886 (2)	0.0620 (3)	0.2988 (2)	0.0360 (8)	
O4	0.27903 (17)	−0.0846 (2)	0.41617 (19)	0.0258 (7)	
O5	0.53149 (17)	0.3356 (3)	0.3676 (2)	0.0269 (7)	

O6	0.38878 (16)	0.3483 (3)	0.30525 (19)	0.0246 (7)	
O1W	0.1846 (2)	0.3148 (3)	0.2723 (3)	0.0501 (9)	
H1	0.173 (3)	0.4081 (16)	0.273 (4)	0.075*	
H2	0.155 (3)	0.264 (4)	0.303 (3)	0.075*	
O2W	0.16551 (17)	0.1042 (3)	0.0844 (2)	0.0344 (8)	
H3	0.131 (2)	0.058 (4)	0.109 (3)	0.052*	
H4	0.1220 (17)	0.115 (4)	0.0161 (13)	0.052*	
O3W	0.34376 (18)	0.1518 (3)	0.1290 (2)	0.0306 (7)	
H5	0.386 (2)	0.213 (3)	0.130 (3)	0.046*	
H6	0.314 (2)	0.120 (4)	0.0594 (14)	0.046*	
C1	0.3347 (3)	0.1398 (4)	0.4788 (3)	0.0244 (9)	
H1A	0.3044	0.1593	0.5186	0.029*	
C2	0.4077 (3)	0.2074 (4)	0.5017 (3)	0.0235 (9)	
C3	0.4660 (3)	0.1831 (4)	0.4463 (3)	0.0214 (9)	
H3A	0.5260	0.1745	0.5008	0.026*	
H3B	0.4497	0.0955	0.4077	0.026*	
C4	0.4613 (3)	0.2976 (4)	0.3683 (3)	0.0181 (9)	
C5	0.2982 (3)	0.0326 (4)	0.3917 (3)	0.0234 (9)	
C6	0.4398 (3)	0.3152 (4)	0.5901 (3)	0.0221 (9)	
O4W	0.5000	−0.033 (2)	0.2500	0.060 (8)	0.20
H7	0.447 (8)	0.01 (2)	0.22 (2)	0.090*	0.20

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0305 (5)	0.0170 (4)	0.0140 (4)	0.000	0.0068 (4)	0.000
Mn2	0.0234 (3)	0.0187 (3)	0.0162 (3)	−0.0010 (3)	0.0075 (3)	0.0022 (3)
O1	0.0338 (18)	0.0360 (18)	0.0361 (17)	−0.0123 (15)	0.0184 (15)	−0.0127 (14)
O2	0.0410 (18)	0.0291 (17)	0.0315 (17)	−0.0117 (14)	0.0246 (16)	−0.0096 (13)
O3	0.068 (2)	0.0178 (15)	0.0192 (16)	−0.0086 (15)	0.0172 (16)	−0.0011 (12)
O4	0.0398 (18)	0.0149 (14)	0.0187 (15)	−0.0076 (13)	0.0095 (14)	0.0001 (12)
O5	0.0249 (16)	0.0294 (16)	0.0327 (16)	0.0038 (13)	0.0184 (14)	0.0082 (13)
O6	0.0226 (16)	0.0228 (15)	0.0184 (14)	0.0004 (12)	0.0002 (13)	0.0020 (12)
O1W	0.082 (3)	0.0256 (18)	0.077 (2)	−0.0053 (19)	0.066 (2)	−0.0007 (18)
O2W	0.0234 (17)	0.050 (2)	0.0237 (16)	−0.0148 (15)	0.0053 (14)	−0.0003 (15)
O3W	0.0298 (18)	0.0356 (18)	0.0264 (16)	−0.0067 (14)	0.0123 (15)	−0.0121 (14)
C1	0.035 (3)	0.017 (2)	0.021 (2)	−0.0002 (19)	0.013 (2)	0.0011 (17)
C2	0.030 (2)	0.017 (2)	0.018 (2)	0.0010 (18)	0.0056 (19)	0.0043 (17)
C3	0.027 (2)	0.018 (2)	0.020 (2)	0.0072 (18)	0.0104 (19)	0.0047 (17)
C4	0.027 (2)	0.013 (2)	0.015 (2)	0.0014 (17)	0.0096 (19)	−0.0040 (16)
C5	0.030 (2)	0.019 (2)	0.018 (2)	−0.0017 (18)	0.0071 (19)	−0.0005 (18)
C6	0.029 (2)	0.016 (2)	0.017 (2)	−0.0005 (18)	0.005 (2)	0.0014 (17)
O4W	0.08 (2)	0.023 (13)	0.042 (15)	0.000	−0.008 (15)	0.000

Geometric parameters (Å, °)

Mn1—O5[i]	2.195 (3)	O5—C4	1.259 (4)
Mn1—O5[ii]	2.195 (3)	O5—Mn1[ii]	2.195 (3)

Mn1—O2	2.248 (3)	O6—C4	1.255 (4)
Mn1—O2^{iii}	2.248 (3)	O1W—H1	0.919 (19)
Mn1—O1	2.332 (3)	O1W—H2	0.95 (5)
Mn1—O1^{iii}	2.332 (3)	O2W—H3	0.92 (4)
Mn1—C6	2.636 (4)	O2W—H4	0.915 (19)
Mn1—C6^{iii}	2.636 (4)	O3W—H5	0.93 (4)
Mn2—O1W	2.137 (3)	O3W—H6	0.92 (1)
Mn2—O3	2.156 (3)	C1—C2	1.313 (5)
Mn2—O4^{iv}	2.183 (2)	C1—C5	1.498 (5)
Mn2—O3W	2.184 (3)	C1—H1A	0.9300
Mn2—O6	2.197 (3)	C2—C6	1.511 (5)
Mn2—O2W	2.213 (3)	C2—C3	1.524 (5)
O1—C6	1.246 (4)	C3—C4	1.521 (5)
O2—C6	1.274 (4)	C3—H3A	0.9700
O3—C5	1.259 (4)	C3—H3B	0.9700
O4—C5	1.260 (4)	O4W—H7	0.928 (11)
O4—Mn2^{v}	2.183 (2)		
O5^{i}—Mn1—O5^{ii}	84.49 (14)	O3W—Mn2—O2W	81.25 (11)
O5^{i}—Mn1—O2	145.92 (10)	O6—Mn2—O2W	163.96 (11)
O5^{ii}—Mn1—O2	96.82 (10)	C6—O1—Mn1	89.6 (2)
O5^{i}—Mn1—O2^{iii}	96.82 (10)	C6—O2—Mn1	92.7 (2)
O5^{ii}—Mn1—O2^{iii}	145.91 (10)	C5—O3—Mn2	137.5 (2)
O2—Mn1—O2^{iii}	100.48 (15)	C5—O4—Mn2^{v}	120.9 (2)
O5^{i}—Mn1—O1	154.37 (10)	C4—O5—Mn1^{ii}	107.5 (2)
O5^{ii}—Mn1—O1	79.91 (10)	C4—O6—Mn2	130.5 (2)
O2—Mn1—O1	57.01 (10)	Mn2—O1W—H1	120 (3)
O2^{iii}—Mn1—O1	85.24 (10)	Mn2—O1W—H2	130 (3)
O5^{i}—Mn1—O1^{iii}	79.91 (10)	H1—O1W—H2	110 (4)
O5^{ii}—Mn1—O1^{iii}	154.37 (10)	Mn2—O2W—H3	117 (2)
O2—Mn1—O1^{iii}	85.24 (10)	Mn2—O2W—H4	134 (3)
O2^{iii}—Mn1—O1^{iii}	57.01 (10)	H3—O2W—H4	95 (3)
O1—Mn1—O1^{iii}	121.24 (15)	Mn2—O3W—H5	111 (3)
O5^{i}—Mn1—C6	170.88 (11)	Mn2—O3W—H6	116 (3)
O5^{ii}—Mn1—C6	89.03 (11)	H5—O3W—H6	107 (3)
O2—Mn1—C6	28.86 (10)	C2—C1—C5	123.1 (4)
O2^{iii}—Mn1—C6	92.15 (11)	C2—C1—H1A	118.4
O1—Mn1—C6	28.19 (10)	C5—C1—H1A	118.4
O1^{iii}—Mn1—C6	103.78 (11)	C1—C2—C6	119.9 (4)
O5^{i}—Mn1—C6^{iii}	89.03 (11)	C1—C2—C3	124.4 (4)
O5^{ii}—Mn1—C6^{iii}	170.88 (11)	C6—C2—C3	115.6 (3)
O2—Mn1—C6^{iii}	92.15 (11)	C4—C3—C2	114.1 (3)
O2^{iii}—Mn1—C6^{iii}	28.86 (10)	C4—C3—H3A	108.7
O1—Mn1—C6^{iii}	103.78 (11)	C2—C3—H3A	108.7

O1^{iii}—Mn1—C6^{iii}	28.19 (10)	C4—C3—H3B	108.7
C6—Mn1—C6^{iii}	98.09 (16)	C2—C3—H3B	108.7
O1W—Mn2—O3	86.19 (12)	H3A—C3—H3B	107.6
O1W—Mn2—O4^{iv}	91.76 (12)	O6—C4—O5	122.1 (3)
O3—Mn2—O4^{iv}	170.60 (10)	O6—C4—C3	120.1 (3)
O1W—Mn2—O3W	173.89 (11)	O5—C4—C3	117.8 (3)
O3—Mn2—O3W	88.53 (11)	O3—C5—O4	123.1 (3)
O4^{iv}—Mn2—O3W	92.97 (11)	O3—C5—C1	119.5 (3)
O1W—Mn2—O6	100.26 (12)	O4—C5—C1	117.4 (3)
O3—Mn2—O6	95.35 (10)	O1—C6—O2	120.5 (3)
O4^{iv}—Mn2—O6	94.04 (10)	O1—C6—C2	117.6 (4)
O3W—Mn2—O6	83.28 (10)	O2—C6—C2	121.9 (4)
O1W—Mn2—O2W	94.79 (13)	O1—C6—Mn1	62.2 (2)
O3—Mn2—O2W	80.06 (11)	O2—C6—Mn1	58.41 (19)
O4^{iv}—Mn2—O2W	90.99 (10)	C2—C6—Mn1	177.6 (3)

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

Hydrogen-bond geometry (Å, °)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—H1$\cdots$O3^{iv}	0.919 (19)	2.05 (4)	2.687 (4)	125 (4)
O1W—H2$\cdots$O2^{vi}	0.93 (5)	1.75 (5)	2.680 (4)	176 (5)
O2W—H3$\cdots$O1^{vii}	0.92 (4)	2.18 (3)	2.843 (4)	129 (3)
O2W—H4$\cdots$O5^{vii}	0.915 (19)	2.011 (11)	2.921 (4)	173 (4)
O3W—H6$\cdots$O4^{viii}	0.92 (1)	1.838 (15)	2.735 (4)	163 (4)
O3W—H5$\cdots$O5^{ix}	0.93 (4)	1.83 (3)	2.751 (4)	179 (4)
O4W—H7$\cdots$O3W	0.92 (1)	2.12 (7)	3.020 (13)	162

Symmetry codes: (iv) −x+1/2, y+1/2, −z+1/2; (vi) −x+1/2, −y+1/2, −z+1; (vii) x−1/2, −y+1/2, z−1/2; (viii) x, −y, z−1/2; (ix) −x+1, y, −z+1/2.

Fig. 1

Fig. 2