metal-organic compounds

Redetermination of poly[μ_2-aqua-diaquabis(μ_3-pyridine-2,6-dicarboxylato)manganese(II)]

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The title compound, $[Mn_2(C_7H_3NO_4)_2(H_2O)_3]_n$, has been synthesized under hydrothermal conditions. In the complex, the Mn atom is seven-coordinated by three symmetry-equivalent pyridine-2,6-dicarboxylate ligands and a water molecule in a pentagonal–bipyramidal coordination environment. A crystallographic twofold rotation axis passes through the bridging water molecule and between adjacent pairs of Mn atoms.

Related literature

For related literature, see: Field *et al.* (2006); Gao *et al.* (2006); Ghosh *et al.* (2004, 2005); Ma, Chen, Chen *et al.* (2003); Ma, Chen, Liu *et al.* (2003); Okabe & Oya (2000); Rueff *et al.* (2002); Wei *et al.* (2005); Zeng *et al.* (2005); Zhao *et al.* (2003).
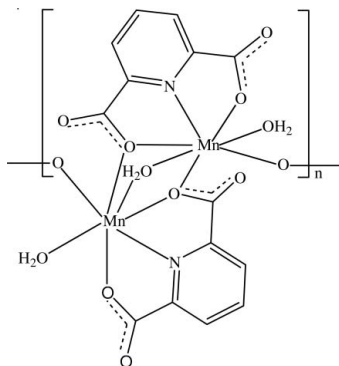
Experimental

Crystal data

$[Mn_2(C_7H_3NO_4)_2(H_2O)_3]$
$M_r = 494.14$

Monoclinic, $C2/c$
$a = 13.1763\ (13)$ Å
$b = 9.7513\ (10)$ Å
$c = 13.1510\ (13)$ Å
$\beta = 96.427\ (2)°$
$V = 1679.1\ (3)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.57$ mm^{-1}
$T = 153\ (2)$ K
$0.39 \times 0.10 \times 0.06$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.836$, $T_{max} = 0.904$

4593 measured reflections
1649 independent reflections
1456 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.075$
$S = 1.05$
1649 reflections
144 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Bruker 1998); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2065).

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supplementary materials

Redetermination of poly[μ_2-aqua-diaquabis(μ_3-pyridine-2,6-dicarboxylato)manganese(II)]

S. Cui, Y. Zhao and J. Zhang

Comment

The chemistry of metal complexes containing paramagnetic metal ions and exhibiting extended structures is at the forefront of modern research, due to these compounds' potential applications in molecular magnetism (Field *et al.*, 2006; Rueff *et al.*, 2002; Zeng *et al.*, 2005). The most useful strategy by which to construct such extended one dimensional systems is to employ appropriate bridging ligands, carboxylate for example, capable of binding metal centers through direct bond formation, promoting magnetic interactions. Pyridine-2,6-dicarboxylate (2,6-pdc^{2-}), which has been used as a ligand in homoleptic coordination polymers and coordination complexes, is a suitable building block for two-dimensional arrays (Zhao *et al.*, 2003; Gao *et al.*, 2006). There are a few examples of manganese complexes of 2,6-pdc (Ma, Chen, Chen *et al.*, 2003; Ma, Chen, Liu *et al.*, 2003; Okabe & Oya, 2000; Wei *et al.*, 2005), although many crystal structures of complexes of 2,6-pdc with divalent ions such as Co^{II}, Ni^{II} and Cu^{II} (Ghosh *et al.*, 2004; Ghosh *et al.*, 2005) have been determined. The reactants we have used are different from those reported previously in the literature in an attempt to obtain a compound analogous to the title complex (I) (Wei *et al.*, 2005). Its crystal structure is presented here. It should be noted that, compound (I) crystallizes in the monoclinic space group *C*2/*c*, while the P-1 space group was previously reported (Wei *et al.*, 2005).

The hydrothermal reaction of Mn(NO$_3$)$_2$, 2,6-pdc and 5-bromo-2,4'-bipyridine (5-Br-2,4'-bpy) did not lead to the expected manganese system with coordinated bpy ligands, but to the unexpected formation of (I). Attempts were made to obtain compound (I) under the same conditions in the absence of bpy ligand. The collected crystals were in poor quality and not suitable for X-ray crystallography.

The crystallographically independent unit and atomic numbering of (I) are shown in Fig. 1, and selected bond distances and angles are given in Table 1. A half of (I) is crystallographically independent with a 2-fold axis through O1w. The asymmetric unit consists of one (O2w) and half water (half O1w), one Mn atom and one 2,6-pdc group. The coordination around the Mn atom is pentagonal-bipyramidal. All water molecules are coordinated with metal atoms: O1w atom as a bridge is connected to two neighbouring Mn atoms, while Ow2 atom is coordinated with Mn atom as terminal ligand. The equatorial belt is formed by one N atom (N1) and four O atoms (O2, O2^{ii}, O3, O1w), and the axial positions are occupied by O3 atom and O2w atom [symmetry codes: (ii)-*x*,-*y*, −*z* + 2]. The Mn—O bond lengths fall in the ranges 2.122 (2)–2.4944 (16) Å, and Mn—N bond length is 2.292 (2) Å. These values are consistent with the corresponding distances in the literature (Wei *et al.*, 2005).

In complex (I), the Mn atom is coordinated by four different O atoms of three *trans* 2,6-pdc ligands, so the complex is extended along *c*-axis, resulting in the formation of one-dimensional supramolecular chains (Fig.2). The water O1w is connected to the atom O1^i by O1w—H1···O1^i within one-dimensional chain[symmetrycodes: (i)-*x*,*y*,-*z* + 3/2]. The water O2w is hydrogen bonded to O4^{iii} and O^{iv} of two neighboring chains through O2w—H2b···O4^{iii} and O2w—H2a···O4^{iv} [symmetry codes: (iii)-*x* + 1/2,*y* − 1/2, −*z* + 3/2; (iv)*x*,-*y*,*z* + 1/2], forming cyclic hydrogen bonded net. Thus, the complex is further assembled into two-dimensional layer by hydrogen-bonding interaction along *b*-axis. Adjacent sheets cross each

supplementary materials

other to give a square hydrogen bonded network, in which are filled 2,6-pdc ligand from neighboring chains (Fig.3). The hydrogen bonding interaction plays an important role in stabilizing the crystal structure.

Experimental

In a typical experiment, H2pdc (0.042 g, 0.25 mmol) in an aqueous solution (6 ml) of NaOH (0.040 g, 1 mmol) was mixed with 5-Br-2,4'-bpy (0.0235 g, 0.1 mmol) in EtOH (2 ml); the mixture was then added to an aqueous solution (2 ml) of 50% $Mn(NO_3)_2$. The new mixture was placed in a 15-ml Teflon-lined autoclave and heated at 423 K for 4 d. The autoclave was then cooled to temperature at a rate of 4 K h^{-1}. Brown block crystals of (I) deposited on the wall of container were collected and air-dried.

Refinement

Hydrogen atoms bound to carbon were placed in calculated positions and refined using a riding model with an isotropic displacement parameter fixed at 1.2 times U_{eq} for the atom to which they are attached. Hydrogen atoms on the water molecule were found in electron-density difference Fourier maps at the stages of the refinement procedure and were refined freely.
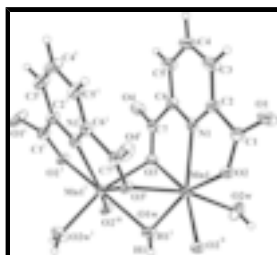
Figures

Fig. 1. Complex (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small of arbitrary radii. [Symmetry codes: (i)-x, y,-z + 3/2; (ii)-x,-y,-z + 2; (iii)-x + 1/2,y − 1/2, −z + 3/2.]
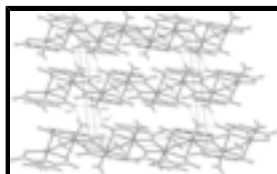
Fig. 2. A perspective view of the hydrogen bonded layer of polymer chains. Hydrogen bonds are drawn as dashed lines. [Symmetry codes: (i)-x, y,-z + 3/2; (iii)-x + 1/2,y − 1/2,-z + 3/2; (iv)x,-y,z + 1/2.]
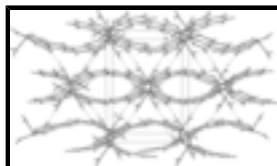
Fig. 3. A view along the c axis of the network structure of complex (I). Hydrogen bonds are drawn as dashed lines.

Poly[μ₂-aqua-diaquabis(μ₃-pyridine-2,6-dicarboxylato)manganese(II)]

Crystal data

$[Mn_2(C_7H_3NO_4)_2(H_2O)_3]$	$F_{000} = 992$
$M_r = 494.14$	$D_x = 1.955$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å

Hall symbol: -C 2yc

$a = 13.1763\ (13)$ Å

$b = 9.7513\ (10)$ Å

$c = 13.1510\ (13)$ Å

$\beta = 96.427\ (2)°$

$V = 1679.1\ (3)$ Å^3

$Z = 4$

Cell parameters from 4593 reflections

$\theta = 2.6–26.0°$

$\mu = 1.57$ mm^{-1}

$T = 153\ (2)$ K

Block, brown

$0.39 \times 0.10 \times 0.06$ mm

Data collection

Siemens SMART CCD area-detector diffractometer	1649 independent reflections
Radiation source: fine-focus sealed tube	1456 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
Detector resolution: 9 pixels mm^{-1}	$\theta_{max} = 26.0°$
$T = 153(2)$ K	$\theta_{min} = 2.6°$
ω scans	$h = -16 \rightarrow 16$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$k = -12 \rightarrow 11$
$T_{min} = 0.836$, $T_{max} = 0.904$	$l = -10 \rightarrow 16$
4593 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.075$	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 1.0348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
1649 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
144 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
Mn1	0.04668 (3)	0.01957 (4)	0.87334 (3)	0.01474 (14)
O3	0.09871 (12)	0.08881 (16)	0.70408 (12)	0.0177 (4)
O4	0.16289 (14)	0.25500 (19)	0.61332 (13)	0.0257 (4)
O2W	0.17185 (16)	−0.1023 (2)	0.93574 (16)	0.0283 (5)
O1	0.10025 (16)	0.29078 (19)	1.13305 (14)	0.0326 (5)
O2	0.04275 (13)	0.11744 (16)	1.02950 (13)	0.0179 (4)
O1W	0.0000	−0.1383 (2)	0.7500	0.0195 (5)
N1	0.11101 (14)	0.2377 (2)	0.87038 (14)	0.0163 (4)

C1	0.08209 (18)	0.2351 (3)	1.04755 (18)	0.0197 (5)
C7	0.13324 (17)	0.2082 (3)	0.69342 (18)	0.0174 (5)
C6	0.13422 (18)	0.3006 (2)	0.78526 (18)	0.0186 (5)
C5	0.1509 (2)	0.4409 (3)	0.7806 (2)	0.0253 (6)
H3	0.1671	0.4817	0.7205	0.030*
C2	0.10824 (19)	0.3133 (2)	0.95497 (19)	0.0201 (5)
C3	0.1234 (2)	0.4546 (3)	0.9564 (2)	0.0274 (6)
H5	0.1204	0.5047	1.0162	0.033*
C4	0.1429 (2)	0.5185 (3)	0.8670 (2)	0.0299 (6)
H4	0.1506	0.6132	0.8650	0.036*
H2A	0.217 (3)	−0.132 (3)	0.911 (3)	0.041 (10)*
H2B	0.166 (3)	−0.141 (3)	0.991 (3)	0.049 (11)*
H1	−0.039 (3)	−0.196 (3)	0.783 (3)	0.053 (11)*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0185 (2)	0.0145 (2)	0.0116 (2)	0.00089 (14)	0.00353 (14)	−0.00022 (14)
O3	0.0200 (8)	0.0171 (9)	0.0167 (9)	−0.0033 (7)	0.0049 (7)	−0.0005 (7)
O4	0.0358 (11)	0.0287 (10)	0.0141 (9)	−0.0114 (8)	0.0102 (8)	−0.0016 (8)
O2W	0.0259 (10)	0.0392 (12)	0.0217 (11)	0.0160 (9)	0.0111 (9)	0.0099 (9)
O1	0.0577 (13)	0.0272 (10)	0.0150 (10)	−0.0202 (9)	0.0129 (9)	−0.0067 (8)
O2	0.0265 (9)	0.0149 (8)	0.0132 (8)	−0.0039 (7)	0.0070 (7)	−0.0017 (7)
O1W	0.0294 (14)	0.0135 (12)	0.0172 (13)	0.000	0.0091 (11)	0.000
N1	0.0177 (10)	0.0201 (11)	0.0117 (10)	−0.0021 (8)	0.0043 (8)	0.0002 (8)
C1	0.0236 (13)	0.0206 (13)	0.0155 (13)	−0.0027 (10)	0.0050 (10)	−0.0003 (10)
C7	0.0147 (11)	0.0223 (13)	0.0154 (13)	−0.0016 (9)	0.0030 (10)	−0.0002 (10)
C6	0.0197 (12)	0.0223 (13)	0.0145 (13)	−0.0026 (10)	0.0047 (10)	0.0017 (10)
C5	0.0360 (15)	0.0229 (14)	0.0180 (14)	−0.0095 (11)	0.0070 (11)	0.0012 (11)
C2	0.0263 (13)	0.0184 (13)	0.0164 (13)	−0.0039 (10)	0.0059 (11)	−0.0010 (10)
C3	0.0388 (16)	0.0230 (14)	0.0219 (14)	−0.0096 (12)	0.0095 (12)	−0.0057 (11)
C4	0.0473 (17)	0.0185 (13)	0.0250 (15)	−0.0119 (12)	0.0093 (13)	−0.0001 (11)

Geometric parameters ($Å$, °)

Mn1—O2W	2.122 (2)	O2—Mn1^{ii}	2.2679 (16)
Mn1—O3^{i}	2.1738 (16)	O1W—Mn1^{i}	2.2707 (17)
Mn1—O2^{ii}	2.2679 (16)	O1W—H1	0.91 (3)
Mn1—O2	2.2704 (17)	N1—C2	1.338 (3)
Mn1—O1W	2.2707 (17)	N1—C6	1.341 (3)
Mn1—N1	2.292 (2)	C1—C2	1.509 (3)
Mn1—O3	2.4944 (16)	C7—C6	1.506 (3)
O3—C7	1.263 (3)	C6—C5	1.388 (3)
O3—Mn1^{i}	2.1738 (16)	C5—C4	1.379 (4)
O4—C7	1.250 (3)	C5—H3	0.9300
O2W—H2A	0.76 (4)	C2—C3	1.391 (3)
O2W—H2B	0.83 (4)	C3—C4	1.380 (4)
O1—C1	1.247 (3)	C3—H5	0.9300

O2—C1	1.271 (3)	C4—H4	0.9300
O2W—Mn1—O3[i]	163.97 (7)	Mn1[ii]—O2—Mn1	109.15 (7)
O2W—Mn1—O2[ii]	83.25 (8)	Mn1—O1W—Mn1[i]	94.63 (9)
O3[i]—Mn1—O2[ii]	87.74 (6)	Mn1—O1W—H1	101 (2)
O2W—Mn1—O2	88.91 (7)	Mn1[i]—O1W—H1	130 (2)
O3[i]—Mn1—O2	100.66 (6)	C2—N1—C6	118.1 (2)
O2[ii]—Mn1—O2	70.85 (7)	C2—N1—Mn1	116.91 (15)
O2W—Mn1—O1W	91.91 (7)	C6—N1—Mn1	123.91 (16)
O3[i]—Mn1—O1W	73.86 (6)	O1—C1—O2	126.5 (2)
O2[ii]—Mn1—O1W	83.50 (5)	O1—C1—C2	118.0 (2)
O2—Mn1—O1W	154.07 (5)	O2—C1—C2	115.5 (2)
O2W—Mn1—N1	104.68 (8)	O4—C7—O3	125.5 (2)
O3[i]—Mn1—N1	90.69 (7)	O4—C7—C6	118.8 (2)
O2[ii]—Mn1—N1	140.61 (6)	O3—C7—C6	115.7 (2)
O2—Mn1—N1	70.80 (6)	N1—C6—C5	122.7 (2)
O1W—Mn1—N1	133.50 (6)	N1—C6—C7	114.4 (2)
O2W—Mn1—O3	102.56 (7)	C5—C6—C7	122.8 (2)
O3[i]—Mn1—O3	79.27 (6)	C4—C5—C6	118.5 (2)
O2[ii]—Mn1—O3	150.96 (6)	C4—C5—H3	120.8
O2—Mn1—O3	136.87 (6)	C6—C5—H3	120.8
O1W—Mn1—O3	68.01 (5)	N1—C2—C3	122.6 (2)
N1—Mn1—O3	66.08 (6)	N1—C2—C1	115.0 (2)
C7—O3—Mn1[i]	122.94 (15)	C3—C2—C1	122.3 (2)
C7—O3—Mn1	119.13 (14)	C4—C3—C2	118.4 (2)
Mn1[i]—O3—Mn1	91.04 (6)	C4—C3—H5	120.8
Mn1—O2W—H2A	131 (3)	C2—C3—H5	120.8
Mn1—O2W—H2B	116 (2)	C5—C4—C3	119.5 (3)
H2A—O2W—H2B	111 (3)	C5—C4—H4	120.2
C1—O2—Mn1[ii]	130.81 (15)	C3—C4—H4	120.2
C1—O2—Mn1	119.90 (15)		
O2W—Mn1—O3—C7	−102.13 (17)	O2W—Mn1—N1—C6	104.24 (19)
O3[i]—Mn1—O3—C7	94.14 (15)	O3[i]—Mn1—N1—C6	−71.14 (19)
O2[ii]—Mn1—O3—C7	159.06 (16)	O2[ii]—Mn1—N1—C6	−158.42 (16)
O2—Mn1—O3—C7	0.0 (2)	O2—Mn1—N1—C6	−172.2 (2)
O1W—Mn1—O3—C7	170.92 (17)	O1W—Mn1—N1—C6	−3.0 (2)
N1—Mn1—O3—C7	−1.45 (15)	O3—Mn1—N1—C6	6.79 (17)
O2W—Mn1—O3—Mn1[i]	128.63 (7)	Mn1[ii]—O2—C1—O1	17.4 (4)
O3[i]—Mn1—O3—Mn1[i]	−35.10 (8)	Mn1—O2—C1—O1	−167.5 (2)
O2[ii]—Mn1—O3—Mn1[i]	29.82 (14)	Mn1[ii]—O2—C1—C2	−162.32 (16)
O2—Mn1—O3—Mn1[i]	−129.28 (7)	Mn1—O2—C1—C2	12.9 (3)
O1W—Mn1—O3—Mn1[i]	41.68 (5)	Mn1[i]—O3—C7—O4	−68.1 (3)
N1—Mn1—O3—Mn1[i]	−130.69 (8)	Mn1—O3—C7—O4	179.19 (18)
O2W—Mn1—O2—C1	100.62 (18)	Mn1[i]—O3—C7—C6	109.6 (2)

O3^i—Mn1—O2—C1	−92.33 (18)	Mn1—O3—C7—C6	−3.1 (3)
O2^{ii}—Mn1—O2—C1	−176.1 (2)	C2—N1—C6—C5	−2.9 (4)
O1W—Mn1—O2—C1	−167.26 (16)	Mn1—N1—C6—C5	165.08 (19)
N1—Mn1—O2—C1	−5.35 (17)	C2—N1—C6—C7	−178.7 (2)
O3—Mn1—O2—C1	−6.7 (2)	Mn1—N1—C6—C7	−10.7 (3)
O2W—Mn1—O2—Mn1^{ii}	−83.24 (9)	O4—C7—C6—N1	−173.6 (2)
O3^i—Mn1—O2—Mn1^{ii}	83.81 (8)	O3—C7—C6—N1	8.5 (3)
O2^{ii}—Mn1—O2—Mn1^{ii}	0.0	O4—C7—C6—C5	10.6 (4)
O1W—Mn1—O2—Mn1^{ii}	8.89 (17)	O3—C7—C6—C5	−167.3 (2)
N1—Mn1—O2—Mn1^{ii}	170.80 (9)	N1—C6—C5—C4	−0.2 (4)
O3—Mn1—O2—Mn1^{ii}	169.44 (6)	C7—C6—C5—C4	175.3 (2)
O2W—Mn1—O1W—Mn1^i	−142.47 (6)	C6—N1—C2—C3	3.3 (4)
O3^i—Mn1—O1W—Mn1^i	45.02 (5)	Mn1—N1—C2—C3	−165.5 (2)
O2^{ii}—Mn1—O1W—Mn1^i	134.55 (5)	C6—N1—C2—C1	−179.7 (2)
O2—Mn1—O1W—Mn1^i	126.10 (13)	Mn1—N1—C2—C1	11.5 (3)
N1—Mn1—O1W—Mn1^i	−30.06 (7)	O1—C1—C2—N1	164.3 (2)
O3—Mn1—O1W—Mn1^i	−39.69 (4)	O2—C1—C2—N1	−16.0 (3)
O2W—Mn1—N1—C2	−87.65 (18)	O1—C1—C2—C3	−18.7 (4)
O3^i—Mn1—N1—C2	96.97 (17)	O2—C1—C2—C3	161.0 (2)
O2^{ii}—Mn1—N1—C2	9.7 (2)	N1—C2—C3—C4	−0.6 (4)
O2—Mn1—N1—C2	−4.08 (17)	C1—C2—C3—C4	−177.4 (3)
O1W—Mn1—N1—C2	165.13 (15)	C6—C5—C4—C3	3.0 (4)
O3—Mn1—N1—C2	174.90 (19)	C2—C3—C4—C5	−2.6 (4)

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

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2W—H2A⋯O4^{iii}	0.76 (4)	1.99 (4)	2.722 (3)	162 (3)
O2W—H2B⋯O4^{iv}	0.83 (4)	1.96 (4)	2.783 (3)	171 (3)
O1W—H1⋯O1^{ii}	0.91 (3)	1.71 (3)	2.603 (2)	169 (3)

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

Fig. 1

Fig. 2

Fig. 3