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Bis(acetato-κ^2O,O')[2,6-bis(1*H*-pyrazol-3-yl-κN^2)pyridine-κN]manganese(II)

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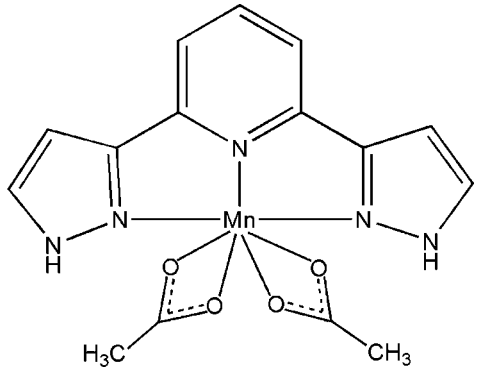
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.117; data-to-parameter ratio = 13.3.

In the title complex, $[Mn(CH_3CO_2)_2(C_{11}H_9N_5)]$, the Mn^{II} atom is coordinated by the pyridine N atom and two pyrazole N atoms from a 2,6-bis(pyrazol-3-yl)pyridine ligand and four O atoms from two bidentate acetate ligands. The complex molecules are linked by intermolecular N—H···O hydrogen bonds into a chain along [010]. π–π interactions between the pyridine rings and between the pyrazole rings [centroid–centroid distances = 3.772 (2) and 3.546 (2) Å] connect the chains.

Related literature

For a related structure, see: Rich *et al.* (2010).



Experimental

Crystal data

$[Mn(C_2H_3O_2)_2(C_{11}H_9N_5)]$
M_r = 384.26
Triclinic, $P\overline{1}$
a = 8.2386 (16) Å
b = 9.4324 (19) Å
c = 11.081 (2) Å
α = 98.32 (3)°
β = 95.01 (3)°
γ = 106.11 (3)°
V = 811.2 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.816, T_{max} = 0.849
5563 measured reflections
3001 independent reflections
2386 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.117
S = 1.10
3001 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mn1—O1	2.480 (2)	Mn1—N2	2.262 (2)
Mn1—O2	2.192 (2)	Mn1—N3	2.235 (2)
Mn1—O3	2.596 (2)	Mn1—N4	2.270 (2)
Mn1—O4	2.160 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O4^{i}	0.86	1.91	2.751 (3)	165
N5—H5B···O2^{ii}	0.86	1.85	2.712 (3)	180

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

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 *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2414).

References

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supporting information

Acta Cryst. (2011). E**67**, m502 [doi:10.1107/S1600536811010506]

Bis(acetato-κ^2O,O')[2,6-bis(1*H*-pyrazol-3-yl-κN^2)pyridine-κN]manganese(II)

Fan Yu and Bao Li

S1. Experimental

2,6-Bis(pyrazol-3-yl)pyridine (0.1 mmol) was dissolved in methanol (2.5 ml) with 0.2 mmol of trimethylamine. $Mn(OAc)_2$ (0.2 mmol) in methanol (2.5 ml) was added into the resulting solution. After stirring at room temperature for 1 h, the resulting yellow solution was put into a tube layered with aether. Yellow crystals were obtained in three days.

S2. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 (aromatic), 0.96 (CH_3) and N—H = 0.86 Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C, N).

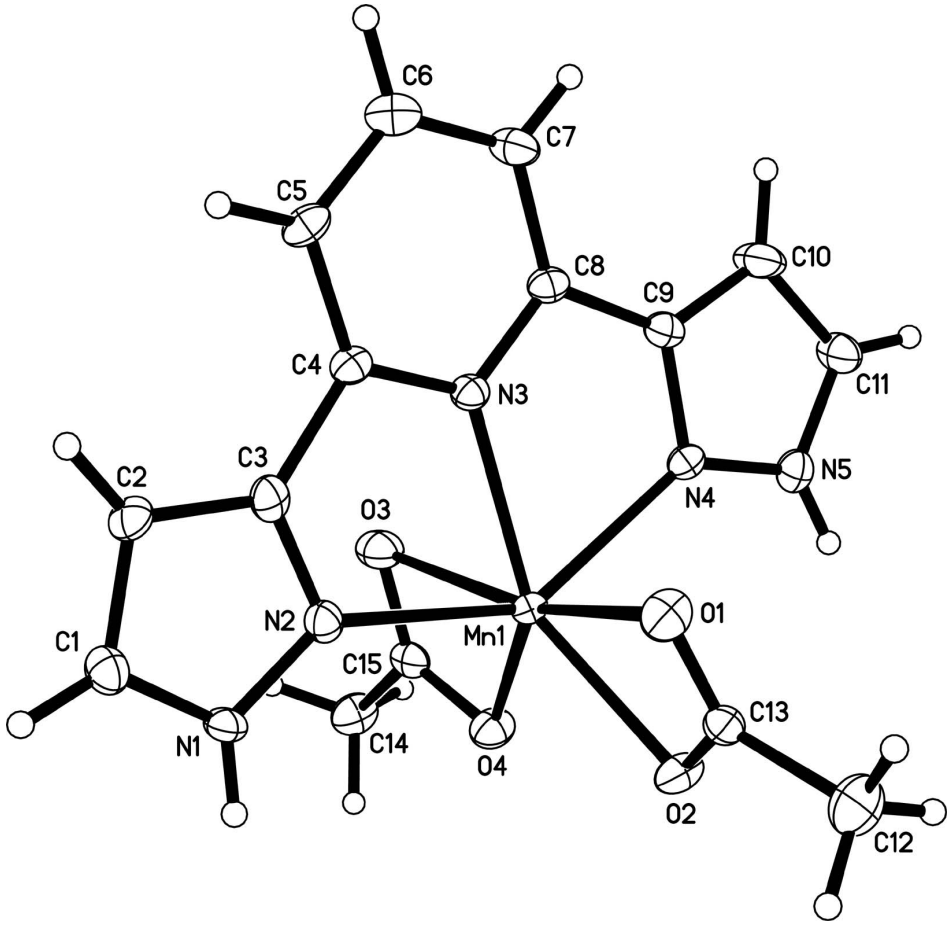

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

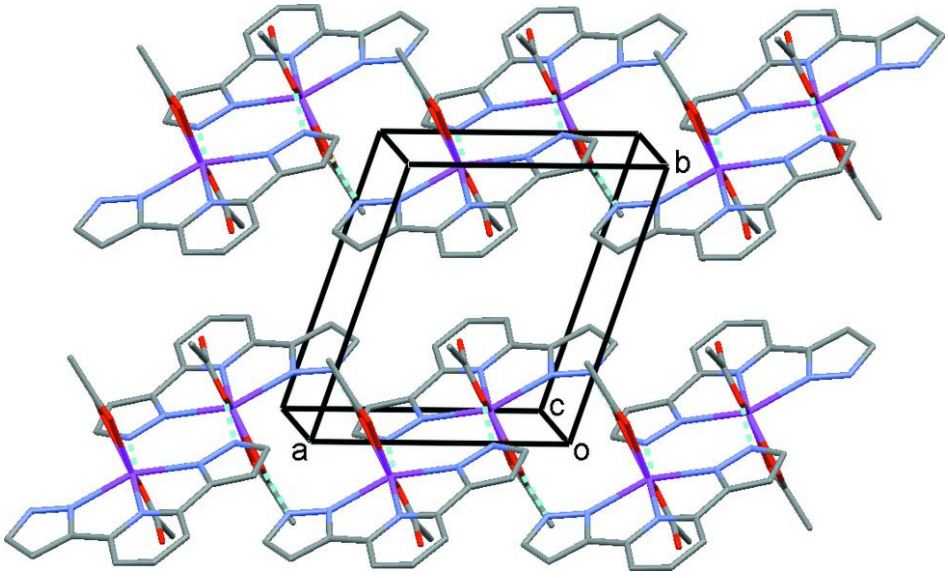

Figure 2

Crystal packing of the title compound, showing the chain structures along the *b* axis. Dashed lines denote hydrogen bonds. H atoms have been omitted for clarity.

Bis(acetato-κ^2O,O')[2,6-bis(1*H*-pyrazol-3-yl- κN^2)pyridine-κN]manganese(II)

Crystal data

$[Mn(C_2H_3O_2)_2(C_{11}H_9N_5)]$
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Hall symbol: -P 1
a = 8.2386 (16) Å
b = 9.4324 (19) Å
c = 11.081 (2) Å
α = 98.32 (3)°
β = 95.01 (3)°
γ = 106.11 (3)°
V = 811.2 (3) Å^3
Z = 2
$F(000)$ = 394
D_x = 1.573 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2386 reflections
θ = 6.1–54.9°
μ = 0.85 mm^{-1}
T = 293 K
Block, yellow
0.30 × 0.20 × 0.20 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} = 0.816, T_{max} = 0.849
5563 measured reflections
3001 independent reflections
2386 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°, θ_{min} = 3.4°
h = −10→10
k = −11→9
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.117$
$S = 1.10$
3001 reflections
226 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
$w = 1/[\sigma^2(F_o^2) + (0.0565P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.67466 (5)	0.89985 (4)	0.81715 (4)	0.01323 (17)
N1	0.3285 (3)	1.0204 (2)	0.7643 (2)	0.0155 (5)
H1B	0.3327	1.0677	0.8375	0.019*
N2	0.4400 (3)	0.9459 (2)	0.7303 (2)	0.0155 (5)
N3	0.6132 (3)	0.7810 (2)	0.6217 (2)	0.0131 (5)
N4	0.8712 (3)	0.7781 (2)	0.7766 (2)	0.0148 (5)
N5	1.0113 (3)	0.7595 (3)	0.8392 (2)	0.0179 (5)
H5B	1.0537	0.8029	0.9135	0.021*
C1	0.2104 (4)	1.0115 (3)	0.6700 (3)	0.0187 (6)
H1A	0.1217	1.0545	0.6732	0.022*
C2	0.2431 (4)	0.9274 (3)	0.5670 (3)	0.0169 (6)
H2A	0.1842	0.9025	0.4877	0.020*
C3	0.3877 (3)	0.8887 (3)	0.6116 (3)	0.0156 (6)
C4	0.4818 (3)	0.7946 (3)	0.5476 (2)	0.0135 (6)
C5	0.4382 (4)	0.7223 (3)	0.4265 (2)	0.0181 (6)
H5A	0.3462	0.7324	0.3771	0.022*
C6	0.5374 (4)	0.6335 (3)	0.3808 (3)	0.0225 (7)
H6A	0.5109	0.5824	0.2999	0.027*
C7	0.6738 (4)	0.6213 (3)	0.4548 (3)	0.0204 (7)
H7A	0.7413	0.5638	0.4244	0.025*
C8	0.7087 (4)	0.6962 (3)	0.5750 (2)	0.0145 (6)
C9	0.8480 (4)	0.6925 (3)	0.6657 (3)	0.0158 (6)
C10	0.9715 (4)	0.6183 (4)	0.6587 (3)	0.0252 (7)
H10A	0.9825	0.5508	0.5922	0.030*
C11	1.0740 (4)	0.6645 (3)	0.7698 (3)	0.0213 (7)
H11A	1.1696	0.6353	0.7926	0.026*
C12	1.0613 (4)	1.3063 (3)	0.8677 (3)	0.0306 (8)
H12A	1.0919	1.3407	0.7931	0.046*
H12B	1.1568	1.2860	0.9100	0.046*
H12C	1.0294	1.3823	0.9194	0.046*
C13	0.9129 (4)	1.1649 (3)	0.8373 (3)	0.0166 (6)
O1	0.8498 (3)	1.1097 (2)	0.7299 (2)	0.0253 (5)
O2	0.8561 (3)	1.1034 (2)	0.92644 (17)	0.0196 (5)
C14	0.3975 (4)	0.6485 (3)	1.0567 (3)	0.0228 (7)

H14A	0.3170	0.5539	1.0197	0.034*
H14B	0.3380	0.7142	1.0935	0.034*
H14C	0.4766	0.6332	1.1188	0.034*
C15	0.4932 (4)	0.7179 (3)	0.9591 (3)	0.0153 (6)
O3	0.4611 (3)	0.6531 (2)	0.85024 (18)	0.0227 (5)
O4	0.6077 (3)	0.8442 (2)	0.99224 (18)	0.0195 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0131 (3)	0.0136 (3)	0.0113 (2)	0.00332 (17)	0.00028 (18)	−0.00105 (16)
N1	0.0176 (13)	0.0184 (12)	0.0118 (12)	0.0079 (10)	0.0042 (10)	0.0006 (9)
N2	0.0136 (13)	0.0139 (12)	0.0192 (13)	0.0045 (10)	0.0024 (10)	0.0029 (10)
N3	0.0139 (12)	0.0139 (12)	0.0114 (12)	0.0035 (10)	0.0023 (10)	0.0024 (9)
N4	0.0146 (12)	0.0180 (12)	0.0110 (12)	0.0050 (10)	−0.0001 (10)	0.0011 (9)
N5	0.0161 (13)	0.0185 (13)	0.0185 (13)	0.0047 (10)	−0.0002 (10)	0.0037 (10)
C1	0.0177 (16)	0.0223 (15)	0.0179 (15)	0.0082 (13)	0.0028 (13)	0.0052 (12)
C2	0.0176 (15)	0.0212 (15)	0.0110 (14)	0.0052 (12)	−0.0009 (12)	0.0031 (11)
C3	0.0128 (14)	0.0119 (14)	0.0216 (16)	0.0020 (11)	0.0035 (12)	0.0039 (11)
C4	0.0158 (15)	0.0142 (14)	0.0099 (14)	0.0021 (11)	0.0026 (12)	0.0038 (11)
C5	0.0221 (16)	0.0204 (15)	0.0103 (14)	0.0053 (13)	−0.0028 (12)	0.0031 (11)
C6	0.0296 (18)	0.0196 (16)	0.0186 (16)	0.0085 (14)	0.0045 (14)	0.0012 (12)
C7	0.0250 (17)	0.0215 (16)	0.0172 (16)	0.0113 (13)	0.0050 (13)	0.0010 (12)
C8	0.0176 (15)	0.0153 (14)	0.0106 (14)	0.0047 (12)	0.0021 (12)	0.0026 (11)
C9	0.0164 (15)	0.0170 (14)	0.0143 (15)	0.0049 (12)	0.0041 (12)	0.0022 (11)
C10	0.0300 (19)	0.0326 (18)	0.0166 (16)	0.0195 (15)	0.0017 (14)	−0.0033 (13)
C11	0.0212 (17)	0.0286 (17)	0.0176 (16)	0.0141 (14)	0.0006 (13)	0.0032 (13)
C12	0.0286 (19)	0.0187 (16)	0.039 (2)	−0.0018 (14)	0.0063 (16)	0.0045 (14)
C13	0.0159 (15)	0.0148 (14)	0.0201 (16)	0.0086 (12)	0.0002 (13)	0.0000 (12)
O1	0.0234 (12)	0.0237 (12)	0.0262 (12)	0.0056 (10)	0.0001 (10)	0.0003 (9)
O2	0.0236 (11)	0.0167 (10)	0.0145 (11)	0.0011 (9)	0.0007 (9)	0.0004 (8)
C14	0.0275 (17)	0.0185 (15)	0.0200 (16)	0.0025 (13)	0.0024 (14)	0.0044 (12)
C15	0.0186 (15)	0.0174 (14)	0.0144 (15)	0.0127 (12)	0.0007 (12)	0.0041 (11)
O3	0.0272 (12)	0.0271 (12)	0.0158 (11)	0.0123 (10)	0.0026 (9)	0.0017 (9)
O4	0.0219 (11)	0.0206 (11)	0.0147 (11)	0.0035 (9)	0.0039 (9)	0.0034 (8)

Geometric parameters (Å, º)

Mn1—O1	2.480 (2)	C5—C6	1.399 (4)
Mn1—O2	2.192 (2)	C5—H5A	0.9300
Mn1—O3	2.596 (2)	C6—C7	1.373 (4)
Mn1—O4	2.160 (2)	C6—H6A	0.9300
Mn1—N2	2.262 (2)	C7—C8	1.380 (4)
Mn1—N3	2.235 (2)	C7—H7A	0.9300
Mn1—N4	2.270 (2)	C8—C9	1.469 (4)
N1—C1	1.341 (4)	C9—C10	1.387 (4)
N1—N2	1.349 (3)	C10—C11	1.370 (4)
N1—H1B	0.8600	C10—H10A	0.9300

N2—C3	1.332 (4)	C11—H11A	0.9300
N3—C4	1.347 (3)	C12—C13	1.510 (4)
N3—C8	1.353 (3)	C12—H12A	0.9600
N4—C9	1.336 (3)	C12—H12B	0.9600
N4—N5	1.361 (3)	C12—H12C	0.9600
N5—C11	1.338 (4)	C13—O1	1.233 (3)
N5—H5B	0.8600	C13—O2	1.275 (3)
C1—C2	1.383 (4)	C14—C15	1.512 (4)
C1—H1A	0.9300	C14—H14A	0.9600
C2—C3	1.410 (4)	C14—H14B	0.9600
C2—H2A	0.9300	C14—H14C	0.9600
C3—C4	1.478 (4)	C15—O3	1.241 (3)
C4—C5	1.382 (4)	C15—O4	1.278 (3)

O4—Mn1—O2	85.32 (8)	N3—C4—C5	122.6 (2)
O4—Mn1—N3	135.59 (8)	N3—C4—C3	112.7 (2)
O2—Mn1—N3	138.38 (8)	C5—C4—C3	124.6 (3)
O4—Mn1—N2	103.71 (8)	C4—C5—C6	117.6 (3)
O2—Mn1—N2	111.90 (8)	C4—C5—H5A	121.2
N3—Mn1—N2	71.44 (8)	C6—C5—H5A	121.2
O4—Mn1—N4	103.09 (8)	C7—C6—C5	120.3 (3)
O2—Mn1—N4	95.79 (8)	C7—C6—H6A	119.8
N3—Mn1—N4	71.19 (8)	C5—C6—H6A	119.8
N2—Mn1—N4	142.63 (8)	C6—C7—C8	118.8 (3)
O4—Mn1—O1	140.27 (8)	C6—C7—H7A	120.6
O2—Mn1—O1	55.33 (7)	C8—C7—H7A	120.6
N3—Mn1—O1	84.13 (8)	N3—C8—C7	122.0 (3)
N2—Mn1—O1	88.11 (8)	N3—C8—C9	112.8 (2)
N4—Mn1—O1	87.66 (8)	C7—C8—C9	125.2 (3)
O4—Mn1—O3	54.13 (7)	N4—C9—C10	109.9 (3)
O2—Mn1—O3	139.25 (7)	N4—C9—C8	117.9 (2)
N3—Mn1—O3	81.62 (7)	C10—C9—C8	132.1 (3)
N2—Mn1—O3	84.46 (7)	C11—C10—C9	106.1 (3)
N4—Mn1—O3	90.63 (7)	C11—C10—H10A	127.0
O1—Mn1—O3	165.39 (6)	C9—C10—H10A	127.0
C1—N1—N2	111.6 (2)	N5—C11—C10	107.3 (3)
C1—N1—H1B	124.2	N5—C11—H11A	126.4
N2—N1—H1B	124.2	C10—C11—H11A	126.4
C3—N2—N1	104.9 (2)	C13—C12—H12A	109.5
C3—N2—Mn1	117.16 (17)	C13—C12—H12B	109.5
N1—N2—Mn1	137.93 (18)	H12A—C12—H12B	109.5
C4—N3—C8	118.8 (2)	C13—C12—H12C	109.5
C4—N3—Mn1	120.55 (17)	H12A—C12—H12C	109.5
C8—N3—Mn1	120.66 (18)	H12B—C12—H12C	109.5
C9—N4—N5	105.9 (2)	O1—C13—O2	121.1 (3)
C9—N4—Mn1	117.09 (18)	O1—C13—C12	121.2 (3)
N5—N4—Mn1	136.93 (17)	O2—C13—C12	117.8 (3)
C11—N5—N4	110.9 (2)	C13—O1—Mn1	85.49 (18)

C11—N5—H5B	124.6	C13—O2—Mn1	97.79 (17)
N4—N5—H5B	124.6	C15—C14—H14A	109.5
N1—C1—C2	108.3 (2)	C15—C14—H14B	109.5
N1—C1—H1A	125.8	H14A—C14—H14B	109.5
C2—C1—H1A	125.8	C15—C14—H14C	109.5
C1—C2—C3	103.0 (3)	H14A—C14—H14C	109.5
C1—C2—H2A	128.5	H14B—C14—H14C	109.5
C3—C2—H2A	128.5	O3—C15—O4	121.3 (3)
N2—C3—C2	112.1 (2)	O3—C15—C14	120.6 (3)
N2—C3—C4	118.0 (2)	O4—C15—C14	118.1 (2)
C2—C3—C4	129.8 (3)	C15—O4—Mn1	101.76 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O4^{i}	0.86	1.91	2.751 (3)	165
N5—H5*B*···O2^{ii}	0.86	1.85	2.712 (3)	180

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