Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Aqua(oxydiacetato-κ^3O,O',O'')(pyridine-2-carboxamide-κ^2N^1,O)copper(II)

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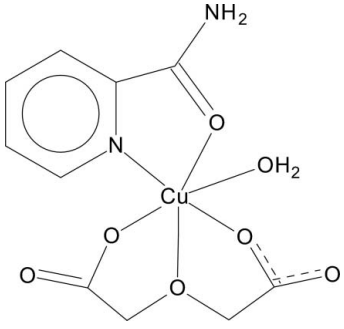
Received 31 October 2007; accepted 14 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.022; wR factor = 0.062; data-to-parameter ratio = 13.6.

The title compound, $[Cu(C_4H_6O_5)(C_6H_2N_2O)(H_2O)]$, has a six-coordinate Cu^{II} atom in a Jahn–Teller-distorted octahedral environment, coordinated by a tridentate oxydiacetate dianion, a bidentate pyridine-2-carboxamide ligand and a water molecule. The oxydiacetate chelates the Cu^{II} atom in a facial configuration.

Related literature

For related structures, see: Sieroń (2004, 2007). For related literature, see: Cremer & Pople (1975); Rao *et al.* (1981); Watanabe *et al.* (1973).



Experimental

Crystal data

$[Cu(C_4H_6O_5)(C_6H_2N_2O)(H_2O)]$
M_r = 335.77
Monoclinic, $P2_1/n$
a = 7.7355 (1) Å
b = 13.2772 (2) Å
c = 12.4147 (2) Å
β = 104.333 (2)°
V = 1235.37 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.80 mm^{-1}
T = 296 K
0.30 × 0.24 × 0.12 mm

Data collection

Kuma KM-4 CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.596, T_{max} = 0.814
13400 measured reflections
2688 independent reflections
2438 reflections with $I > 2\sigma(I)$
R_{int} = 0.010

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.062
S = 1.06
2688 reflections
197 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O2^{i}	0.87 (2)	2.11 (2)	2.946 (2)	161 (2)
N2—H2···O5^{ii}	0.81 (2)	2.50 (2)	2.985 (2)	120 (2)
N2—H2···O6^{ii}	0.81 (2)	2.20 (2)	2.966 (2)	158 (2)
O7—H71···O6^{iii}	0.72 (3)	2.09 (3)	2.804 (3)	175 (3)
O7—H72···O2^{iv}	0.74 (4)	2.49 (4)	3.225 (2)	171 (4)
C3—H3···O6^{ii}	0.93	2.59	3.474 (2)	159
C5—H5···O3^{v}	0.93	2.60	3.251 (2)	128
C6—H6···O1^{vi}	0.93	2.35	3.248 (2)	162
C9—H9*B*···O3^{i}	0.97	2.50	3.399 (3)	154

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+1, y, z$; (iv) $-x+2, -y+2, -z+1$; (v) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (vi) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2003); molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2044).

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supplementary materials

Acta Cryst. (2007). E**63**, m3087 [**doi:10.1107/S1600536807059144**]

Aqua(oxydiacetato-κ^3O,O',O'')(pyridine-2-carboxamide-κ^2N^1,O)copper(II)

L. Sieron

Comment

The present work is a continuation of earlier studies of the preparation, and structure of copper(II) complexes with pyridine-2-carboxamide ($C_6H_6N_2O$, pca) and dicarboxylic acids (Sieroń, 2004; 2007).

The structure of the title compound, (I), is shown in Fig. 1. The Cu^{II} atom shows a typical Jahn-Teller distorted octahedral environment. In the basal plane Cu is bound to O and N atoms of pca [1.979 (1) and 2.013 (1) Å for Cu1–O1 and Cu1–N1, respectively], to two terminal carboxylate O atoms from the oda ligand [1.944 (1) and 1.958 (1) Å for Cu1–O2 and Cu1–O5, respectively]. The apical positions are occupied by the central O atom of oda [Cu1–O4 = 2.413 (1) Å] and by the water ligand [Cu1–O7 = 2.306 (2) Å]. The octahedral (4 + 2) coordination is distinctly deformed, with the O4–Cu1–O7 angle between the axial bonds measuring to 159.59 (6)°.

The tridentate oda dianion chelates to the Cu^{II} atom in a facial coordination mode *via* O2, O4 and O5. The Cu1/O2/C7/C8/O4 ring is essentially planar with only atom C7 being displaced by 0.076 (3) Å out of the mean plane of the other atoms. The Cu1/O4/C9/C10/O5 ring is twisted about the Cu—O4 bond, with the puckering defined by Q(2) = 0.3236 (12) Å and φ(2)= 190.0 (3) ° (Cremer & Pople, 1975) and the pseudorotation parameters P = 348.9 (3) and τ(*M*) = 26.1 (1) ° (Rao *et al.*, 1981).

The individual carboxylate ions are differently involved in the intermolecular hydrogen-bond system. In the C7/O2/O3 group, only O2 is engaged in hydrogen bonding (as an unsymmetrical bifurcated acceptor). The C10/O5/O6 group forms intermolecular hydrogen bonds in which both O5 and O6 (bifurcatedly) are engaged. This causes distinctly different delocalization of π-bonds in both carboxylic groups. The bonds C7—O2 [1.288 (2) Å] and C7—O3 [1.223 (2) Å] are differentiated, while C10—O5 [1.262 (2) Å] and C10—O6 [1.246 (2) Å] are very similar.

Neighbouring Cu^{II} complex molecules are also linked through π···π stacking interactions, with distances between ring centroids $Cg\cdots Cg(2-x, 1-y, 1-z)$ of 3.7350 (9) Å.

Experimental

A mixture of 2-pyridinecarbonitrile (2 mmol) and copper(II) oxydiacetate (2 mmol) in water (60 ml) was heated to boiling. When the solution became dark blue, indicating the copper-assisted hydrolysis of 2-pyridinecarbonitrile to pyridine-2-carboxamide (Watanabe *et al.*, 1973), it was filtered and allowed to cool to room temperature. After a few days, blue crystals of the title compound were obtained.

Refinement

The amine and water H atoms were located in a difference Fourier synthesis and their positions and isotropic displacement parameters were refined freely. The remaining H atoms were positioned with idealized geometry, with C–H = 0.93 or 0.97 Å, and refined with fixed isotropic displacement parameters using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

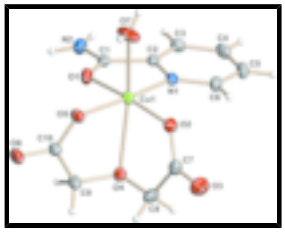

Fig. 1. The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Aqua(oxydiacetato-κ^3*O*,*O*',*O*'')(pyridine-2-carboxamide- κ^2*N*^{1},*O*)copper(II)

Crystal data

$[Cu(C_4H_6O_5)(C_6H_2N_2O)(H_2O)]$	F_{000} = 684
M_r = 335.77	D_x = 1.805 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7383 reflections
a = 7.7355 (1) Å	θ = 2.7–29.9º
b = 13.2772 (2) Å	μ = 1.80 mm^{-1}
c = 12.4147 (2) Å	T = 296 K
β = 104.333 (2)º	Prism, blue
V = 1235.37 (3) Å^3	0.30 × 0.24 × 0.12 mm
Z = 4	

Data collection

Kuma KM-4 CCD diffractometer	2688 independent reflections
Monochromator: graphite	2438 reflections with $I > 2\sigma(I)$
Detector resolution: 8.2356 pixels mm^{-1}	R_{int} = 0.010
T = 296 K	θ_{max} = 27.0º
ω scans	θ_{min} = 2.8º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	h = −9→9
T_{min} = 0.596, T_{max} = 0.814	k = −16→16
13400 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.022$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.5556P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
2688 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
197 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
Cu1	0.91871 (2)	0.79729 (1)	0.46233 (2)	0.0278 (1)
O1	0.82820 (17)	0.72202 (9)	0.32210 (10)	0.0361 (4)
O2	0.99275 (16)	0.85784 (10)	0.60908 (10)	0.0371 (4)
O3	0.9346 (2)	0.89120 (13)	0.77194 (12)	0.0595 (5)
O4	0.68592 (16)	0.74097 (9)	0.54645 (10)	0.0340 (3)
O5	0.72887 (15)	0.89632 (9)	0.41005 (11)	0.0354 (4)
O6	0.43811 (17)	0.92043 (12)	0.35059 (12)	0.0495 (4)
O7	1.1011 (3)	0.90533 (14)	0.39538 (19)	0.0637 (7)
N1	1.08345 (18)	0.67767 (10)	0.49316 (11)	0.0279 (4)
N2	0.8586 (2)	0.58362 (13)	0.22552 (13)	0.0368 (5)
C1	0.9078 (2)	0.64115 (12)	0.31296 (13)	0.0280 (4)
C2	1.0604 (2)	0.61205 (12)	0.40834 (13)	0.0268 (4)
C3	1.1611 (2)	0.52483 (13)	0.41424 (15)	0.0343 (5)
C4	1.2872 (2)	0.50461 (14)	0.51251 (16)	0.0391 (6)
C5	1.3100 (2)	0.57096 (14)	0.60005 (16)	0.0393 (5)
C6	1.2065 (2)	0.65726 (13)	0.58795 (14)	0.0336 (5)
C7	0.8996 (2)	0.84925 (13)	0.68138 (14)	0.0354 (5)

C8	0.7381 (3)	0.7809 (2)	0.65578 (16)	0.0530 (7)
C9	0.5314 (2)	0.78558 (15)	0.47609 (16)	0.0393 (6)
C10	0.5693 (2)	0.87439 (13)	0.40789 (14)	0.0327 (5)
H1	0.758 (3)	0.5959 (17)	0.1771 (19)	0.045 (6)*
H2	0.913 (3)	0.5324 (19)	0.2210 (18)	0.042 (6)*
H3	1.14450	0.48120	0.35400	0.0410*
H4	1.35600	0.44640	0.51920	0.0470*
H5	1.39390	0.55800	0.66640	0.0470*
H6	1.22250	0.70230	0.64690	0.0400*
H8A	0.76150	0.72500	0.70770	0.0640*
H8B	0.63800	0.81820	0.66980	0.0640*
H9A	0.45340	0.80800	0.52160	0.0470*
H9B	0.46780	0.73450	0.42570	0.0470*
H71	1.187 (4)	0.906 (2)	0.383 (2)	0.064 (9)*
H72	1.072 (4)	0.958 (3)	0.398 (3)	0.091 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0264 (1)	0.0288 (1)	0.0271 (1)	0.0030 (1)	0.0047 (1)	−0.0014 (1)
O1	0.0380 (7)	0.0355 (6)	0.0293 (6)	0.0073 (5)	−0.0018 (5)	−0.0024 (5)
O2	0.0359 (6)	0.0421 (7)	0.0321 (6)	−0.0048 (5)	0.0061 (5)	−0.0076 (5)
O3	0.0683 (10)	0.0699 (10)	0.0408 (8)	−0.0023 (8)	0.0146 (7)	−0.0230 (7)
O4	0.0342 (6)	0.0335 (6)	0.0326 (6)	−0.0013 (5)	0.0053 (5)	0.0042 (5)
O5	0.0277 (6)	0.0325 (6)	0.0473 (7)	0.0038 (5)	0.0116 (5)	0.0102 (5)
O6	0.0296 (6)	0.0592 (9)	0.0576 (8)	0.0065 (6)	0.0071 (6)	0.0241 (7)
O7	0.0475 (10)	0.0430 (9)	0.1135 (16)	0.0028 (7)	0.0446 (10)	0.0180 (9)
N1	0.0264 (7)	0.0295 (7)	0.0270 (7)	0.0000 (5)	0.0051 (5)	0.0013 (5)
N2	0.0400 (9)	0.0366 (8)	0.0308 (7)	0.0006 (7)	0.0033 (7)	−0.0056 (6)
C1	0.0285 (8)	0.0306 (8)	0.0257 (7)	−0.0023 (6)	0.0085 (6)	0.0014 (6)
C2	0.0253 (7)	0.0293 (7)	0.0271 (7)	−0.0025 (6)	0.0088 (6)	0.0016 (6)
C3	0.0333 (9)	0.0318 (8)	0.0402 (9)	0.0009 (7)	0.0139 (7)	−0.0022 (7)
C4	0.0310 (9)	0.0328 (9)	0.0537 (11)	0.0064 (7)	0.0109 (8)	0.0085 (8)
C5	0.0310 (9)	0.0413 (10)	0.0405 (9)	0.0015 (7)	−0.0007 (7)	0.0107 (8)
C6	0.0317 (8)	0.0354 (9)	0.0299 (8)	−0.0013 (7)	0.0006 (7)	0.0015 (7)
C7	0.0384 (9)	0.0347 (9)	0.0314 (8)	0.0075 (7)	0.0057 (7)	−0.0031 (7)
C8	0.0476 (12)	0.0834 (16)	0.0287 (9)	−0.0130 (11)	0.0110 (8)	0.0006 (10)
C9	0.0289 (9)	0.0457 (10)	0.0419 (10)	−0.0035 (7)	0.0060 (7)	0.0116 (8)
C10	0.0295 (8)	0.0356 (8)	0.0330 (8)	0.0013 (7)	0.0077 (7)	0.0034 (7)

Geometric parameters (Å, °)

Cu1—O1	1.9789 (12)	N2—H1	0.87 (2)
Cu1—O2	1.9435 (12)	N2—H2	0.81 (2)
Cu1—O4	2.4132 (13)	C1—C2	1.501 (2)
Cu1—O5	1.9582 (12)	C2—C3	1.387 (2)
Cu1—O7	2.306 (2)	C3—C4	1.387 (3)
Cu1—N1	2.0128 (14)	C4—C5	1.376 (3)
O1—C1	1.257 (2)	C5—C6	1.385 (2)

O2—C7	1.288 (2)	C7—C8	1.513 (3)
O3—C7	1.223 (2)	C9—C10	1.522 (3)
O4—C8	1.420 (2)	C3—H3	0.93
O4—C9	1.423 (2)	C4—H4	0.93
O5—C10	1.262 (2)	C5—H5	0.93
O6—C10	1.246 (2)	C6—H6	0.93
O7—H71	0.72 (3)	C8—H8A	0.97
O7—H72	0.74 (4)	C8—H8B	0.97
N1—C2	1.344 (2)	C9—H9A	0.97
N1—C6	1.345 (2)	C9—H9B	0.97
N2—C1	1.305 (2)		
O1—Cu1—O2	172.55 (5)	N1—C2—C3	122.40 (15)
O1—Cu1—O4	94.87 (5)	C1—C2—C3	125.32 (15)
O1—Cu1—O5	88.54 (5)	N1—C2—C1	112.15 (14)
O1—Cu1—O7	96.42 (7)	C2—C3—C4	118.13 (16)
O1—Cu1—N1	80.69 (5)	C3—C4—C5	119.71 (16)
O2—Cu1—O4	78.51 (5)	C4—C5—C6	119.11 (17)
O2—Cu1—O5	93.20 (5)	N1—C6—C5	121.77 (16)
O2—Cu1—O7	90.91 (7)	O2—C7—O3	124.44 (16)
O2—Cu1—N1	97.03 (5)	O2—C7—C8	118.83 (15)
O4—Cu1—O5	76.87 (5)	O3—C7—C8	116.71 (16)
O4—Cu1—O7	159.59 (6)	O4—C8—C7	116.71 (17)
O4—Cu1—N1	100.27 (5)	O4—C9—C10	114.56 (13)
O5—Cu1—O7	86.47 (7)	O6—C10—C9	117.13 (15)
O5—Cu1—N1	168.63 (5)	O5—C10—O6	123.58 (16)
O7—Cu1—N1	98.30 (7)	O5—C10—C9	119.28 (15)
Cu1—O1—C1	115.87 (11)	C2—C3—H3	121
Cu1—O2—C7	122.07 (11)	C4—C3—H3	121
Cu1—O4—C8	103.42 (12)	C3—C4—H4	120
Cu1—O4—C9	102.05 (9)	C5—C4—H4	120
C8—O4—C9	115.36 (15)	C4—C5—H5	120
Cu1—O5—C10	120.09 (11)	C6—C5—H5	120
Cu1—O7—H72	111 (3)	N1—C6—H6	119
H71—O7—H72	108 (3)	C5—C6—H6	119
Cu1—O7—H71	140 (2)	O4—C8—H8A	108
C2—N1—C6	118.86 (14)	O4—C8—H8B	108
Cu1—N1—C2	114.05 (11)	C7—C8—H8A	108
Cu1—N1—C6	127.08 (11)	C7—C8—H8B	108
C1—N2—H2	120.0 (16)	H8A—C8—H8B	107
H1—N2—H2	120 (2)	O4—C9—H9A	109
C1—N2—H1	119.4 (15)	O4—C9—H9B	109
N2—C1—C2	121.08 (15)	C10—C9—H9A	109
O1—C1—N2	121.79 (15)	C10—C9—H9B	109
O1—C1—C2	117.12 (14)	H9A—C9—H9B	108
O4—Cu1—O1—C1	−101.07 (12)	Cu1—O1—C1—N2	178.58 (13)
O5—Cu1—O1—C1	−177.75 (12)	Cu1—O1—C1—C2	−0.16 (18)
O7—Cu1—O1—C1	95.97 (13)	Cu1—O2—C7—O3	−175.11 (14)
N1—Cu1—O1—C1	−1.43 (12)	Cu1—O2—C7—C8	6.6 (2)

O4—Cu1—O2—C7	−2.54 (13)	Cu1—O4—C8—C7	5.4 (2)
O5—Cu1—O2—C7	73.36 (13)	C9—O4—C8—C7	−105.2 (2)
O7—Cu1—O2—C7	159.88 (14)	Cu1—O4—C9—C10	−20.20 (16)
N1—Cu1—O2—C7	−101.65 (13)	C8—O4—C9—C10	91.13 (19)
O1—Cu1—O4—C8	174.68 (12)	Cu1—O5—C10—O6	−160.48 (14)
O1—Cu1—O4—C9	−65.25 (11)	Cu1—O5—C10—C9	18.0 (2)
O2—Cu1—O4—C8	−1.89 (12)	Cu1—N1—C2—C1	−3.65 (17)
O2—Cu1—O4—C9	118.18 (11)	Cu1—N1—C2—C3	−179.72 (13)
O5—Cu1—O4—C8	−97.97 (13)	C6—N1—C2—C1	174.91 (14)
O5—Cu1—O4—C9	22.11 (10)	C6—N1—C2—C3	−1.2 (2)
O7—Cu1—O4—C8	−61.9 (2)	Cu1—N1—C6—C5	178.63 (12)
O7—Cu1—O4—C9	58.2 (2)	C2—N1—C6—C5	0.3 (2)
N1—Cu1—O4—C8	93.28 (13)	O1—C1—C2—N1	2.6 (2)
N1—Cu1—O4—C9	−146.65 (10)	O1—C1—C2—C3	178.53 (16)
O1—Cu1—O5—C10	72.95 (13)	N2—C1—C2—N1	−176.16 (15)
O2—Cu1—O5—C10	−99.81 (13)	N2—C1—C2—C3	−0.2 (3)
O4—Cu1—O5—C10	−22.39 (12)	N1—C2—C3—C4	1.3 (2)
O7—Cu1—O5—C10	169.48 (14)	C1—C2—C3—C4	−174.25 (15)
O1—Cu1—N1—C2	2.90 (11)	C2—C3—C4—C5	−0.5 (2)
O1—Cu1—N1—C6	−175.52 (15)	C3—C4—C5—C6	−0.3 (3)
O2—Cu1—N1—C2	175.73 (11)	C4—C5—C6—N1	0.4 (3)
O2—Cu1—N1—C6	−2.69 (15)	O2—C7—C8—O4	−8.3 (3)
O4—Cu1—N1—C2	96.20 (11)	O3—C7—C8—O4	173.30 (18)
O4—Cu1—N1—C6	−82.22 (14)	O4—C9—C10—O5	6.2 (2)
O7—Cu1—N1—C2	−92.31 (12)	O4—C9—C10—O6	−175.28 (15)
O7—Cu1—N1—C6	89.28 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1···O2^{i}	0.87 (2)	2.11 (2)	2.946 (2)	161 (2)
N2—H2···O5^{ii}	0.81 (2)	2.50 (2)	2.985 (2)	120 (2)
N2—H2···O6^{ii}	0.81 (2)	2.20 (2)	2.966 (2)	158 (2)
O7—H71···O6^{iii}	0.72 (3)	2.09 (3)	2.804 (3)	175 (3)
O7—H72···O2^{iv}	0.74 (4)	2.49 (4)	3.225 (2)	171 (4)
C3—H3···O6^{ii}	0.93	2.59	3.474 (2)	159
C5—H5···O3^{v}	0.93	2.60	3.251 (2)	128
C6—H6···O1^{vi}	0.93	2.35	3.248 (2)	162
C9—H9B···O3^{i}	0.97	2.50	3.399 (3)	154

Symmetry codes: (i) *x*−1/2, −*y*+3/2, *z*−1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) *x*+1, *y*, *z*; (iv) −*x*+2, −*y*+2, −*z*+1; (v) −*x*+5/2, *y*−1/2, −*z*+3/2; (vi) *x*+1/2, −*y*+3/2, *z*+1/2.

Fig. 1