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Poly[(μ-1*H*-benzimidazole-5,6-dicarboxylato)lead(II)]

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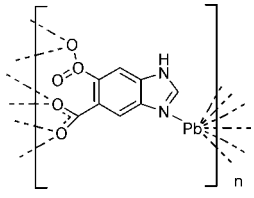
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.008 Å; R factor = 0.042; wR factor = 0.120; data-to-parameter ratio = 11.0.

The crystal structure of the two-dimensional polymeric title compound, $[Pb(C_9H_4N_2O_4)]_n$, comprises one crystallographically independent Pb^{II} atom and one fully deprotonated 1*H*-benzimidazole-5,6-dicarboxylate (H_2L) ligand. The Pb^{II} atom is seven-coordinated by six O atoms and one N atom from the H_2L ligands, giving a capped octahedral coordination geometry. The structure is a layered two-dimensional coordination polymer extending parallel to (100) with N—H···O hydrogen bonds interactions between the layers, stabilizing the crystal structure.

Related literature

For applications of metal-organic frameworks, see: Li *et al.* (2007). For related structures, see: Gao *et al.* (2008); Lo *et al.*. (2007); Wang *et al.* (2009); Wei *et al.* (2008);Yao *et al.* (2008); Zhai (2009).



Experimental

Crystal data

$[Pb(C_9H_4N_2O_4)]$
M_r = 411.34
Monoclinic, $P2_1/c$
a = 13.127 (2) Å
b = 9.5571 (14) Å
c = 6.7557 (10) Å
β = 99.587 (2)°
V = 835.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 20.19 mm^{-1}
T = 273 K
0.30 × 0.30 × 0.27 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.003, T_{max} = 0.004
3954 measured reflections
1458 independent reflections
1273 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.08
1458 reflections
133 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 3.24 e Å^{-3}
$\Delta\rho_{min}$ = −2.83 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O4^{i}	0.86	2.02	2.723 (12)	138

Symmetry code: (i) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

The authors acknowledge the Chan Xue Yan Cooperative Special Project of Guangdong Province and the Ministry of Science and Technology of PRC (project No. 2010B090400184).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2009).

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supporting information

Acta Cryst. (2011). E**67**, m755 [doi:10.1107/S1600536811017065]

Poly[(*μ*-1*H*-benzimidazole-5,6-dicarboxylato)lead(II)]

Jinhua Chen, Chun Zheng, Yuezhu Wang, Tingting Yun and Yifan Luo

S1. Comment

In recent years, metal-organic frameworks (MOF) based on supramolecular chemistry and crystal engineering have attracted extensive attention not only due to their diverse topologies and intriguing structures but also owing to their interesting physical and chemical properties, such as photoluminescence, magnetism, ferroelectricity, gas storage, ion exchange and catalysis, Li *et al.* (2007). N-Heterocyclic multicarboxylic acids have been widely used to construct MOF for their potential application. 1*H*-benzimidazole-5,6-dicarboxylic acid possesses two nitrogen atoms of imidazole ring and four oxygen atoms of carboxylate groups, and might be used as versatile linker in constructing coordination polymers with abundant hydrogen bonds. Several coordination polymers fomed by this ligand have been reported recently: Gao *et al.* (2008); Lo *et al.* (2007); Wang *et al.* (2009); Wei *et al.* (2008); Yao *et al.* (2008); Zhai (2009). Herein we report the synthesis and crystal structure of the title complex of $(C_9H_4N_2O_4Pb)_n$, Fig. 1. This is a layered 2D-coordination polymer structure with H-bonds interactions between the layers which is shown in Fig. 2.

S2. Experimental

A mixture of $Pb(CH_3COO)_2$ (0.6 mmol), H_2L(0.6 mmol) and water (13 ml) was added to a 25 ml teflon-lined stainless container, which was heated to 430K and held at that temperature for 3 days. After cooling to room temperature, yellow crystals were recovered by filtration.

S3. Refinement

H atoms of water and hydroxyl were located in Fourier difference maps and refined with isotropic displacement parameters set at 1.5 times those of the parent O atoms. the refinement using a riding-model approximation [C–H = 0.93, O–H = 0.84 and N—H = 0.86 Å] with U_{iso}(H) = 1.2 U_{eq}(C,*N*) or 1.5Ueq(O).

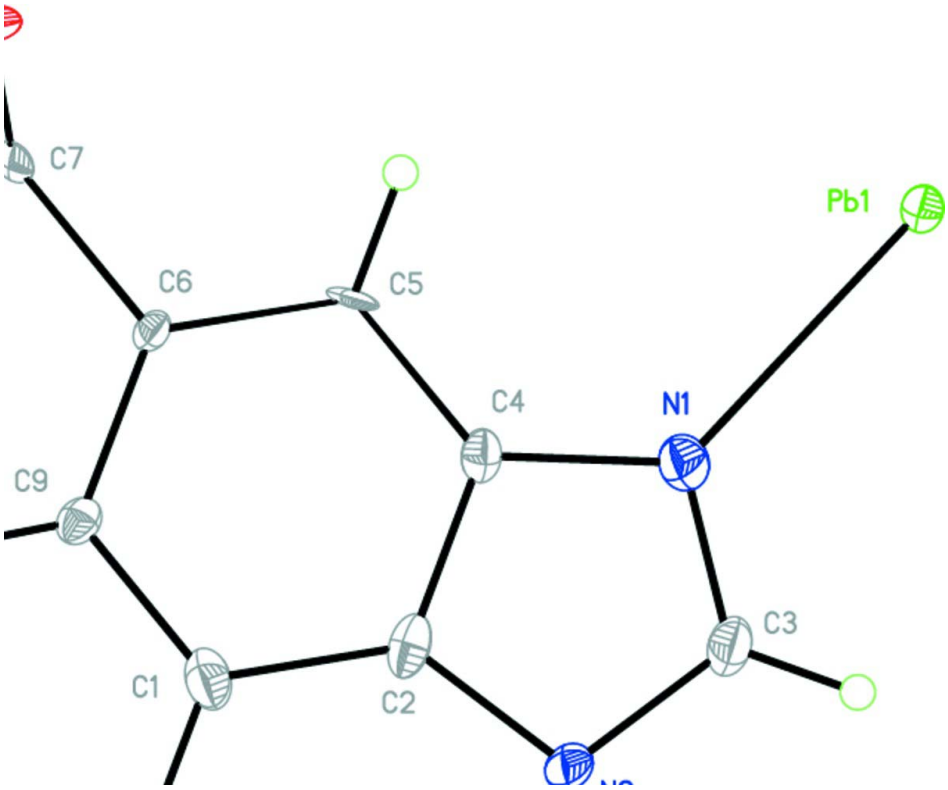

Figure 1

The structure of the title compound, showing the atomic numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids.

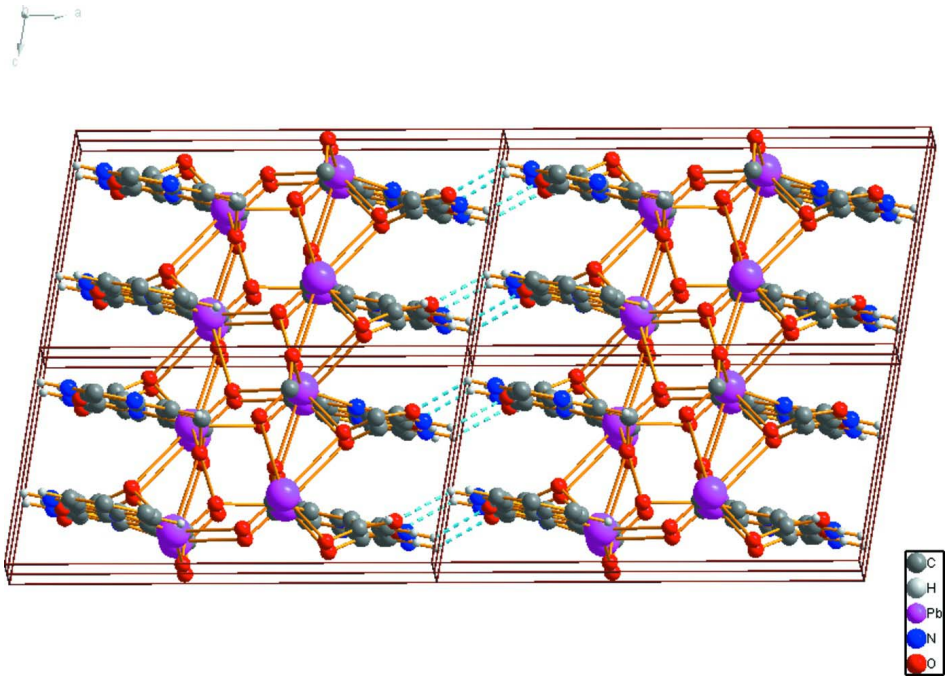

Figure 2

The packing diagram of the title compound, with H atoms omitted for clarity. Hydrogen bonds are shown as dashed lines.

Poly[(*μ*-1*H*-benzimidazole-5,6-dicarboxylato)lead(II)]

Crystal data

$[Pb(C_9H_4N_2O_4)]$
$M_r = 411.34$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.127$ (2) Å
$b = 9.5571$ (14) Å
$c = 6.7557$ (10) Å
$\beta = 99.587$ (2)°
$V = 835.7$ (2) Å^3
$Z = 4$
$F(000) = 744.0$
$D_x = 3.269$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2747 reflections
$\theta = 2.7$–$28.4°$
$\mu = 20.19$ mm^{-1}
$T = 273$ K
Block, yellow
0.30 × 0.30 × 0.27 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.003$, $T_{max} = 0.004$
3954 measured reflections
1458 independent reflections
1273 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -15 \rightarrow 15$
$k = -11 \rightarrow 8$
$l = -7 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.120$
$S = 1.08$
1458 reflections
133 parameters
12 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
$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 3.24$ e Å^{-3}
$\Delta\rho_{min} = -2.83$ e Å^{-3}

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. The number of independent reflections and the number of reflections used in the refinement are not the same, because we use 'omit -3 50′ to enhance the′_diffrn_measured_fraction_theta_full′.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C4	0.7560 (4)	0.3072 (4)	0.2539 (9)	0.019 (2)
C5	0.6729 (3)	0.2152 (5)	0.2241 (10)	0.0164 (19)
H5	0.6058	0.2496	0.1959	0.020*
C6	0.6901 (4)	0.0717 (4)	0.2362 (9)	0.0152 (18)
C9	0.7904 (4)	0.0203 (4)	0.2783 (9)	0.0169 (19)
C1	0.8736 (3)	0.1123 (6)	0.3081 (9)	0.025 (3)
H1	0.9407	0.0779	0.3363	0.030*
C2	0.8564 (4)	0.2558 (5)	0.2959 (9)	0.021 (2)
Pb1	0.62381 (3)	0.62780 (3)	0.17812 (5)	0.0172 (2)
N1	0.7597 (7)	0.4523 (8)	0.2560 (13)	0.0252 (19)
C3	0.8566 (8)	0.4844 (11)	0.2927 (15)	0.025 (2)
H3	0.8810	0.5759	0.3003	0.029*
N2	0.9199 (8)	0.3693 (7)	0.3195 (14)	0.021 (2)
H2	0.9863	0.3690	0.3459	0.025*
C8	0.8123 (9)	−0.1314 (8)	0.3226 (17)	0.020 (2)
O4	0.8944 (6)	−0.1832 (8)	0.2949 (13)	0.036 (2)
C7	0.6000 (7)	−0.0282 (8)	0.1935 (12)	0.0146 (19)
O2	0.5921 (6)	−0.1031 (6)	0.0387 (11)	0.0220 (16)
O1	0.5389 (5)	−0.0325 (6)	0.3196 (9)	0.0184 (14)
O3	0.7406 (4)	−0.2011 (6)	0.3876 (9)	0.0167 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C4	0.024 (5)	0.013 (4)	0.019 (5)	−0.001 (4)	0.002 (4)	0.001 (3)
C5	0.006 (4)	0.021 (4)	0.022 (4)	0.005 (3)	0.002 (3)	0.002 (3)
C6	0.014 (5)	0.012 (4)	0.021 (5)	−0.003 (3)	0.007 (4)	0.000 (3)
C9	0.018 (5)	0.017 (4)	0.017 (5)	−0.003 (4)	0.007 (4)	−0.001 (3)
C1	0.030 (6)	0.017 (5)	0.030 (6)	0.005 (3)	0.011 (5)	0.001 (3)
C2	0.033 (6)	0.015 (5)	0.016 (5)	−0.006 (4)	0.008 (4)	−0.002 (4)
Pb1	0.0188 (3)	0.0151 (3)	0.0172 (3)	−0.00085 (11)	0.0019 (2)	−0.00061 (10)
N1	0.026 (5)	0.021 (4)	0.029 (5)	0.001 (4)	0.008 (4)	−0.003 (3)
C3	0.029 (6)	0.016 (5)	0.028 (6)	−0.004 (4)	0.003 (5)	−0.001 (4)
N2	0.016 (5)	0.019 (4)	0.031 (5)	−0.004 (3)	0.010 (4)	−0.001 (3)
C8	0.013 (6)	0.019 (5)	0.027 (6)	0.001 (3)	0.003 (5)	−0.006 (3)
O4	0.021 (4)	0.021 (4)	0.066 (6)	0.000 (3)	0.011 (4)	0.004 (4)
C7	0.013 (5)	0.014 (4)	0.014 (5)	0.004 (3)	−0.006 (4)	0.005 (3)
O2	0.030 (4)	0.017 (3)	0.021 (4)	0.003 (3)	0.010 (3)	−0.003 (3)
O1	0.010 (3)	0.032 (3)	0.013 (3)	−0.001 (2)	0.003 (3)	0.002 (2)
O3	0.010 (3)	0.018 (3)	0.021 (3)	0.001 (2)	0.000 (3)	0.003 (2)

Geometric parameters (Å, º)

C4—N1	1.387 (8)	Pb1—O1^{iv}	2.653 (6)
C4—C5	1.389 (7)	Pb1—O2^{i}	2.746 (6)

C4—C2	1.391 (7)	N1—C3	1.292 (13)
C5—C6	1.390 (7)	C3—N2	1.371 (13)
C5—H5	0.9300	C3—H3	0.9300
C6—C9	1.390 (7)	N2—H2	0.8600
C6—C7	1.510 (10)	C8—O4	1.228 (13)
C9—C1	1.390 (7)	C8—O3	1.289 (11)
C9—C8	1.498 (9)	C7—O2	1.258 (11)
C1—C2	1.390 (7)	C7—O1	1.265 (11)
C1—H1	0.9300	O2—Pb1^{iv}	2.549 (7)
C2—N2	1.362 (9)	O2—Pb1^{v}	2.746 (6)
Pb1—N1	2.442 (8)	O1—Pb1^{vi}	2.630 (6)
Pb1—O3^{i}	2.511 (6)	O1—Pb1^{ii}	2.653 (6)
Pb1—O2^{ii}	2.549 (7)	O3—Pb1^{v}	2.511 (6)
Pb1—O1^{iii}	2.630 (6)		

N1—C4—C5	131.3 (5)	N1—Pb1—O2^{i}	141.3 (2)
N1—C4—C2	108.7 (5)	O3^{i}—Pb1—O2^{i}	68.1 (2)
C5—C4—C2	120.0 (4)	O2^{ii}—Pb1—O2^{i}	112.01 (18)
C4—C5—C6	120.0 (4)	O1^{iii}—Pb1—O2^{i}	118.1 (2)
C6—C5—H5	120.0	O1^{iv}—Pb1—O2^{i}	89.52 (19)
C4—C5—H5	120.0	C3—N1—C4	105.7 (7)
C9—C6—C5	120.0 (4)	C3—N1—Pb1	122.6 (6)
C9—C6—C7	120.0 (4)	C4—N1—Pb1	131.4 (5)
C5—C6—C7	119.9 (4)	N1—C3—N2	113.0 (9)
C1—C9—C6	120.1 (4)	N1—C3—H3	123.5
C1—C9—C8	117.6 (5)	N2—C3—H3	123.5
C6—C9—C8	121.8 (5)	C2—N2—C3	106.1 (8)
C2—C1—H1	120.0	C2—N2—H2	126.9
C9—C1—H1	120.0	C3—N2—H2	126.9
C9—C1—C2	120.0 (4)	O4—C8—O3	123.6 (8)
N2—C2—C1	133.6 (5)	O4—C8—C9	120.2 (8)
N2—C2—C4	106.4 (5)	O3—C8—C9	116.2 (8)
C1—C2—C4	120.0 (4)	O2—C7—O1	124.6 (8)
N1—Pb1—O3^{i}	88.3 (2)	O2—C7—C6	118.2 (8)
N1—Pb1—O2^{ii}	87.7 (2)	O1—C7—C6	117.2 (7)
O3^{i}—Pb1—O2^{ii}	72.7 (2)	C7—O2—Pb1^{iv}	147.5 (6)
N1—Pb1—O1^{iii}	99.4 (2)	C7—O2—Pb1^{v}	105.1 (5)
O3^{i}—Pb1—O1^{iii}	142.76 (18)	Pb1^{iv}—O2—Pb1^{v}	101.6 (2)
O2^{ii}—Pb1—O1^{iii}	71.3 (2)	C7—O1—Pb1^{vi}	126.3 (5)
N1—Pb1—O1^{iv}	98.2 (2)	C7—O1—Pb1^{ii}	114.1 (5)
O3^{i}—Pb1—O1^{iv}	149.59 (19)	Pb1^{vi}—O1—Pb1^{ii}	114.4 (2)
O2^{ii}—Pb1—O1^{iv}	136.9 (2)	C8—O3—Pb1^{v}	123.8 (6)
O1^{iii}—Pb1—O1^{iv}	65.6 (2)		

N1—C4—C5—C6	−177.8 (6)	O1^{iii}—Pb1—N1—C4	14.3 (7)
C2—C4—C5—C6	0.0	O1^{iv}—Pb1—N1—C4	−52.2 (7)
C4—C5—C6—C9	0.0	O2^{i}—Pb1—N1—C4	−151.8 (5)
C4—C5—C6—C7	−176.9 (6)	C4—N1—C3—N2	−1.0 (11)

C5—C6—C9—C1	0.0	Pb1—N1—C3—N2	−175.9 (7)
C7—C6—C9—C1	176.9 (6)	C1—C2—N2—C3	−178.7 (6)
C5—C6—C9—C8	170.9 (7)	C4—C2—N2—C3	0.4 (9)
C7—C6—C9—C8	−12.2 (8)	N1—C3—N2—C2	0.4 (12)
C6—C9—C1—C2	0.0	C1—C9—C8—O4	−32.8 (12)
C8—C9—C1—C2	−171.2 (7)	C6—C9—C8—O4	156.1 (8)
C9—C1—C2—N2	179.1 (9)	C1—C9—C8—O3	147.9 (7)
C9—C1—C2—C4	0.0	C6—C9—C8—O3	−23.2 (11)
N1—C4—C2—N2	−1.1 (7)	C5—C6—C7—O2	112.1 (7)
C5—C4—C2—N2	−179.3 (6)	C9—C6—C7—O2	−64.9 (8)
N1—C4—C2—C1	178.2 (5)	C5—C6—C7—O1	−69.5 (8)
C5—C4—C2—C1	0.0	C9—C6—C7—O1	113.6 (7)
C5—C4—N1—C3	179.3 (6)	O1—C7—O2—Pb1^{iv}	150.4 (8)
C2—C4—N1—C3	1.3 (8)	C6—C7—O2—Pb1^{iv}	−31.3 (15)
C5—C4—N1—Pb1	−6.5 (9)	O1—C7—O2—Pb1^{v}	−65.2 (9)
C2—C4—N1—Pb1	175.5 (5)	C6—C7—O2—Pb1^{v}	113.1 (6)
O3^{i}—Pb1—N1—C3	−29.0 (8)	O2—C7—O1—Pb1^{vi}	−94.0 (9)
O2^{ii}—Pb1—N1—C3	−101.8 (8)	C6—C7—O1—Pb1^{vi}	87.7 (7)
O1^{iii}—Pb1—N1—C3	−172.4 (7)	O2—C7—O1—Pb1^{ii}	113.2 (8)
O1^{iv}—Pb1—N1—C3	121.2 (8)	C6—C7—O1—Pb1^{ii}	−65.2 (7)
O2^{i}—Pb1—N1—C3	21.6 (10)	O4—C8—O3—Pb1^{v}	−74.3 (13)
O3^{i}—Pb1—N1—C4	157.6 (7)	C9—C8—O3—Pb1^{v}	105.0 (7)
O2^{ii}—Pb1—N1—C4	84.8 (7)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{vii}	0.86	2.02	2.723 (12)	138

Symmetry code: (vii) −*x*+2, *y*+1/2, −*z*+1/2.