

2-(Morpholin-4-ylmethyl)isoindole-1,3-dione

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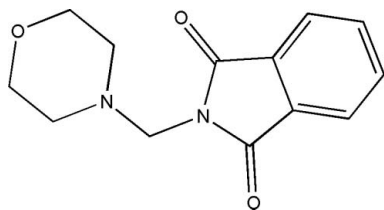
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.044; wR factor = 0.145; data-to-parameter ratio = 21.9.

In the title compound, $\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}_3$, the morpholine ring adopts the usual chair conformation. The crystal structure is stabilized by weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bond interactions.

Related literature

For related literature, see: Allen (2002); Allen *et al.* (1987); Bailleux *et al.* (1993); Couture *et al.* (1997, 1998); Fisher & Wyvratt (1990); Lima *et al.* (2002); Liu *et al.* (2004); Orzeszka *et al.* (2000); Ramnathan *et al.* (1996); Yoshioka (1995).



Experimental

Crystal data

$\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}_3$
 $M_r = 246.26$
Monoclinic, $P2_1/c$
 $a = 9.3891$ (6) Å
 $b = 5.4617$ (3) Å
 $c = 23.5796$ (16) Å
 $\beta = 92.209$ (2)°

$V = 1208.27$ (13) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 293$ (2) K
 $0.30 \times 0.22 \times 0.22$ mm

Data collection

Bruker APEXII diffractometer	15502 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2004)	3753 independent reflections
$T_{\min} = 0.971$, $T_{\max} = 0.979$	2518 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.145$
 $S = 1.03$
3753 reflections
171 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4A}\cdots\text{O3}^i$	0.93	2.60	3.424 (2)	149
$\text{C9}-\text{H9A}\cdots\text{O2}$	0.978 (16)	2.553 (14)	2.9025 (16)	100.9 (9)

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

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2 and SAINT-NT (Bruker, 2004); data reduction: SAINT-NT and XPREP (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: PLATON (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2525).

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supplementary materials

Acta Cryst. (2007). E63, o4284 [doi:10.1107/S1600536807048738]

2-(Morpholin-4-ylmethyl)isoindole-1,3-dione

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Comment

Morpholine is used as an important chemical intermediate in the preparation of pesticides. Drugs containing the morpholine ring have established activities that include the reduction of blood sugar and lipid levels (Yoshioka, 1995), and amelioration of obesity and insulin resistance (Fisher & Wyvrat, 1990). Owing to their pharmacological activities the morpholine derivatives have received a great deal of attention in respect of their synthesis and crystal structures. Phthalimides and N-substituted phthalimides are an important class of compounds because of their interesting biological activities (Lima *et al.*, 2002; Orzeszka *et al.*, 2000; Bailleux *et al.*, 1993).

Phthalimides have also served as starting materials and intermediates for synthesis of alkaloids (Couture *et al.*, 1998) and pharmacophores (Couture *et al.*, 1997).

The molecular structure of the title compound is illustrated in Fig. 1.

In the morpholine ring the average C—N, C—C and C—O bond distances [1.457 (2), 1.504 (2), 1.421 (2) Å] are in good agreement with earlier reports (Ramnathan *et al.*, 1996). The morpholine ring adopts the usual chair conformation. This is in good agreement with structural data available from version 5.14 of the Cambridge Structural Database (Allen, 2002). The geometry of the phthalimide ring system is close to that in the related compound 4-(1,3-dioxoisoindolin-2-yl)benzaldehyde (Liu *et al.*, 2004).

The sum of the angles around N1 is 358.60 (10)° indicating sp^2 hybridization. However the N1—C1 [1.399 (2) Å] and N1—C8 [1.402 (2) Å] distances are intermediate between the average C_{ar} —N sp^3 (pyramidal) [1.419 (17) Å] and C_{ar} —N sp^2 (planar) [1.353 (7) Å] distances reported by Allen *et al.* (1987).

The crystal structure is stabilized by weak C—H...O hydrogen bonds (Table 1).

Experimental

Phthalimide (14.7 g, 0.1 mole) taken in a 250 ml beaker was dissolved in 20 ml dimethylformamide and 9.5 ml of 37% (w/v) aqueous formaldehyde (0.1 mole) was added and stirred well. Morpholine (9.0 ml, 0.1 mole) was slowly added to the beaker with stirring. The clear solution became oily. The oily mixture on continuous stirring gave the colourless solid product. The solid product was washed with cold water and finally with diethyl ether. The crude product was recrystallized from ethanol. It melts at 114°C.

Refinement

All H atoms were refined with fixed individual displacement parameters [$U(H) = 1.2 U_{eq}(C)$] using a riding model with C—H(aromatic) = 0.93 Å. The two methylene H atoms were freely refined.

Figures

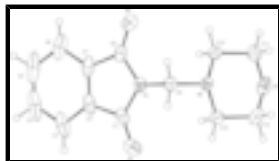


Fig. 1. The structure of the title compound showing the atom numbering scheme with 30% probability displacement ellipsoids.

2-(Morpholin-4-ylmethyl)isoindole-1,3-dione

Crystal data

$C_{13}H_{14}N_2O_3$

$M_r = 246.26$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 9.3891\ (6)\ \text{\AA}$

$b = 5.4617\ (3)\ \text{\AA}$

$c = 23.5796\ (16)\ \text{\AA}$

$\beta = 92.209\ (2)^\circ$

$V = 1208.27\ (13)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 520$

$D_x = 1.354\ \text{Mg m}^{-3}$

Melting point: 114 K

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5593 reflections

$\theta = 1.7\text{--}31.0^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Prism, colorless

$0.30 \times 0.22 \times 0.22\ \text{mm}$

Data collection

Bruker APEXII
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293\ (2)\ \text{K}$

ω and φ scans

Absorption correction: multi-scan
(SADABS; Bruker, 2004)

$T_{\min} = 0.971$, $T_{\max} = 0.979$

15502 measured reflections

3753 independent reflections

2518 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 31.0^\circ$

$\theta_{\min} = 1.7^\circ$

$h = -13 \rightarrow 13$

$k = -7 \rightarrow 7$

$l = -33 \rightarrow 33$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.145$

$S = 1.03$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 0.1528P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.003$

3753 reflections $\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$
 171 parameters $\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$
 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 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.53689 (11)	-0.2316 (2)	0.06952 (5)	0.0644 (4)
O2	0.83043 (11)	0.4355 (2)	0.07666 (4)	0.0618 (3)
O3	0.82872 (11)	-0.1431 (2)	0.27481 (4)	0.0616 (4)
N1	0.67568 (11)	0.11172 (19)	0.08750 (4)	0.0430 (3)
N2	0.66236 (10)	0.11859 (18)	0.19243 (4)	0.0375 (3)
C1	0.62829 (15)	-0.0907 (3)	0.05571 (5)	0.0484 (4)
C2	0.71093 (16)	-0.0865 (3)	0.00319 (5)	0.0572 (5)
C3	0.7080 (2)	-0.2493 (4)	-0.04214 (7)	0.0810 (7)
C4	0.7964 (3)	-0.1936 (6)	-0.08606 (8)	0.1082 (10)
C5	0.8805 (3)	0.0147 (6)	-0.08507 (8)	0.1069 (9)
C6	0.88466 (19)	0.1762 (4)	-0.03932 (7)	0.0804 (7)
C7	0.79708 (16)	0.1177 (3)	0.00476 (5)	0.0575 (5)
C8	0.77630 (14)	0.2498 (3)	0.05890 (5)	0.0474 (4)
C9	0.60573 (13)	0.2024 (2)	0.13835 (5)	0.0417 (3)
C10	0.81102 (12)	0.1807 (3)	0.20460 (5)	0.0455 (4)
C11	0.85198 (16)	0.1099 (3)	0.26483 (6)	0.0592 (5)
C12	0.68315 (16)	-0.2018 (3)	0.26299 (6)	0.0584 (5)
C13	0.63978 (15)	-0.1416 (2)	0.20251 (6)	0.0493 (4)
H3A	0.65007	-0.38755	-0.04295	0.0972*
H4A	0.79922	-0.29876	-0.11700	0.1298*
H5A	0.93613	0.04779	-0.11596	0.1282*
H6A	0.94246	0.31458	-0.03839	0.0965*
H9A	0.6128 (14)	0.381 (3)	0.1371 (6)	0.048 (4)*
H9B	0.5058 (16)	0.150 (3)	0.1337 (6)	0.048 (4)*
H10A	0.82499	0.35520	0.19949	0.0546*
H10B	0.87098	0.09469	0.17858	0.0546*
H11A	0.95183	0.14768	0.27247	0.0711*
H11B	0.79643	0.20552	0.29068	0.0711*
H12A	0.62398	-0.11068	0.28840	0.0700*

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H12B	0.66817	-0.37498	0.26971	0.0700*
H13A	0.69587	-0.23740	0.17689	0.0592*
H13B	0.54008	-0.18188	0.19539	0.0592*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0630 (6)	0.0573 (7)	0.0717 (7)	0.0000 (5)	-0.0109 (5)	-0.0117 (5)
O2	0.0655 (6)	0.0595 (6)	0.0608 (6)	-0.0033 (5)	0.0090 (5)	0.0098 (5)
O3	0.0570 (6)	0.0753 (7)	0.0528 (6)	0.0141 (5)	0.0057 (4)	0.0212 (5)
N1	0.0499 (6)	0.0448 (6)	0.0343 (5)	0.0069 (4)	0.0036 (4)	-0.0027 (4)
N2	0.0392 (5)	0.0383 (5)	0.0352 (5)	0.0018 (4)	0.0053 (4)	-0.0002 (4)
C1	0.0546 (7)	0.0486 (7)	0.0411 (6)	0.0166 (6)	-0.0102 (5)	-0.0056 (5)
C2	0.0682 (9)	0.0679 (9)	0.0346 (6)	0.0358 (7)	-0.0094 (6)	-0.0042 (6)
C3	0.1056 (13)	0.0921 (13)	0.0432 (8)	0.0564 (11)	-0.0238 (8)	-0.0191 (8)
C4	0.141 (2)	0.148 (2)	0.0343 (8)	0.0961 (18)	-0.0133 (10)	-0.0177 (11)
C5	0.1146 (18)	0.169 (2)	0.0385 (9)	0.0920 (18)	0.0198 (10)	0.0219 (12)
C6	0.0766 (10)	0.1193 (15)	0.0467 (8)	0.0509 (11)	0.0190 (7)	0.0288 (9)
C7	0.0620 (8)	0.0761 (10)	0.0345 (6)	0.0342 (8)	0.0048 (5)	0.0101 (6)
C8	0.0489 (7)	0.0546 (8)	0.0388 (6)	0.0134 (6)	0.0035 (5)	0.0098 (5)
C9	0.0439 (6)	0.0431 (6)	0.0383 (6)	0.0084 (5)	0.0048 (5)	-0.0027 (5)
C10	0.0421 (6)	0.0508 (7)	0.0438 (7)	-0.0042 (5)	0.0045 (5)	0.0046 (5)
C11	0.0522 (7)	0.0769 (10)	0.0481 (8)	-0.0025 (7)	-0.0041 (6)	0.0049 (7)
C12	0.0638 (8)	0.0591 (9)	0.0532 (8)	0.0003 (7)	0.0154 (6)	0.0170 (7)
C13	0.0535 (7)	0.0430 (7)	0.0518 (7)	-0.0061 (5)	0.0058 (6)	0.0038 (5)

Geometric parameters (\AA , $^\circ$)

O1—C1	1.2068 (18)	C7—C8	1.4858 (19)
O2—C8	1.2025 (19)	C10—C11	1.5074 (19)
O3—C11	1.420 (2)	C12—C13	1.504 (2)
O3—C12	1.4210 (18)	C3—H3A	0.9300
N1—C1	1.3987 (18)	C4—H4A	0.9300
N1—C8	1.4018 (17)	C5—H5A	0.9300
N1—C9	1.4748 (15)	C6—H6A	0.9300
N2—C9	1.4374 (15)	C9—H9A	0.978 (16)
N2—C10	1.4542 (15)	C9—H9B	0.983 (15)
N2—C13	1.4577 (15)	C10—H10A	0.9700
C1—C2	1.4867 (18)	C10—H10B	0.9700
C2—C3	1.390 (2)	C11—H11A	0.9700
C2—C7	1.377 (2)	C11—H11B	0.9700
C3—C4	1.386 (3)	C12—H12A	0.9700
C4—C5	1.385 (4)	C12—H12B	0.9700
C5—C6	1.393 (3)	C13—H13A	0.9700
C6—C7	1.387 (2)	C13—H13B	0.9700
O1...C13	3.2825 (18)	C4...H9B ⁱ	3.021 (15)
O1...C2 ⁱ	3.3263 (18)	C8...H10B	3.0500
O2...C1 ⁱⁱ	3.2358 (19)	C9...H12A ^{ix}	2.9900

O2...C10	3.3336 (16)	C12...H4A ^{vii}	2.9900
O2...C2 ⁱⁱ	3.3054 (19)	C13...H9A ^{iv}	3.035 (16)
O3...N2	2.8323 (14)	H3A...O1 ⁱⁱⁱ	2.7800
O1...H9B	2.599 (16)	H4A...O3 ^x	2.6000
O1...H13A	2.8900	H4A...C12 ^x	2.9900
O1...H3A ⁱⁱⁱ	2.7800	H5A...H10B ^{viii}	2.5000
O1...H9A ^{iv}	2.727 (16)	H6A...O2 ^v	2.7200
O2...H9A	2.553 (14)	H9A...O1 ⁱⁱ	2.727 (16)
O2...H6A ^v	2.7200	H9A...O2	2.553 (14)
O3...H11A ^{vi}	2.6400	H9A...C13 ⁱⁱ	3.035 (16)
O3...H4A ^{vii}	2.6000	H9A...H10A	2.4300
N2...O3	2.8323 (14)	H9A...H13A ⁱⁱ	2.4000
N1...H10B	2.7700	H9B...O1	2.599 (16)
N1...H13A	2.8400	H9B...H13B	2.3400
C1...O2 ^{iv}	3.2358 (19)	H9B...H12A ^{ix}	2.6000
C1...C13	3.4702 (19)	H9B...C3 ⁱ	2.941 (15)
C1...C2 ⁱ	3.559 (2)	H9B...C4 ⁱ	3.021 (15)
C2...O1 ⁱ	3.3263 (18)	H10A...H9A	2.4300
C2...O2 ^{iv}	3.3054 (19)	H10A...H13A ⁱⁱ	2.5800
C2...C1 ⁱ	3.559 (2)	H10B...N1	2.7700
C3...C6 ^{iv}	3.549 (3)	H10B...C8	3.0500
C5...C8 ^{viii}	3.563 (3)	H10B...H13A	2.4500
C5...C7 ^{viii}	3.582 (3)	H10B...H5A ^{viii}	2.5000
C6...C7 ^{viii}	3.462 (2)	H11A...O3 ^{xi}	2.6400
C6...C3 ⁱⁱ	3.549 (3)	H11B...H12A	2.3700
C6...C6 ^{viii}	3.395 (3)	H12A...H11B	2.3700
C7...C6 ^{viii}	3.462 (2)	H12A...C9 ^{xii}	2.9900
C7...C5 ^{viii}	3.582 (3)	H12A...H9B ^{xii}	2.6000
C8...C10	3.4591 (17)	H13A...O1	2.8900
C8...C5 ^{viii}	3.563 (3)	H13A...N1	2.8400
C10...C8	3.4591 (17)	H13A...C1	3.0100
C10...O2	3.3336 (16)	H13A...H9A ^{iv}	2.4000
C13...O1	3.2825 (18)	H13A...H10A ^{iv}	2.5800
C13...C1	3.4702 (19)	H13A...H10B	2.4500
C1...H13A	3.0100	H13B...H9B	2.3400
C3...H9B ⁱ	2.941 (15)		
C11—O3—C12	109.87 (11)	C5—C4—H4A	119.00
C1—N1—C8	111.95 (10)	C4—C5—H5A	119.00
C1—N1—C9	123.97 (10)	C6—C5—H5A	119.00
C8—N1—C9	122.68 (10)	C5—C6—H6A	122.00
C9—N2—C10	114.85 (9)	C7—C6—H6A	122.00
C9—N2—C13	113.83 (10)	N1—C9—H9A	106.1 (8)
C10—N2—C13	109.86 (10)	N1—C9—H9B	105.3 (9)

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O1—C1—N1	125.05 (12)	N2—C9—H9A	108.7 (8)
O1—C1—C2	129.35 (14)	N2—C9—H9B	109.0 (9)
N1—C1—C2	105.59 (12)	H9A—C9—H9B	110.6 (12)
C1—C2—C3	129.44 (15)	N2—C10—H10A	110.00
C1—C2—C7	108.36 (12)	N2—C10—H10B	110.00
C3—C2—C7	122.20 (14)	C11—C10—H10A	110.00
C2—C3—C4	116.1 (2)	C11—C10—H10B	110.00
C3—C4—C5	121.7 (2)	H10A—C10—H10B	108.00
C4—C5—C6	122.2 (2)	O3—C11—H11A	109.00
C5—C6—C7	115.8 (2)	O3—C11—H11B	109.00
C2—C7—C6	122.06 (14)	C10—C11—H11A	109.00
C2—C7—C8	108.65 (12)	C10—C11—H11B	109.00
C6—C7—C8	129.29 (15)	H11A—C11—H11B	108.00
O2—C8—N1	124.74 (12)	O3—C12—H12A	109.00
O2—C8—C7	129.87 (13)	O3—C12—H12B	109.00
N1—C8—C7	105.39 (12)	C13—C12—H12A	109.00
N1—C9—N2	116.95 (10)	C13—C12—H12B	109.00
N2—C10—C11	109.52 (11)	H12A—C12—H12B	108.00
O3—C11—C10	111.75 (12)	N2—C13—H13A	110.00
O3—C12—C13	111.09 (12)	N2—C13—H13B	110.00
N2—C13—C12	109.39 (11)	C12—C13—H13A	110.00
C2—C3—H3A	122.00	C12—C13—H13B	110.00
C4—C3—H3A	122.00	H13A—C13—H13B	108.00
C3—C4—H4A	119.00		
C12—O3—C11—C10	-58.12 (14)	N1—C1—C2—C3	178.32 (16)
C11—O3—C12—C13	58.81 (14)	N1—C1—C2—C7	-2.42 (16)
C8—N1—C1—C2	2.55 (15)	C1—C2—C7—C6	-178.17 (15)
C8—N1—C1—O1	-176.23 (14)	C3—C2—C7—C8	-179.25 (15)
C9—N1—C1—O1	-9.5 (2)	C7—C2—C3—C4	-0.4 (3)
C1—N1—C9—N2	95.41 (14)	C1—C2—C3—C4	178.78 (19)
C8—N1—C9—N2	-99.23 (13)	C1—C2—C7—C8	1.42 (17)
C1—N1—C8—C7	-1.72 (15)	C3—C2—C7—C6	1.2 (2)
C1—N1—C8—O2	178.10 (13)	C2—C3—C4—C5	-1.2 (4)
C9—N1—C8—O2	11.2 (2)	C3—C4—C5—C6	2.0 (4)
C9—N1—C8—C7	-168.67 (11)	C4—C5—C6—C7	-1.2 (4)
C9—N1—C1—C2	169.30 (11)	C5—C6—C7—C8	-179.85 (18)
C10—N2—C13—C12	57.89 (13)	C5—C6—C7—C2	-0.3 (3)
C9—N2—C13—C12	-171.72 (11)	C6—C7—C8—O2	-0.2 (3)
C10—N2—C9—N1	59.89 (14)	C2—C7—C8—O2	-179.71 (15)
C13—N2—C9—N1	-67.98 (13)	C6—C7—C8—N1	179.66 (16)
C9—N2—C10—C11	173.24 (11)	C2—C7—C8—N1	0.10 (16)
C13—N2—C10—C11	-56.92 (14)	N2—C10—C11—O3	57.48 (15)
O1—C1—C2—C7	176.30 (15)	O3—C12—C13—N2	-59.08 (15)
O1—C1—C2—C3	-3.0 (3)		

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $x, y+1, z$; (iii) $-x+1, -y-1, -z$; (iv) $x, y-1, z$; (v) $-x+2, -y+1, -z$; (vi) $-x+2, y-1/2, -z+1/2$; (vii) $x, -y-1/2, z+1/2$; (viii) $-x+2, -y, -z$; (ix) $-x+1, y+1/2, -z+1/2$; (x) $x, -y-1/2, z-1/2$; (xi) $-x+2, y+1/2, -z+1/2$; (xii) $-x+1, y-1/2, -z+1/2$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C4—H4A···O3 ^x	0.9300	2.6000	3.424 (2)	149.00
C9—H9A···O2	0.978 (16)	2.553 (14)	2.9025 (16)	100.9 (9)

Symmetry codes: (x) *x*, $-y-1/2$, $z-1/2$.

Fig. 1

