Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(Pyrrolidin-1-ylmethyl)isoindoline-1,3-dione

P. Sakthivel,[a] P. S. Joseph,[b]* A. Sebastiyan,[c] M. Yosuva Suvaikin[c] and M. Ramesh[c]

[a]Department of Physics, Urumu Dhanalakshmi College, Tiruchirappalli 620 019, India, [b]Department of Physics, Periyar E.V.R. College, Tiruchirappalli 620 023, India, and [c]Department of Chemistry, Urumu Dhanalakshmi College, Tiruchirappalli 620 019, India
Correspondence e-mail: sakthi2udc@yahoo.com

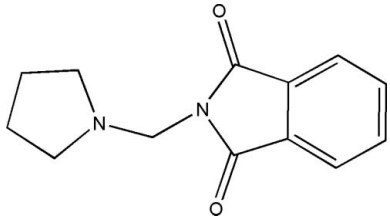
Received 7 October 2007; accepted 15 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.133; data-to-parameter ratio = 17.8.

In the title compound, $C_{13}H_{14}N_2O_2$, the pyrrolidine ring adopts an envelope conformation. The crystal structure is stabilized by C—H···O and C—H···N hydrogen bonds.

Related literature

For related literature, see: Abdul Ajees *et al.* (2002); Amal Raj *et al.* (2003); Bailleux *et al.* (1993); Couture *et al.* (1997, 1998); Cremer & Pople (1975); Kolocouris *et al.* (1994); Lima *et al.* (2002); Obniska & Zagorska (2003); Obniska *et al.* (2005); Orzeszka *et al.* (2000); Stylianakis *et al.* (2003); Suzuki *et al.* (1994).



Experimental

Crystal data

$C_{13}H_{14}N_2O_2$
M_r = 230.26
Orthorhombic, $P2_12_12_1$
a = 9.0609 (3) Å
b = 10.0777 (3) Å
c = 13.0192 (3) Å
V = 1188.82 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.30 × 0.22 × 0.20 mm

Data collection

Bruker Kappa-APEX2 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.974, T_{max} = 0.983
10764 measured reflections
2752 independent reflections
1943 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.134
S = 1.03
2752 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···O2^{i}	0.93	2.51	3.340 (2)	149
C5—H5A···N2^{ii}	0.93	2.54	3.405 (2)	155

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

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: *ORTEP-32* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

The authors thank Professor A. Sebastiyan for providing the sample for the X-ray study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2534).

References

Abdul Ajees, A., Manikandan, S. & Raghunathan, R. (2002). *Acta Cryst.* E**58**, o802–o804.
Amal Raj, A., Raghunathan, R., Sridevikumari, M. R. & Raman, N. (2003). *Bioorg. Med. Chem.* **11**, 407–419.
Bailleux, V., VallCe, L., Nuyts, J. P. & Vamecq, J. (1993). *Biomed. Pharmacother.* **47**, 4634–4637.
Bruker (2004). *APEX2* (Version 1.22), *SAINT-NT* (Version 6.0) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Couture, A., Deniau, E., Grandclaudon, P. & Hoarau, C. (1998). *J. Org. Chem.* **63**, 3128–132.
Couture, A., Deniau, E., Woisel, P. & GrandClauden, P. (1997). *Synthesis*, **63**, 1469–1445.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Kolocouris, N., Foscolos, G. B., Kolocouris, A., Marakos, P., Pouli, N., Fytas, G., Ikeda, S. & De Clercq, E. (1994). *J. Med. Chem.* **37**, 2896–2902.
Lima, L. M., Castro, P., Machado, A. L., Frage, C. A. M., Lugniur, C., Moraes, V. L. G. & Barreiro, E. J. (2002). *Bioorg. Med. Chem.* **10**, 3067–3073.
Obniska, J., Jurczyk, S., Zejc, A., Kaminski, K., Tatarczynska, E. & Stachowicz, K. (2005). *Pharmacol. Rep.* **57**, 170–175.
Obniska, J. & Zagorska, A. (2003). *Farmaco*, **58**, 1227–1234.
Orzeszka, A., Kaminsaka, B., Orzesko, G. & Stareerciak, J. (2000). *Farmaco*, **55**, 619–623.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stylianakis, I., Kolocouris, A., Kolocouris, N., Fytas, G., Foscolos, G. B., Padalko, E., Neyts, J. & De Clereq, E. (2003). *Bioorg. Med. Chem. Lett.* **13**, 1699–1703.
Suzuki, H. M., Soyagi, S. & Kibayahi, C. (1994). *Tetrahedron Lett.* **35**, 6119–6122.

  doi:10.1107/S1600536807050519

supplementary materials

Acta Cryst. (2007). E**63**, o4388 [**doi:10.1107/S1600536807050519**]

2-(Pyrrolidin-1-ylmethyl)isoindoline-1,3-dione

P. Sakthivel, P. S. Joseph, A. Sebastiyan, M. Y. Suvaikin and M. Ramesh

Comment

Substitituted pyrrolidine compounds have been found to have antimicrobial antifungal activity against various pathogens except Basillus substilis (Amal Raj *et al.*, 2003). Pyrrolidine derivatives possess anti-influenza virus (Stylianakis *et al.*, 2003), anticonvulsant (Obniska & Zagorska, 2003; Obniska *et al.*, 2005), and other antiviral (Kolocouris *et al.*, 1994) activities. 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) pharmacophores (Couture *et al.*, 1997). Several optically active pyrrolidine compounds have been used as intermediates in controlled asymmetric synthesis (Suzuki *et al.*, 1994). In view of its importance and to obtain more detailed information of the structure and conformation of the title compound, its crystal structure was determined.

All C—C and C—N bond lengths in the pyrrolidine ring are comparable with values in related pyrrolidine derivatives (Abdul Ajees *et al.*, 2002).

The sum of the angles at N2 of the pyrrolidine ring (340.69°) is in accordance with sp^3 hybridization. The pyrrolidine ring adopts an envelope conformation and puckering parameters q_2=0.3772 (2)Å and φ_2 = 359.7 (4)° (Cremer & Pople,1975). Atom N2 deviates by 0.248 (2)Å from the least squares plane through the remaining four C atoms (C10/C11/C12/C13) of the ring.

The pyrrolidine ring makes a dihedral angle of 78.72 (8)° with the isoindole-1–3-dione ring. The molecular structure is stabilized by C—H···O and C—H···N interactions (Table 2 and Fig 2.).

Experimental

The title compound is synthesized by the Manich condensation of phthalimide (14.71 g, 0.1 mol), 37% aqueous formaldehyde (7.5 ml, 0.1 mol) and pyrrolidone (8.2 ml, 0.1 mol) at 5°C. It was recrystalized from ethanol. The sample melts at 106–107°C.

Refinement

All the hydrogen atoms were geometrically fixed and allowed to ride on their parent atoms with C—H=0.93 − 0.96 Å, and U_{iso}=1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for H atoms. The absolute structure was determined using 1957 Friedal pairs.

Figures

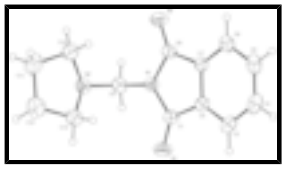


Fig. 1. : The structure of the title compound showing the atom numbering scheme with 50% probability dispalcement ellipsoids.

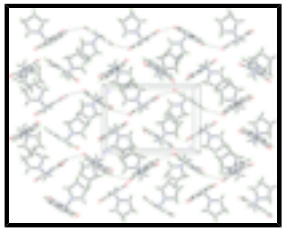


Fig. 2. : View of intermolecular C—H.·O and C—H.·N interactions in the title compound.

2-(Pyrrolidin-1-ylmethyl)isoindoline-1,3-dione

Crystal data

$C_{13}H_{14}N_2O_2$	Least Squares Treatment of 25 SET4 setting angles.
$M_r = 230.26$	$D_x = 1.287$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 3270 reflections
$a = 9.0609$ (3) Å	$\theta = 2.3$–26.9º
$b = 10.0777$ (3) Å	$\mu = 0.09$ mm^{-1}
$c = 13.0192$ (3) Å	$T = 293$ (2) K
$V = 1188.82$ (6) Å^3	Prism, colorless
$Z = 4$	0.30 × 0.22 × 0.20 mm
$F_{000} = 488$	

Data collection

Bruker Kappa-APEX2 diffractometer	2752 independent reflections
Radiation source: fine focus sealed tube	1943 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 293$(2) K	$\theta_{max} = 34.2$º
ω and φ scans	$\theta_{min} = 2.6$º
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -12\rightarrow14$
$T_{min} = 0.974$, $T_{max} = 0.983$	$k = -13\rightarrow15$
10764 measured reflections	$l = -20\rightarrow20$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.134$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
2752 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
155 parameters	Extinction coefficient: 0.017 (4)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1957 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter:
Hydrogen site location: inferred from neighbouring sites	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.18398 (17)	0.21647 (14)	−0.06749 (9)	0.0629 (4)
O2	0.43688 (14)	0.14885 (13)	0.23098 (8)	0.0539 (4)
N1	0.30783 (15)	0.21825 (12)	0.08729 (9)	0.0410 (3)
N2	0.22703 (15)	0.43629 (14)	0.15153 (11)	0.0458 (4)
C1	0.23597 (17)	0.15773 (17)	0.00464 (10)	0.0427 (4)
C2	0.24128 (18)	0.01370 (17)	0.02426 (10)	0.0420 (4)
C3	0.1829 (2)	−0.0904 (2)	−0.03067 (13)	0.0574 (6)
C4	0.2072 (3)	−0.2164 (2)	0.00767 (17)	0.0692 (7)
C5	0.2855 (3)	−0.2374 (2)	0.09740 (18)	0.0687 (7)
C6	0.3435 (2)	−0.13266 (18)	0.15237 (15)	0.0536 (5)
C7	0.32003 (17)	−0.00686 (15)	0.11436 (10)	0.0403 (4)
C8	0.36506 (15)	0.12407 (15)	0.15516 (11)	0.0396 (4)
C9	0.33321 (18)	0.36197 (15)	0.09495 (12)	0.0444 (4)
C10	0.2215 (2)	0.4163 (2)	0.26207 (13)	0.0620 (6)
C11	0.0869 (3)	0.4946 (4)	0.29372 (18)	0.0900 (10)
C12	−0.0082 (3)	0.5043 (4)	0.19898 (18)	0.0905 (10)
C13	0.0746 (2)	0.4311 (2)	0.11634 (15)	0.0612 (6)
H3A	0.12962	−0.07660	−0.09079	0.0689*
H4A	0.16982	−0.28910	−0.02784	0.0830*
H5A	0.29935	−0.32358	0.12106	0.0824*
H6A	0.39631	−0.14643	0.21269	0.0642*

H9A	0.42910	0.37592	0.12627	0.0533*
H9B	0.33773	0.39790	0.02590	0.0533*
H10A	0.30976	0.45017	0.29506	0.0744*
H10B	0.21039	0.32302	0.27884	0.0744*
H11A	0.03441	0.44943	0.34846	0.1079*
H11B	0.11495	0.58223	0.31751	0.1079*
H12A	−0.10374	0.46376	0.21084	0.1084*
H12B	−0.02286	0.59635	0.17971	0.1084*
H13A	0.04060	0.34015	0.11058	0.0734*
H13B	0.06364	0.47467	0.05035	0.0734*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0758 (9)	0.0638 (8)	0.0492 (6)	0.0015 (8)	−0.0174 (6)	0.0122 (5)
O2	0.0591 (7)	0.0564 (7)	0.0462 (5)	−0.0071 (6)	−0.0155 (5)	0.0043 (5)
N1	0.0463 (7)	0.0364 (6)	0.0402 (5)	−0.0019 (5)	−0.0041 (5)	0.0042 (4)
N2	0.0445 (6)	0.0416 (7)	0.0514 (6)	−0.0014 (6)	−0.0012 (6)	0.0003 (5)
C1	0.0437 (7)	0.0471 (8)	0.0373 (6)	−0.0010 (6)	−0.0024 (6)	0.0030 (5)
C2	0.0434 (7)	0.0445 (8)	0.0382 (6)	−0.0015 (6)	0.0016 (5)	−0.0022 (5)
C3	0.0637 (11)	0.0584 (10)	0.0502 (8)	−0.0085 (9)	−0.0011 (8)	−0.0144 (7)
C4	0.0835 (14)	0.0493 (11)	0.0747 (12)	−0.0092 (11)	0.0059 (11)	−0.0199 (9)
C5	0.0834 (14)	0.0378 (9)	0.0848 (13)	0.0019 (10)	0.0067 (12)	0.0005 (9)
C6	0.0600 (10)	0.0418 (8)	0.0589 (9)	0.0041 (8)	−0.0001 (8)	0.0068 (7)
C7	0.0419 (7)	0.0384 (7)	0.0407 (6)	−0.0001 (6)	0.0010 (5)	0.0027 (5)
C8	0.0380 (6)	0.0424 (7)	0.0383 (6)	−0.0014 (6)	−0.0005 (5)	0.0054 (5)
C9	0.0432 (7)	0.0384 (7)	0.0516 (7)	−0.0055 (6)	0.0033 (6)	0.0075 (6)
C10	0.0626 (11)	0.0704 (12)	0.0531 (9)	0.0027 (10)	−0.0013 (8)	−0.0048 (8)
C11	0.0835 (16)	0.115 (2)	0.0715 (13)	0.0182 (17)	0.0118 (12)	−0.0226 (14)
C12	0.0615 (13)	0.120 (2)	0.0900 (16)	0.0255 (16)	0.0038 (12)	−0.0157 (17)
C13	0.0477 (9)	0.0724 (12)	0.0634 (10)	0.0053 (9)	−0.0076 (8)	−0.0028 (9)

Geometric parameters (Å, °)

O1—C1	1.2059 (19)	C11—C12	1.508 (4)
O2—C8	1.2084 (18)	C12—C13	1.505 (4)
N1—C1	1.3978 (19)	C3—H3A	0.9300
N1—C8	1.3966 (19)	C4—H4A	0.9300
N1—C9	1.4699 (19)	C5—H5A	0.9300
N2—C9	1.425 (2)	C6—H6A	0.9300
N2—C10	1.454 (2)	C9—H9A	0.9700
N2—C13	1.456 (2)	C9—H9B	0.9700
C1—C2	1.475 (2)	C10—H10A	0.9700
C2—C3	1.375 (2)	C10—H10B	0.9700
C2—C7	1.389 (2)	C11—H11A	0.9700
C3—C4	1.382 (3)	C11—H11B	0.9700
C4—C5	1.383 (3)	C12—H12A	0.9700
C5—C6	1.379 (3)	C12—H12B	0.9700
C6—C7	1.377 (2)	C13—H13A	0.9700

C7—C8	1.480 (2)	C13—H13B	0.9700
C10—C11	1.510 (4)		
O1···C13	3.375 (2)	C13···C2^{i}	3.575 (2)
O1···C9^{i}	3.295 (2)	C13···C1	3.441 (3)
O2···C10	3.352 (2)	C1···H13A	2.9000
O2···C6^{ii}	3.334 (2)	C2···H11A^{ix}	3.0700
O2···C3^{iii}	3.340 (2)	C2···H13B^{v}	3.0800
O1···H9A^{i}	2.6100	C6···H12A^{ix}	2.9700
O1···H9B	2.6000	C7···H13B^{v}	3.0900
O2···H9A	2.6600	C7···H12A^{ix}	3.0200
O2···H3A^{iii}	2.5100	C8···H10B	2.9300
O2···H10B	2.7700	H3A···O2^{vi}	2.5100
O2···H6A^{ii}	2.6600	H5A···N2^{vii}	2.5400
N2···C5^{iv}	3.405 (2)	H6A···O2^{viii}	2.6600
N1···H10B	2.8500	H9A···O2	2.6600
N1···H13A	2.7300	H9A···H10A	2.5600
N2···H5A^{iv}	2.5400	H9A···O1^{v}	2.6100
C1···C13	3.441 (3)	H9B···O1	2.6000
C1···C13^{v}	3.563 (2)	H10A···H9A	2.5600
C2···C13^{v}	3.575 (2)	H10B···O2	2.7700
C3···O2^{vi}	3.340 (2)	H10B···N1	2.8500
C5···N2^{vii}	3.405 (2)	H10B···C8	2.9300
C6···O2^{viii}	3.334 (2)	H11A···C2^{x}	3.0700
C8···C10	3.508 (2)	H12A···C6^{x}	2.9700
C9···O1^{v}	3.295 (2)	H12A···C7^{x}	3.0200
C10···O2	3.352 (2)	H13A···N1	2.7300
C10···C8	3.508 (2)	H13A···C1	2.9000
C13···C1^{i}	3.563 (2)	H13B···C2^{i}	3.0800
C13···O1	3.375 (2)	H13B···C7^{i}	3.0900
C1—N1—C8	111.31 (12)	C5—C4—H4A	119.00
C1—N1—C9	123.71 (12)	C4—C5—H5A	119.00
C8—N1—C9	124.65 (12)	C6—C5—H5A	119.00
C9—N2—C10	117.53 (14)	C5—C6—H6A	121.00
C9—N2—C13	117.33 (14)	C7—C6—H6A	121.00
C10—N2—C13	105.89 (14)	N1—C9—H9A	108.00
O1—C1—N1	124.56 (16)	N1—C9—H9B	108.00
O1—C1—C2	129.11 (15)	N2—C9—H9A	108.00
N1—C1—C2	106.32 (12)	N2—C9—H9B	108.00
C1—C2—C3	130.40 (14)	H9A—C9—H9B	107.00
C1—C2—C7	108.06 (13)	N2—C10—H10A	111.00
C3—C2—C7	121.54 (16)	N2—C10—H10B	111.00
C2—C3—C4	116.85 (17)	C11—C10—H10A	111.00
C3—C4—C5	121.83 (19)	C11—C10—H10B	111.00
C4—C5—C6	121.11 (19)	H10A—C10—H10B	109.00

C5—C6—C7	117.33 (18)	C10—C11—H11A	111.00
C2—C7—C6	121.34 (15)	C10—C11—H11B	111.00
C2—C7—C8	108.17 (13)	C12—C11—H11A	111.00
C6—C7—C8	130.48 (14)	C12—C11—H11B	111.00
O2—C8—N1	125.19 (14)	H11A—C11—H11B	109.00
O2—C8—C7	128.76 (14)	C11—C12—H12A	111.00
N1—C8—C7	106.05 (12)	C11—C12—H12B	111.00
N1—C9—N2	116.58 (13)	C13—C12—H12A	111.00
N2—C10—C11	103.03 (16)	C13—C12—H12B	111.00
C10—C11—C12	105.8 (2)	H12A—C12—H12B	109.00
C11—C12—C13	105.6 (2)	N2—C13—H13A	111.00
N2—C13—C12	103.32 (17)	N2—C13—H13B	111.00
C2—C3—H3A	122.00	C12—C13—H13A	111.00
C4—C3—H3A	122.00	C12—C13—H13B	111.00
C3—C4—H4A	119.00	H13A—C13—H13B	109.00
C8—N1—C1—O1	−175.81 (15)	N1—C1—C2—C3	177.47 (17)
C9—N1—C1—O1	−2.0 (2)	C3—C2—C7—C6	0.3 (2)
C8—N1—C1—C2	3.08 (16)	C1—C2—C7—C6	−179.93 (14)
C9—N1—C1—C2	176.87 (13)	C1—C2—C7—C8	0.79 (17)
C9—N1—C8—C7	−176.32 (13)	C1—C2—C3—C4	179.79 (18)
C1—N1—C9—N2	94.98 (17)	C7—C2—C3—C4	−0.4 (3)
C8—N1—C9—N2	−92.06 (18)	C3—C2—C7—C8	−179.03 (15)
C1—N1—C8—C7	−2.60 (16)	C2—C3—C4—C5	0.5 (3)
C1—N1—C8—O2	177.17 (14)	C3—C4—C5—C6	−0.3 (4)
C9—N1—C8—O2	3.5 (2)	C4—C5—C6—C7	0.1 (3)
C10—N2—C9—N1	69.20 (19)	C5—C6—C7—C2	−0.1 (3)
C13—N2—C10—C11	−39.5 (2)	C5—C6—C7—C8	179.03 (18)
C9—N2—C13—C12	173.19 (19)	C2—C7—C8—N1	1.04 (16)
C10—N2—C13—C12	39.7 (2)	C2—C7—C8—O2	−178.72 (15)
C13—N2—C9—N1	−58.89 (19)	C6—C7—C8—O2	2.1 (3)
C9—N2—C10—C11	−172.84 (18)	C6—C7—C8—N1	−178.15 (16)
O1—C1—C2—C3	−3.7 (3)	N2—C10—C11—C12	23.4 (3)
N1—C1—C2—C7	−2.33 (17)	C10—C11—C12—C13	0.2 (3)
O1—C1—C2—C7	176.49 (17)	C11—C12—C13—N2	−23.6 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3A···O2^{vi}	0.9300	2.5100	3.340 (2)	149.00
C5—H5A···N2^{vii}	0.9300	2.5400	3.405 (2)	155.00

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

Fig. 1

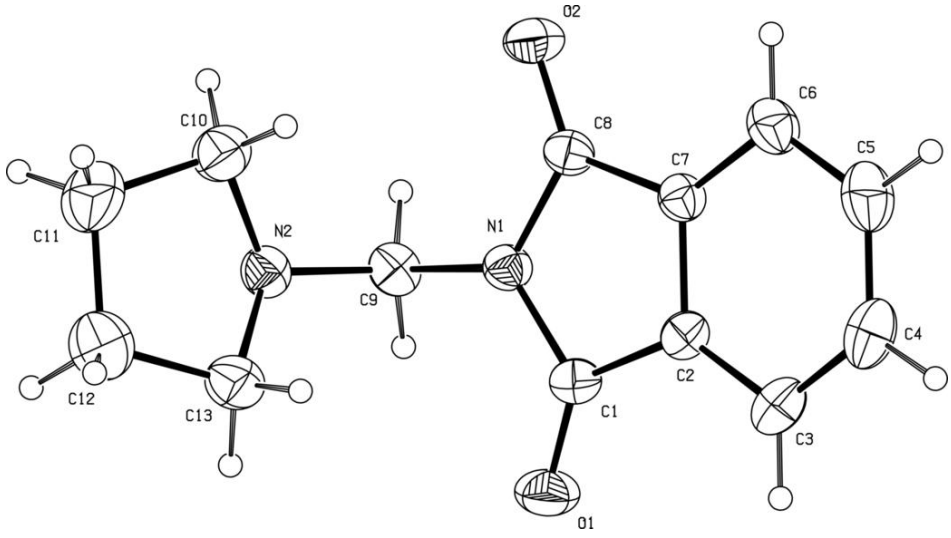


Fig. 2