electronic reprint

Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

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S. Thamotharan,[a] V. Parthasarathi,[a]* P. Gupta,[b] D. P. Jindal,[b]† P. Piplani[b] and Anthony Linden[c]

[a]Department of Physics, Bharathidasan University, Tiruchirappalli 620 024, India, [b]University Institute of Pharmaceutical Sciences, Panjab University, Chandigarh 160 014, India, and [c]Institute of Organic Chemistry, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

† Deceased

Correspondence e-mail: vpsarati@yahoo.com

Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.128
Data-to-parameter ratio = 13.6

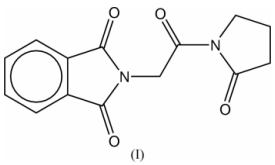
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 June 2003
Accepted 18 June 2003
Online 30 June 2003

The title compound, $C_{14}H_{12}N_2O_4$, is a potential antiamnesic agent. The pyrrolidinone ring has an envelope conformation. The dihedral angle between the *N*-substituted phthalimide moiety and the pyrrolidinone ring is 77.16 (5)°. In the solid state, symmetry-related molecules are linked by weak intermolecular C—H···O interactions, forming a continuous chain.

Comment

The conformations of molecules with antiamnesic activity have attracted considerable interest (Amato *et al.*, 1991), and the structure determination of the title compound, (I), was carried out to continue the investigation of a new class of antiamnesic agents (Thamotharan, Parthasarathi, Malik *et al.*, 2003; Thamotharan, Parthasarathi, Gupta *et al.*, 2003).



(I)

Fig. 1 shows the molecular structure of (I) with the atom-numbering scheme. The geometric parameters of the *N*-substituted phthalimide moiety in (I) are almost the same as those in 2-(5-chloropyridin-2-yl)-2,3-dihydro-1*H*-isoindole-1,3-dione (Holband *et al.*, 2001). The angles C5—C4—C9 [117.2 (2)°] and C6—C7—C8 [117.4 (2)°] are significantly smaller than the other angles in the benzene ring. Similar observations have been made in related structures (Christensen & Thom, 1971, and references therein). This angular distortion can be explained by the strain caused by fusion with the five-membered ring.

In (I), the five-membered pyrrolidinone ring exhibits an envelope conformation, with atom C15 as the flap, a pseudo-rotation angle Δ = 270.3 (2)° and a maximum torsion angle φ_m = 30.7 (1)° for the atom sequence N12—C13—C14—C15—C16 (Rao *et al.*, 1981). The dihedral angle between the *N*-substituted phthalimide moiety and the pyrrolidinone ring is 77.16 (5)°. The planar central moiety, N2—C10—C11—N12, is oriented at angles of 7.62 (11) and 84.67 (10)° with respect to the pyrrolidinone and *N*-substituted phthalimide moieties, respectively.

In the crystal structure, atom C15 acts as a donor for a weak intermolecular C—H···O interaction with carbonyl atom O1 of an adjacent molecule. This interaction links the molecules into a chain, which runs parallel to the *b* axis and has a graph-set motif of *C*(9) (Bernstein *et al.*, 1995). Atom C16 has a weak intermolecular C—H···O interaction with carbonyl atom O13

of a different adjacent molecule. This interaction also links the molecules into a chain, which runs parallel to the *b* axis and has a graph-set motif of *C*(5) (Table 1) (Bernstein *et al.*, 1995). A short intermolecular contact is observed, O3···C1^{i} 2.883 (3) Å [symmetry code: (i) $\frac{1}{2}-x, y+\frac{1}{2}, z$].

Experimental

A solution of (1,3-dioxo-1,3-dihydroisoindole-2-yl)acetyl chloride (1.0 g) in dichloromethane was stirred with pyrrolidinone. The dichloromethane was removed and crushed ice was added to the contents. The solid material obtained was filtered off and crystallized from methanol to afford crystals of (I) (yield 0.81 g, 66.5%; m.p. 473 K).

Crystal data

$C_{14}H_{12}N_2O_4$
$M_r = 272.26$
Orthorhombic, *Pbca*
$a = 10.7480\ (2)$ Å
$b = 8.3280\ (1)$ Å
$c = 27.9084\ (4)$ Å
$V = 2498.06\ (7)$ Å^3
$Z = 8$
$D_x = 1.448$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2839 reflections
$\theta = 2.0$–$26.0°$
$\mu = 0.11$ mm^{-1}
$T = 160\ (2)$ K
Plate, colourless
0.18 × 0.18 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
ω scans with κ offsets
Absorption correction: none
29914 measured reflections
2459 independent reflections
1620 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 26.0°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 10$
$l = -34 \rightarrow 0$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.129$
$S = 1.03$
2459 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0681P)^2 + 0.4733P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H152···O1^{i}	0.99	2.44	3.426 (3)	175
C16—H162···O13^{ii}	0.99	2.56	3.261 (3)	128

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

All H atoms were placed in geometrically idealized positions (C—H = 0.95–0.99 Å) and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

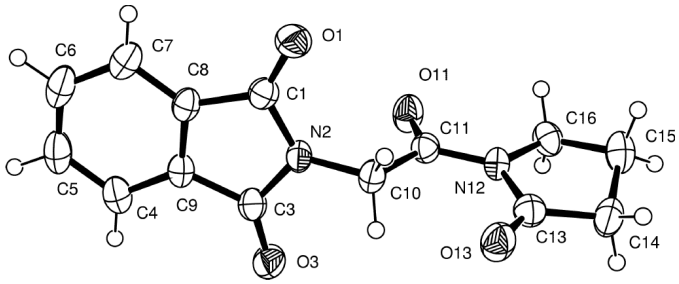


Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Version 1.07; Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

ST thanks the X-ray Crystallography Facility, Institute of Organic Chemistry, University of Zurich, Switzerland, for providing access to the facility during his visit in August 2002.

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