organic papers

2-[(2-Oxopyrrolidin-1-yl)carbonylmethyl]-2,3-dihydro-1H-isoindole-1,3-dione: an antiamnesic agent

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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 anti-amnesic agents (Thamotharan, Parthasarathi, Malik *et al.*, 2003; Thamotharan, Parthasarathi, Gupta *et al.*, 2003).
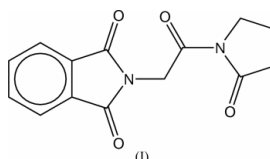

(I)

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-1H-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 $\Delta = 270.3$ (2)° and a maximum torsion angle $\varphi_m = 30.7$ (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$\cdots$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

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

Data collection

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

Refinement

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C15—H152$\cdots$O1^i	0.99	2.44	3.426 (3)	175
C16—H162$\cdots$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 $U_{iso}(H) = 1.2U_{eq}(C)$.
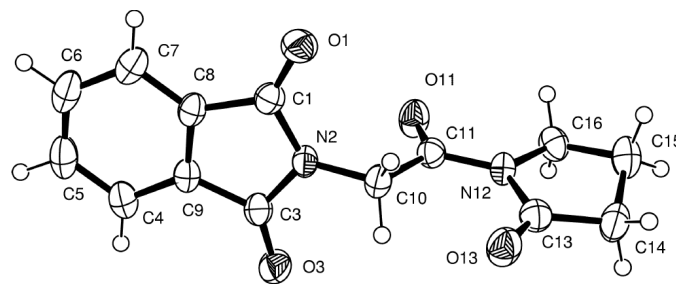

Figure 1
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

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).

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