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Structure of 3-(3,5-Dimethylpiperidino)-*N*-(*p*-chlorophenyl)succinimide

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Abstract

In the title molecule, 3-(3,5-dimethylpiperidino)-1-(4-chlorophenyl)-2,5-pyrrolidinedione (1), the *N*-(*p*-chlorophenyl) substituent is rotated by 68.8° relative to the succinimide plane. The piperidyl ring has a chair conformation with all substituents in equatorial positions; the conformation around the piperidino–succinimide C–N bond is staggered.

Comment

The title compound was prepared in the framework of our structural and conformational studies (Joseph-Nathan, Mendoza & Garcia G., 1972, 1974; Soriano-García, Toscano, Mendoza, García G., Guzmán, Alemán & Huipe N., 1990; Mendoza, Garcia G., Guzmán, Gutierrez & Chavez, 1991) of some 3-(1-cycloalkylamine)succinimides derived by condensation reactions from maleimides or isomaleimides and cycloalkylamines.

The chemical structure of (1) as well as its molecular stereochemistry are unequivocally established by the present X-ray investigation. The central succinimide moiety is planar within 0.004 Å. Its N atom [N(2)] has a planar-trigonal bond configuration with the *N*-(*p*-chlorophenyl) substituent, rotated by 68.8°

around the C(10)—N(2) bond, out of the succinimide plane. The dimethylpiperidine substituent has a chair conformation with both methyl groups and the succinimide moiety in equatorial positions. The conformation around the N(1)—C(8) bond is staggered; all relevant torsion angles are close to 60 and 180°. The piperidine N(1) atom has a trigonal-pyramidal bond configuration; its displacement from the plane of three neighbouring atoms is 0.422 (4) Å.

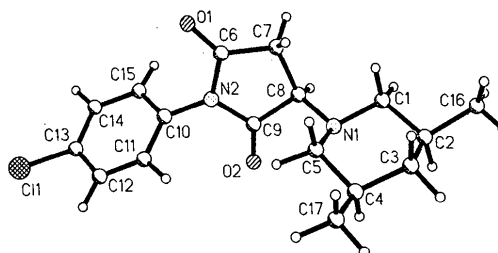


Fig. 1. General view of the title molecule (1).

Experimental

Crystal data

$C_{17}H_{21}ClN_2O_2$

$M_r = 320.8$

Monoclinic

$P2_1/c$

$a = 8.804 (3) \text{ \AA}$

$b = 6.472 (2) \text{ \AA}$

$c = 29.075 (12) \text{ \AA}$

$\beta = 94.75 (2)^\circ$

$V = 1651.0 (3) \text{ \AA}^3$

$Z = 4$

$D_x = 1.291 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

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

Data collection

Siemens P3/PC diffractometer

$\theta/2\theta$ scans

Absorption correction:

none

6095 measured reflections

5773 independent reflections

1176 observed reflections

$[F > 6.0\sigma(F)]$

Refinement

Refinement on F

Final $R = 0.052$

$wR = 0.064$

$S = 2.16$

1176 reflections

262 parameters

H atoms refined isotropically

with fixed $U_{iso} = 0.05 \text{ \AA}^2$

$w = 1/\sigma^2(F)$

Cell parameters from 24 reflections

$\theta = 12-13^\circ$

$\mu = 0.240 \text{ mm}^{-1}$

$T = 153 \text{ K}$

Needles

$0.4 \times 0.2 \times 0.1 \text{ mm}$

Colourless

Crystal source: from hexane-ethyl acetate solution (2/3)

$R_{int} = 0.049$

$\theta_{max} = 30^\circ$

$h = 0 \rightarrow 13$

$k = 0 \rightarrow 9$

$l = -42 \rightarrow 43$

2 standard reflections

monitored every 98

reflections

intensity variation: $\pm 1.8\%$

$(\Delta/\sigma)_{max} = 0.333$

$\Delta\rho_{max} = 0.40 \text{ e \AA}^{-3}$

$\Delta\rho_{min} = -0.29 \text{ e \AA}^{-3}$

Atomic scattering factors

from *International Tables*

for *X-ray Crystallography*

(1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2)
$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	y	z	U_{eq}
Cl(1)	0.2122 (3)	0.2497 (4)	0.0577 (1)	0.043 (1)
O(1)	0.3922 (6)	-0.4067 (9)	0.2281 (2)	0.031 (2)
O(2)	0.0428 (6)	0.0606 (10)	0.2712 (2)	0.037 (2)
N(1)	0.1881 (7)	-0.1111 (10)	0.3580 (2)	0.024 (2)
N(2)	0.2200 (6)	-0.1508 (10)	0.2406 (2)	0.021 (2)
C(1)	0.1974 (9)	-0.2382 (15)	0.3999 (3)	0.025 (2)
C(2)	0.2038 (10)	-0.1125 (14)	0.4431 (3)	0.033 (3)
C(3)	0.3433 (10)	0.0288 (14)	0.4441 (3)	0.033 (3)
C(4)	0.3469 (9)	0.1567 (14)	0.4001 (3)	0.031 (3)
C(5)	0.3275 (9)	0.0162 (14)	0.3577 (3)	0.026 (3)
C(6)	0.3071 (8)	-0.3249 (12)	0.2535 (3)	0.024 (3)
C(7)	0.2746 (10)	-0.3854 (13)	0.3010 (3)	0.029 (3)
C(8)	0.1555 (9)	-0.2278 (15)	0.3166 (3)	0.027 (3)
C(9)	0.1281 (8)	-0.0859 (14)	0.2747 (3)	0.027 (3)
C(10)	0.2162 (9)	-0.0529 (13)	0.1967 (3)	0.024 (3)
C(11)	0.2756 (9)	0.1433 (12)	0.1920 (3)	0.025 (3)
C(12)	0.2724 (8)	0.2387 (15)	0.1511 (3)	0.027 (3)
C(13)	0.2113 (9)	0.1334 (14)	0.1123 (3)	0.031 (3)
C(14)	0.1502 (9)	-0.0647 (13)	0.1148 (3)	0.025 (3)
C(15)	0.1520 (8)	-0.1590 (14)	0.1576 (3)	0.026 (3)
C(16)	0.2134 (12)	-0.2593 (20)	0.4854 (3)	0.046 (3)
C(17)	0.4914 (9)	0.2846 (15)	0.3999 (3)	0.034 (3)

Table 2. Geometric parameters (\AA , $^\circ$)

Cl(1)—C(13)	1.758 (9)	C(3)—C(4)	1.53 (1)
O(1)—C(6)	1.22 (1)	C(4)—C(5)	1.53 (1)
O(2)—C(9)	1.21 (1)	C(4)—C(17)	1.52 (1)
N(1)—C(1)	1.47 (1)	C(6)—C(7)	1.49 (1)
N(1)—C(5)	1.48 (1)	C(7)—C(8)	1.56 (1)
N(1)—C(8)	1.43 (1)	C(8)—C(9)	1.53 (1)
N(2)—C(6)	1.40 (1)	C(10)—C(15)	1.41 (1)
N(2)—C(9)	1.40 (1)	C(11)—C(12)	1.34 (1)
N(2)—C(10)	1.42 (1)	C(12)—C(13)	1.39 (1)
C(1)—C(2)	1.50 (1)	C(13)—C(14)	1.39 (1)
C(2)—C(3)	1.53 (1)	C(14)—C(15)	1.38 (1)
C(2)—C(16)	1.55 (1)		
C(1)—N(1)—C(5)	109.1 (6)	C(6)—C(7)—C(8)	106.5 (7)
C(1)—N(1)—C(8)	113.3 (7)	N(1)—C(8)—C(7)	119.9 (6)
C(5)—N(1)—C(8)	113.5 (6)	N(1)—C(8)—C(9)	111.1 (7)
C(6)—N(2)—C(9)	112.9 (6)	C(7)—C(8)—C(9)	103.2 (6)
C(6)—N(2)—C(10)	124.9 (7)	O(2)—C(9)—N(2)	124.6 (7)
C(9)—N(2)—C(10)	122.1 (6)	O(2)—C(9)—C(8)	126.6 (7)
N(1)—C(1)—C(2)	112.9 (7)	N(2)—C(9)—C(8)	108.8 (7)
C(1)—C(2)—C(3)	108.4 (7)	N(2)—C(10)—C(11)	121.0 (7)
C(1)—C(2)—C(16)	109.3 (8)	N(2)—C(10)—C(15)	119.1 (7)
C(3)—C(2)—C(16)	111.1 (7)	C(11)—C(10)—C(15)	119.9 (7)
C(2)—C(3)—C(4)	112.3 (7)	C(10)—C(11)—C(12)	121.9 (8)
C(3)—C(4)—C(5)	110.1 (7)	C(11)—C(12)—C(13)	118.3 (9)
C(3)—C(4)—C(17)	112.0 (7)	Cl(1)—C(13)—C(12)	119.6 (7)
C(5)—C(4)—C(17)	111.0 (7)	Cl(1)—C(13)—C(14)	118.2 (6)
N(1)—C(5)—C(4)	111.4 (7)	C(12)—C(13)—C(14)	122.2 (8)
O(1)—C(6)—N(2)	122.8 (7)	C(13)—C(14)—C(15)	118.5 (8)
O(1)—C(6)—C(7)	128.7 (7)	C(10)—C(15)—C(14)	119.0 (8)
N(2)—C(6)—C(7)	108.5 (7)		

All calculations were performed with *SHELXTL-PC* (Sheldrick, 1990) programs on an IBM PC/AT computer

Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71116 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: VS1003]