

Table 2. Bond lengths (Å) and angles (°) with standard deviations in parentheses

Mo—Mo	3.051 (1)	Mo—C(7)	2.25 (1)
Mo—Cl(1)	2.38 (2)	C—C	1.403 (fixed)
Mo—Cl(2)	2.50 (1)	B—F(1)	1.57 (5)
Mo—Cl(2)'	2.47 (1)	B—F(2)	1.29 (4)
Mo—Cl(3)	2.49 (2)	B—F(3)	1.47 (4)
Mo—Cl(3)'	2.55 (2)	B—F(4)	1.40 (4)
Mo—Cl(4)	2.42 (2)	B—F(5)	1.42 (4)
Mo—C(1)	2.26 (2)		
Mo—C(2)	2.25 (2)	Mo—Cl(1)—Mo'	79.7 (8)
Mo—C(3)	2.28 (2)	Mo—Cl(2)—Mo'	75.7 (4)
Mo—C(4)	2.28 (2)	Mo—Cl(3)—Mo'	74.4 (5)
Mo—C(5)	2.26 (2)	Mo—Cl(4)—Mo'	78.1 (8)
Mo—C(6)	2.28 (1)	C—C—C	128.57 (fixed)

Br(OH)₂ bridged species indicates that the Mo—Mo distance is mainly controlled by the nature of the bridging atoms.

The average Mo—C distance (2.265 Å) is similar to that in the Br(OH)₂-bridged ion (2.25 Å). It is clear from the thermal parameters and Fig. 1 that the ring has high thermal motion, both circumferentially and by pivoting about the Mo atom.

The packing (Fig. 2) shows no unusual interactions and appears to be dominated by contact between the spherical BF₄⁻ ions and the elongated cations.

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5-Chloro-1-{3-[4-(4-fluorobenzoyl)piperidino]propyl}-1,3-dihydro-2H-benzimidazol-2-one

BY M. H. J. KOCH

Research Laboratories, Janssen Pharmaceutica, B-2340 Beerse, Belgium

AND J. P. DECLERCQ,* G. GERMAIN AND M. VAN MEERSSCHE

Laboratoire de Chimie Physique et de Cristallographie, Université de Louvain, 1 place L. Pasteur, B-1348 Louvain-la-Neuve, Belgium

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Abstract. C₂₂H₂₃ClFN₃O₂, *M_r* = 415.88; triclinic, *P* $\bar{1}$; *a* = 8.084 (2), *b* = 12.621 (3), *c* = 10.259 (2) Å, α = 87.10 (2), β = 87.87 (2), γ = 86.56 (2)°; 25 °C; *Z* = 2. The molecules are linked by hydrogen bonds between the amide groups of the benzimidazolone moiety: N(5)···O(7), 2.82 Å [O(7): 2 - *x*, 1 - *y*, -*z*].

Introduction. The title compound is a new potent neuroleptic drug. Transparent colourless crystals were obtained by cooling a saturated solution in hot isopropanol. The experimental conditions used for data

collection are given in Table 1. The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). Anisotropic block-diagonal least-squares refinement (Ahmed, Hall, Pippy & Huber, 1966) gave a final $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ of 0.09 for all observed

Table 1. Experimental conditions

Instrument: Syntex P2₁ diffractometer
 Source: Cu *K*α; λ = 1.5418 Å; ω scan; θ_{max} = 55 °
 Confidence level: 2.5
 Total number of independent reflexions: 2631
 Total observed: 2267

* Chargé de Recherches du Fonds National de la Recherche Scientifique.

Table 2. Final positional parameters ($\times 10^4$) (with standard deviations in parentheses)

	x	y	z
Cl(1)	6615 (1)	5503 (1)	6213 (1)
C(2)	7987 (3)	5931 (2)	4985 (3)
C(3)	8151 (3)	5389 (2)	3844 (2)
C(4)	9306 (3)	5752 (2)	2911 (2)
N(5)	9761 (2)	5393 (1)	1669 (2)
C(6)	10955 (3)	6036 (2)	1126 (2)
O(7)	11596 (2)	5973 (1)	12 (2)
N(8)	11232 (2)	6773 (1)	2006 (2)
C(9)	10244 (3)	6609 (2)	3125 (2)
C(10)	10077 (3)	7139 (2)	4268 (2)
C(11)	8928 (3)	6796 (2)	5224 (3)
C(12)	12502 (3)	7566 (2)	1815 (2)
C(13)	14093 (3)	7172 (2)	2502 (3)
C(14)	15404 (3)	7994 (2)	2435 (3)
N(15)	15918 (2)	8349 (2)	1100 (2)
C(16)	16972 (3)	9227 (2)	1182 (3)
C(17)	17543 (3)	9649 (2)	-150 (3)
C(18)	18514 (3)	8752 (2)	-882 (2)
C(19)	17381 (4)	7851 (2)	-976 (3)
C(20)	16779 (4)	7469 (2)	417 (3)
C(21)	19118 (3)	9156 (2)	-2211 (2)
O(22)	18198 (3)	9770 (2)	-2852 (2)
C(23)	20779 (3)	8852 (2)	-2752 (2)
C(24)	21434 (3)	9484 (2)	-3780 (2)
C(25)	23038 (4)	9224 (2)	-4291 (3)
C(26)	23886 (3)	8345 (2)	-3804 (2)
F(27)	25444 (2)	8131 (1)	-4306 (2)
C(28)	23297 (3)	7702 (2)	-2800 (3)
C(29)	21726 (3)	7969 (2)	-2256 (2)

reflexions. The scattering factors used are those given in *International Tables for X-ray Crystallography* (1962). The final coordinates are given in Table 2.*

Discussion. The conformation of the molecule and the numbering scheme are shown in Fig. 1 and the bond distances and angles in Table 3.

The torsion angles defining the conformation are given in Table 4. The molecules form centrosymmetric hydrogen-bonded dimers as described in the *Abstract*.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32714 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

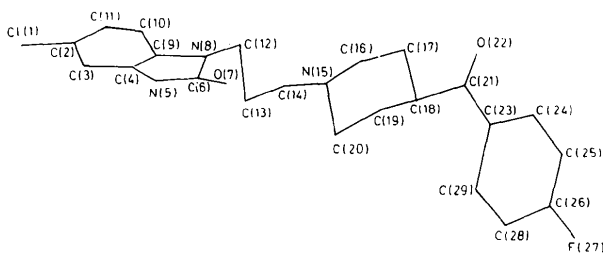


Fig. 1. Conformation and numbering scheme of $C_{22}H_{23}N_3O_2FCl$.

Table 3. Bond distances (Å) and angles ($^\circ$) (with standard deviations in parentheses)

Cl(1)—C(2)	1.735 (3)	Cl(1)—C(2)—C(3)	119.2 (2)
C(2)—C(3)	1.383 (4)	Cl(1)—C(2)—C(11)	117.7 (2)
C(2)—C(11)	1.404 (4)	C(3)—C(2)—C(11)	123.1 (2)
C(3)—C(4)	1.392 (3)	C(2)—C(3)—C(4)	116.4 (2)
C(4)—N(5)	1.403 (3)	C(3)—C(4)—N(5)	130.7 (2)
C(4)—C(9)	1.388 (3)	C(3)—C(4)—C(9)	121.5 (2)
N(5)—C(6)	1.383 (3)	N(5)—C(4)—C(9)	107.8 (2)
C(6)—O(7)	1.241 (3)	C(4)—N(5)—C(6)	107.9 (2)
C(6)—N(8)	1.362 (3)	N(5)—C(6)—O(7)	125.5 (2)
N(8)—C(9)	1.388 (3)	N(5)—C(6)—N(8)	107.7 (2)
N(8)—C(12)	1.477 (3)	O(7)—C(6)—N(8)	126.8 (2)
C(9)—C(10)	1.377 (3)	C(6)—N(8)—C(9)	110.0 (2)
C(10)—C(11)	1.397 (4)	C(6)—N(8)—C(12)	124.0 (2)
C(12)—C(13)	1.534 (4)	C(9)—N(8)—C(12)	125.9 (2)
C(13)—C(14)	1.524 (4)	C(4)—C(9)—N(8)	106.6 (2)
C(14)—N(15)	1.473 (3)	C(4)—C(9)—C(10)	121.7 (2)
N(15)—C(16)	1.445 (3)	N(8)—C(9)—C(10)	131.7 (2)
N(15)—C(20)	1.469 (4)	C(9)—C(10)—C(11)	118.4 (2)
C(16)—C(17)	1.509 (4)	C(2)—C(11)—C(10)	119.0 (2)
C(17)—C(18)	1.549 (4)	N(8)—C(12)—C(13)	110.4 (2)
C(18)—C(19)	1.511 (4)	C(12)—C(13)—C(14)	112.9 (2)
C(18)—C(21)	1.505 (3)	C(13)—C(14)—N(15)	114.4 (2)
C(19)—C(20)	1.555 (4)	C(14)—N(15)—C(16)	108.3 (2)
C(21)—O(22)	1.226 (3)	C(14)—N(15)—C(20)	110.5 (2)
C(21)—C(23)	1.471 (3)	C(16)—N(15)—C(20)	111.3 (2)
C(23)—C(24)	1.398 (3)	N(15)—C(16)—C(17)	111.8 (2)
C(23)—C(29)	1.399 (3)	C(16)—C(17)—C(18)	109.6 (2)
C(24)—C(25)	1.407 (4)	C(17)—C(18)—C(19)	107.9 (2)
C(25)—C(26)	1.353 (4)	C(17)—C(18)—C(21)	110.7 (2)
C(26)—F(27)	1.360 (3)	C(19)—C(18)—C(21)	111.6 (2)
C(26)—C(28)	1.368 (4)	C(18)—C(19)—C(20)	109.7 (2)
C(28)—C(29)	1.397 (4)	N(15)—C(20)—C(19)	110.6 (2)
		C(18)—C(21)—O(22)	118.7 (2)
		C(18)—C(21)—C(23)	122.2 (2)
		O(22)—C(21)—C(23)	119.1 (2)
		C(21)—C(23)—C(24)	118.4 (2)
		C(21)—C(23)—C(29)	122.2 (2)
		C(24)—C(23)—C(29)	119.4 (2)
		C(23)—C(24)—C(25)	119.4 (2)
		C(24)—C(25)—C(26)	119.0 (3)
		C(25)—C(26)—F(27)	117.3 (2)
		C(25)—C(26)—C(28)	123.6 (3)
		F(27)—C(26)—C(28)	119.0 (2)
		C(26)—C(28)—C(29)	117.9 (2)
		C(23)—C(29)—C(28)	120.6 (2)

Table 4. Torsion angles ($^\circ$) defining the conformation of $C_{22}H_{23}N_3O_2FCl$

C(9)—N(8)—C(12)—C(13)	78
N(8)—C(12)—C(13)—C(14)	-175
C(12)—C(13)—C(14)—N(15)	-58
C(13)—C(14)—N(15)—C(16)	172
C(14)—N(15)—C(16)—C(17)	-179
N(15)—C(16)—C(17)—C(18)	-59
C(16)—C(17)—C(18)—C(21)	-179
C(17)—C(18)—C(21)—O(22)	-40
C(17)—C(18)—C(21)—C(23)	139
C(18)—C(21)—C(23)—C(24)	-161

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4-(*p*-Chlorophenyl)-4-hydroxy-*N,N*, γ -trimethyl- α,α -diphenyl-1-piperidinebutyramide

BY J. P. DECLERCQ,* G. GERMAIN AND M. VAN MEERSSCHE

Laboratoire de Chimie Physique et de Cristallographie, Université de Louvain, 1 place L. Pasteur, B-1348 Louvain-la-Neuve, Belgium

AND M. H. J. KOCH

Research Laboratories, Janssen Pharmaceutica, B-2340 Beerse, Belgium

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Abstract. C₃₀H₃₅N₂O₂Cl, $M_r = 491.05$; monoclinic, $P2_1/c$; $a = 8.991$ (2), $b = 14.303$ (3), $c = 20.758$ (5) Å, $\beta = 95.07$ (2); 25°C; $Z = 4$. Each molecule is involved in two hydrogen bonds: O(14)···O(19), 2.84 Å [O(19): $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$], and O(19)···O(14) [O(14): $1 - x, y - \frac{1}{2}, z$].

Introduction. The title compound is related to the potent antidiarrhoeal drug loperamide (Germain, Declercq, Van Meerssche & Koch, 1977).

Transparent colourless crystals were obtained by evaporation of a solution in ethanol. The experimental conditions used for data collection are given in Table 1. The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). Anisotropic block-diagonal least-squares refinement (Ahmed, Hall, Pippy & Huber, 1966) gave a final $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ of 0.09 for all observed reflexions. The scattering factors used are those given in *International Tables for X-ray*

Table 2. Final positional parameters ($\times 10^4$) (with standard deviations in parentheses)

	<i>x</i>	<i>y</i>	<i>z</i>
Cl(1)	7481 (1)	9370 (1)	8666 (0)
C(2)	8809 (3)	7823 (2)	8229 (1)
C(3)	8828 (3)	6869 (2)	8074 (1)
C(4)	7597 (3)	6298 (2)	8158 (1)
C(5)	6335 (3)	6696 (2)	8395 (1)
C(6)	6282 (4)	7639 (2)	8543 (1)
C(7)	7520 (4)	8188 (2)	8460 (1)
C(8)	7705 (3)	5257 (2)	8013 (1)
C(9)	8390 (3)	4747 (2)	8623 (1)
C(10)	8442 (3)	3692 (2)	8521 (1)
N(11)	6933 (2)	3343 (1)	8352 (1)
C(12)	6320 (3)	3744 (2)	7735 (1)
C(13)	6161 (3)	4799 (2)	7802 (1)
O(14)	8700 (2)	5106 (1)	7515 (1)
C(15)	6864 (3)	2313 (2)	8390 (1)
C(16)	5267 (3)	1936 (2)	8436 (1)
C(17)	4384 (2)	2267 (2)	9018 (1)
C(18)	2982 (3)	1616 (2)	8976 (1)
O(19)	2861 (2)	981 (1)	8574 (1)
N(20)	1900 (2)	1726 (2)	9379 (1)
C(21)	1856 (3)	2437 (2)	9882 (1)
C(22)	601 (3)	1093 (2)	9296 (2)
C(23)	5378 (3)	2095 (2)	9637 (1)
C(24)	6562 (3)	2709 (2)	9832 (1)
C(25)	7559 (3)	2511 (2)	10370 (1)
C(26)	7429 (3)	1689 (2)	10719 (1)
C(27)	6281 (3)	1083 (2)	10532 (1)
C(28)	5242 (3)	1275 (2)	10002 (1)
C(29)	3784 (2)	3277 (2)	8905 (1)
C(30)	2900 (3)	3459 (2)	8337 (1)
C(31)	2280 (3)	4341 (2)	8203 (1)
C(32)	2544 (3)	5054 (2)	8651 (1)
C(33)	3383 (3)	4877 (2)	9226 (1)
C(34)	3991 (3)	3996 (2)	9348 (1)
C(35)	7503 (3)	1804 (2)	7802 (1)

Table 1. Experimental conditions

Instrument: Syntex *P2*, diffractometer
 Source: Cu $K\alpha$; $\lambda = 1.5418$ Å; ω - 2θ scan; $\theta_{\max} = 55^\circ$
 Confidence level: 2.5
 Total number of independent reflexions: 3343
 Total observed: 2547

* Chargé de Recherches du Fonds National de la Recherche Scientifique.