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6-Methoxy-1′-methyl-4′-phenylchroman-3-spiro-3′-pyrrolidine-2′-spiro-3″(2″*H*)-indole-2″,4-dione

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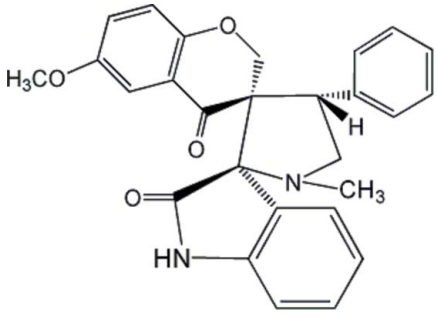
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.115; data-to-parameter ratio = 17.7.

The title compound, $C_{27}H_{24}N_2O_4$, has been synthesized as a potential pharmacologically active compound. All bond lengths and angles are within normal ranges and the molecules are linked into centrosymmetric $R_2^2(14)$ dimers by a simple N—H···O interaction. The packing is stabilized through intermolecular N—H···O hydrogen bonds and van der Waals interactions.

Related literature

For related literature, see: Abdul Ajees *et al.* (2001); Bernstein *et al.* (1995); Deshong & Leginus (1983); Fujimori (1990); Henrickson & Silva (1962); James *et al.* (1991).



Experimental

Crystal data

$C_{27}H_{24}N_2O_4$
M_r = 440.48
Monoclinic, $P2_1/n$
a = 9.2244 (2) Å
b = 26.1163 (5) Å
c = 9.3506 (2) Å
β = 103.233 (1)°
V = 2192.81 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.23 × 0.21 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.899, T_{max} = 0.987
27791 measured reflections
5379 independent reflections
3670 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.02
5379 reflections
304 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.878 (18)	2.167 (19)	3.0401 (16)	172.8 (16)

Symmetry code: (i) $-x+1, -y, -z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Department of Chemistry, IIT Madras, Chennai, India, for the single-crystal X-ray diffraction data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2097).

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supplementary materials

Acta Cryst. (2007). E**63**, o3794 [**doi:10.1107/S1600536807038755**]

6-Methoxy-1'-methyl-4'-phenylchroman-3-spiro-3'-pyrrolidine-2'-spiro-3''(2''*H*)-indole-2'',4-dione

T. Augustine, C. C. Kanakam, R. Suresh, Y. Christurajan and V. Ramkumar

Comment

Spiroheterocycles represent an important class of naturally occurring substances characterized by their highly pronounced biological activities·(James *et al.*, 1991) Highly substituted pyrrolidines have gained much prominence since they form the central skeleton of many natural products and pharmacologically active compounds. (Deshong & Leginus, 1983). Pyrrolidine and oxindole alkaloids (Fujimori, 1990) constitute another class of compounds with significant biological activity which are normally found in rhyncophylline, corynoxeine, nitraphylline, vincatine, horsifiline,*etc* (Henrickson & Silva, 1962).

In the crystal structure of the title compound, $C_{27}H_{24}N_2O_4$, the chromanone moiety consists of a methoxy benzene ring fused with a six membered heterocyclic ring which adopts a sofa conformation (Abdul Ajees *et al.*, 2001). The five membered spiropyrrolidine ring is in an envelope conformation. The oxindole and phenyl rings attached to the five membered rings are nearly perpendicular to each other. The molecules are linked into centrosymmetric $R_2^2(14)$ dimmer by a simple N—H···O interaction (Bernstein *et al.*, 1995)

Experimental

A mixture of Isatin (1*H*-indole-2,3-dione) (1 mmol, 0.082 g), Sarcosine (2-methylaminoacetic acid) (1 mmol, 0.046 g) and the dipolarophile (3-arylidene-4-chromanone) (1 mmol, 0.2 g) in aqueous methanol (20 ml) was refluxed for 5 h and was subsequently monitored by TLC for the disappearance of starting materials. The solvent was removed under reduced pressure and the crude product was purified by column chromatography using silica gel and hexane–ethyl acetate (5:1) as eluent to give the cycloadduct.

Refinement

All the H atoms were geometrically fixed at chemically meaningful positions. The hydrogen atoms of the phenyl ring were allowed to ride at a distance of 0.93 Å from the parent carbons and their thermal parameter were fixed at 1.2 times that of the parent atom.

The secondary CH_2 H atoms were fixed at a distance of 0.97 Å from the parent atom and their thermal parameters were fixed at 1.2 times the parent atom.

The CH_3 H atoms attached to Nitrogen were fixed at a distance of 0.96 Å from the parent atom and their thermal parameters were fixed at 1.5 times the parent atom. similarly the CH_3 H atoms attached to Oxygen were fixed at a distance of 0.96 Å from the parent atom and their thermal parameters were fixed at 1.5 times the parent atom.

Figures

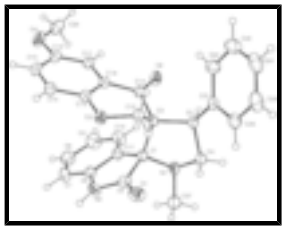

Fig. 1. *ORTEP* representation of the molecule showing the atom numbering scheme. Thermal ellipsoids are drawn with 30% probability.

Fig. 2. Packing diagram of title compound projected down the C-axis

6-Methoxy-1'-methyl-4'-phenylchroman-3-spiro-3'-pyrrolidine-2'-spiro-3''(2''H)- indole-2'',4-dione

Crystal data

$C_{27}H_{24}N_2O_4$	F_{000} = 928
M_r = 440.48	D_x = 1.334 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8137 reflections
a = 9.2244 (2) Å	θ = 2.4–26.8º
b = 26.1163 (5) Å	μ = 0.09 mm^{-1}
c = 9.3506 (2) Å	T = 295 (2) K
β = 103.2330 (10)º	Rectangular, colourless
V = 2192.81 (8) Å^3	0.23 × 0.21 × 0.15 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	5379 independent reflections
Radiation source: fine-focus sealed tube	3670 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 295(2) K	θ_{max} = 28.4º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (Blessing, 1995)	h = −11→12
T_{min} = 0.899, T_{max} = 0.987	k = −34→34
27791 measured reflections	l = −12→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.486P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
5379 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
304 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances,angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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.

The reflections with Bragg angle less than 2.4° could not be collected due to the hinderence of the beam stop. This lead to the absence of 14 low angle reflections from the measured data. As *b* axis length is quite large (26.116 Å) for the wave length used (0.71073 Å),it became unavoidable. Except for these missing low angle reflections, the data set is complete with in 50° two theta.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.25225 (16)	0.09504 (5)	0.02539 (14)	0.0343 (3)
C2	0.34793 (15)	0.14452 (5)	0.00669 (13)	0.0312 (3)
C3	0.23382 (16)	0.17999 (5)	−0.09708 (14)	0.0338 (3)
H3	0.1920	0.2025	−0.0330	0.041*
C4	0.11035 (18)	0.14375 (6)	−0.16772 (16)	0.0445 (4)
H4A	0.0178	0.1619	−0.2058	0.053*
H4B	0.1367	0.1242	−0.2463	0.053*
C5	0.30377 (17)	0.04717 (5)	−0.05042 (16)	0.0401 (3)
C6	0.31749 (17)	0.02527 (5)	0.18915 (16)	0.0392 (3)
C7	0.3394 (2)	−0.00243 (6)	0.31793 (19)	0.0552 (4)
H7	0.3771	−0.0356	0.3237	0.066*
C8	0.3033 (2)	0.02077 (7)	0.43793 (19)	0.0640 (5)
H8	0.3183	0.0031	0.5264	0.077*
C9	0.2459 (2)	0.06933 (8)	0.4293 (2)	0.0639 (5)
H9	0.2210	0.0840	0.5111	0.077*
C10	0.2246 (2)	0.09686 (7)	0.29919 (18)	0.0512 (4)
H10	0.1848	0.1297	0.2932	0.061*

C11	0.26312 (16)	0.07498 (5)	0.17921 (15)	0.0366 (3)
C12	0.40941 (16)	0.16912 (5)	0.15696 (14)	0.0343 (3)
C13	0.48437 (16)	0.13335 (5)	−0.05463 (15)	0.0364 (3)
H13A	0.4520	0.1199	−0.1535	0.044*
H13B	0.5375	0.1651	−0.0601	0.044*
C14	0.74957 (18)	0.08581 (6)	0.26498 (18)	0.0462 (4)
H14	0.8021	0.0620	0.2227	0.055*
C15	0.79350 (18)	0.09709 (6)	0.41191 (19)	0.0514 (4)
H15	0.8757	0.0805	0.4693	0.062*
C16	0.71684 (18)	0.13301 (6)	0.47627 (16)	0.0452 (4)
C17	0.59566 (17)	0.15788 (6)	0.39204 (15)	0.0403 (3)
H17	0.5452	0.1824	0.4342	0.048*
C18	0.54837 (16)	0.14622 (5)	0.24221 (15)	0.0348 (3)
C19	0.62592 (16)	0.11033 (5)	0.18011 (15)	0.0369 (3)
C20	0.6949 (2)	0.17725 (8)	0.69199 (18)	0.0620 (5)
H20A	0.7026	0.2104	0.6497	0.093*
H20B	0.7393	0.1783	0.7954	0.093*
H20C	0.5918	0.1679	0.6772	0.093*
C21	0.29494 (16)	0.21463 (5)	−0.19882 (15)	0.0356 (3)
C22	0.38359 (19)	0.25574 (6)	−0.14124 (19)	0.0512 (4)
H22	0.4076	0.2608	−0.0401	0.061*
C23	0.4371 (2)	0.28933 (7)	−0.2299 (2)	0.0655 (5)
H23	0.4968	0.3166	−0.1882	0.079*
C24	0.4031 (2)	0.28291 (7)	−0.3794 (2)	0.0645 (5)
H24	0.4397	0.3056	−0.4393	0.077*
C25	0.3146 (2)	0.24280 (8)	−0.4395 (2)	0.0660 (5)
H25	0.2905	0.2382	−0.5408	0.079*
C26	0.2605 (2)	0.20884 (6)	−0.34931 (17)	0.0523 (4)
H26	0.2000	0.1818	−0.3914	0.063*
C27	−0.0093 (2)	0.06977 (7)	−0.0786 (2)	0.0661 (5)
H27A	−0.1068	0.0841	−0.1136	0.099*
H27B	−0.0073	0.0499	0.0081	0.099*
H27C	0.0145	0.0482	−0.1532	0.099*
N1	0.10004 (14)	0.11104 (5)	−0.04404 (14)	0.0428 (3)
N2	0.33944 (15)	0.00992 (5)	0.05262 (14)	0.0447 (3)
O1	0.30669 (15)	0.04317 (4)	−0.17904 (12)	0.0583 (3)
O2	0.34710 (13)	0.20420 (4)	0.20365 (11)	0.0502 (3)
O3	0.58380 (11)	0.09720 (4)	0.03378 (10)	0.0406 (2)
O4	0.76976 (14)	0.14063 (5)	0.62380 (12)	0.0631 (4)
H2	0.369 (2)	−0.0207 (7)	0.0335 (18)	0.056 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0353 (8)	0.0335 (7)	0.0331 (7)	0.0026 (6)	0.0057 (6)	0.0026 (5)
C2	0.0316 (7)	0.0319 (7)	0.0283 (6)	0.0027 (5)	0.0034 (5)	0.0017 (5)
C3	0.0340 (8)	0.0341 (7)	0.0312 (7)	0.0030 (6)	0.0031 (6)	0.0031 (5)
C4	0.0405 (9)	0.0435 (8)	0.0434 (8)	−0.0033 (7)	−0.0028 (7)	0.0106 (6)

C5	0.0416 (9)	0.0377 (8)	0.0408 (8)	−0.0044 (6)	0.0089 (6)	−0.0043 (6)
C6	0.0375 (8)	0.0360 (7)	0.0423 (8)	−0.0003 (6)	0.0052 (6)	0.0051 (6)
C7	0.0607 (12)	0.0438 (9)	0.0566 (10)	0.0029 (8)	0.0042 (8)	0.0178 (8)
C8	0.0752 (14)	0.0695 (12)	0.0444 (9)	−0.0103 (10)	0.0080 (9)	0.0191 (9)
C9	0.0805 (14)	0.0718 (13)	0.0456 (10)	−0.0028 (10)	0.0274 (9)	0.0062 (9)
C10	0.0603 (11)	0.0508 (9)	0.0486 (9)	0.0088 (8)	0.0251 (8)	0.0042 (7)
C11	0.0359 (8)	0.0366 (7)	0.0377 (7)	0.0028 (6)	0.0088 (6)	0.0067 (6)
C12	0.0360 (8)	0.0350 (7)	0.0309 (7)	0.0034 (6)	0.0059 (6)	0.0001 (5)
C13	0.0372 (8)	0.0371 (7)	0.0342 (7)	0.0035 (6)	0.0068 (6)	0.0017 (6)
C14	0.0381 (9)	0.0403 (8)	0.0555 (9)	0.0088 (7)	0.0010 (7)	−0.0036 (7)
C15	0.0391 (9)	0.0468 (9)	0.0577 (10)	0.0070 (7)	−0.0110 (7)	0.0040 (7)
C16	0.0424 (9)	0.0450 (8)	0.0400 (8)	−0.0017 (7)	−0.0076 (7)	0.0000 (6)
C17	0.0397 (9)	0.0397 (8)	0.0373 (7)	0.0019 (6)	0.0001 (6)	−0.0027 (6)
C18	0.0324 (8)	0.0347 (7)	0.0343 (7)	0.0009 (6)	0.0017 (6)	0.0001 (5)
C19	0.0325 (8)	0.0356 (7)	0.0395 (7)	−0.0003 (6)	0.0020 (6)	−0.0011 (6)
C20	0.0552 (12)	0.0884 (14)	0.0374 (9)	−0.0034 (10)	0.0002 (8)	−0.0058 (9)
C21	0.0361 (8)	0.0329 (7)	0.0364 (7)	0.0063 (6)	0.0056 (6)	0.0056 (5)
C22	0.0531 (11)	0.0486 (9)	0.0514 (9)	−0.0090 (8)	0.0108 (8)	0.0020 (7)
C23	0.0593 (12)	0.0541 (11)	0.0840 (14)	−0.0137 (9)	0.0184 (10)	0.0117 (10)
C24	0.0611 (12)	0.0623 (12)	0.0771 (13)	0.0105 (10)	0.0303 (10)	0.0346 (10)
C25	0.0859 (15)	0.0689 (12)	0.0454 (10)	0.0115 (11)	0.0198 (9)	0.0215 (9)
C26	0.0691 (12)	0.0464 (9)	0.0386 (8)	−0.0006 (8)	0.0066 (8)	0.0062 (7)
C27	0.0445 (11)	0.0580 (11)	0.0868 (14)	−0.0137 (8)	−0.0037 (9)	0.0233 (10)
N1	0.0331 (7)	0.0415 (7)	0.0501 (7)	−0.0029 (5)	0.0016 (5)	0.0129 (5)
N2	0.0542 (9)	0.0291 (6)	0.0512 (8)	0.0048 (6)	0.0128 (6)	−0.0010 (6)
O1	0.0835 (9)	0.0523 (7)	0.0413 (6)	−0.0062 (6)	0.0193 (6)	−0.0107 (5)
O2	0.0557 (7)	0.0523 (6)	0.0382 (6)	0.0214 (5)	0.0016 (5)	−0.0078 (5)
O3	0.0389 (6)	0.0404 (5)	0.0406 (5)	0.0098 (4)	0.0053 (4)	−0.0045 (4)
O4	0.0609 (8)	0.0731 (8)	0.0417 (6)	0.0111 (6)	−0.0166 (6)	−0.0063 (6)

Geometric parameters (Å, °)

C1—N1	1.4663 (18)	C14—C15	1.372 (2)
C1—C11	1.5124 (18)	C14—C19	1.388 (2)
C1—C5	1.5638 (19)	C14—H14	0.9300
C1—C2	1.5970 (19)	C15—C16	1.392 (2)
C2—C13	1.5258 (19)	C15—H15	0.9300
C2—C12	1.5309 (18)	C16—O4	1.3685 (18)
C2—C3	1.5620 (18)	C16—C17	1.374 (2)
C3—C4	1.511 (2)	C17—C18	1.4022 (19)
C3—C21	1.5123 (19)	C17—H17	0.9300
C3—H3	0.9800	C18—C19	1.3847 (19)
C4—N1	1.4583 (18)	C19—O3	1.3774 (16)
C4—H4A	0.9700	C20—O4	1.414 (2)
C4—H4B	0.9700	C20—H20A	0.9600
C5—O1	1.2136 (17)	C20—H20B	0.9600
C5—N2	1.3558 (19)	C20—H20C	0.9600
C6—C7	1.379 (2)	C21—C26	1.378 (2)
C6—C11	1.387 (2)	C21—C22	1.382 (2)

C6—N2	1.3964 (19)	C22—C23	1.374 (2)
C7—C8	1.381 (3)	C22—H22	0.9300
C7—H7	0.9300	C23—C24	1.371 (3)
C8—C9	1.369 (3)	C23—H23	0.9300
C8—H8	0.9300	C24—C25	1.367 (3)
C9—C10	1.388 (2)	C24—H24	0.9300
C9—H9	0.9300	C25—C26	1.393 (2)
C10—C11	1.376 (2)	C25—H25	0.9300
C10—H10	0.9300	C26—H26	0.9300
C12—O2	1.2147 (16)	C27—N1	1.461 (2)
C12—C18	1.4726 (19)	C27—H27A	0.9600
C13—O3	1.4384 (16)	C27—H27B	0.9600
C13—H13A	0.9700	C27—H27C	0.9600
C13—H13B	0.9700	N2—H2	0.878 (18)
N1—C1—C11	111.60 (11)	C15—C14—H14	120.4
N1—C1—C5	112.75 (11)	C19—C14—H14	120.4
C11—C1—C5	101.15 (11)	C14—C15—C16	120.98 (14)
N1—C1—C2	102.60 (10)	C14—C15—H15	119.5
C11—C1—C2	117.80 (11)	C16—C15—H15	119.5
C5—C1—C2	111.37 (11)	O4—C16—C17	124.37 (15)
C13—C2—C12	105.13 (11)	O4—C16—C15	115.76 (14)
C13—C2—C3	112.11 (11)	C17—C16—C15	119.86 (14)
C12—C2—C3	112.14 (11)	C16—C17—C18	119.74 (14)
C13—C2—C1	114.24 (11)	C16—C17—H17	120.1
C12—C2—C1	109.69 (10)	C18—C17—H17	120.1
C3—C2—C1	103.71 (10)	C19—C18—C17	119.58 (13)
C4—C3—C21	116.86 (11)	C19—C18—C12	121.14 (12)
C4—C3—C2	103.50 (11)	C17—C18—C12	119.06 (12)
C21—C3—C2	116.76 (11)	O3—C19—C18	121.99 (12)
C4—C3—H3	106.3	O3—C19—C14	117.46 (13)
C21—C3—H3	106.3	C18—C19—C14	120.55 (13)
C2—C3—H3	106.3	O4—C20—H20A	109.5
N1—C4—C3	101.52 (11)	O4—C20—H20B	109.5
N1—C4—H4A	111.5	H20A—C20—H20B	109.5
C3—C4—H4A	111.5	O4—C20—H20C	109.5
N1—C4—H4B	111.5	H20A—C20—H20C	109.5
C3—C4—H4B	111.5	H20B—C20—H20C	109.5
H4A—C4—H4B	109.3	C26—C21—C22	117.43 (14)
O1—C5—N2	125.84 (14)	C26—C21—C3	123.00 (13)
O1—C5—C1	126.59 (13)	C22—C21—C3	119.50 (13)
N2—C5—C1	107.52 (12)	C23—C22—C21	121.54 (17)
C7—C6—C11	121.86 (14)	C23—C22—H22	119.2
C7—C6—N2	128.65 (14)	C21—C22—H22	119.2
C11—C6—N2	109.47 (12)	C24—C23—C22	120.48 (18)
C6—C7—C8	117.69 (16)	C24—C23—H23	119.8
C6—C7—H7	121.2	C22—C23—H23	119.8
C8—C7—H7	121.2	C25—C24—C23	119.24 (16)
C9—C8—C7	121.33 (16)	C25—C24—H24	120.4
C9—C8—H8	119.3	C23—C24—H24	120.4

C7—C8—H8	119.3	C24—C25—C26	120.14 (17)
C8—C9—C10	120.46 (17)	C24—C25—H25	119.9
C8—C9—H9	119.8	C26—C25—H25	119.9
C10—C9—H9	119.8	C21—C26—C25	121.17 (16)
C11—C10—C9	119.22 (16)	C21—C26—H26	119.4
C11—C10—H10	120.4	C25—C26—H26	119.4
C9—C10—H10	120.4	N1—C27—H27A	109.5
C10—C11—C6	119.40 (13)	N1—C27—H27B	109.5
C10—C11—C1	131.16 (13)	H27A—C27—H27B	109.5
C6—C11—C1	109.40 (12)	N1—C27—H27C	109.5
O2—C12—C18	122.46 (12)	H27A—C27—H27C	109.5
O2—C12—C2	122.69 (12)	H27B—C27—H27C	109.5
C18—C12—C2	114.84 (11)	C4—N1—C27	115.06 (13)
O3—C13—C2	112.44 (11)	C4—N1—C1	106.76 (11)
O3—C13—H13A	109.1	C27—N1—C1	115.48 (12)
C2—C13—H13A	109.1	C5—N2—C6	112.41 (12)
O3—C13—H13B	109.1	C5—N2—H2	123.1 (11)
C2—C13—H13B	109.1	C6—N2—H2	124.4 (11)
H13A—C13—H13B	107.8	C19—O3—C13	113.90 (10)
C15—C14—C19	119.28 (14)	C16—O4—C20	117.03 (13)
N1—C1—C2—C13	−131.28 (11)	C1—C2—C13—O3	−57.31 (15)
C11—C1—C2—C13	105.74 (13)	C19—C14—C15—C16	−0.6 (3)
C5—C1—C2—C13	−10.42 (15)	C14—C15—C16—O4	179.25 (15)
N1—C1—C2—C12	111.00 (12)	C14—C15—C16—C17	−0.3 (3)
C11—C1—C2—C12	−11.98 (16)	O4—C16—C17—C18	−178.35 (15)
C5—C1—C2—C12	−128.14 (12)	C15—C16—C17—C18	1.2 (2)
N1—C1—C2—C3	−8.95 (13)	C16—C17—C18—C19	−1.1 (2)
C11—C1—C2—C3	−131.93 (12)	C16—C17—C18—C12	173.62 (14)
C5—C1—C2—C3	111.90 (12)	O2—C12—C18—C19	−172.56 (14)
C13—C2—C3—C4	104.93 (13)	C2—C12—C18—C19	8.73 (19)
C12—C2—C3—C4	−137.07 (12)	O2—C12—C18—C17	12.8 (2)
C1—C2—C3—C4	−18.80 (13)	C2—C12—C18—C17	−165.90 (12)
C13—C2—C3—C21	−24.98 (16)	C17—C18—C19—O3	179.60 (13)
C12—C2—C3—C21	93.02 (14)	C12—C18—C19—O3	5.0 (2)
C1—C2—C3—C21	−148.71 (11)	C17—C18—C19—C14	0.2 (2)
C21—C3—C4—N1	169.87 (12)	C12—C18—C19—C14	−174.45 (14)
C2—C3—C4—N1	40.03 (14)	C15—C14—C19—O3	−178.76 (14)
N1—C1—C5—O1	56.5 (2)	C15—C14—C19—C18	0.7 (2)
C11—C1—C5—O1	175.82 (15)	C4—C3—C21—C26	−10.6 (2)
C2—C1—C5—O1	−58.19 (19)	C2—C3—C21—C26	112.71 (16)
N1—C1—C5—N2	−121.14 (13)	C4—C3—C21—C22	166.10 (14)
C11—C1—C5—N2	−1.84 (15)	C2—C3—C21—C22	−70.64 (17)
C2—C1—C5—N2	124.15 (12)	C26—C21—C22—C23	−0.7 (2)
C11—C6—C7—C8	0.8 (3)	C3—C21—C22—C23	−177.56 (16)
N2—C6—C7—C8	−177.26 (16)	C21—C22—C23—C24	0.2 (3)
C6—C7—C8—C9	0.9 (3)	C22—C23—C24—C25	0.3 (3)
C7—C8—C9—C10	−1.0 (3)	C23—C24—C25—C26	−0.3 (3)
C8—C9—C10—C11	−0.6 (3)	C22—C21—C26—C25	0.8 (2)
C9—C10—C11—C6	2.2 (2)	C3—C21—C26—C25	177.49 (15)

C9—C10—C11—C1	179.56 (16)	C24—C25—C26—C21	−0.3 (3)
C7—C6—C11—C10	−2.4 (2)	C3—C4—N1—C27	−178.03 (14)
N2—C6—C11—C10	176.04 (14)	C3—C4—N1—C1	−48.48 (14)
C7—C6—C11—C1	179.73 (14)	C11—C1—N1—C4	162.45 (12)
N2—C6—C11—C1	−1.85 (17)	C5—C1—N1—C4	−84.51 (14)
N1—C1—C11—C10	−55.2 (2)	C2—C1—N1—C4	35.40 (14)
C5—C1—C11—C10	−175.36 (16)	C11—C1—N1—C27	−68.24 (17)
C2—C1—C11—C10	63.1 (2)	C5—C1—N1—C27	44.80 (18)
N1—C1—C11—C6	122.33 (13)	C2—C1—N1—C27	164.71 (13)
C5—C1—C11—C6	2.20 (15)	O1—C5—N2—C6	−176.80 (15)
C2—C1—C11—C6	−119.38 (13)	C1—C5—N2—C6	0.88 (17)
C13—C2—C12—O2	141.65 (14)	C7—C6—N2—C5	178.87 (16)
C3—C2—C12—O2	19.57 (19)	C11—C6—N2—C5	0.59 (18)
C1—C2—C12—O2	−95.10 (16)	C18—C19—O3—C13	17.24 (19)
C13—C2—C12—C18	−39.64 (15)	C14—C19—O3—C13	−163.30 (13)
C3—C2—C12—C18	−161.72 (12)	C2—C13—O3—C19	−53.20 (15)
C1—C2—C12—C18	83.61 (14)	C17—C16—O4—C20	−1.0 (2)
C12—C2—C13—O3	62.99 (13)	C15—C16—O4—C20	179.47 (15)
C3—C2—C13—O3	−174.93 (10)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O3^{i}	0.878 (18)	2.167 (19)	3.0401 (16)	172.8 (16)

Symmetry codes: (i) −*x*+1, −*y*, −*z*.

Fig. 1

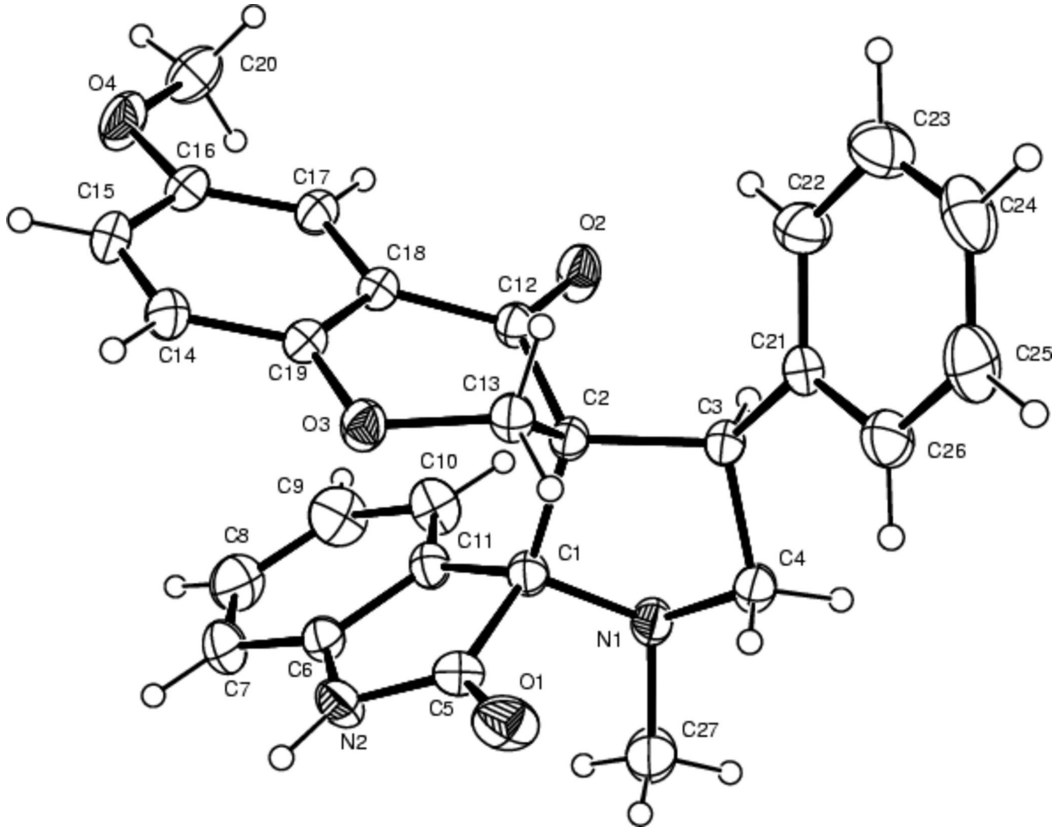
O4
C20
C16
C17
C15
C18
O2
C12
C14
C19
C13
C2
C3
O3
C10
C9
C11
C1
C4
C8
N1
C6
C7
C5
O1
N2
C27
C23
C22
C24
C21
C25
C26

Fig. 2