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1-Acetyl-2,6-bis(4-methoxyphenyl)-3-methyl-4-piperidone

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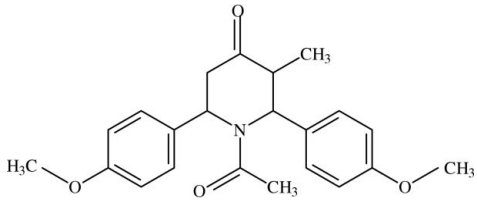
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.058; wR factor = 0.202; data-to-parameter ratio = 26.0.

The piperidine ring in the title molecule, $C_{22}H_{25}NO_4$, adopts a boat conformation. The bond lengths and angles in the vicinity of the N atom reflect the expected delocalization of electrons in this part of the molecule. The crystal structure is stabilized by weak intermolecular C—H···O and C—H···π interactions.

Related literature

For related literature, see: Comins *et al.* (2001); Nardelli (1995); Roques *et al.* (1981); Wang & Wuorola (1992).



Experimental

Crystal data

$C_{22}H_{25}NO_4$
M_r = 367.43
Monoclinic, $P2_1/c$
a = 17.2799 (5) Å
b = 10.6783 (3) Å
c = 10.5702 (3) Å
β = 90.951 (1)°
V = 1950.1 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.15 × 0.10 × 0.10 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: none
48723 measured reflections
6336 independent reflections
4237 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.202
S = 1.03
6336 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C20—O4	1.231 (2)	C20—C21	1.500 (2)
C20—N1	1.361 (2)		
C20—N1—C6	117.40 (12)	C6—N1—C2	120.00 (11)
C20—N1—C2	122.17 (12)		

Table 2
Hydrogen-bond geometry (Å, °).

Cg is the centroid of ring atoms C14–C19.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O4^{i}	0.98	2.55	3.511 (2)	167
C5—H5B···Cg^{i}	0.97	2.70	3.634 (2)	162

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2463).

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supplementary materials

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1-Acetyl-2,6-bis(4-methoxyphenyl)-3-methyl-4-piperidone

T. Kavitha, S. Ponnuswamy, K. Kaileshwaran and M. N. Ponnuswamy

Comment

Various piperidine derivatives are found to possess pharmacological activities and form an essential part of the molecular structure of important drugs. The piperidine ring function is a feature of antidepressant, antirrhythmic, antithrombogenic, spasmolytic, tranquilizing and blood cholesterol-lowering activities (Comins *et al.*, 2001). Piperidine derivatives, namely 4-piperidones, are synthetic intermediates in the preparation of various alkaloids and pharmaceutical products (Wang & Wuorola, 1992). The molecular structure of the title compound is shown in Fig. 1. The bond lengths N1—C20 = 1.362 (2)Å and O4—C20 = 1.232 (2)Å show that there is a possibility of resonance between the atoms N1, C2O and O4 due to the delocalization of the hetero π electrons of the carbonyl group. The sum of the bond angles around N1 in the molecule is 359.6 (1)° which confirms that the atom N1 is in the sp^2 hybridized state. Other bond lengths and bond angles agree well with the average values reported in the literature (Roques *et al.*, 1981). The two benzene rings are oriented equatorially with respect to piperidine moiety and are at an angle of 64.63 (5)° with respect to each other. A study on asymmetry parameters, least-squares planes and torsion angles show that the piperidine ring adopts boat conformation (Q_T =0.6531 (2); Nardelli, 1995). The atoms C3 and C6 deviate by 0.5436 (2)Å and 0.5825 (2) Å, respectively, from the mean plane constituted by atoms C2, N1, C5 and C4 atoms. The methyl group substituted at position C-3 of the piperidine ring is oriented equatorially as can be seen from the torsion angle C5—C4—C3—C7 of −168.69 (16)°.

The packing of the molecules is shown in Fig. 3. In the crystal structure, molecules are stabilized by weak C—H···O and C—H···π intermolecular interactions..

Experimental

The condensation reaction involving *p*-methoxybenzaldehyde, ammonium acetate and ethyl methyl ketone in ethanol afforded 3-methyl-2,6-di(*p*-methoxyphenyl)piperidine-4-one (PM3MPO). The condensation reation between PM3MPO and acetic anhydride in benzene medium at 373 K yielded *N*-acetyl-3-methyl-2,6-di(*p*-methoxyphenyl)piperidine-4-one (APM3MPO). The crystals were formed by the slow evaporation method using ethanol as solvent.

Refinement

H atoms were placed at idealized positions and allowed to ride on their parent atoms, with C—H = 0.93–0.98 and U_{iso}(H) = 1.2–1.5U_{eq}(C).

Figures

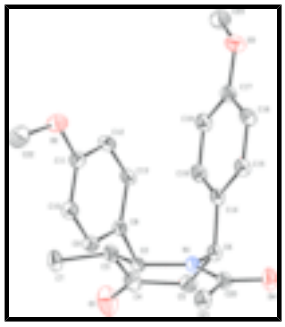

Fig. 1. The molecular structure drawn with 20% probability ellipsoids.

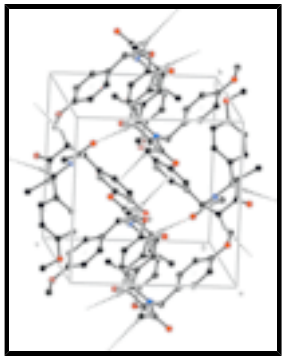

Fig. 2. The packing of the title compound with hydrogen bonds shown as dashed lines.

1-Acetyl-2,6-bis(4-methoxyphenyl)-3-methyl-4-piperidone

Crystal data

$C_{22}H_{25}NO_4$	F_{000} = 784
M_r = 367.43	D_x = 1.251 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6336 reflections
a = 17.2799 (5) Å	θ = 1.2–31.2°
b = 10.6783 (3) Å	μ = 0.09 mm^{-1}
c = 10.5702 (3) Å	T = 293 (2) K
β = 90.951 (1)°	Block, colourless
V = 1950.1 (1) Å^3	0.15 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker Kappa APEXII diffractometer	4237 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.028
Monochromator: graphite	θ_{max} = 31.2°
T = 293(2) K	θ_{min} = 1.2°
ω and Φ scan	h = −25→24
Absorption correction: none	k = −15→15

48723 measured reflections
6336 independent reflections

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.058$

$wR(F^2) = 0.202$

$S = 1.03$

6336 reflections

244 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1024P)^2 + 0.5597P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.41$ e Å^{-3}

$\Delta\rho_{min} = -0.34$ e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C2	0.24134 (8)	0.42425 (14)	−0.08397 (13)	0.0384 (3)
H2	0.2265	0.3800	−0.1619	0.046*
C3	0.32592 (9)	0.46922 (16)	−0.09782 (15)	0.0453 (3)
H3	0.3366	0.5264	−0.0271	0.054*
C4	0.38377 (10)	0.36388 (19)	−0.08614 (17)	0.0540 (4)
C5	0.36909 (10)	0.27017 (17)	0.01597 (16)	0.0500 (4)
H5A	0.4158	0.2611	0.0672	0.060*
H5B	0.3582	0.1897	−0.0230	0.060*
C6	0.30243 (9)	0.30384 (15)	0.10221 (14)	0.0416 (3)
H6	0.2893	0.2268	0.1474	0.050*
C7	0.33568 (13)	0.5451 (2)	−0.21867 (18)	0.0637 (5)
H7A	0.2977	0.6108	−0.2219	0.096*
H7B	0.3288	0.4913	−0.2908	0.096*
H7C	0.3866	0.5810	−0.2194	0.096*
C8	0.18951 (9)	0.53827 (14)	−0.07312 (13)	0.0394 (3)
C9	0.13810 (10)	0.56948 (15)	−0.16958 (15)	0.0453 (3)
H9	0.1319	0.5154	−0.2379	0.054*
C10	0.09535 (10)	0.68025 (16)	−0.16688 (16)	0.0483 (4)
H10	0.0602	0.6988	−0.2317	0.058*
C11	0.10588 (9)	0.76218 (15)	−0.06678 (16)	0.0460 (3)
C12	0.15667 (11)	0.73131 (17)	0.03122 (15)	0.0505 (4)
H12	0.1632	0.7857	0.0993	0.061*
C13	0.19733 (10)	0.62084 (16)	0.02835 (14)	0.0466 (4)
H13	0.2307	0.6008	0.0953	0.056*
C14	0.31855 (8)	0.40173 (15)	0.20338 (13)	0.0404 (3)
C15	0.25926 (9)	0.43286 (16)	0.28652 (14)	0.0451 (3)
H15	0.2112	0.3946	0.2766	0.054*
C16	0.27017 (9)	0.51809 (17)	0.38202 (16)	0.0485 (4)

H16	0.2297	0.5369	0.4358	0.058*
C17	0.34164 (10)	0.57669 (16)	0.39885 (14)	0.0463 (3)
C18	0.40139 (10)	0.54699 (17)	0.31849 (16)	0.0497 (4)
H18	0.4495	0.5851	0.3289	0.060*
C19	0.38947 (9)	0.46045 (17)	0.22259 (15)	0.0470 (4)
H19	0.4301	0.4411	0.1695	0.056*
C20	0.16813 (10)	0.26840 (16)	0.04235 (15)	0.0465 (4)
C21	0.10092 (11)	0.2842 (2)	−0.04786 (18)	0.0569 (4)
H21A	0.1145	0.3423	−0.1131	0.085*
H21B	0.0571	0.3156	−0.0030	0.085*
H21C	0.0881	0.2048	−0.0852	0.085*
C22	0.02875 (14)	0.9225 (2)	−0.1635 (2)	0.0736 (6)
H22A	0.0066	1.0024	−0.1434	0.110*
H22B	−0.0118	0.8650	−0.1867	0.110*
H22C	0.0635	0.9318	−0.2328	0.110*
C23	0.41925 (13)	0.7143 (2)	0.5244 (2)	0.0688 (5)
H23A	0.4145	0.7712	0.5941	0.103*
H23B	0.4373	0.7589	0.4518	0.103*
H23C	0.4555	0.6495	0.5465	0.103*
N1	0.23407 (7)	0.33491 (12)	0.02276 (11)	0.0394 (3)
O1	0.43862 (10)	0.3541 (2)	−0.15422 (18)	0.0973 (7)
O2	0.07009 (8)	0.87548 (13)	−0.05605 (13)	0.0624 (4)
O3	0.34637 (8)	0.66045 (14)	0.49598 (12)	0.0619 (4)
O4	0.16286 (8)	0.19646 (14)	0.13284 (13)	0.0661 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0427 (7)	0.0427 (7)	0.0299 (6)	−0.0040 (6)	0.0024 (5)	0.0008 (5)
C3	0.0444 (8)	0.0524 (8)	0.0394 (7)	−0.0066 (6)	0.0072 (6)	0.0027 (6)
C4	0.0422 (8)	0.0694 (11)	0.0506 (9)	0.0012 (8)	0.0087 (7)	0.0020 (8)
C5	0.0483 (9)	0.0537 (9)	0.0481 (8)	0.0065 (7)	0.0028 (7)	−0.0023 (7)
C6	0.0422 (7)	0.0455 (7)	0.0372 (7)	−0.0004 (6)	0.0001 (5)	0.0042 (6)
C7	0.0672 (12)	0.0723 (12)	0.0521 (10)	−0.0096 (10)	0.0148 (9)	0.0169 (9)
C8	0.0424 (7)	0.0424 (7)	0.0336 (6)	−0.0031 (6)	0.0037 (5)	0.0016 (5)
C9	0.0495 (8)	0.0476 (8)	0.0386 (7)	−0.0027 (7)	−0.0028 (6)	−0.0030 (6)
C10	0.0451 (8)	0.0518 (9)	0.0479 (8)	0.0012 (7)	−0.0050 (6)	0.0017 (7)
C11	0.0427 (8)	0.0445 (8)	0.0511 (9)	0.0010 (6)	0.0092 (6)	0.0007 (6)
C12	0.0588 (10)	0.0537 (9)	0.0391 (8)	0.0004 (7)	0.0056 (7)	−0.0091 (7)
C13	0.0551 (9)	0.0520 (8)	0.0325 (7)	0.0016 (7)	−0.0004 (6)	−0.0005 (6)
C14	0.0375 (7)	0.0493 (8)	0.0343 (6)	−0.0007 (6)	−0.0005 (5)	0.0051 (6)
C15	0.0362 (7)	0.0581 (9)	0.0409 (7)	−0.0034 (6)	0.0005 (6)	0.0019 (6)
C16	0.0412 (8)	0.0618 (10)	0.0426 (8)	0.0021 (7)	0.0041 (6)	−0.0010 (7)
C17	0.0483 (8)	0.0515 (8)	0.0390 (7)	−0.0007 (7)	−0.0041 (6)	0.0014 (6)
C18	0.0410 (8)	0.0619 (10)	0.0460 (8)	−0.0095 (7)	−0.0008 (6)	0.0019 (7)
C19	0.0377 (7)	0.0623 (9)	0.0411 (7)	−0.0036 (7)	0.0040 (6)	0.0005 (7)
C20	0.0470 (8)	0.0524 (8)	0.0403 (7)	−0.0112 (7)	0.0021 (6)	0.0020 (6)
C21	0.0476 (9)	0.0711 (12)	0.0520 (9)	−0.0169 (8)	−0.0033 (7)	0.0073 (8)

C22	0.0713 (13)	0.0596 (12)	0.0898 (15)	0.0170 (10)	−0.0029 (11)	0.0083 (11)
C23	0.0722 (13)	0.0694 (13)	0.0644 (12)	−0.0161 (10)	−0.0084 (10)	−0.0079 (10)
N1	0.0401 (6)	0.0442 (6)	0.0339 (6)	−0.0049 (5)	0.0004 (4)	0.0041 (5)
O1	0.0634 (9)	0.1290 (16)	0.1007 (13)	0.0277 (10)	0.0411 (9)	0.0362 (12)
O2	0.0584 (8)	0.0557 (7)	0.0731 (9)	0.0128 (6)	0.0013 (6)	−0.0073 (6)
O3	0.0603 (8)	0.0707 (8)	0.0546 (7)	−0.0054 (6)	−0.0020 (6)	−0.0160 (6)
O4	0.0647 (8)	0.0794 (9)	0.0541 (7)	−0.0250 (7)	−0.0019 (6)	0.0240 (6)

Geometric parameters (Å, °)

C2—N1	1.484 (2)	C12—H12	0.9300
C2—C8	1.517 (2)	C13—H13	0.9300
C2—C3	1.548 (2)	C14—C19	1.388 (2)
C2—H2	0.9800	C14—C15	1.401 (2)
C3—C4	1.508 (3)	C15—C16	1.370 (2)
C3—C7	1.524 (2)	C15—H15	0.9300
C3—H3	0.9800	C16—C17	1.393 (2)
C4—O1	1.204 (2)	C16—H16	0.9300
C4—C5	1.497 (3)	C17—O3	1.363 (2)
C5—C6	1.524 (2)	C17—C18	1.385 (2)
C5—H5A	0.9700	C18—C19	1.385 (2)
C5—H5B	0.9700	C18—H18	0.9300
C6—N1	1.476 (2)	C19—H19	0.9300
C6—C14	1.518 (2)	C20—O4	1.231 (2)
C6—H6	0.9800	C20—N1	1.361 (2)
C7—H7A	0.9600	C20—C21	1.500 (2)
C7—H7B	0.9600	C21—H21A	0.9600
C7—H7C	0.9600	C21—H21B	0.9600
C8—C9	1.382 (2)	C21—H21C	0.9600
C8—C13	1.393 (2)	C22—O2	1.423 (3)
C9—C10	1.395 (2)	C22—H22A	0.9600
C9—H9	0.9300	C22—H22B	0.9600
C10—C11	1.383 (2)	C22—H22C	0.9600
C10—H10	0.9300	C23—O3	1.412 (2)
C11—O2	1.364 (2)	C23—H23A	0.9600
C11—C12	1.386 (2)	C23—H23B	0.9600
C12—C13	1.374 (2)	C23—H23C	0.9600
N1—C2—C8	113.64 (11)	C12—C13—C8	121.16 (15)
N1—C2—C3	111.30 (12)	C12—C13—H13	119.4
C8—C2—C3	108.53 (12)	C8—C13—H13	119.4
N1—C2—H2	107.7	C19—C14—C15	117.00 (14)
C8—C2—H2	107.7	C19—C14—C6	124.42 (14)
C3—C2—H2	107.7	C15—C14—C6	118.54 (13)
C4—C3—C7	112.50 (15)	C16—C15—C14	121.79 (15)
C4—C3—C2	112.73 (14)	C16—C15—H15	119.1
C7—C3—C2	111.22 (14)	C14—C15—H15	119.1
C4—C3—H3	106.6	C15—C16—C17	120.22 (15)
C7—C3—H3	106.6	C15—C16—H16	119.9
C2—C3—H3	106.6	C17—C16—H16	119.9

O1—C4—C5	121.18 (18)	O3—C17—C18	125.19 (15)
O1—C4—C3	122.86 (17)	O3—C17—C16	115.65 (15)
C5—C4—C3	115.95 (14)	C18—C17—C16	119.16 (15)
C4—C5—C6	114.36 (14)	C19—C18—C17	119.90 (15)
C4—C5—H5A	108.7	C19—C18—H18	120.0
C6—C5—H5A	108.7	C17—C18—H18	120.0
C4—C5—H5B	108.7	C18—C19—C14	121.92 (15)
C6—C5—H5B	108.7	C18—C19—H19	119.0
H5A—C5—H5B	107.6	C14—C19—H19	119.0
N1—C6—C14	112.45 (12)	O4—C20—N1	121.10 (15)
N1—C6—C5	108.57 (12)	O4—C20—C21	119.84 (15)
C14—C6—C5	116.89 (13)	N1—C20—C21	119.07 (14)
N1—C6—H6	106.1	C20—C21—H21A	109.5
C14—C6—H6	106.1	C20—C21—H21B	109.5
C5—C6—H6	106.1	H21A—C21—H21B	109.5
C3—C7—H7A	109.5	C20—C21—H21C	109.5
C3—C7—H7B	109.5	H21A—C21—H21C	109.5
H7A—C7—H7B	109.5	H21B—C21—H21C	109.5
C3—C7—H7C	109.5	O2—C22—H22A	109.5
H7A—C7—H7C	109.5	O2—C22—H22B	109.5
H7B—C7—H7C	109.5	H22A—C22—H22B	109.5
C9—C8—C13	117.92 (14)	O2—C22—H22C	109.5
C9—C8—C2	120.72 (13)	H22A—C22—H22C	109.5
C13—C8—C2	121.08 (13)	H22B—C22—H22C	109.5
C8—C9—C10	121.57 (15)	O3—C23—H23A	109.5
C8—C9—H9	119.2	O3—C23—H23B	109.5
C10—C9—H9	119.2	H23A—C23—H23B	109.5
C11—C10—C9	119.29 (15)	O3—C23—H23C	109.5
C11—C10—H10	120.4	H23A—C23—H23C	109.5
C9—C10—H10	120.4	H23B—C23—H23C	109.5
O2—C11—C10	124.80 (16)	C20—N1—C6	117.40 (12)
O2—C11—C12	115.53 (15)	C20—N1—C2	122.17 (12)
C10—C11—C12	119.67 (15)	C6—N1—C2	120.00 (11)
C13—C12—C11	120.36 (15)	C11—O2—C22	117.96 (15)
C13—C12—H12	119.8	C17—O3—C23	118.00 (16)
C11—C12—H12	119.8		
N1—C2—C3—C4	44.06 (17)	N1—C6—C14—C15	55.01 (18)
C8—C2—C3—C4	169.83 (13)	C5—C6—C14—C15	−178.42 (14)
N1—C2—C3—C7	171.48 (14)	C19—C14—C15—C16	0.5 (2)
C8—C2—C3—C7	−62.75 (17)	C6—C14—C15—C16	178.40 (15)
C7—C3—C4—O1	11.1 (3)	C14—C15—C16—C17	0.0 (3)
C2—C3—C4—O1	137.8 (2)	C15—C16—C17—O3	179.61 (15)
C7—C3—C4—C5	−168.74 (16)	C15—C16—C17—C18	−0.4 (3)
C2—C3—C4—C5	−42.0 (2)	O3—C17—C18—C19	−179.75 (16)
O1—C4—C5—C6	173.8 (2)	C16—C17—C18—C19	0.3 (3)
C3—C4—C5—C6	−6.4 (2)	C17—C18—C19—C14	0.3 (3)
C4—C5—C6—N1	50.56 (19)	C15—C14—C19—C18	−0.7 (2)
C4—C5—C6—C14	−77.90 (18)	C6—C14—C19—C18	−178.39 (15)
N1—C2—C8—C9	−124.80 (15)	O4—C20—N1—C6	8.9 (2)

C3—C2—C8—C9	110.81 (16)	C21—C20—N1—C6	−171.52 (15)
N1—C2—C8—C13	61.28 (18)	O4—C20—N1—C2	−178.67 (15)
C3—C2—C8—C13	−63.11 (17)	C21—C20—N1—C2	1.0 (2)
C13—C8—C9—C10	0.3 (2)	C14—C6—N1—C20	−105.61 (16)
C2—C8—C9—C10	−173.76 (14)	C5—C6—N1—C20	123.47 (15)
C8—C9—C10—C11	1.5 (2)	C14—C6—N1—C2	81.74 (16)
C9—C10—C11—O2	177.08 (16)	C5—C6—N1—C2	−49.18 (18)
C9—C10—C11—C12	−2.1 (2)	C8—C2—N1—C20	67.01 (18)
O2—C11—C12—C13	−178.30 (15)	C3—C2—N1—C20	−170.11 (14)
C10—C11—C12—C13	1.0 (3)	C8—C2—N1—C6	−120.70 (14)
C11—C12—C13—C8	0.9 (3)	C3—C2—N1—C6	2.18 (18)
C9—C8—C13—C12	−1.5 (2)	C10—C11—O2—C22	−10.6 (3)
C2—C8—C13—C12	172.55 (15)	C12—C11—O2—C22	168.60 (18)
N1—C6—C14—C19	−127.30 (16)	C18—C17—O3—C23	−5.4 (3)
C5—C6—C14—C19	−0.7 (2)	C16—C17—O3—C23	174.52 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O4^{i}	0.98	2.55	3.511 (2)	167
C5—H5B···Cg^{i}	0.97	2.70	3.634 (2)	162

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2.

Fig. 1

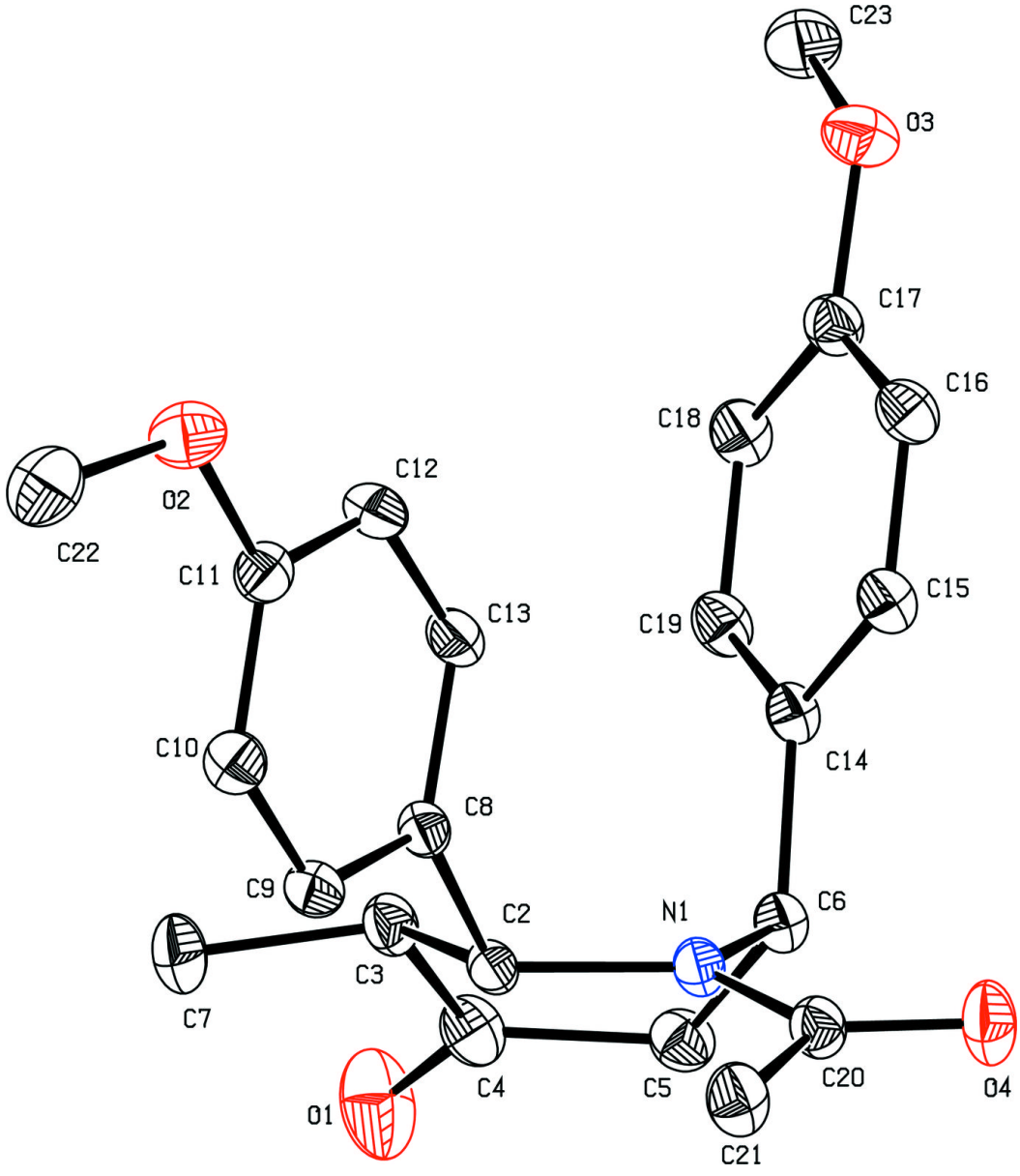
C23
O3
C17
C16
C18
C12
O2
C22
C11
C15
C13
C19
C10
C14
C8
C9
C2
N1
C6
C3
C7
C4
C5
C20
O4
O1
C21

Fig. 2