Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Methoxy-2-methylanilino)-1,2-diphenylethanone

Hakan Arslan,[a,b]* Oztekin Algul,[c] Selin Zirek,[c] Ozden Tari,[c] Aydın Demircan[d] and Kenneth I. Hardcastle[a]

[a]Department of Chemistry, Emory University, Atlanta, GA 30322, USA, [b]Department of Chemistry, Faculty of Arts and Science, Mersin University, Mersin, TR 33343, Turkey, [c]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mersin University, Mersin, TR 33169, Turkey, and [d]Department of Chemistry, Faculty of Arts and Sciences, Nigde University, Nigde, TR 51240, Turkey
Correspondence e-mail: hakan.arslan.acad@gmail.com

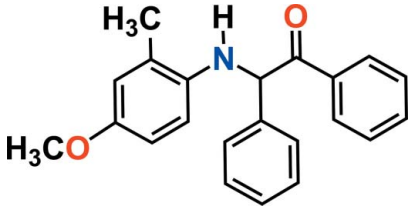
Received 26 April 2011; accepted 27 April 2011

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 18.2.

The title compound, $C_{22}H_{21}NO_2$, was synthesized from 4-methoxy-2-methylaniline and 2-hydroxy-1,2-diphenylethanone. In the title compound, the C—C—C—N—C backbone adopts an all-*trans* conformation. The crystal structure is stabilized by weak intermolecular C—H···O hydrogen-bond interactions.

Related literature

For the synthesis and similar structures, see: Au & Tafeenko (1986, 1987); Batsanov *et al.*, (2006). For general background to these structures, see: Batsanov *et al.* (2006); Abdulla *et al.* (1985). For bond-length data, see: Allen *et al.* (1987). For geometrical analysis, see: Bruno *et al.* (2002).



Experimental

Crystal data

$C_{22}H_{21}NO_2$
M_r = 331.40
Monoclinic, $P2_1/c$
a = 12.570 (12) Å
b = 8.009 (8) Å
c = 18.091 (17) Å
β = 100.544 (15)°
V = 1791 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 K
0.21 × 0.19 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.984, T_{max} = 0.988
28799 measured reflections
4122 independent reflections
2935 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 1.05
4122 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O1^{i}	0.95	2.48	3.352 (4)	153

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

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008), *OLEX2*, *publCIF* (Westrip, 2010) and *Mercury* (Macrae *et al.*, 2006).

This work was supported by the Mersin University Research Fund [Project No. BAP-SBE FK (SZ) 2008–8 YL].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5030).

References

Abdulla, R. F., Boyd, D. B., Jones, N. D. & Swartzendruber, J. K. (1985). *J. Org. Chem.* **50**, 3502–3505.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Au, O. & Tafeenko, V. (1986). *Rev. Cubana Quim.* **2**, 65–74.
Au, O. & Tafeenko, V. (1987). *Rev. Cubana Quim.* **3**, 79–86.
Batsanov, A. S., Goeta, A. E., Howard, J. A. K., Soto, B. & Au-Alvarez, O. (2006). *Acta Cryst.* C**62**, o304–o306.
Bruker (2008). *APEX2*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E**67**, o1303 [doi:10.1107/S1600536811015960]

2-(4-Methoxy-2-methylanilino)-1,2-diphenylethanone

Hakan Arslan, Oztekin Algul, Selin Zirek, Ozden Tari, Aydın Demircan and Kenneth I. Hardcastle

S1. Comment

A few 1-arylanilinoethanone derivatives have been structurally charactized because of their importance in synthesis or because of their interesting charge-transfer properties (Abdulla *et al.*, 1985). We found only four structurally similar compounds (Au & Tafeenko, 1987; Au & Tafeenko, 1986; Batsanov *et al.*, 2006) in the Cambridge Structural Database (CSD CONQUEST 1.11, B4; Bruno *et al.*, 2002).

Compound **I** was synthesized by the HCl acid-catalyzed reaction of a benzoin derivative to 4-methoxy-2-methylaniline (Scheme 1) resulting in the title compound, 2-((4-methoxy-2-methylphenyl)amino)-1,2-diphenylethanone, **I**, Figure 1, its structure was determined by X-ray crystallography.

The molecular structure of the title compound contains two phenyl rings and one substituted aniline ring connected by a –C(O)—C– linker. The dihedral angle between the two phenyl rings is 87.78 (7) ° and the dihedral angle between the substitute aniline and phenyl rings are 55.30 (7) and 84.57 (7) °, respectively. In adition, in the title compound, the C2—C1—C8—N1—C15 backbone adopts an all-*trans* conformation (Au & Tafeenko, 1987; Au & Tafeenko, 1986; Batsanov *et al.*, 2006).

The C—N bond lengths C8—N1 and C15—N1 are shorter than the normal C—N single-bond length of about 1.48 Å. The shortening of these C—N bonds reveals the effects of some conjugation in this part of the molecule. All other bond lengths fall within the expected ranges (Allen *et al.*, 1987).

Intramolecular hydrogen bonding N1–H1A···O1 with N–H 0.88 Å, H···O 2.22 Å, N–H···O 107 ° results in the formation of a five membered ring in the O1—C1—C8—N1–H1A plane. The crystal packing is dominated by weak intermolecular C11—H11A···O1 (x, 1 + y, z) hydrogen bonds, with H···O = 2.48 Å and a C—H···O angle of 153 ° (Figure 2).

S2. Experimental

A mixture of 4-methoxy-2-methylaniline (15 mmol), 2-hydroxy-1,2-diphenylethanone (5 mmol) and 1 ml conc. HCl in 20 ml of ethanol were refluxed for 5 h (Figure 3). After reaction was complete, the mixture was allowed to cool to room temperature, poured into cold water (20 ml) and finally extracted with CH_2Cl_2 (3x15 ml). The organic layer was dried over magnesium sulfate and the solvent removed under reduced pressure to yield a crude product that was purified by recrystallization in ethyl acetate. 2-((4-methoxy-2-methylphenyl)amino)-1,2-diphenylethanone: Yield: 1.20 g, 46%. *M*.p.: 110–112 °C. ^{1}H NMR (DMSO-d_6) δ: 8.18–8.16 (d, 2H, Ar—H (C3, C7)), 7.62 (t, 1H, Ar—H (C5)), 7.56–7.49 (m, 4H, Ar—H (C4, C6, C11, C13)), 7.30–7.26 (m, 2H, Ar—H (C10, C14)), 7.16 (t, 1H, Ar—H (C12)), 6.70–6.68 (d, *J*=4.8 Hz, 1H, Ar—H (C19)), 6.67 (s, 1H, Ar—H (C17)), 6.57–6.55 (d, *J*=8 Hz, 1H, Ar—H (C20)), 6.46–6.44 (d, *J*=8 Hz, 1H, Ar—H (C8)), 5.19–5.17 (d, *J*=8 Hz, 1H, NH), 3.60 (s, 3H, OCH_3), 2.22 (s, 3H, CH_3). ^{13}C NMR (400 MHz, p.p.m.) δ: 17.5 (CH_3), 55.1 (OCH_3), 61.5 (C8), 111.2 (C19), 112.5 (C20), 116.4 (C17), 123.9 (C16), 127.6, 128.1, 128.6, 128.7, 128.8 (C), 133.7 (C5), 134.7 (C2), 138.1 (C9), 138.3 (C15), 151.1 (C18), 197.6 (C9). Anal. Calc. for $C_{22}H_{21}NO_2$: C, 79.73; H, 6.39; N,

4.23%. Found: C, 79.70; H, 6.21; N, 4.19%.

S3. Refinement

H atom positions were clearly derived from difference Fourier maps and refined using a riding model, fixing the bond lengths at 0.98 and 0.95 Å for CH_3 and CH(aromatic), respectively. The displacement parameters of the H atoms were constrained with U_{iso}(H) = 1.2U_{eq} (C) or 1.5U_{eq} (methyl C).

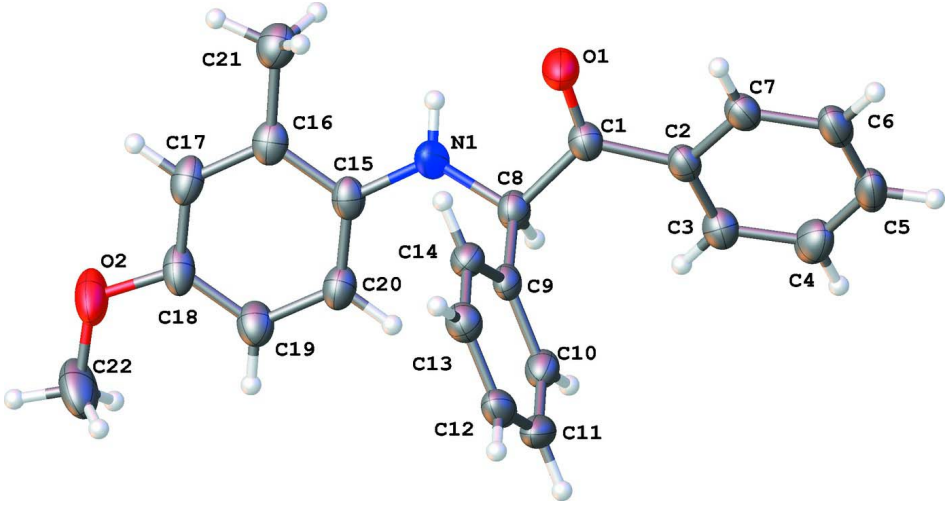


Figure 1

The molecular structure of (I), showing ellipsoids at the 50% probability level.

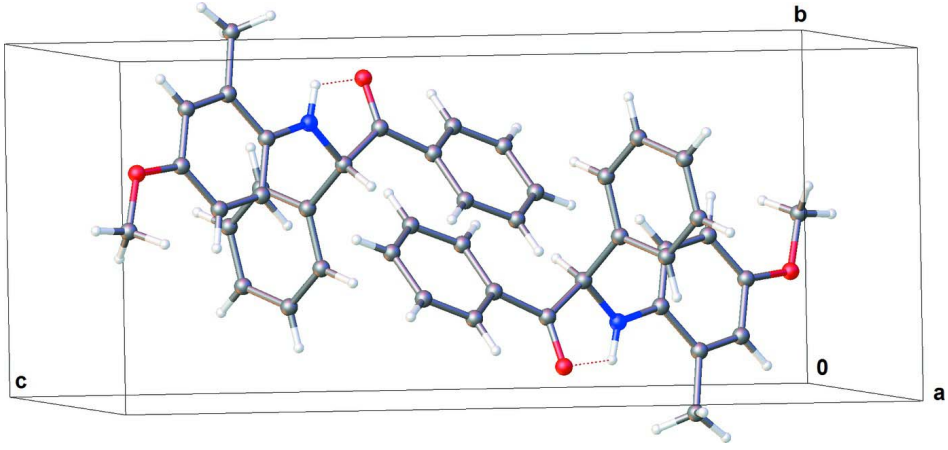


Figure 2

The molecular packing of (I). The hydrogen bonds are shown as dashed lines.

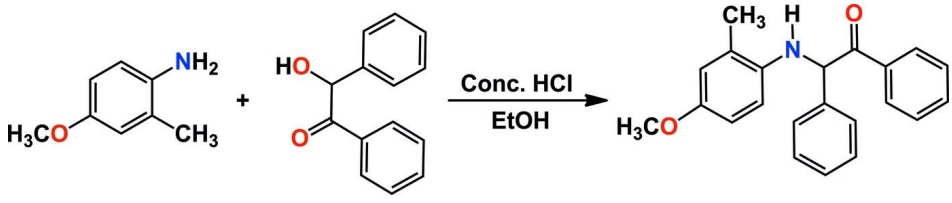


Figure 3

Synthesis of the title compound.

2-(4-Methoxy-2-methylanilino)-1,2-diphenylethanone

Crystal data

$C_{22}H_{21}NO_2$
M_r = 331.40
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 12.570 (12) Å
b = 8.009 (8) Å
c = 18.091 (17) Å
β = 100.544 (15)°
V = 1791 (3) Å^3
Z = 4
$F(000)$ = 704
D_x = 1.229 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4852 reflections
θ = 2.3–24.5°
μ = 0.08 mm^{-1}
T = 173 K
Block, yellow
0.21 × 0.19 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.984, T_{max} = 0.988
28799 measured reflections
4122 independent reflections
2935 reflections with $I > 2\sigma(I)$
R_{int} = 0.055
θ_{max} = 27.5°, θ_{min} = 1.7°
h = −16→16
k = −10→10
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 1.05
4122 reflections
226 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.4229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.004
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.70413 (11)	0.71666 (18)	0.13255 (8)	0.0336 (3)

C2	0.65511 (11)	0.79413 (17)	0.05905 (7)	0.0314 (3)
C3	0.70228 (12)	0.92642 (19)	0.02686 (8)	0.0380 (3)
H3A	0.7667	0.9764	0.0533	0.046*
C4	0.65510 (14)	0.9856 (2)	−0.04399 (8)	0.0453 (4)
H4A	0.6879	1.0748	−0.0662	0.054*
C5	0.56034 (14)	0.9144 (2)	−0.08206 (8)	0.0436 (4)
H5A	0.5286	0.9546	−0.1305	0.052*
C6	0.51179 (13)	0.7853 (2)	−0.05009 (8)	0.0420 (4)
H6A	0.4460	0.7385	−0.0761	0.050*
C7	0.55897 (12)	0.72392 (18)	0.01989 (8)	0.0361 (3)
H7A	0.5260	0.6339	0.0414	0.043*
C8	0.78651 (11)	0.81396 (18)	0.19059 (8)	0.0339 (3)
H8A	0.8385	0.8744	0.1644	0.041*
C9	0.72052 (11)	0.94044 (17)	0.22728 (7)	0.0297 (3)
C10	0.72302 (12)	1.11045 (18)	0.21167 (8)	0.0370 (3)
H10A	0.7685	1.1508	0.1790	0.044*
C11	0.65930 (13)	1.22179 (18)	0.24361 (9)	0.0421 (4)
H11A	0.6615	1.3376	0.2327	0.051*
C12	0.59250 (12)	1.16418 (19)	0.29135 (8)	0.0396 (4)
H12A	0.5489	1.2403	0.3129	0.048*
C13	0.58976 (12)	0.99566 (19)	0.30736 (8)	0.0378 (3)
H13A	0.5441	0.9557	0.3399	0.045*
C14	0.65372 (11)	0.88458 (18)	0.27584 (8)	0.0334 (3)
H14A	0.6519	0.7691	0.2875	0.040*
C15	0.91952 (11)	0.72896 (19)	0.30593 (8)	0.0330 (3)
C16	0.95263 (11)	0.59902 (19)	0.35825 (8)	0.0346 (3)
C17	1.02943 (11)	0.6351 (2)	0.42183 (8)	0.0393 (4)
H17A	1.0524	0.5485	0.4570	0.047*
C18	1.07393 (12)	0.7936 (2)	0.43580 (8)	0.0412 (4)
C19	1.04216 (12)	0.9204 (2)	0.38448 (8)	0.0409 (4)
H19A	1.0725	1.0289	0.3929	0.049*
C20	0.96492 (11)	0.88712 (19)	0.32004 (8)	0.0375 (3)
H20A	0.9429	0.9745	0.2851	0.045*
C21	0.90500 (13)	0.4262 (2)	0.34587 (9)	0.0442 (4)
H21A	0.9374	0.3535	0.3875	0.066*
H21B	0.9201	0.3810	0.2985	0.066*
H21C	0.8266	0.4318	0.3435	0.066*
C22	1.19345 (16)	0.9696 (3)	0.52047 (11)	0.0690 (6)
H22A	1.2440	0.9640	0.5686	0.103*
H22B	1.1358	1.0496	0.5244	0.103*
H22C	1.2322	1.0058	0.4810	0.103*
N1	0.84386 (10)	0.69119 (16)	0.24129 (7)	0.0412 (3)
H1A	0.8302	0.5852	0.2308	0.049*
O1	0.67637 (9)	0.57676 (13)	0.14827 (6)	0.0477 (3)
O2	1.14758 (10)	0.80923 (17)	0.50230 (6)	0.0612 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0331 (7)	0.0372 (8)	0.0294 (7)	−0.0008 (6)	0.0026 (6)	−0.0002 (6)
C2	0.0323 (7)	0.0345 (8)	0.0264 (7)	0.0029 (6)	0.0024 (6)	−0.0041 (6)
C3	0.0388 (8)	0.0420 (8)	0.0318 (8)	−0.0004 (7)	0.0030 (6)	−0.0009 (6)
C4	0.0585 (10)	0.0449 (9)	0.0338 (8)	0.0049 (8)	0.0114 (7)	0.0045 (7)
C5	0.0558 (10)	0.0458 (9)	0.0256 (7)	0.0141 (8)	−0.0022 (7)	−0.0025 (6)
C6	0.0435 (9)	0.0450 (9)	0.0326 (8)	0.0067 (7)	−0.0062 (7)	−0.0089 (7)
C7	0.0386 (8)	0.0360 (8)	0.0318 (7)	0.0014 (6)	0.0013 (6)	−0.0056 (6)
C8	0.0314 (7)	0.0377 (8)	0.0299 (7)	−0.0001 (6)	−0.0013 (6)	0.0027 (6)
C9	0.0279 (7)	0.0321 (7)	0.0252 (7)	−0.0033 (6)	−0.0055 (5)	0.0023 (5)
C10	0.0399 (8)	0.0347 (8)	0.0331 (7)	−0.0082 (6)	−0.0024 (6)	0.0067 (6)
C11	0.0503 (9)	0.0265 (7)	0.0418 (8)	−0.0024 (7)	−0.0121 (7)	0.0012 (6)
C12	0.0401 (8)	0.0371 (8)	0.0362 (8)	0.0056 (7)	−0.0076 (7)	−0.0060 (6)
C13	0.0381 (8)	0.0399 (8)	0.0337 (7)	−0.0025 (7)	0.0023 (6)	−0.0008 (6)
C14	0.0373 (8)	0.0288 (7)	0.0314 (7)	−0.0032 (6)	−0.0006 (6)	0.0029 (6)
C15	0.0260 (7)	0.0444 (8)	0.0281 (7)	0.0042 (6)	0.0033 (5)	0.0017 (6)
C16	0.0279 (7)	0.0453 (9)	0.0315 (7)	0.0023 (6)	0.0084 (6)	0.0050 (6)
C17	0.0302 (7)	0.0542 (10)	0.0333 (8)	0.0001 (7)	0.0047 (6)	0.0151 (7)
C18	0.0297 (8)	0.0616 (10)	0.0295 (7)	−0.0071 (7)	−0.0016 (6)	0.0101 (7)
C19	0.0351 (8)	0.0499 (9)	0.0356 (8)	−0.0089 (7)	0.0011 (6)	0.0052 (7)
C20	0.0337 (8)	0.0445 (9)	0.0323 (7)	0.0018 (7)	0.0007 (6)	0.0082 (6)
C21	0.0437 (9)	0.0476 (9)	0.0407 (8)	−0.0011 (7)	0.0062 (7)	0.0079 (7)
C22	0.0614 (12)	0.0892 (15)	0.0463 (10)	−0.0308 (11)	−0.0170 (9)	0.0086 (10)
N1	0.0441 (7)	0.0359 (7)	0.0371 (7)	0.0081 (6)	−0.0094 (6)	−0.0035 (5)
O1	0.0572 (7)	0.0424 (6)	0.0380 (6)	−0.0124 (5)	−0.0057 (5)	0.0068 (5)
O2	0.0565 (7)	0.0759 (9)	0.0411 (6)	−0.0243 (7)	−0.0179 (6)	0.0195 (6)

Geometric parameters (Å, º)

C1—O1	1.2226 (19)	C12—H12A	0.9500
C1—C2	1.494 (2)	C13—C14	1.390 (2)
C1—C8	1.544 (2)	C13—H13A	0.9500
C2—C3	1.393 (2)	C14—H14A	0.9500
C2—C7	1.402 (2)	C15—C20	1.394 (2)
C3—C4	1.393 (2)	C15—N1	1.399 (2)
C3—H3A	0.9500	C15—C16	1.417 (2)
C4—C5	1.385 (2)	C16—C17	1.390 (2)
C4—H4A	0.9500	C16—C21	1.509 (2)
C5—C6	1.380 (2)	C17—C18	1.391 (2)
C5—H5A	0.9500	C17—H17A	0.9500
C6—C7	1.386 (2)	C18—O2	1.383 (2)
C6—H6A	0.9500	C18—C19	1.385 (2)
C7—H7A	0.9500	C19—C20	1.399 (2)
C8—N1	1.4443 (19)	C19—H19A	0.9500
C8—C9	1.535 (2)	C20—H20A	0.9500
C8—H8A	1.0000	C21—H21A	0.9800

C9—C10	1.392 (2)	C21—H21B	0.9800
C9—C14	1.395 (2)	C21—H21C	0.9800
C10—C11	1.393 (2)	C22—O2	1.422 (2)
C10—H10A	0.9500	C22—H22A	0.9800
C11—C12	1.389 (2)	C22—H22B	0.9800
C11—H11A	0.9500	C22—H22C	0.9800
C12—C13	1.382 (2)	N1—H1A	0.8800

O1—C1—C2	119.92 (13)	C12—C13—H13A	120.0
O1—C1—C8	119.27 (13)	C14—C13—H13A	120.0
C2—C1—C8	120.77 (13)	C13—C14—C9	120.87 (14)
C3—C2—C7	119.18 (14)	C13—C14—H14A	119.6
C3—C2—C1	123.38 (13)	C9—C14—H14A	119.6
C7—C2—C1	117.39 (13)	C20—C15—N1	122.87 (13)
C2—C3—C4	120.09 (15)	C20—C15—C16	119.00 (14)
C2—C3—H3A	120.0	N1—C15—C16	118.12 (14)
C4—C3—H3A	120.0	C17—C16—C15	118.33 (15)
C5—C4—C3	119.99 (16)	C17—C16—C21	120.70 (13)
C5—C4—H4A	120.0	C15—C16—C21	120.97 (14)
C3—C4—H4A	120.0	C16—C17—C18	122.38 (14)
C6—C5—C4	120.41 (15)	C16—C17—H17A	118.8
C6—C5—H5A	119.8	C18—C17—H17A	118.8
C4—C5—H5A	119.8	O2—C18—C19	125.58 (15)
C5—C6—C7	120.02 (15)	O2—C18—C17	115.06 (13)
C5—C6—H6A	120.0	C19—C18—C17	119.35 (14)
C7—C6—H6A	120.0	C18—C19—C20	119.34 (15)
C6—C7—C2	120.30 (15)	C18—C19—H19A	120.3
C6—C7—H7A	119.9	C20—C19—H19A	120.3
C2—C7—H7A	119.9	C15—C20—C19	121.61 (14)
N1—C8—C9	114.91 (13)	C15—C20—H20A	119.2
N1—C8—C1	106.44 (13)	C19—C20—H20A	119.2
C9—C8—C1	106.20 (12)	C16—C21—H21A	109.5
N1—C8—H8A	109.7	C16—C21—H21B	109.5
C9—C8—H8A	109.7	H21A—C21—H21B	109.5
C1—C8—H8A	109.7	C16—C21—H21C	109.5
C10—C9—C14	118.68 (13)	H21A—C21—H21C	109.5
C10—C9—C8	121.58 (13)	H21B—C21—H21C	109.5
C14—C9—C8	119.71 (13)	O2—C22—H22A	109.5
C9—C10—C11	120.40 (15)	O2—C22—H22B	109.5
C9—C10—H10A	119.8	H22A—C22—H22B	109.5
C11—C10—H10A	119.8	O2—C22—H22C	109.5
C12—C11—C10	120.28 (15)	H22A—C22—H22C	109.5
C12—C11—H11A	119.9	H22B—C22—H22C	109.5
C10—C11—H11A	119.9	C15—N1—C8	124.59 (13)
C13—C12—C11	119.71 (14)	C15—N1—H1A	117.7
C13—C12—H12A	120.1	C8—N1—H1A	117.7
C11—C12—H12A	120.1	C18—O2—C22	117.49 (13)
C12—C13—C14	120.05 (15)		

O1—C1—C2—C3	−160.36 (14)	C11—C12—C13—C14	0.1 (2)
C8—C1—C2—C3	22.1 (2)	C12—C13—C14—C9	−0.6 (2)
O1—C1—C2—C7	17.0 (2)	C10—C9—C14—C13	0.8 (2)
C8—C1—C2—C7	−160.60 (12)	C8—C9—C14—C13	−177.33 (12)
C7—C2—C3—C4	−1.2 (2)	C20—C15—C16—C17	0.0 (2)
C1—C2—C3—C4	176.15 (14)	N1—C15—C16—C17	178.73 (13)
C2—C3—C4—C5	0.9 (2)	C20—C15—C16—C21	179.37 (13)
C3—C4—C5—C6	0.3 (2)	N1—C15—C16—C21	−1.9 (2)
C4—C5—C6—C7	−1.3 (2)	C15—C16—C17—C18	0.4 (2)
C5—C6—C7—C2	1.0 (2)	C21—C16—C17—C18	−178.96 (14)
C3—C2—C7—C6	0.2 (2)	C16—C17—C18—O2	178.75 (13)
C1—C2—C7—C6	−177.25 (13)	C16—C17—C18—C19	−0.8 (2)
O1—C1—C8—N1	21.30 (18)	O2—C18—C19—C20	−178.70 (14)
C2—C1—C8—N1	−161.10 (12)	C17—C18—C19—C20	0.8 (2)
O1—C1—C8—C9	−101.58 (16)	N1—C15—C20—C19	−178.65 (14)
C2—C1—C8—C9	76.02 (16)	C16—C15—C20—C19	0.0 (2)
N1—C8—C9—C10	135.07 (14)	C18—C19—C20—C15	−0.4 (2)
C1—C8—C9—C10	−107.56 (15)	C20—C15—N1—C8	−14.1 (2)
N1—C8—C9—C14	−46.83 (17)	C16—C15—N1—C8	167.24 (13)
C1—C8—C9—C14	70.54 (15)	C9—C8—N1—C15	−57.18 (19)
C14—C9—C10—C11	−0.5 (2)	C1—C8—N1—C15	−174.41 (13)
C8—C9—C10—C11	177.64 (12)	C19—C18—O2—C22	1.2 (2)
C9—C10—C11—C12	−0.1 (2)	C17—C18—O2—C22	−178.33 (16)
C10—C11—C12—C13	0.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1	0.88	2.22	2.609 (3)	107
C11—H11*A*···O1^{i}	0.95	2.48	3.352 (4)	153

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