Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Methylpiperidin-1-yl)isobenzofuran-1(3*H*)-one

Orhan Büyükgüngör[a] and Mustafa Odabaşoğlu[b]*

[a]Department of Physics, Faculty of Arts & Science, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey, and [b]Department of Chemistry, Faculty of Arts & Science, Ondokuz Mayıs University, TR-55139 Kurupelit Samsun, Turkey

Correspondence e-mail: muodabas@omu.edu.tr

Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.141
Data-to-parameter ratio = 16.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

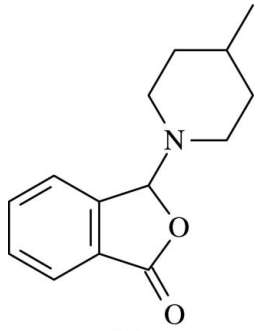
The crystal structure of the title compound, $C_{14}H_{17}NO_2$, is stabilized by three intermolecular C—H···O hydrogen bonds and one π–π interaction. C—H···O hydrogen bonds generate an edge-fused $[R_3^3(13)R_4^2(14)R_3^3(13)]$ ring motif.

Received 9 June 2006
Accepted 14 June 2006

3-Substituted phthalides, Part XII

Comment

The present work is part of a structural study of compounds of 3-substituted phthalides and we report here the structure of 3-(4-methylpiperidin-1-yl)isobenzofuran-1(3*H*)-one, (I) (Fig. 1).



(I)

The phthalide group (C1–C8/O2) is essentially planar, the largest deviation from the mean plane being 0.033 (1) Å for atom O2. The six-membered N1/C9–C13 ring has a chair conformation, as evidenced by the puckering parameters (Cremer & Pople, 1975) Φ_2 = 223 (4)°, Q_2 = 176.04 (3)° and Q_T = 0.564 (2) Å.

The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds (Table 1) and also by π–π interactions. The intermolecular C—H···O hydrogen bonds generate an

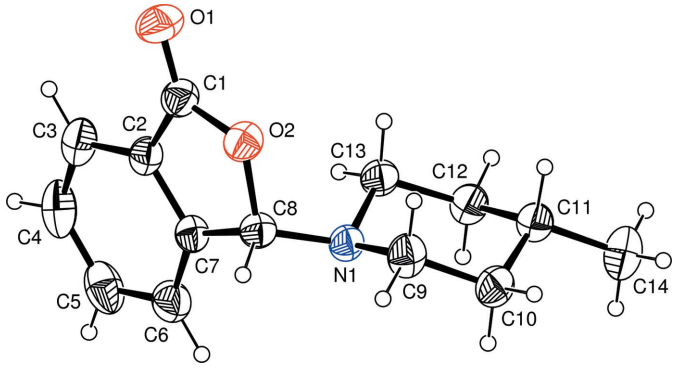


Figure 1
A view of (I), showing the atomic numbering scheme, with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as spheres of arbitrary radii.

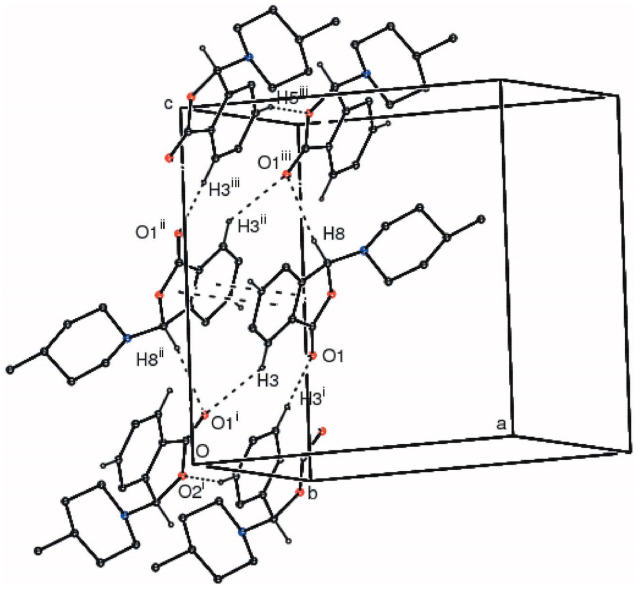


Figure 2
A packing diagram for (I), showing the N—H···O, C—H···π and π–π interactions, represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $-x$, $y+\frac{1}{2}$, $-z+\frac{1}{2}$; (ii) $-x$, $-y+1$, $-z+1$; (iii) x, $-y+\frac{3}{2}$, $z+\frac{1}{2}$.]

$[R_3^3(13)R_4^2(14)R_3^3(13)]$ ring motif (Etter, 1990). The π–π interaction occurs between the six- and five-membered rings of the phthalide system at $(-x, 2-y, -z)$, with a centroid-to-centroid distance of 3.6654 (14) Å and a plane-to-plane separation of 3.500 Å.

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006) using phthalaldehydic acid and 4-methylpiperidine as starting materials (yield 80%; m.p. 371–372 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a dimethylformamide solution at room temperature.

Crystal data

$C_{14}H_{17}NO_2$
M_r = 231.29
Monoclinic, $P2_1/c$
a = 12.7916 (11) Å
b = 8.0661 (11) Å
c = 12.3650 (11) Å
β = 90.266 (7)°
V = 1275.8 (2) Å^3
Z = 4
D_x = 1.204 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
Prism, colorless
0.62 × 0.49 × 0.33 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.954, T_{max} = 0.976
17106 measured reflections
2504 independent reflections
1663 reflections with $I > 2\sigma(I)$
R_{int} = 0.101
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.142
S = 1.10
2504 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.1775P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0097 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	0.93	2.58	3.314 (3)	136
C5—H5···O2^{ii}	0.93	2.55	3.449 (3)	162
C8—H8···O1^{iii}	0.98	2.53	3.479 (3)	164

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y-1, z$; (iii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

All H atoms were treated as riding on their parent atoms, with C—H = 0.93 Å for aromatic H atoms, 0.98 Å for methine H atoms and 0.97 Å for methylene H atoms [all U_{iso}(H) = 1.2U_{eq}(C)], and C—H = 0.96 Å for methyl H atoms [U_{iso}(H) = 1.5U_{eq}(C)].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS-2 diffractometer (purchased under grant F.279 of the University Research Fund).

References

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Odabaşoğlu, M. & Büyükgüngör, O. (2006). *Acta Cryst.* E**62**, o1879–o1881.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (2002). *X-AREA* (Version 1.18) and *X-RED32* (Version 1.04). Stoe & Cie, Darmstadt, Germany.