Acta Cryst. (1999). C**55**, 587-588

2-Benzoyl-1-naphthyl benzoate

KANDASAMY CHINNAKALI,[a]† HOONG-KUN FUN,[b] KAMARAJ SRIRAGHAVAN[c] AND VAYALAKKAVOOR T. RAMAKRISHNAN[c]

[a]Department of Physics, Anna University, Chennai 600 025, India, [b]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [c]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India. E-mail: hkfun@usm.my

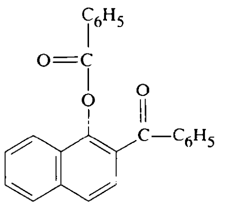
(*Received 17 November 1998; accepted 15 December 1998*)

Abstract

In the title compound, $C_{24}H_{16}O_3$, the naphthalene ring system is slightly distorted from planarity. The benzoyl and benzoate phenyl rings form dihedral angles of 58.22 (8) and 85.69 (6)°, respectively, with the attached benzene ring.

Comment

Naphthalene derivatives are widely used as intermediates in the synthesis of several polycyclic phenols which are useful antifibrillatory agents, disinfectants and water softeners (Hauck *et al.*, 1977). The 1,2-disubstituted derivatives of naphthalene are useful in the synthesis of the subunits of daunomycinone and adriamycin anticancer drugs (Crouse *et al.*, 1981). The crystal structure determination of the title compound, (I), was carried out in order to elucidate the molecular conformation.



(I)

The bond lengths observed in the naphthalene ring system are comparable with the reported mean values (Allen *et al.*, 1987), except for C8—C9 [1.454 (4) Å] and C5—C10 [1.450 (4) Å], which are slightly longer. The mean C—C distance in the phenyl rings is 1.379 (4) Å. The naphthalene ring system is nearly planar, with the fused benzene rings forming a dihedral angle of 3.26 (9)°. The benzene ring comprised of atoms C1–C4, C9 and C10 makes dihedral angles of 58.22 (8) and 85.69 (6)° with the benzoyl and benzoate phenyl rings, respectively. The conformation of the attachment of the benzoyl and benzoate substituents to the naphthyl ring system is better described by the torsion angles C3—C2—C11—C12 [−39.1 (3)] and C2—C1—O2—C18 [96.2 (2)°], respectively. The C2—C11—C12—C13 torsion angle [155.7 (2)°] shows how the benzoyl phenyl ring is oriented. In the solid state, the screw-related molecules are linked through weak C21—H21···O3($\frac{1}{2}-x$, $y-\frac{1}{2}$, $\frac{1}{2}-z$) hydrogen bonds.

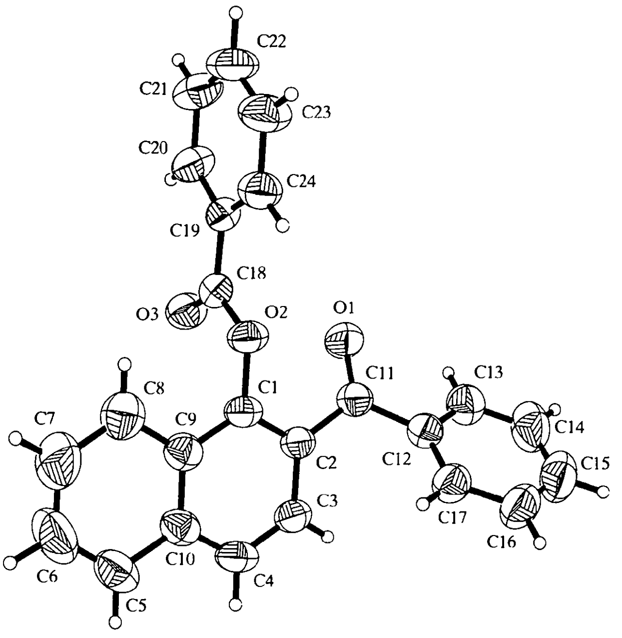


Fig. 1. The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

Treatment of 2-benzoyl-1-naphthol (0.5 g, 2 mmol) with benzoyl chloride (0.28 g, 2 mmol) in the presence of two equivalents of pyridine (0.31 g, 4 mmol) using dry benzene (50 ml) as a solvent provided the title compound.

Crystal data

$C_{24}H_{16}O_3$
$M_r = 352.37$
Monoclinic
$P2_1/n$
$a = 10.6629$ (4) Å
$b = 9.8546$ (4) Å
$c = 17.5982$ (8) Å
$\beta = 94.249$ (1)°
$V = 1844.11$ (13) Å^3
$Z = 4$
$D_x = 1.269$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 4068 reflections
$\theta = 2.99$–28.50°
$\mu = 0.083$ mm^{-1}
$T = 293$ (2) K
Parallelepiped
0.36 × 0.36 × 0.24 mm
Yellow

---

† Visiting Postdoctoral Fellow, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia.

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
12 365 measured reflections
4651 independent reflections
2922 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.045$
$\theta_{\rm max} = 28.5°$
$h = -14 \rightarrow 14$
$k = 0 \rightarrow 13$
$l = 0 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.180$
$S = 1.142$
4208 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 0.7524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.20$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 1997)
Extinction coefficient: 0.0040 (12)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected bond lengths (Å)*

O1—C11	1.221 (3)	C4—C10	1.402 (4)
O2—C18	1.364 (3)	C5—C6	1.388 (5)
O2—C1	1.407 (3)	C5—C10	1.450 (4)
O3—C18	1.199 (3)	C6—C7	1.376 (5)
C1—C2	1.378 (3)	C7—C8	1.406 (5)
C1—C9	1.402 (3)	C8—C9	1.454 (4)
C2—C3	1.410 (3)	C9—C10	1.412 (3)
C2—C11	1.493 (3)	C11—C12	1.495 (3)
C3—C4	1.364 (3)	C18—C19	1.479 (3)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···O3$^{\rm i}$	0.93	2.52	3.398 (4)	156

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

The data collection covered over a hemisphere of reciprocal space by a combination of three sets of exposures; each set had a different φ angle (0, 88 and 180°) for the crystal and each exposure of 10 s covered 0.3° in ω. The crystal-to-detector distance was 4 cm and the detector swing angle was −35°. Crystal decay was monitored by repeating 30 initial frames at the end of data collection and analysing the intensity of duplicate reflections, and was found to be negligible.

Data collection: *SMART* (Siemens, 1996). Cell refinement: *SAINT* (Siemens, 1996). Data reduction: *SAINT*. Program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997). Program(s) used to refine structure: *SHELXTL*. Molecular graphics: *SHELXTL*. Software used to prepare material for publication: *SHELXTL* and *PARST* (Nardelli, 1995).

The authors would like to thank the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 190-9609-2801. KC thanks the Universiti Sains Malaysia for a Visiting Postdoctoral Fellowship.

References

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.
Crouse, D. J., Hurlbut, S. L. & Wheeler, D. M. S. (1981). *J. Org. Chem.* **46**, 374–378.
Hauck, F. P., Cimarusti, C. M. & Sundeen, J. E. (1977). *Chem. Abstr.* **86**, 43447U.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (1997). *SHELXTL. Structure Determination Software Programs*. Version 5.10. Bruker Analytical X-ray Systems Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. *Area Detector Control and Integration Software*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1396). Services for accessing these data are described at the back of the journal.

Acta Cryst. (1999). C**55**, 588-590

2-Hydroxy-5-methyl-2-oxo-6-phenyl-4-phosphonomethyl-1,4,2-oxazoniaphosphorinane†

JEAN-FRANÇOIS SAINT-CLAIR,[a] FABRICE SIMÉON,[a] DIDIER VILLEMIN[a] AND MARIE-THÉRÈSE AVERBUCH-POUCHOT[b]

[a]*Ecole Nationale Supérieure d'Ingénieurs de Caen (ISMRA), Université de Caen, UMR CNRS 6507, 6 Boulevard du Maréchal Juin, 14050 Caen, France, and* [b]*LEDSS, UMR CNRS 5616, Université Joseph Fourier, BP53, 38041 Grenoble CEDEX 9, France. E-mail: marie-therese.averbuch@ujf-grenoble.fr*

(*Received 16 September 1998; accepted 3 December 1998*)

Abstract

The title compound, $C_{11}H_{17}NO_6P_2$, crystallizes as a racemic zwitterion in the space group $Pca2_1$. The molecules are interlinked by O—H···O and N—H···O hydrogen bonds.

Comment

Our ongoing investigation of aminophosphonates as supports for organic–inorganic materials (Ortiz-Avila *et al.*, 1994) led us to study procedures to prepare new achiral and chiral compounds of this kind. Moreover, these compounds are known either as analogues of natural amino acids exhibiting biological activities (Engel, 1977, 1987) or for their extraordinary chelating properties (Schwarzenbach *et al.*, 1948).

The main route to these compounds is a Mannich-type reaction first used by Fields (1952), but Moedritzer & Irani (1966) improved this reaction so that it proceeds almost quantitatively in most cases. Benzylamine

---

† Zwitterionic name: 5-methyl-2-oxido-2-oxo-6-phenyl-1,4,2-oxazoniaphosphorinan-4-ylmethylphosphonic acid.

Acta Crystallographica Section C
ISSN 0108-2701 © 1999