Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Nitrophenylimino)-1,2-diphenylethanone

Shao-Fa Sun,[a] Rong-Ming Ma[a] and Seik Weng Ng[b]*

[a]Department of Chemistry and Life Science, Xianning College, Xianning, Hubei 437005, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.059
wR factor = 0.160
Data-to-parameter ratio = 16.3

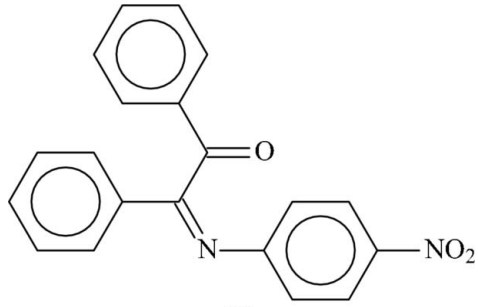
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 13 July 2006
Accepted 14 July 2006

The O═C—C═N sequence of atoms in the title molecule [alternative name: 2,3-diphenyl-4-(4-nitrophenyl)-1-oxa-4-azabutadiene], $C_{20}H_{14}N_2O_3$, adopts a *gauche* conformation, with an O═C—C═N torsion angle of 88.9 (1)°.

Comment

Dibenzoyl condenses with a primary amine to form a mono-imino Schiff base such as, for example, 2-(phenylimino)-1,2-diphenylethanone, $(C_6H_5)C(=O)C(C_6H_5)(=NC_6H_5)$; this compound has a molecular structure which contributes to the understanding of *peri*-selectivity in cycloadditions. In this compound, the ═C═O and ═C═N— functional groups are almost perpendicular to each other [O═C—C═N torsion angle = 84.5 (2)°; Guner *et al.*, 2000].



(I)

In the title molecular structure, (I) (Fig. 1), the addition of an electron-withdrawing nitro substituent to the phenylimino unit does not lead to a change either in the C═N distance [1.277 (2) Å, compared with 1.278 (2) Å found in the parent molecule] or in the bond lengths and angles in other parts of the molecule, although the O═C—C═N torsion angle is slightly different [O1—C7—C8—N1 torsion angle = 88.9 (1)°].

Experimental

4-Nitroaniline (2.00 g, 14.5 mmol) and dibenzoyl (2.99 g, 14.2 mmol) were dissolved in ethanol (35 ml) along with formic acid (1 ml). The solution was refluxed for 6 h. The solvent was then removed and the pure product obtained upon recrystallization from a 1:1 ethanol–chloroform mixture (35 ml) in 80% yield. Crystals of (I) were grown from ethanol as solvent. CHN elemental analysis: calculated for $C_{20}H_{14}O_3N_2$: C 72.72, H 4.27, N 8.48%; found: C 72.68, H 4.19, N 8.60%.

Crystal data

$C_{20}H_{14}N_2O_3$
M_r = 330.33
Monoclinic, $P2_1/c$
a = 8.8265 (7) Å
b = 11.5590 (9) Å
c = 16.365 (1) Å
β = 101.323 (1)°
V = 1637.1 (2) Å^3
Z = 4
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 292 (2) K
Block, yellow
0.36 × 0.23 × 0.19 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
8569 measured reflections
3684 independent reflections
2574 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.160
S = 1.01
3684 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.086P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

H atoms were placed in calculated positions, with C—H 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), and were included in the refinement in the riding-model approximation.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

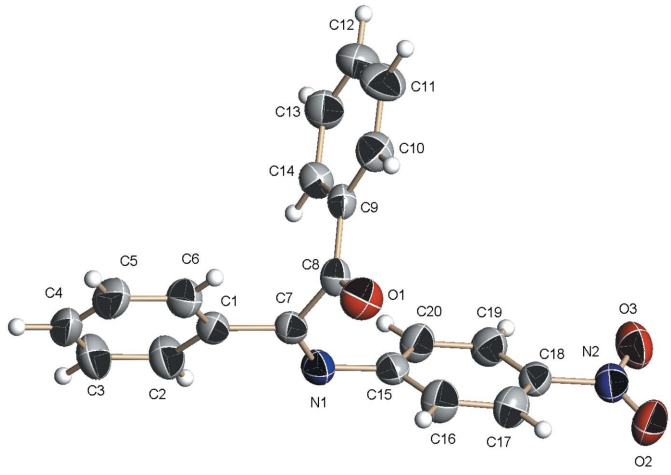


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

The authors thank Xianning College and the University of Malaya for supporting this study.

References

Bruker (2003). *SAINT* (Version 6.54a) and *SMART* (Version 6.54a). Bruker AXS Inc., Madison, Wisconsin, USA.
Guner, V., Kabak, M. & Elerman, Y. (2000). *J. Mol. Struct.* **526**, 151–157.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.