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N-(1,2-Diphenyl-2-oxoethylidene)-benzenamine *N*-oxide

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Key indicators

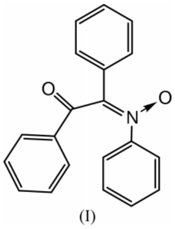
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.045
wR factor = 0.125
Data-to-parameter ratio = 18.6

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

The title compound, $C_{20}H_{15}NO_2$, crystallizes in a monoclinic unit cell with two independent molecules in the asymmetric unit. The configurations of three phenyl rings are determined by the sp^2 C and N atoms of the ethylideneamine group.

Comment

Nitrone compounds are important synthetic reagents for 1,3-dipolar cycloaddition reactions. Some nitrones are also good spin traps used in electron spin resonance (ESR) experiments. The title nitrone compound was prepared in order to examine the mechanism of formation of the *N*,*N*-dibenzoylaniline product in the photo-induced reactions of nitroarenes with diphenylacetylene (Tian & Xu, 2003). We report here the results of an X-ray crystallographic analysis of the title compound, (I), which was undertaken to establish its configuration.



(I)

There are two molecules *A* and *B* in the asymmetric unit, and these are related by a local pseudo-twofold rotation axis (Fig. 1). The bond lengths and angles of both molecules *A* and *B* (Fig. 1) agree with each other, and are within normal ranges (Allen *et al.*, 1987).

In both molecules, the configurations of the three phenyl rings are determined by the sp^2 state of atoms of the ethylideneamine group (C7, C8 and N1). The oxide atom O2 lies in the C7/C8/N1 plane. The phenyl rings attached at atoms C7, C8 and N1 make dihedral angles of 75.2 (1), 35.3 (1) and 64.3 (1)°, respectively, with the ethylideneamine plane in molecule *A*, and 78.0 (1), 35.7 (1) and 65.8 (1)° in molecule *B*. The phenyl rings attached at C8 and N1 are nearly orthogonal to each other, with dihedral angles of 80.6 (1) and 78.8 (1)° in molecules *A* and *B*, respectively.

In the benzoyl moiety, the carbonyl group (C7═O1) is twisted out of the plane of the aromatic ring, so that atom O1 deviates by 0.572 (1) and 0.490 (1) Å in molecules *A* and *B*, respectively. The C6/C7/C8/O1 plane makes an angle of 23.1 (1) and 27.4 (1)° in molecules *A* and *B*, respectively. The twist angles of the carbonyl group in this compound are comparable to that in the another benzoyl derivative [22.1 (1)°; Usman *et al.*, 2001].

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Experimental

The title compound was prepared by the oxidation of the corresponding imine with *m*-chloroperbenzoic acid in chloroform, and was isolated by column chromatography on silica gel with petroleum ether–ethyl acetate as eluants. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

Crystal data

$C_{20}H_{15}NO_2$
$M_r = 301.33$
Monoclinic, $P2_1/c$
$a = 11.2399\ (5)$ Å
$b = 14.7231\ (7)$ Å
$c = 19.6858\ (9)$ Å
$\beta = 105.754\ (1)^\circ$
$V = 3135.4\ (2)$ Å^3
$Z = 8$

$D_x = 1.277$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7892 reflections
$\theta = 2.3$–28.3°
$\mu = 0.08$ mm^{-1}
$T = 293\ (2)$ K
Block, light yellow
$0.46 \times 0.42 \times 0.38$ mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.963$, $T_{\max} = 0.969$
19 495 measured reflections

7725 independent reflections
5330 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 28.3^\circ$
$h = -14 \rightarrow 13$
$k = -19 \rightarrow 13$
$l = -24 \rightarrow 26$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.125$
$S = 1.02$
7725 reflections
415 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.567P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1*A*—C7*A*	1.2109 (15)	O1*B*—C7*B*	1.2135 (16)
O2*A*—N1*A*	1.2848 (14)	O2*B*—N1*B*	1.2893 (15)
N1*A*—C8*A*	1.3160 (16)	N1*B*—C8*B*	1.3151 (18)
C7*A*—C8*A*	1.5114 (17)	C7*B*—C8*B*	1.5206 (19)
O2*A*—N1*A*—C8*A*—C7*A*	175.77 (13)	O2*B*—N1*B*—C8*B*—C7*B*	177.04 (14)

All H atoms were geometrically fixed and treated as riding on their parent C atoms, with C—H distances of 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

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, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

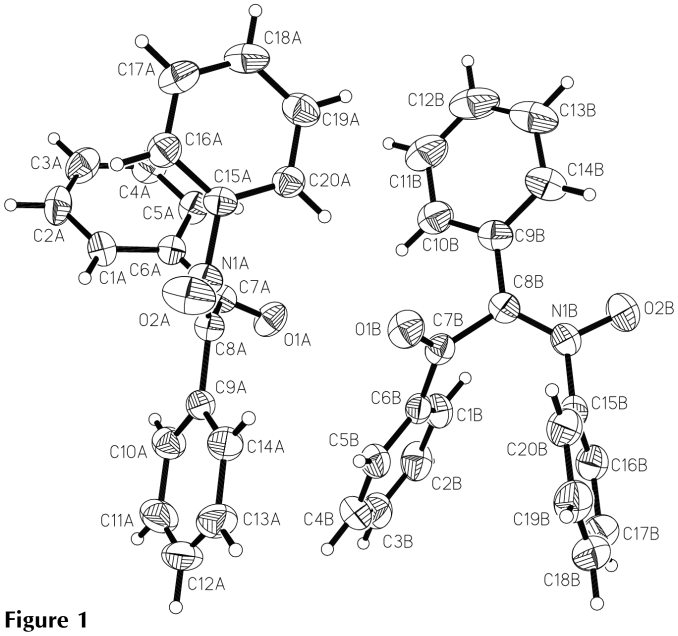

Figure 1
The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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