Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,2-Diphenyl-2-{[1-(quinoxalin-3-yl)propylidene]-hydrazono}ethanone

Qi-Kui Liu, Jian-Ping Ma, Ru-Qi Huang and Yu-Bin Dong*

College of Chemistry, Chemical, Engineering and Materials Science, Shandong Normal University, Jinan 250014, People's Republic of China

Correspondence e-mail: yubindong@sdnu.edu.cn

Received 8 March 2007
Accepted 9 April 2007

Key indicators

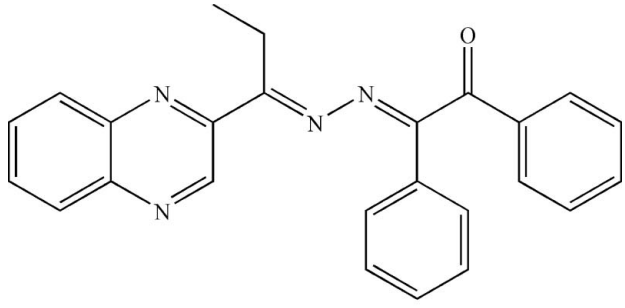
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.124
Data-to-parameter ratio = 13.3

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

The title compound, $C_{25}H_{20}N_4O$, has a non-planar molecular structure. The two benzene rings of the benzil unit make a dihedral angle of 83.64 (8)°.

Comment

Schiff base compounds have been used in preparing coordination polymers (Dong *et al.*, 2000). As part of our ongoing investigation of polymeric complexes (Dong *et al.*, 2005), we recently prepared the title compound, (I), involving a quinoxaline group, and have determined its crystal structure.



(I)

The molecular structure of (I) is shown in Fig. 1. The three aromatic ring systems in (I) are twisted relative to each other. The dihedral angle between the C13-benzene and C20-benzene rings is 83.64 (8)°, the angle between the C13-benzene and quinoxaline ring systems is 15.40 (4)°, and the angle between the C20-benzene and quinoxaline ring systems is 74.80 (5)°

Experimental

1-[1-(Quinoxalin-3-yl)propylidene]hydrazine (2.2 g, 10 mmol) was dissolved in ethanol (15 ml), followed by dropwise addition of benzil (2.1 g, 10 mmol) dissoled in ethanol (10 ml). After two drops of formic acid were added, the mixture was stirred at room temperature for 12 h. After removal of the solvent under vacuum, the residue was extracted with dichloromethane and washed with water several times. The organic phase was dried over $MgSO_4$ and filtered. Yellow crystals of (I) formed in about one week.

Crystal data

$C_{25}H_{20}N_4O$
M_r = 392.45
Monoclinic, $P2_1/c$
a = 8.1587 (18) Å
b = 13.703 (3) Å
c = 18.660 (4) Å
β = 99.991 (3)°
V = 2054.5 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.38 × 0.18 × 0.13 mm

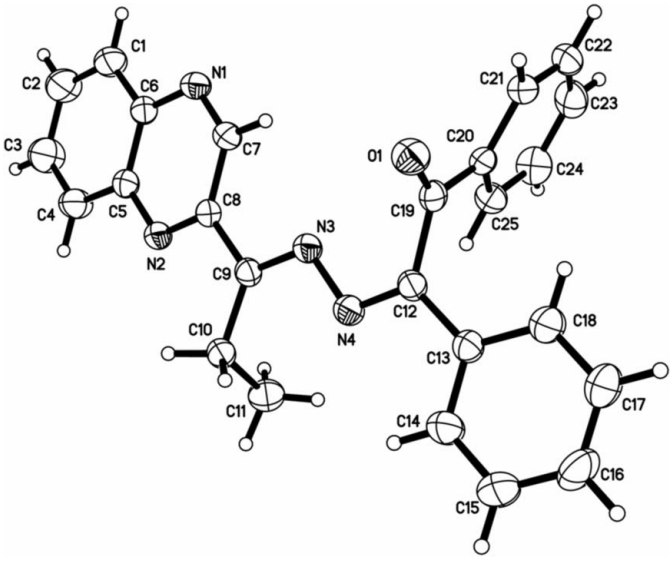


Figure 1
Molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms are drawn as small spheres of arbitrary radius.

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.990
10445 measured reflections
3617 independent reflections
2607 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.124
S = 1.02
3617 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

H atoms were included in calculated positions and refined as riding using a riding model with C—H = 0.93–0.97 Å. For aromatic ring systems and methylene groups U_{iso}(H) = 1.2U_{eq}(C); for methyl groups U_{iso}(H) = 1.5U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (Nos. 20671060, 20371030 and 20335030), and Shangdong Natural Science Foundation (Nos. Z2004B01, J06D05 and 2006BS04040) for support.

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