

2-(2,6-Diisopropylphenylamino)cyclohex-1-enyl  
phenyl ketoneGuo-Qiu Gui,<sup>a</sup> Feng Bao,<sup>a</sup>  
Xing-Qiang Lü,<sup>a</sup> Qing Wu<sup>a</sup> and  
Seik Weng Ng<sup>b\*</sup><sup>a</sup>School of Chemistry and Chemical Engineering,  
Sun Yat-Sen University, Guangzhou 510275,  
People's Republic of China, and <sup>b</sup>Department of  
Chemistry, University of Malaya, 50603 Kuala  
Lumpur, Malaysia

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

## Key indicators

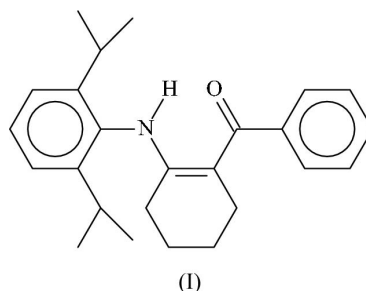
Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.130  
Data-to-parameter ratio = 9.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.The two independent molecules of the title compound,  
 $\text{C}_{25}\text{H}_{31}\text{NO}$ , are linked by a pair of weak hydrogen bonds  
across a non-crystallographic inversion center in the mono-  
clinic space group  $Cc$ .

Received 11 March 2005

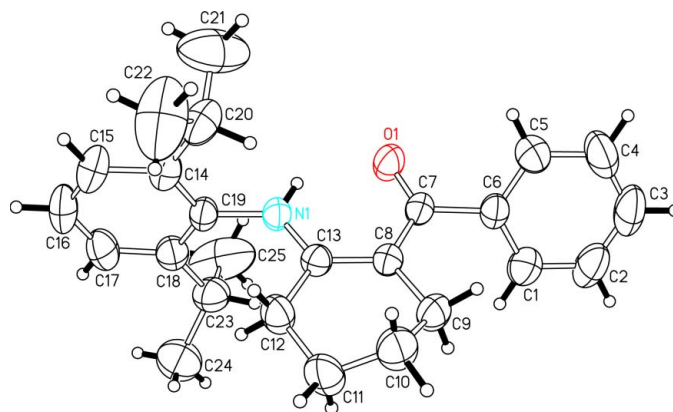
Accepted 14 March 2005

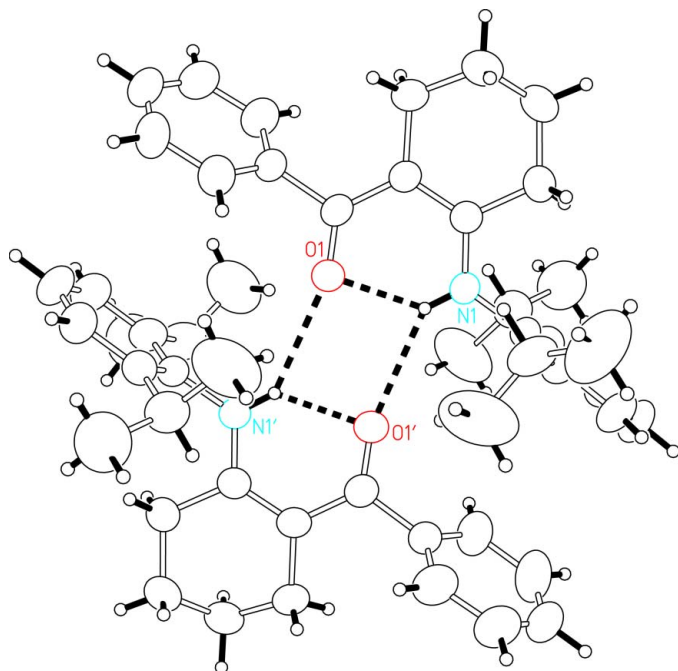
Online 25 March 2005

## Comment

A previous report (Gao *et al.*, 2005) describes the structure of  
a sterically crowded Schiff base; the compound features  
diisopropyl substituents in the 2,6-positions of the aromatic  
ring that is bonded to the imino N atom. The condensation of  
2,6-diisopropylphenylamine with 2-benzoylcyclohexanone  
probably yielded the expected Schiff base; however, the imine  
had isomerized to an amine, (I) (Fig. 1). The same amine was  
obtained even if the ratio of the amine reagent was raised to  
3:1. The two independent molecules are linked by a pair of  
weak hydrogen bonds across a non-crystallographic inversion  
center (Table 1 and Fig. 2).

## Experimental

2-Benzoylcyclohexanone (3.10 g, 0.015 mol), 2,6-diisopropylphenyl-  
amine (3.00 ml, 0.015 mol) and a catalytic amount of *p*-toluene-**Figure 1**  
ORTEP plot (Johnson, 1976) of one of the two independent molecules  
of (I). Displacement ellipsoids are drawn at the 50% probability level and  
H atoms are shown as spheres of arbitrary radii.



**Figure 2**  
ORTEP plot (Johnson, 1976) illustrating the arrangement of the two independent molecules across a non-crystallographic center of inversion.

sulfonic acid were heated in toluene (50 ml) in a Dean–Stark water separator. When the water was removed after about a day, the solvent was evaporated to give a product that was recrystallized from hexane in about 80% yield (m.p. 388 K). Elemental analysis calculated for  $C_{25}H_{31}NO$ : C 82.98, H 8.64, N 3.87%; found: C 82.86, H 8.76, N 3.75%.

#### Crystal data

$C_{25}H_{31}NO$   
 $M_r = 361.51$   
Monoclinic,  $Cc$   
 $a = 9.815$  (1) Å  
 $b = 23.404$  (3) Å  
 $c = 18.777$  (2) Å  
 $\beta = 92.002$  (2)°  
 $V = 4310.5$  (9) Å<sup>3</sup>  
 $Z = 8$

#### Data collection

Bruker SMART area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: none  
13505 measured reflections  
4703 independent reflections

$D_x = 1.114$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 946 reflections  
 $\theta = 1.7$ – $27.1$ °  
 $\mu = 0.07$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
Block, pale yellow  
0.50 × 0.48 × 0.45 mm

4021 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.015$   
 $\theta_{max} = 27.1$ °  
 $h = -12 \rightarrow 12$   
 $k = -29 \rightarrow 30$   
 $l = -23 \rightarrow 12$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.130$   
 $S = 1.03$   
4703 reflections  
487 parameters  
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0842P)^2 + 0.6097P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.27$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.14$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1n\cdots O1$	0.85	1.93	2.598 (2)	135
$N1-H1n\cdots O1'$	0.85	2.51	3.204 (3)	140
$N1'-H1'n\cdots O1'$	0.85	1.96	2.614 (3)	133
$N1'-H1'n\cdots O1$	0.85	2.51	3.206 (3)	140

In the absence of significant anomalous scattering effects, Friedel pairs were merged and the calculation of the Flack (1983) parameter was suppressed. The carbon-bound H atoms were placed at calculated positions ( $C-H = 0.93$  Å aromatic H atoms, 0.97 Å for methylene H atoms and 0.96 Å for methyl H atoms) and were included in the refinement in the riding-model approximation, with  $U_{iso}(H)$  values set at 1.2 times  $U_{eq}$  of the parent C atoms, except for the methyl H atoms, for which this was set at 1.5 times  $U_{eq}$ . The nitrogen-bound H atoms were similarly treated [ $N-H = 0.85$  Å and  $U_{iso}(H) = 1.2U_{eq}(N)$ ].

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP II* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

The authors thank Sun-Yat Sen University and the University of Malaya for supporting this study.

#### References

- Bruker (2001). *SAINTE* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.  
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
Gao, H.-Y., Lü, X.-Q., Bao, F., Wu, Q. & Ng, S. W. (2005). *Acta Cryst.* **E61**, o1068–o1069.  
Johnson, C. K. (1976). *ORTEP II*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.  
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.