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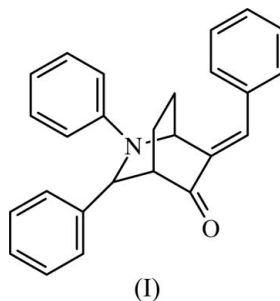
## Key indicators

Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.068  
 $wR$  factor = 0.145  
Data-to-parameter ratio = 13.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.6-[(*Z*)-Benzylidene]-2,3-diphenyl-2-azabicyclo[2.2.2]-octan-5-one

The title compound,  $\text{C}_{26}\text{H}_{23}\text{NO}$ , was obtained from the Diels–Alder reaction of *N*-benzylideneaniline and cyclohexen-2-one catalyzed by zirconium tetrachloride. The molecule is the *Z* isomer. All three six-membered rings in the 2-azabicyclo[2.2.2]octane system adopt the expected boat conformation. In the crystal packing, the phenyl groups are aggregated in hydrophobic layers at  $y = 0$  and  $\frac{1}{2}$ .

## Comment

Recently, we have published structures of 2-azabicyclo[2.2.2]octane derivatives (Ravikumar *et al.*, 2005*a,b*). In continuation of this work, we report here the crystal structure of the title compound (I).



In all essential details, the molecular geometry of (I) (Table 1 and Fig. 1) is in good agreement with that of similar structures (Shi & Xu, 2001; Shi *et al.*, 2002). The present structure is the *Z* isomer, as shown by the C5–C6–C21–C22 torsion angle of  $175.3(2)^\circ$ . As observed in the previous structures, the C1–C6–C21 and C6–C21–C22 bond angles are distorted, as a consequence of double-bond strain.

As expected, all three six-membered rings of the azabicyclo[2.2.2] system adopt a boat conformation with puckering parameters (Cremer & Pople, 1975)  $q_2 = 0.828(3)^\circ$ ,  $q_3 = -0.003(2)^\circ$ ,  $Q_T = 0.828(3)^\circ$ ,  $\varphi_2 = -69.3(2)^\circ$  and  $\theta_2 = 90.2(2)^\circ$  for N2/C3/C4/C8/C7/C1;  $q_2 = 0.836(2)^\circ$ ,  $q_3 = 0.012(2)^\circ$ ,  $Q_T = 0.836(2)^\circ$ ,  $\varphi_2 = 171.7(2)^\circ$  and  $\theta_2 = 89.2(2)^\circ$  for C1/C7/C8/C4/C5/C6;  $q_2 = 0.819(3)^\circ$ ,  $q_3 = 0.007(2)^\circ$ ,  $Q_T = 0.819(3)^\circ$ ,  $\varphi_2 = 174.6(2)^\circ$  and  $\theta_2 = 89.5(2)^\circ$  for C1/C6/C5/C4/C3/N2.

In the absence of hydrogen-bond donating groups, the crystal packing is stabilized purely by van der Waals forces. The phenyl groups are aggregated in hydrophobic layers at  $y = 0$  and  $\frac{1}{2}$  (Fig. 2).

## Experimental

To a solution of *N*-benzylideneaniline (5.5 mmol) in  $\text{CH}_2\text{Cl}_2$  (5 ml) at room temperature were sequentially added  $\text{ZrCl}_4$  (10 mol%) and

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cyclohexen-2-one (5.5 mmol), and the mixture was stirred for 6 h. After completion of the reaction as indicated by thin-layer chromatography, it was quenched with water; the mixture was diluted with  $\text{CH}_2\text{Cl}_2$  (20 ml) and washed with water (10 ml). The aqueous layer was extracted with  $\text{CH}_2\text{Cl}_2$  ( $2 \times 10$  ml). The combined organic layers were dried over  $\text{Na}_2\text{SO}_4$  and concentrated *in vacuo* to yield a dark-brown residue, which was purified by column chromatography using 2–10% ethyl acetate in hexane as eluant.

#### Crystal data

$\text{C}_{26}\text{H}_{23}\text{NO}$	$D_x = 1.238 \text{ Mg m}^{-3}$
$M_r = 365.45$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3275 reflections
$a = 10.1554$ (9) Å	$\theta = 2.4\text{--}21.4^\circ$
$b = 16.5088$ (15) Å	$\mu = 0.08 \text{ mm}^{-1}$
$c = 11.7903$ (11) Å	$T = 273$ (2) K
$\beta = 97.154$ (2)°	Block, colorless
$V = 1961.3$ (3) Å <sup>3</sup>	$0.21 \times 0.13 \times 0.08 \text{ mm}$
$Z = 4$	

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer	2759 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.043$
Absorption correction: none	$\theta_{\text{max}} = 25.0^\circ$
18504 measured reflections	$h = -12 \rightarrow 12$
3437 independent reflections	$k = -19 \rightarrow 19$
	$l = -14 \rightarrow 13$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.6492P]$
$R[F^2 > 2\sigma(F^2)] = 0.068$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.145$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.18$	$\Delta\rho_{\text{max}} = 0.18 \text{ e \AA}^{-3}$
3437 reflections	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
253 parameters	
H-atom parameters constrained	

**Table 1**

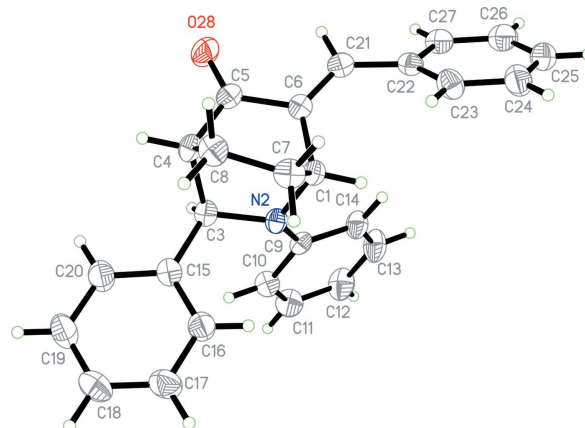
Selected geometric parameters (Å, °).

C5–O28	1.220 (3)	C6–C21	1.329 (3)
C21–C6–C1	129.5 (2)	C6–C21–C22	129.9 (2)

H atoms were included in calculated positions and refined as riding, with C–H distances in the range 0.93–0.98 Å and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

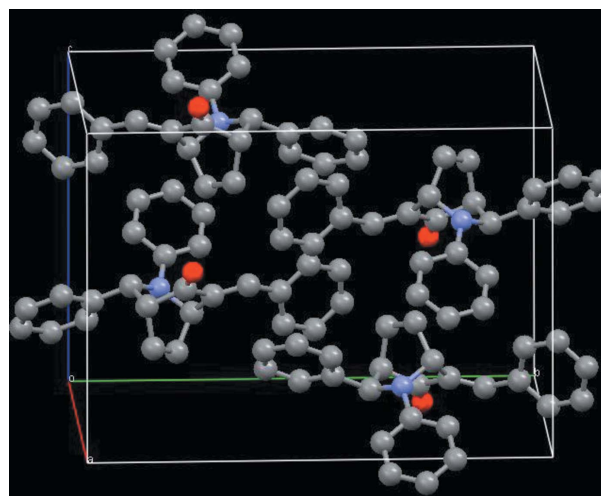
Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990) and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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**Figure 1**

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.



**Figure 2**

A packing diagram for (I), viewed approximately down the  $a$  axis. H atoms have been omitted for clarity.

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