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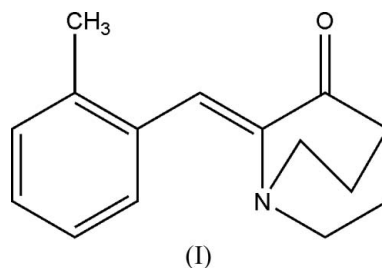
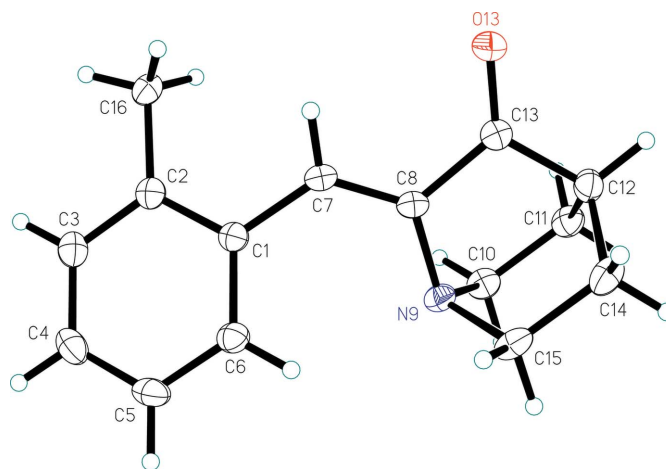
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Key indicators

Single-crystal X-ray study
 $T = 90\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.039
 wR factor = 0.107
Data-to-parameter ratio = 17.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(Z)-2-(2-Methylbenzylidene)-1-azabicyclo-
[2.2.2]octan-3-one**The title compound, $\text{C}_{15}\text{H}_{17}\text{NO}$, has been synthesized by base-catalyzed condensation of 2-methylbenzaldehyde with 1-azabicyclo[2.2.2]octan-3-one and crystallization of the product with ethyl acetate. The geometry around the $\text{C}=\text{C}$ bond is *Z*.Received 6 November 2006
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Comment

The title compound, (I), was prepared by base-catalyzed condensation of 2-methylbenzaldehyde with 1-azabicyclo[2.2.2]octan-3-one and the product was crystallized from ethyl acetate to afford a single geometrical isomer. The present X-ray crystallographic determination was carried out in order to determine both the geometry and the conformation of the molecule.

Fig. 1 shows a view of (I) and selected geometric parameters are presented in Table 1. The C1—C7 bond is in a *trans* disposition with respect to the C8—C13 bond. Deviations from ideal bond-angle geometry around the Csp^2 atoms of the double bonds are observed. The bond angles N9—C8—C13,**Figure 1**

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

C7=C8–N9 and C8=C7–C1 (Table 1) are distorted because of the steric hindrance of the double bond linking the 2-methylphenyl ring with the azabicyclic moiety. These deviations significantly contribute to the relief of the intramolecular non-bonded interactions present in this portion of the molecule. The C6–C1–C7=C8 torsion angle indicates the deviation of the double bond from the plane of the benzene ring. However, the C1–C7 bond length suggests conjugation of the C7=C8 bond π electrons with those of the 2-methylphenyl ring (Wilson, 1992).

Experimental

The title compound was prepared according to the previously reported procedure of Sonar *et al.* (2003). Crystallization from ethyl acetate afforded yellow crystals.

Crystal data

C ₁₅ H ₁₇ NO	$Z = 4$
$M_r = 227.30$	$D_x = 1.285 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 6.6514 (1) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 22.3378 (5) \text{ \AA}$	$T = 90.0 (2) \text{ K}$
$c = 8.0734 (2) \text{ \AA}$	Block, yellow
$\beta = 101.6068 (10)^\circ$	$0.32 \times 0.28 \times 0.28 \text{ mm}$
$V = 1175.00 (4) \text{ \AA}^3$	

Data collection

Nonius KappaCCD diffractometer	4984 measured reflections
ω scans	2688 independent reflections
Absorption correction: multi-scan (SCALEPACK; Otwinowski & Minor, 1997)	2099 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.975$, $T_{\max} = 0.978$	$R_{\text{int}} = 0.021$
	$\theta_{\max} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 0.2705P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.04$	$\Delta\rho_{\max} = 0.28 \text{ e \AA}^{-3}$
2688 reflections	$\Delta\rho_{\min} = -0.20 \text{ e \AA}^{-3}$
155 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1–C7	1.4678 (16)	C8–C13	1.4966 (16)
C2–C16	1.5029 (16)	N9–C10	1.4826 (15)
C7–C8	1.3374 (16)	O13–C13	1.2194 (14)
C8–N9	1.4427 (14)		
C1–C2–C16	121.44 (10)	C8–N9–C10	108.50 (9)
C8–C7–C1	127.53 (11)	O13–C13–C8	124.44 (11)
C7–C8–N9	124.50 (10)	O13–C13–C12	125.28 (11)
C7–C8–C13	121.91 (11)	C8–C13–C12	110.24 (10)
N9–C8–C13	113.53 (10)		
C6–C1–C7–C8	34.30 (18)	C7–C8–C13–O13	–2.39 (18)
C1–C7–C8–C13	177.27 (10)		

H atoms were found in difference Fourier maps and subsequently placed in idealized positions with constrained C–H distances of 1.00 \AA ($R_3\text{CH}$), 0.99 \AA ($R_2\text{CH}_2$), 0.98 \AA ($R\text{CH}_3$) and 0.95 \AA (C_{sp^2}). $U_{\text{iso}}(\text{H})$ values were set to either 1.5 U_{eq} of the attached C atom (CH_3) or 1.2 U_{eq} for all other H atoms.

Data collection: COLLECT (Nonius, 1999); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: DENZO-SMN (Otwinowski & Minor, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL (Sheldrick, 1995); software used to prepare material for publication: SHELXL97 (Sheldrick, 1997) and local procedures.

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