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s_natarajan50@yahoo.com**Key indicators**

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.063

wR factor = 0.192

Data-to-parameter ratio = 14.8

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**3-Acetyl-2-(4-methylphenyl)cyclohex-2-en-1-one oxime**

In the title compound, $\text{C}_{15}\text{H}_{17}\text{NO}_2$, the six-membered cyclohexene ring has an envelope conformation. The structure is stabilized by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds and weak van der Waals interactions. There are no $\text{C}-\text{H}\cdots\pi$ or $\pi-\pi$ interactions between the two ring systems; however, there is an intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond.

Comment

Oximes and related compounds have found widespread use as drugs and pesticides and, as a result, are commonly encountered in the environment (Milne *et al.*, 1995). Oxidation of oximes can result in the formation of reactive oxygen species (ROS) such as iminoxyl radicals, which are deemed harmful to organisms (de Lijser *et al.*, 2002; Rosen *et al.*, 2002; Halliwell *et al.*, 1999). The X-ray crystal structure determination of the title compound, (I), was undertaken to study the influence of steric and electronic factors on the configuration and conformation of the substituents in the compound.

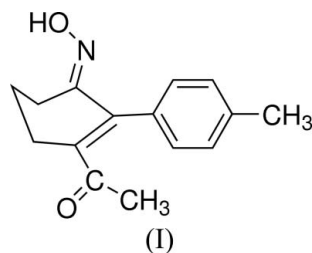


Fig. 1 shows the structure of (I), with the atom-numbering scheme. The present X-ray diffraction analysis indicates that the oxime six-membered ring is in an envelope conformation, with atom C5 deviating by $0.620(5) \text{ \AA}$ from the mean plane formed by the other C atoms (C1, C6, C4, C3 and C2). Intramolecular interactions determine the conformation of the oximino hydroxyl, the rotameric preference of the aryl ring and that of the acetyl group. In order to avoid $A^{1,3}$ strain between the hydroxyl group and the aryl ring, the hydroxyl function prefers an *anti* conformation with respect to the aryl substituent at C2. On the other hand, the *cis*-oriented acetyl and the aryl ring planes make a dihedral angle of $57.31(1)^\circ$. The substituted methylphenyl ring and the acetyl group are twisted by $60.0(1)$ and $43.4(2)^\circ$, respectively, from the mean plane formed by the C atoms (C1, C6, C4, C3 and C2). In spite of this, the geometrical parameters of the oxime fragment show standard values (Table 1) (Chertanova *et al.*, 1994).

Fig. 2 shows the packing of molecules of (I), viewed down the *a* axis. In the present structure, two cyclohexanone oxime

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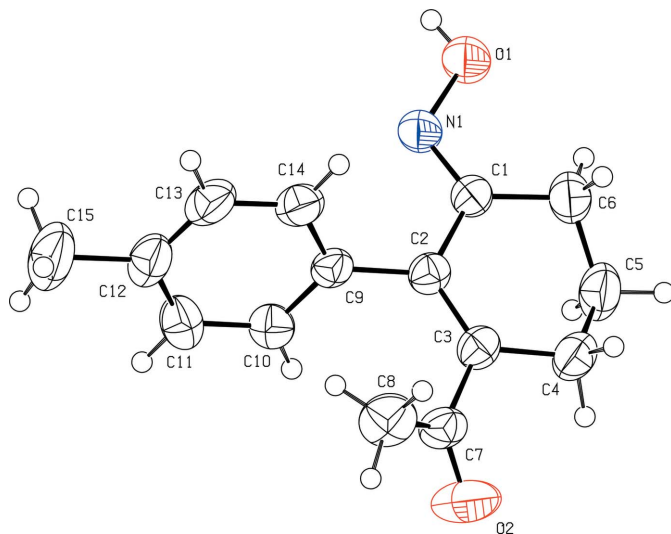


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

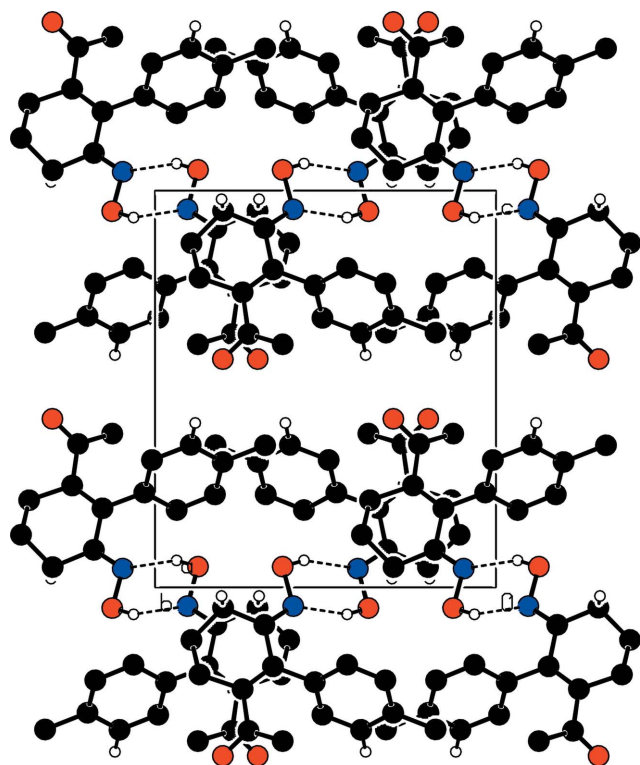


Figure 2
Packing of the molecules of (I), viewed down the *a* axis. H atoms not involved in the hydrogen bonds (dashed lines) have been omitted for clarity.

molecules form layered centrosymmetric dimers through an O—H···N hydrogen bond (Table 2 and Fig. 2) repeated along the *bc* plane. Many such layers extending along the *a* axis give a three-dimensional pattern. In addition, an intermolecular C—H···O interaction is observed.

Experimental

A mixture of 6-acetyl-1-(4-methylphenyl)cyclohexene (0.3 mol), acetic acid (100 ml) and *n*-butyl nitrite (35 ml) was cooled below 263 K. Concentrated hydrochloric acid (35 ml) was then added dropwise with stirring while maintaining the temperature below 263 K. After the addition was complete, the mixture was stirred for a further period of 4 h at the same temperature. The precipitated solid was filtered, washed with cold methanol and dried in air to yield the nitrosochloride adduct as a white powder. This was suspended in pyridine (30 ml) and warmed to 338 K. A vigorous exothermic reaction took place and the entire solid dissolved. The mixture was kept at 343 K for 10 min, cooled and acidified with dilute hydrochloric acid. The resultant solid was filtered off, washed with water and recrystallized from alcohol to give the title compound (yield 57%). Elemental analysis calculated: C 74.05, H 7.04, N 5.76%; found: C 74.15, H 7.03, N 5.80%.

Crystal data

C₁₅H₁₇NO₂
M_r = 243.30
 Monoclinic, *P*₂₁/*a*
a = 9.205 (4) Å
b = 11.311 (4) Å
c = 13.489 (5) Å
 β = 102.19 (3)°
V = 1372.7 (9) Å³

Z = 4
D_x = 1.177 Mg m⁻³
 Mo *K*α radiation
 μ = 0.08 mm⁻¹
T = 293 (2) K
 Block, colourless
 0.28 × 0.14 × 0.12 mm

Data collection

Nonius MACH3 four-circle diffractometer
 ω scans
 Absorption correction: ψ scan (North *et al.*, 1968)
 T_{\min} = 0.987, T_{\max} = 0.991
 2574 measured reflections

2407 independent reflections
 1584 reflections with *I* > 2σ(*I*)
 R_{int} = 0.049
 θ_{\max} = 25.0°
 3 standard reflections
 frequency: 60 min
 intensity decay: none

Refinement

Refinement on *F*²
 $R[F^2 > 2\sigma(F^2)]$ = 0.063
 $wR(F^2)$ = 0.192
 S = 1.02
 2407 reflections
 163 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1097P)^2 + 0.2444P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.28 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{Å}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···N1 ⁱ	0.82	2.11	2.798 (3)	142
C11—H11···O2 ⁱⁱ	0.93	2.53	3.439 (4)	163

Symmetry code: (i) $-x, -y + 1, -z$; (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + 1$.

All H atoms were positioned geometrically and were allowed to ride on their parent atoms [C—H = 0.93–0.97 Å and O—H = 0.82 Å; $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{O})$].

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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