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3-Cyano-3-methyl-5-phenylcyclohexanone

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In the title molecule, $C_{14}H_{15}NO$, the cyclohexane ring adopts a chair conformation. The cyano group and the methyl group have axial and equatorial orientations, respectively. The phenyl ring has an equatorial orientation.

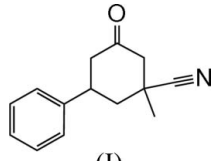
Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.095
Data-to-parameter ratio = 12.0

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

Comment

The present X-ray diffraction study of the title compound, (I), was undertaken to determine how the conformation of the system is affected by the substitution of cyano and methyl groups at position 3 and a phenyl ring at position 5 of the cyclohexanone.



(I)

The molecular structure of (I) is shown in Fig. 1. The cyclohexane ring adopts a chair conformation. The cyano group and the methyl group at position 3 have axial and equatorial orientations, respectively. The phenyl ring at position 5 has an equatorial orientation. The mean plane of atoms C2/C3/C5/C6 and the phenyl ring make a dihedral angle of 83.8 (1)°.

Experimental

A mixture of 3-methyl-5-phenylcyclohex-2-enone (3.72 g, 0.02 mol), potassium cyanide (2.6 g, 0.04 mol), ammonium chloride (1.59 g, 0.03 mol), dimethylformamide (50 ml) and water (2 ml) was heated with stirring for 16–18 h at 353 K. The reaction mixture was then cooled to room temperature and poured into water. The product was extracted with CH_2Cl_2 (3 × 10 ml) and the organic layer was dried, evaporated and purified by column chromatography (hexane–EtOAc, 4.5:1 v/v). The yield of the isolated product was 2.5 g (75%).

Crystal data

$C_{14}H_{15}NO$
M_r = 213.27
Orthorhombic, *Aba*2
a = 11.5745 (3) Å
b = 17.5499 (5) Å
c = 11.2629 (3) Å
V = 2287.85 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 160 (1) K
0.35 × 0.33 × 0.28 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
24679 measured reflections
1755 independent reflections
1527 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$	1 restraint
$wR(F^2) = 0.095$	H-atom parameters constrained
$S = 1.05$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
1755 reflections	$\Delta\rho_{min} = -0.20$ e Å^{-3}
146 parameters	

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C). In the absence of significant anomalous scattering, Friedel pairs were merged.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

The data collection was carried out by Dr A. Linden of the Institute of Organic Chemistry at the University of Zurich; his help is gratefully acknowledged by Dr A. Thiruvalluvar.

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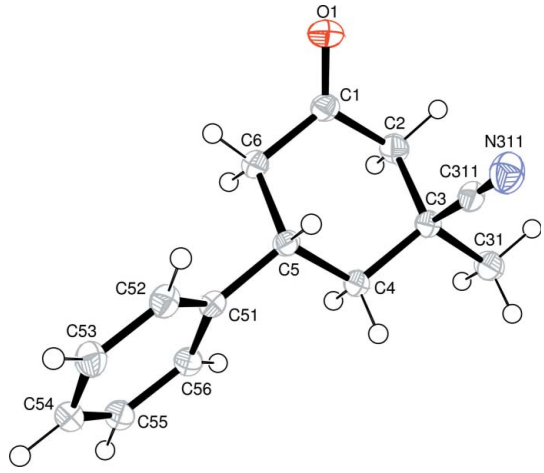

Figure 1
The molecular structure of (I), showing the atom-numbering scheme and with displacement ellipsoids drawn at the 50% probability level.

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