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1-Naphthyl-4-phenylcyclohexene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.066
wR factor = 0.221
Data-to-parameter ratio = 14.4

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

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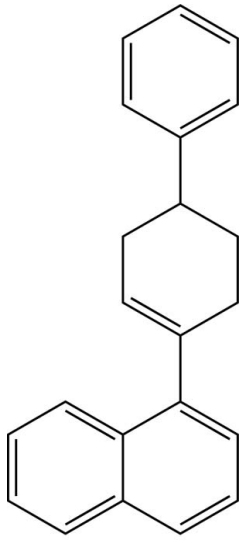
In the title compound, $C_{22}H_{20}$, the central cyclohexene ring is in a slightly distorted half-chair conformation and the structure is stabilized by C—H···π interactions.

Comment

Alkenes undergo co-halogenation reactions to afford bifunctional compounds which serve as potential synthons towards the synthesis of various heterocyclic compounds (Rodriguez & Dulcere, 1993). The regio/stereoselectivity of such addition reactions is governed by various factors, one being the structural features of the alkene. We were interested in investigating some of the structural features in the title compound, (I), which may alter the regio/stereoselectivity in addition reactions. In particular, we hoped to examine the rotameric preference of the naphthyl ring system attached to one of the olefinic carbons in (I).



(I)

The slightly distorted half-chair conformation of the cyclohexene ring is confirmed by the puckering analysis [q_2 = 0.195 (2) Å, φ_2 = 329 (2)°, q_3 = 0.099 (3) Å; Cremer & Pople, 1975] (Fig. 1). The r.m.s. deviations from the phenyl and naphthyl planes are 0.0057 and 0.0022 Å, respectively and these ring systems subtend an angle of 33.3 (1)° with one another.

The crystal structure of (I) is stabilized by C—H···π interactions (Fig. 2). There are four intermolecular C—H···π interactions (Desiraju & Steiner, 1999) in the structure of (I). Atoms C3 and C9 interact with the C1–C6 benzene ring

(centroid *Cg*1), while C12 and C18 interact with the C17–C22 ring (centroid *Cg*4) (Table 2).

Experimental

A solution of 4-phenylcyclohexanone (25 mmol) in dry diethyl ether (25 ml) was added dropwise to a stirred solution of naphthylmagnesium bromide, prepared from magnesium turnings (25 mmol) and 1-bromonaphthalene (25 mmol) in dry diethyl ether (50 ml). The stirring was continued for 1 h, then the Grignard complex was decomposed with ice-cold water. The ether layer was decanted, and washed repeatedly with dilute sodium bicarbonate solution and water. It was dried with anhydrous sodium sulfate and the solvent evaporated to yield 1-naphthyl-4-phenylcyclohexanol. 1-Naphthyl-4-phenylcyclohexanol (1.5 mmol) was mixed with 20% sulfuric acid/acetic acid (5 ml). It was kept over a water bath with occasional swirling for 1 h. Two layers separated immediately. The mixture was cooled and added to an excess of cold water. The organic layer was separated, washed free of acid with water and then with saturated sodium bicarbonate solution; it was then dried over anhydrous calcium chloride and the solvent evaporated to give 1-naphthyl-4-phenylcyclohexene. This was purified by column chromatography on silica gel with petroleum ether (333–353 K) as eluent. Crystals suitable for the X-ray investigation were obtained from the resulting solution. Yield: 62%. Elemental analysis: Anal. Calc. C, 92.91%; H, 7.09%. Found. C, 92.98%; H, 7.05%.

Crystal data

$C_{22}H_{20}$
M_r = 284.38
Monoclinic, $P2_1/c$
a = 17.1942 (11) Å
b = 7.4769 (6) Å
c = 13.7953 (8) Å
β = 112.99 (2)°
V = 1632.4 (3) Å^3
Z = 4
D_x = 1.157 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
Block, colourless
0.21 × 0.18 × 0.15 mm

Data collection

Nonius MACH3 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.940, T_{max} = 0.989
3495 measured reflections
2866 independent reflections
1864 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.0°
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.221
S = 1.04
2866 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1087P)^2 + 0.9808P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ <0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected torsion angles (°).

C1—C6—C7—C8	−68.6 (6)	C8—C7—C12—C11	−29.4 (7)
C12—C7—C8—C9	20.9 (8)	C9—C10—C13—C22	−71.8 (4)

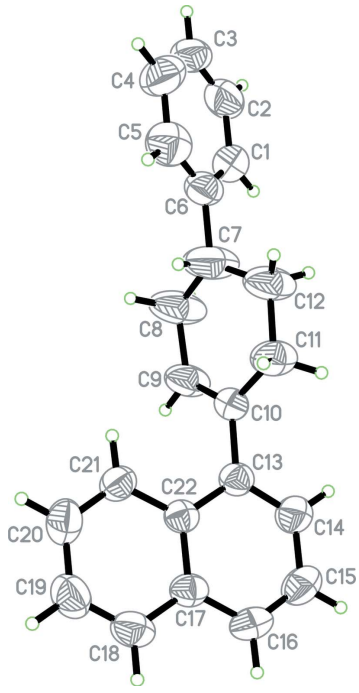


Figure 1
The molecular structure of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids.

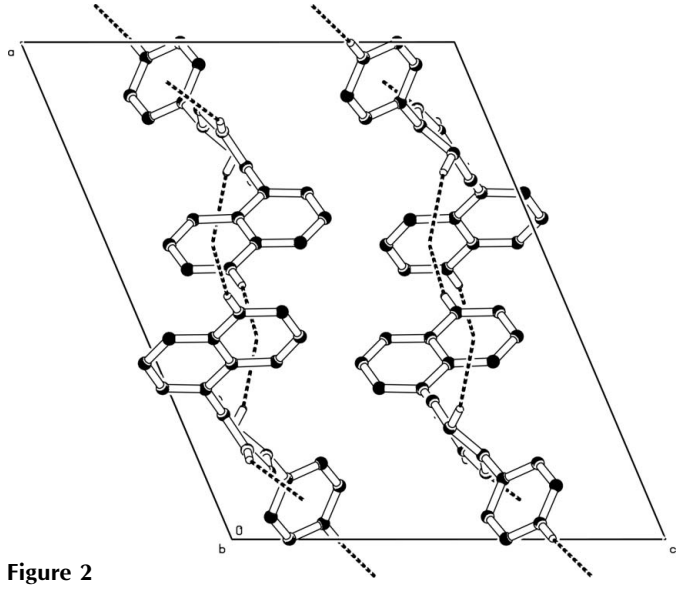


Figure 2
Packing of the molecules, viewed down the *b* axis. H atoms have been omitted..

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 benzene ring and *Cg*4 is the centroid of the C17–C22 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···*Cg*1^{i}	0.93	2.69	3.616 (4)	176
C9—H9···*Cg*1^{ii}	0.93	2.98	3.787 (5)	146
C12—H12*A*···*Cg*4^{iii}	0.97	2.81	3.746 (3)	163
C18—H18···*Cg*4^{iv}	0.93	2.71	3.616 (4)	166

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

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93/0.96/0.97/0.98 Å and U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL/PC* (Bruker, 2000); program(s) used to refine structure: *SHELXTL/PC*; molecular graphics: *SHELXTL/PC* and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL/PC*.

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