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2-(1-Naphthylimino)-1-acenaphthen-1-one

Alexandre C. Silvino,[a]* Leonardo C. Ferreira,[b] Marcos L. Dias,[a] Carlos Alberto L. Filgueiras,[b] Manfredo Hörner,[c] Lorenzo do C. Visentin[c] and Jairo Bordinhao[b]

[a]Instituto de Macromoleculas Eloisa Mano, Universidade Federal do Rio de Janeiro, Caixa Postal 68525, 21945-970 Rio de Janeiro, RJ, Brazil, [b]Instituto de Quimica, Universidade Federal do Rio de Janeiro, Caixa Postal 68563, 21949-900 Rio de Janeiro, RJ, Brazil, and [c]Departamento de Quimica, Universidade Federal de Santa Maria, Caixa Postal 5071, 97110-900 Santa Maria, RS, Brazil

Correspondence e-mail:
alexandresilvino@terra.com.br

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In the title compound, $C_{22}H_{13}NO$, the angle between the acenaphthenyl and naphthyl ring systems is 83.56 (3)°. In the crystal structure, the molecules aggregate *via* π–π stacking and $C—H\cdots\pi$(arene) interactions.

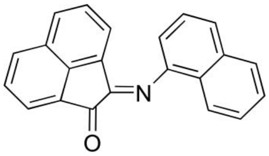
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.111
Data-to-parameter ratio = 12.8

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

Comment

There is increasing interest in the design and development of new catalyst systems for olefin polymerization. Numerous catalysts have been employed in alkene polymerization, among which α-diimine complexes of transition metals, the so-called Brookhart catalysts, are the best known (Rix & Brookhart, 1995). Many studies have addressed the direct influence of the electronic and steric features of the α-diimine ligand systems on the polymer molecular weight and tacticity. However, little is known about the actual catalytic performance of α-iminoketone complexes towards olefin polymerization (Macchioni *et al.*, 2004).



(I)

Recently, we reported the structure of 2-(2,6-diisopropylphenylimino)-1-phenyl-1-one, an α-iminoketone containing a bulky side group (Ferreira *et al.*, 2006). It has already been shown that the bulkiness of the aryl groups in the α-diimine ligands plays an important role in many alkene polymerizations, allowing the preparation of a range of linear and branched polyethylenes (Morokuma *et al.*, 1998). In the context of our interest in α-iminoketones, we describe here the preparation and structural features of 2-(1-naphthylimino)-1-acenaphthene-1-one, (I) (Fig. 1). The most important feature in the molecular structure of (I) is the conformation about the N1—C13 bond; the planar naphthyl and acenaphthenyl units have an interplanar angle of 83.56 (3)° due to steric hindrance. All atoms in both planar aromatic systems lie within 0.01Å of their respective mean planes.

The C═O and C═N bond lengths of 1.215 (2) and 1.278 (2)Å, respectively, are similar to those in related α-imino-ketones, *e.g.* 2-(2,6-diisopropylphenylimino)-1-phenylpropane-one [C═O = 1.247 (19) and C═N 1.274 (19)Å; Ferreira *et al.*, 2006], and 2-(phenylimino)-1,2-diphenylethanone [1.214 (2) and 1.278 (2)Å; Güner *et al.*, 2000], and literature values (Allen *et al.*, 1987). Additionally, a comparison of the C═N and $C_{aryl}—N$ bond lengths in (I) with literature values (Allen *et al.*, 1987) suggests no delocalization of the π electrons involving the C=N—C group with the naphthyl ring system. Furthermore, the C2—C1—N1—C13 and O1—C2—C1—N1 torsion angles are 177.17 (15) and 2.6 (3)°, respectively.

The crystal packing in (I) shows π–π stacking involving parallel-displaced acenaphtenyl rings along the [101] plane. The shortest distance between these neighboring fragments is 3.509 (5) Å and involves the C7 and C8^{i} atoms [symmetry code: (i) $1 - x, -y, 1 - z$]. There are also C—H$\cdots\pi$ contacts between the naphthyl and acenaphtenyl rings of adjacent molecules forming pairs along the crystallographic direction [010]. The distance between the donor atom (D) C6 and the acceptor atom (A) C21^{i} is 3.719 (3) Å and the distance between H6 and C21^{i} is 2.81 (2) Å. The angle in the C6—H6$\cdots$C21^{i} interaction (non-classical) is 165°.

Experimental

1-Naphthylamine (0.56 g, 4.0 mmol) was added at room temperature to an ethanol solution (50 ml) of acenaphthenequinone (0.73 g, 4.0 mmol) in the presence of a catalytic amount of formic acid. After 24 h of magnetic stirring, the solution was concentrated to 25 ml by evaporating the solvent under vacuum and the crude red product was isolated by filtration, washed with cold ethanol and dried under vacuum. Red block-shaped crystals suitable for X-ray diffraction were obtained by recrystallization from CH_2Cl_2 (yield 1.13 g, 92%).

Crystal data

$C_{22}H_{13}NO$
$M_r = 307.33$
Monoclinic, $P2_1/c$
$a = 8.2350\ (7)$ Å
$b = 15.4991\ (13)$ Å
$c = 11.9910\ (12)$ Å
$\beta = 100.387\ (3)^\circ$
$V = 1505.4\ (2)$ Å^3
$Z = 4$
$D_x = 1.356$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 295\ (2)$ K
Block, red
0.36 × 0.25 × 0.20 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: none
12556 measured reflections
2788 independent reflections
1698 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.056$
$\theta_{\rm max} = 25.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.111$
$S = 1.01$
2788 reflections
218 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.16$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0062 (16)

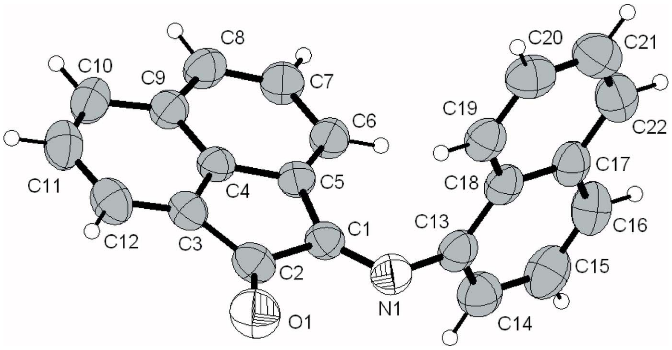


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids.

H atoms were treated as riding atoms in the refinement, with C—H bond lengths fixed at 0.93 Å and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(aromatic C)..

Data collection: *COSMO/APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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: *WinGX* (Farrugia, 1999).

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