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4-Nitrophenanthrene

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Key indicators

Single-crystal X-ray study
T = 169 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.110
Data-to-parameter ratio = 10.2

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

This study at 168 K shows that in the crystal structure of $C_{14}H_9NO_2$, the plane of the nitro group is inclined at 72.2 (7)° to the plane of the attached six-membered ring. The phenanthrene system is significantly non-planar.

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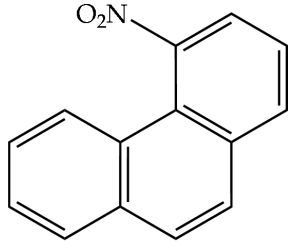
Comment

As part of a study directed towards relating NMR chemical shifts to the degree of conjugation of substituents in phenanthrene, the structure of 4-nitrophenanthrene, (I) (Fig. 1), has been determined. The angle between the NO_2 and phenanthrene planes indicates that there will be reduced conjugation. This angle of 72.2 (7)° can be compared with the value of 60.7° obtained by calculation using *SPARTAN* (Wavefunction, 1995).



(I)

Experimental

A mixture of isomers was obtained by nitration of phenanthrene with nitric acid in benzene following the method of Heaney *et al.* (1965). After chromatography of the mixture, 4-nitrophenanthrene was obtained pure and was crystallized as yellow prisms from hexane.

Crystal data

$C_{14}H_9NO_2$
M_r = 223.23
Monoclinic, $P2_1/c$
a = 8.061 (2) Å
b = 12.449 (3) Å
c = 11.132 (3) Å
β = 109.73 (1)°
V = 1051.5 (5) Å^3
Z = 4
D_x = 1.41 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5719 reflections
θ = 2.5–26.4°
μ = 0.10 mm^{-1}
T = 168 (2) K
Prism, pale yellow
0.72 × 0.46 × 0.26 mm

Data collection

Bruker SMART $P4$ diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.78, T_{max} = 0.98
13 110 measured reflections
2135 independent reflections
1945 reflections with $F^2>0$
R_{int} = 0.028
θ_{max} = 26.4°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 15$
$l = -13 \rightarrow 13$

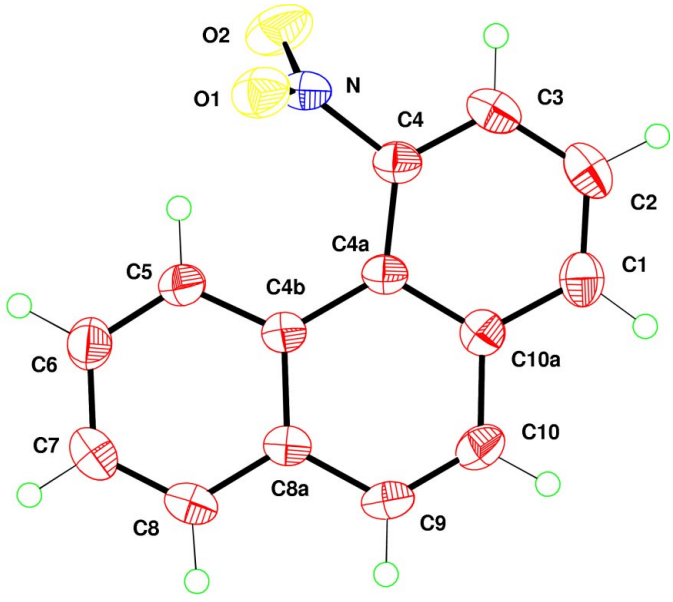


Figure 1
The molecular structure of 4-nitrophenanthrene showing 50% probability displacement ellipsoids.

Refinement

Refinement on F^2
$R(F) = 0.049$
$wR(F^2) = 0.11$
$S = 0.99$
1943 reflections
190 parameters

All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.06F_o^2)^2 + 0.5F_o^2]$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å).

N—O1	1.226 (2)	C3—C4	1.371 (2)
N—O2	1.230 (2)	C4—C4a	1.420 (2)
N—C4	1.488 (2)		

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1996); data reduction: *SAINT* and *Xtal*3.4 *ADDREF SORTRF* (Hall *et al.*, 1995); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *Xtal*3.4 *CRYLSQ*; molecular graphics: *Xtal*3.4; software used to prepare material for publication: *Xtal*3.4 *BONDLA CIFIO*.

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