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1-(Methoxymethyl)pyrene

Tobias Gruber, Wilhelm Seichter and Edwin Weber*

Institut für Organische Chemie, TU Bergakademie Freiberg, Leipziger Strasse 29, D-09596 Freiberg/Sachsen, Germany

Correspondence e-mail:
edwin.weber@chemie.tu-freiberg.de

Key indicators
Single-crystal X-ray study
T = 93 K
Mean σ(C–C) = 0.001 Å
R factor = 0.046
wR factor = 0.142
Data-to-parameter ratio = 21.6

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

The title compound, $C_{18}H_{14}O$, crystallizes with aromatic π–π stacking interactions.

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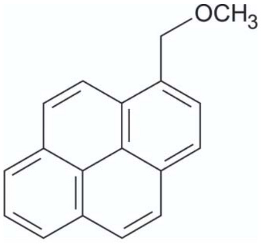
Comment

With their particular electronic, optical and geometric properties, pyrene and its derivatives (Garcia-Cruz *et al.*, 2004; Takahashi *et al.*, 2004; Borisevich *et al.*, 1992) have attracted considerable recent interest. This is demonstrated in a great number of applications including host–guest (Vögtle, 1996) and metal coordination chemistry (Arrais *et al.*, 2004), as well as fluorescent sensor development (Bren, 2001). Although pyrenes with a functional side arm are important building blocks in this respect, reports on corresponding crystal structures are limited (Foss & Stevens, 1985; Olszak *et al.*, 1989). Here, we describe the structure of 1-(methoxymethyl)pyrene, (I), a new example of this type of compound.



(I)

The pyrene part of the molecule shows no significant deviations of bond lengths and angles compared with those of the unsubstituted analogue (Camerman & Trotter, 1965; Allmann, 1970; Hazell *et al.*, 1972; Kai *et al.*, 1978), and is almost planar. The largest deviation from the mean plane through the carbon framework of the pyrene unit is 0.042 (1) Å for atom C1. The torsion angle C2—C1—C17—O1 is 15.1 (1)°, indicating that the methoxymethyl group is turned away from the aromatic plane, while the C—C—O—C fragment itself exhibits a nearly ideal anti-periplanar conformation [179.7 (1)°].

Due to the aromatic nature of the molecule, the crystal packing of (I) is dominated by arene–arene supramolecular contacts. In contrast to the unsubstituted pyrene, which forms face-to-face dimers packed in a herringbone fashion, the crystal structure of (I) is characterized by molecular stacks which are stabilized by offset face-to-face interactions. Within the stacks, the mean distance between consecutive molecules is 3.5 Å. The molecules of neighboring stacks are inclined to each other at an angle of 86.47 (3)°. Hence the compound has an overall packing structure resembling the pattern found in the solid state structures of many aromatic compounds (Desiraju, 1989).

Experimental

The title compound, (I), was synthesized from commercially available pyrene-1-carbaldehyde, which was initially reduced with sodium borohydride in boiling methanol, following an analogous procedure described for the reduction of anthracene-9-carbaldehyde (Steward, 1960), to yield the intermediate compound 1-(hydroxymethyl)pyrene. This was transformed into 1-(bromomethyl)pyrene by the usual bromination with phosphorus tribromide in chloroform (Okamoto *et al.*, 1990). Subsequent treatment with boiling methanol and recrystallization of the product from the same solvent yielded 60% of compound (I) as colorless needles (m.p. 322–323 K). ^{1}H NMR spectroscopic data (400 MHz, CDCl$_3$): δ 8.32 (*d*, ArH, 1H), 8.13 (*m*, ArH, 4H), 8.02 (*m*, ArH, 4H), 5.14 (*s*, CH$_2$OH, 2H), 3.49 (*s*, CH$_3$, 3H).

Crystal data

$C_{18}H_{14}O$
$M_r = 246.29$
Monoclinic, $P2_1/n$
$a = 4.7220$ (10) Å
$b = 20.087$ (4) Å
$c = 12.824$ (3) Å
$\beta = 91.13$ (3)°
$V = 1216.1$ (5) Å^3

$Z = 4$
$D_x = 1.345$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 93$ (2) K
Prism, colorless
0.41 × 0.20 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{\min} = 0.906$, $T_{\max} = 0.986$

19573 measured reflections
3712 independent reflections
2920 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.027$
$\theta_{\max} = 30.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.142$
$S = 0.97$
3712 reflections
172 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0988P)^2 + 0.1716P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.48$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}

H atoms were positioned geometrically (C—H = 0.95–0.99) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 times $U_{\text{eq}}(\text{C})$.

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2003); software used to prepare material for publication: *SHELXTL*.

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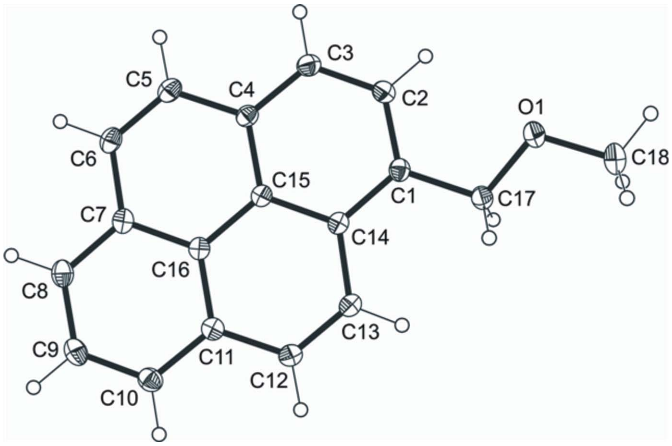

Figure 1
Perspective view of (I), showing 50% probability displacement ellipsoids for the non-H atoms.

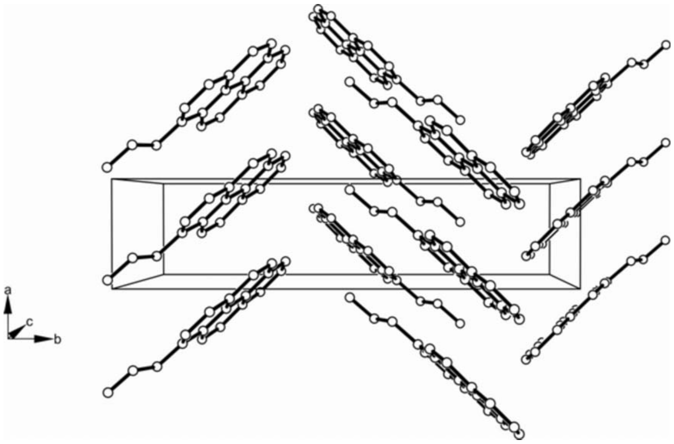

Figure 2
Packing diagram of (I), viewed down the *c* axis. H atoms have been omitted.

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