Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Bromopyrene

Robert E. Taylor,[a] Paul R. Raithby[a,b]* and Simon J. Teat[a]

[a]Department of Chemistry, University of Bath, Bath BA2 7AY, England, and [b]CCLRC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England

Correspondence e-mail: p.r.raithby@bath.ac.uk

Key indicators

Single-crystal synchrotron study
T = 200 K
Mean σ(C–C) = 0.007 Å
R factor = 0.046
wR factor = 0.126
Data-to-parameter ratio = 12.3

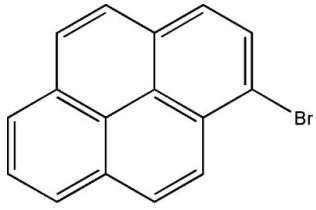
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 20 March 2006
Accepted 22 March 2006.

1-Bromopyrene, $C_{16}H_9Br$, is a planar, fused aromatic organic compound. The molecule is approximately planar with an r.m.s. deviation of 0.0243 Å for the ring C atoms and 0.0261 Å for all non-H atoms. A herringbone packing motif based on π-π interactions is observed, with a perpendicular distance between adjacent stacked molecules of 3.519 Å.

Comment

We report here the structural characterization of the title compound, (I), which is a planar, fused aromatic organic compound. Its structure was determined to establish whether π–π stacking occurred in the solid state, and to relate the nature of the packing to some of the physical properties of the material, including triboluminescence. Similar fused aromatic compounds have exhibited π–π interactions (Desiraju & Gavezzotti, 1989) which, we believe, may be a requirement for aromatic materials to show triboluminescent activity (Sweeting *et al.*, 1997).



(I)

The molecule (Fig. 1) is shown to be approximately planar, with an r.m.s. deviation of 0.0243 Å for the ring C atoms and 0.0261 Å for all non-H atoms. A herringbone packing motif based on π-π interactions is observed (Fig. 2), with a perpendicular distance between adjacent stacked molecules of 3.519 Å. No C—H···π contacts shorter than 2.91 Å are observed.

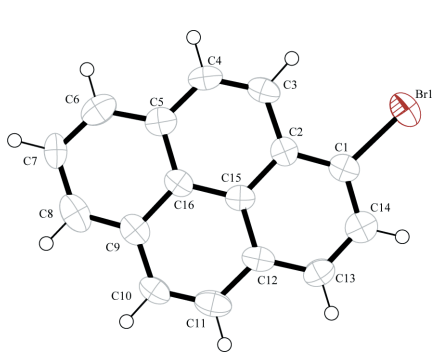


Figure 1
The molecular structure of (I) with atom labels and 50% probability ellipsoids for non-H atoms.

Experimental

1-Bromopyrene was purchased as a yellow powder from the Aldrich Chemical Company. Small orange crystals suitable for X-ray diffraction were grown by slow evaporation of a solution in benzene stored at 278 K.

Crystal data

$C_{16}H_9Br$
M_r = 281.14
Monoclinic, $P2_1/c$
a = 14.530 (3) Å
b = 3.9490 (8) Å
c = 20.277 (4) Å
β = 108.163 (3)°
V = 1105.5 (4) Å^3
Z = 4
D_x = 1.689 Mg m^{-3}
Synchrotron radiation
λ = 0.6775 Å
Cell parameters from 1772 reflections
θ = 2.8–23.3°
μ = 3.69 mm^{-1}
T = 200 (2) K
Block, orange
0.05 × 0.05 × 0.03 mm

Data collection

Bruker APEX-II CCD diffractometer
Narrow–frame ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.817, T_{max} = 0.895
7895 measured reflections
1888 independent reflections
1284 reflections with $I > 2\sigma(I)$
R_{int} = 0.149
θ_{max} = 24.7°
$h = -17 \rightarrow 17$
$k = -4 \rightarrow 4$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.126
S = 0.95
1888 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

H atoms were constrained as riding atoms, with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The value of R_{int} is rather high due to the poor quality of the crystal, which required the use of synchrotron radiation for any diffraction to be observed.

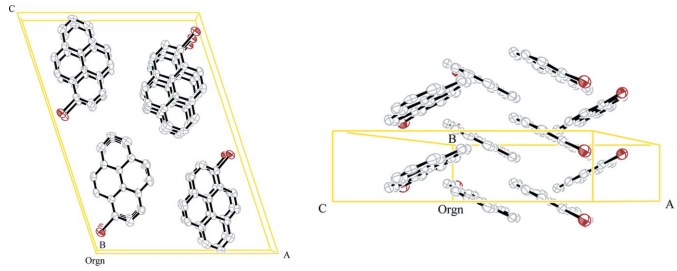


Figure 2
Two views of the packing, perpendicular to (010) and to (001), with 50% probability ellipsoids for non-H atoms. H atoms have been omitted for clarity.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); 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* publication routines (Farrugia, 1999).

We thank the EPSRC and the CCLRC Centre for Molecular Structure and Dynamics for funding.

References

Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Desiraju, G. R. & Gavezzotti, A. (1989). *Acta Cryst.* B**45**, 473–482.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sweeting, L. M., Rheingold, A. L., Gingerich, J. M., Rutter, A. W., Spence, R. A., Cox, C. D. & Kim, T. J. (1997). *Chem. Mater.* **9**, 1103–1115.

supporting information

Acta Cryst. (2006). E**62**, o1604–o1605 [https://doi.org/10.1107/S160053680601052X]

1-Bromopyrene

Robert E. Taylor, Paul R. Raithby and Simon J. Teat

(I)

Crystal data

$C_{16}H_9Br$
$M_r = 281.14$
Monoclinic, $P2_1/c$
$a = 14.530$ (3) Å
$b = 3.9490$ (8) Å
$c = 20.277$ (4) Å
$\beta = 108.163$ (3)°
$V = 1105.5$ (4) Å^3
$Z = 4$
$F(000) = 560$
$D_x = 1.689$ Mg m^{-3}
Synchrotron radiation, $\lambda = 0.6775$ Å
Cell parameters from 1772 reflections
$\theta = 2.8$–$23.3°$
$\mu = 3.69$ mm^{-1}
$T = 200$ K
Block, orange
0.05 × 0.05 × 0.03 mm

Data collection

Bruker APEX-II CCD diffractometer
narrow–frame ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.817$, $T_{max} = 0.895$
7895 measured reflections
1888 independent reflections
1284 reflections with $I > 2\sigma(I)$
$R_{int} = 0.149$
$\theta_{max} = 24.7°$, $\theta_{min} = 2.1°$
$h = -17 \rightarrow 17$
$k = -4 \rightarrow 4$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.126$
$S = 0.95$
1888 reflections
154 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1723 (3)	0.1059 (12)	0.1548 (2)	0.0396 (11)
C2	0.1812 (3)	0.1333 (11)	0.2249 (2)	0.0351 (11)

C3	0.1100 (3)	0.2885 (10)	0.2515 (3)	0.0402 (11)
H3	0.0537	0.3879	0.2201	0.048*
C4	0.1221 (4)	0.2940 (11)	0.3195 (3)	0.0432 (12)
H4	0.0726	0.3928	0.3346	0.052*
C5	0.2034 (4)	0.1631 (11)	0.3696 (3)	0.0416 (12)
C6	0.2178 (4)	0.1619 (12)	0.4423 (3)	0.0508 (14)
H6	0.1672	0.2513	0.4576	0.061*
C7	0.2964 (4)	0.0459 (10)	0.4911 (2)	0.0382 (12)
H7	0.3034	0.0608	0.5392	0.046*
C8	0.3709 (4)	−0.1054 (13)	0.4657 (3)	0.0541 (15)
H8	0.4265	−0.2003	0.4986	0.065*
C9	0.3644 (4)	−0.1172 (12)	0.3960 (3)	0.0409 (12)
C10	0.4363 (4)	−0.2660 (11)	0.3704 (3)	0.0428 (12)
H10	0.4931	−0.3593	0.4023	0.051*
C11	0.4251 (4)	−0.2762 (11)	0.3024 (3)	0.0483 (13)
H11	0.4754	−0.3715	0.2876	0.058*
C12	0.3405 (3)	−0.1496 (11)	0.2511 (3)	0.0390 (12)
C13	0.3274 (4)	−0.1702 (11)	0.1800 (3)	0.0414 (12)
H13	0.3762	−0.2694	0.1641	0.05*
C14	0.2428 (4)	−0.0451 (11)	0.1323 (3)	0.0449 (13)
H14	0.2338	−0.0641	0.0839	0.054*
C15	0.2672 (3)	0.0006 (10)	0.2747 (2)	0.0339 (11)
C16	0.2778 (3)	0.0149 (10)	0.3464 (2)	0.0349 (11)
Br1	0.06020 (4)	0.26841 (12)	0.08553 (2)	0.0523 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.035 (3)	0.032 (2)	0.050 (3)	−0.006 (2)	0.009 (2)	−0.002 (2)
C2	0.037 (3)	0.026 (2)	0.040 (3)	−0.0095 (19)	0.010 (2)	−0.0001 (18)
C3	0.028 (2)	0.030 (2)	0.057 (3)	−0.003 (2)	0.006 (2)	−0.004 (2)
C4	0.035 (3)	0.036 (3)	0.062 (3)	0.000 (2)	0.022 (2)	−0.007 (2)
C5	0.039 (3)	0.033 (2)	0.054 (3)	−0.009 (2)	0.016 (3)	−0.006 (2)
C6	0.059 (4)	0.038 (3)	0.065 (4)	−0.011 (2)	0.033 (3)	−0.012 (2)
C7	0.056 (3)	0.027 (2)	0.027 (2)	−0.014 (2)	0.006 (2)	0.0023 (18)
C8	0.056 (4)	0.040 (3)	0.054 (3)	−0.011 (3)	−0.002 (3)	0.011 (2)
C9	0.041 (3)	0.030 (2)	0.048 (3)	−0.008 (2)	0.008 (2)	0.005 (2)
C10	0.034 (3)	0.034 (3)	0.053 (3)	0.003 (2)	0.004 (2)	0.005 (2)
C11	0.034 (3)	0.035 (3)	0.075 (4)	−0.002 (2)	0.015 (3)	0.000 (2)
C12	0.031 (3)	0.027 (2)	0.059 (3)	−0.0024 (18)	0.014 (2)	0.001 (2)
C13	0.040 (3)	0.038 (3)	0.051 (3)	−0.009 (2)	0.021 (2)	−0.007 (2)
C14	0.048 (3)	0.032 (3)	0.055 (3)	−0.011 (2)	0.018 (3)	−0.004 (2)
C15	0.030 (2)	0.026 (2)	0.047 (3)	−0.0077 (18)	0.014 (2)	−0.0018 (18)
C16	0.030 (3)	0.026 (2)	0.045 (3)	−0.0083 (19)	0.007 (2)	0.0007 (18)
Br1	0.0461 (4)	0.0499 (4)	0.0509 (4)	−0.0028 (3)	0.0007 (2)	0.0080 (3)

Geometric parameters (Å, º)

C1—C14	1.381 (7)	C8—C9	1.389 (7)
C1—C2	1.392 (6)	C8—H8	0.950
C1—Br1	1.900 (5)	C9—C10	1.429 (7)
C2—C15	1.438 (6)	C9—C16	1.441 (6)
C2—C3	1.444 (7)	C10—C11	1.338 (7)
C3—C4	1.334 (7)	C10—H10	0.950
C3—H3	0.950	C11—C12	1.431 (7)
C4—C5	1.395 (7)	C11—H11	0.950
C4—H4	0.950	C12—C13	1.397 (7)
C5—C6	1.424 (7)	C12—C15	1.425 (6)
C5—C16	1.433 (6)	C13—C14	1.396 (7)
C6—C7	1.336 (7)	C13—H13	0.950
C6—H6	0.950	C14—H14	0.950
C7—C8	1.463 (7)	C15—C16	1.414 (6)
C7—H7	0.950		
C14—C1—C2	121.9 (5)	C8—C9—C10	123.9 (5)
C14—C1—Br1	117.1 (4)	C8—C9—C16	117.8 (5)
C2—C1—Br1	121.0 (4)	C10—C9—C16	118.2 (4)
C1—C2—C15	118.2 (4)	C11—C10—C9	121.2 (4)
C1—C2—C3	124.4 (4)	C11—C10—H10	119.4
C15—C2—C3	117.4 (4)	C9—C10—H10	119.4
C4—C3—C2	120.8 (4)	C10—C11—C12	122.7 (5)
C4—C3—H3	119.6	C10—C11—H11	118.7
C2—C3—H3	119.6	C12—C11—H11	118.7
C3—C4—C5	123.8 (5)	C13—C12—C15	119.7 (4)
C3—C4—H4	118.1	C13—C12—C11	122.7 (5)
C5—C4—H4	118.1	C15—C12—C11	117.6 (5)
C4—C5—C6	125.0 (5)	C14—C13—C12	120.1 (5)
C4—C5—C16	117.8 (4)	C14—C13—H13	119.9
C6—C5—C16	117.1 (5)	C12—C13—H13	119.9
C7—C6—C5	125.7 (5)	C1—C14—C13	120.5 (5)
C7—C6—H6	117.1	C1—C14—H14	119.7
C5—C6—H6	117.1	C13—C14—H14	119.7
C6—C7—C8	115.8 (4)	C16—C15—C12	120.5 (4)
C6—C7—H7	122.1	C16—C15—C2	119.9 (4)
C8—C7—H7	122.1	C12—C15—C2	119.5 (4)
C9—C8—C7	123.2 (5)	C15—C16—C5	120.2 (4)
C9—C8—H8	118.4	C15—C16—C9	119.7 (4)
C7—C8—H8	118.4	C5—C16—C9	120.2 (4)