

## 1-Bromopyrene

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## Key indicators

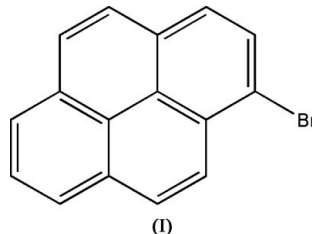
Single-crystal synchrotron study  
 $T = 200\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$   
 $R$  factor = 0.046  
 $wR$  factor = 0.126  
Data-to-parameter ratio = 12.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

1-Bromopyrene,  $\text{C}_{16}\text{H}_9\text{Br}$ , is a planar, fused aromatic organic compound. The molecule is approximately planar with an r.m.s. deviation of  $0.0243\text{ \AA}$  for the ring C atoms and  $0.0261\text{ \AA}$  for all non-H atoms. A herringbone packing motif based on  $\pi$ - $\pi$  interactions is observed, with a perpendicular distance between adjacent stacked molecules of  $3.519\text{ \AA}$ .

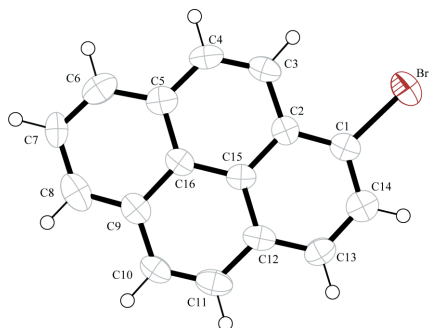
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## Comment

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  $\pi$ - $\pi$  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  $\pi$ - $\pi$  interactions (Desiraju & Gavezzotti, 1989) which, we believe, may be a requirement for aromatic materials to show triboluminescent activity (Sweeting *et al.*, 1997).



The molecule (Fig. 1) is shown to be approximately planar, with an r.m.s. deviation of  $0.0243\text{ \AA}$  for the ring C atoms and  $0.0261\text{ \AA}$  for all non-H atoms. A herringbone packing motif based on  $\pi$ - $\pi$  interactions is observed (Fig. 2), with a perpendicular distance between adjacent stacked molecules of  $3.519\text{ \AA}$ . No  $\text{C}-\text{H}\cdots\pi$  contacts shorter than  $2.91\text{ \AA}$  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  
 $\beta = 108.163$  (3)°  
 $V = 1105.5$  (4) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.689$  Mg m<sup>-3</sup>

Synchrotron radiation  
 $\lambda = 0.6775$  Å  
 Cell parameters from 1772 reflections  
 $\theta = 2.8\text{--}23.3^\circ$   
 $\mu = 3.69$  mm<sup>-1</sup>  
 $T = 200$  (2) K  
 Block, orange  
 $0.05 \times 0.05 \times 0.03$  mm

### Data collection

Bruker APEX-II CCD diffractometer  
 Narrow-frame  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.817$ ,  $T_{\max} = 0.895$   
 7895 measured reflections

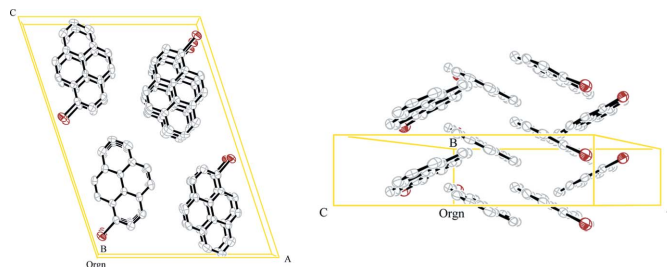
1888 independent reflections  
 1284 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.149$   
 $\theta_{\text{max}} = 24.7^\circ$   
 $h = -17 \rightarrow 17$   
 $k = -4 \rightarrow 4$   
 $l = -23 \rightarrow 23$

### 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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.66$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.67$  e Å<sup>-3</sup>

H atoms were constrained as riding atoms, with C—H = 0.95 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The value of  $R_{\text{int}}$  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).

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