

## 10,10'-Dibromo-9,9'-bianthryl

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## Key indicators

Single-crystal X-ray study

T = 298 K

Mean  $\sigma(\text{C}-\text{C}) = 0.012 \text{ \AA}$ 

R factor = 0.064

wR factor = 0.175

Data-to-parameter ratio = 13.3

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

In the title compound,  $\text{C}_{28}\text{H}_{16}\text{Br}_2$ , the two anthryl moieties are almost perpendicular to each other; the dihedral angles between the anthryl planes are  $89.42(9)$  and  $82.36(7)^\circ$  in the two independent molecules, one of which lies on a crystallographic twofold rotation axis. An interesting feature of the crystal structure is the presence of  $\text{C}-\text{H}\cdots\pi$  interactions.

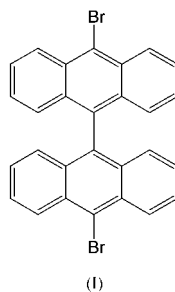
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## Comment

Photo-induced charge separation in molecular systems is a process in which there is considerable interest because of the importance of the electron/charge-transfer process in photosynthesis and solar energy conversion. Symmetric bianthryl derivatives are attractive candidates for the study of charge separation on photo-excitation through symmetry breaking (Piet *et al.*, 2001). Taking this into consideration, we have initiated studies on various bianthryl derivatives, such as the title compound, (I), and 10,10'-dicyano-9,9'-bianthryl. Since the dihedral angle between the two anthryl moieties controls the extent of charge separation in bianthryl derivatives, we have determined the crystal structure of (I).



The asymmetric unit contains a complete molecule, together with half a molecule; this second molecule lies on a crystallographic twofold rotation axis. Apart from finding that the two anthryl moieties are almost perpendicular to one another [the dihedral angles are  $89.42(9)$  and  $82.36(7)^\circ$  in the two independent molecules], we observe that the crystal structure is stabilized by weak  $\text{C}-\text{H}\cdots\pi$  intermolecular interactions involving an aromatic  $\text{C}-\text{H}$  of one molecule and the aromatic ring of an adjacent molecule. The distance between the H atom to the centroid of the aromatic ring varies between 2.75 and 3.10  $\text{\AA}$ .

## Experimental

Bianthryl was synthesized according to the procedure reported by Bell & Waring (1949). Bianthryl was then treated with bromine at 273 K to obtain the title compound, following the procedure

suggested by Müller & Baumgarten (1995). Crystals suitable for X-ray diffraction were grown by slow evaporation of a solution of (I) in chloroform–methanol (1:4).

#### Crystal data

$C_{28}H_{16}Br_2$	$D_x = 1.669 \text{ Mg m}^{-3}$
$M_r = 512.23$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 25 reflections
$a = 24.818 (6) \text{ \AA}$	$\theta = 9.4\text{--}10.5^\circ$
$b = 20.677 (4) \text{ \AA}$	$\mu = 3.99 \text{ mm}^{-1}$
$c = 14.473 (5) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 124.59 (2)^\circ$	Rectangular block, brown
$V = 6114 (3) \text{ \AA}^3$	$0.58 \times 0.46 \times 0.40 \text{ mm}$
$Z = 12$	

#### Data collection

Enraf–Nonius MACH3 four-circle diffractometer	$R_{\text{int}} = 0.034$
$\omega$ scans	$\theta_{\text{max}} = 25.0^\circ$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$h = 0 \rightarrow 29$
$T_{\text{min}} = 0.127$ , $T_{\text{max}} = 0.203$	$k = 0 \rightarrow 24$
5669 measured reflections	$l = -17 \rightarrow 14$
5380 independent reflections	3 standard reflections
3109 reflections with $I > 2\sigma(I)$	frequency: 90 min
	intensity decay: none

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 27.1434P]$
$R[F^2 > 2\sigma(F^2)] = 0.064$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.175$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.60 \text{ e \AA}^{-3}$
5380 reflections	$\Delta\rho_{\text{min}} = -0.74 \text{ e \AA}^{-3}$
406 parameters	
H-atom parameters constrained	

**Table 1**

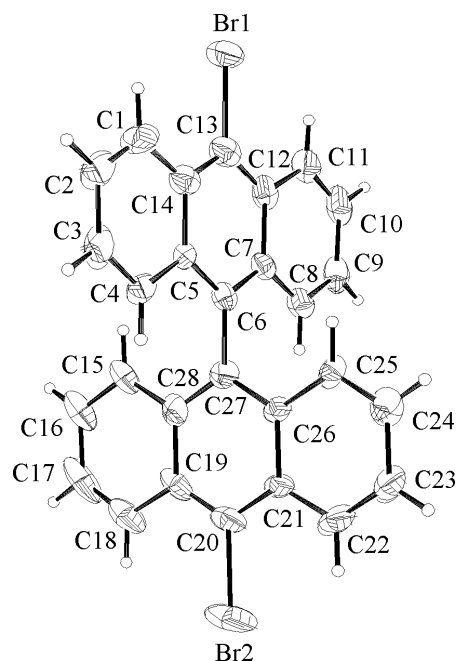
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Br3–C41	1.895 (7)	C6–C7	1.391 (9)
Br2–C20	1.896 (7)	C6–C27	1.496 (8)
Br1–C13	1.889 (7)	C26–C27	1.416 (9)
C5–C6	1.415 (9)	C27–C28	1.379 (9)
C6–C7–C8	122.8 (6)	C20–C21–C22	125.5 (7)
C14–C13–Br1	119.4 (6)	C28–C27–C6	119.7 (6)
C12–C13–Br1	118.1 (6)	C26–C27–C6	119.1 (5)
C19–C20–Br2	117.4 (6)		

All H atoms were positioned geometrically and treated as riding, with a C–H distance of 0.93  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

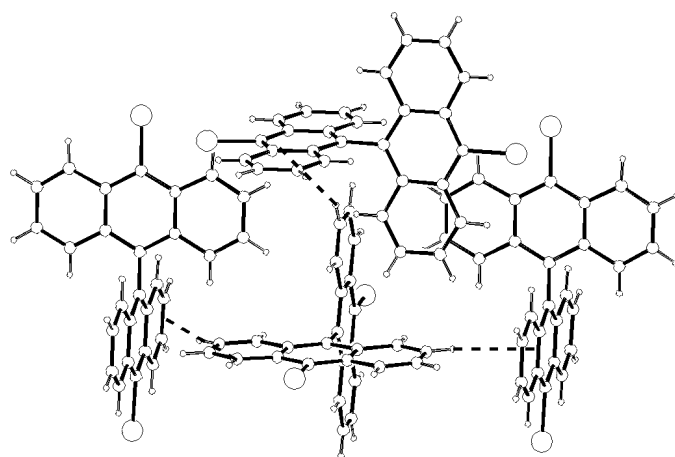
Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *WinGX* (Farrugia, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (Version 6a; McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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**Figure 1**

The structure of one independent molecule of the title compound, showing 40% displacement ellipsoids and atom-labelling scheme.



**Figure 2**

Various C–H... $\pi$  interactions in the crystal structure of the title compound.

## References

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