Tetrahedron Letters No.46, pp. 4129-4131, 1965. Pergamon Press Ltd.
Printed in Great Britain.

THE CONFORMATION OF 9,9' - BIANTHRYL

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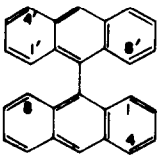
(Received 20 September 1965)

It is well known that the ultraviolet absorption of 9,9'-bianthryl (I) (1) is practically identical with that of anthracene. This absence of conjugation between the two rings is best explained by the non-planarity of the molecule, caused by the mutual interference between the hydrogen atoms in the 1,8,1'8' - positions. Indeed, 9,9' - bianthryl is a tetra-ortho-substituted biphenyl and should, therefore, be non-planar. Models show the interaction to be so strong that the molecule would be rigid (apart from oscillations of the two halves around the positions of lowest energy which have been disregarded in this study).

It seemed, thus, interesting to measure the angle between the two anthracene systems in I, using the dipole moments of suitably substituted 9,9'-bianthryls as a means for the determination of this angle. 2,2'-Dichloro -,2,2'-difluoro - and 2,2'-dibromo - 9,9'-bianthryl have been employed for this purpose.

2,2'-Dichloro - 9,9'-bianthryl (m.p.289°) had been prepared before (2) by reduction of 2-chloroanthrone. Analogously, reduction of 2-fluoroanthrone (3) gave 2,2'-difluoro - 9,9'-bianthryl (from cyclohexane, m.p. 283°, yield, 61%) (Anal.Found: C,86.1; H,4.1; F,9.6. $C_{28}H_{16}F_2$ requires C,86.2; H,4.1; F,9.7%) and reduction of 2-bromoanthrone (4) gave 2,2'-dibromo - 9,9'-bianthryl (from benzene - cyclohexane,m.p. 300-302° ; yield, 51%) (Anal.Found : C,65.8; H,3.1; Br, 31.7. $C_{28}H_{16}Br_2$ requires C,65.6; H,3.1; Br, 31.2%).

The experimental data are summarized in the Table (5). From the dipole moments, the angles between the two halves of the molecule of I follow to be : 85° for the fluoro -, 62° for the chloro - and 76° for the bromo-derivative.



I

Table

- 9,9' - bianthryl	UV-spectrum; λ[mμ] (log ε) (in chloroform)			μ(D±0.02)
2,2' - Difluoro -	257(5.16)	320^{s} (3.47)	336(3.75)	2.18
	355(3.96)	374(4.15)	395(4.25)	
2,2' - Dichloro -	263(5.32)	325^{s}(3.60)	340(3.80)	2.51
	357(3.99)	376(4.16)	397(4.23)	
2,2' - Dibromo -	268(5.27)	325^{s}(3.53)	340(3.75)	2.69
	357(3.93)	376(4.11)	397(4.10)	

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5. The dipole moments were measured in benzene solution at 30°. The method adopted for the calculations was that of J.F.Halverstad and W.D.Kumler, J.Amer.Chem.Soc., 64 , 2988 (1942).