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Dicyclobuta[*a*,*c*]anthracene

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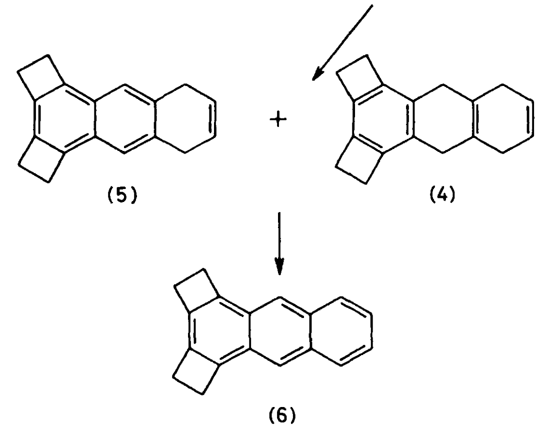
Summary The synthesis and spectroscopic properties of dicyclobuta[*a*,*c*]anthracene are described.

Although benzene and naphthalene have been annelated with two[1] and even three[2] small rings, the annelation of the polyacenes has proved more difficult. Thus, it has not yet been possible to prepare a cyclopropa-anthracene,[3] and only anthracenes[4] and phenanthrenes[5] with one 4-membered ring joined to a benzene ring have been synthesised. This increase in difficulty of annelation may arise from the non-equivalence of Kekulé structures with a concomitant preference for one ring to maintain an aromatic sextet.[3] We now report the synthesis of dicyclobuta[*a*,*c*]anthracene (**6**), a polyacene with increased ring strain and the first to have one benzene ring annelated by two 4-membered rings.



(1) (2) (3)

a; R = Me
b; R = H

(5) (4)

(6)

The dibromide (**1**)[2b] was treated with the dianion (**2**) (prepared from the corresponding diester and $\mathrm{Pr^i_2NLi}$)[6] in tetrahydrofuran (THF) to give the adduct (**3a**) as white crystals (57%), m.p. 140—143 °C.† Hydrolysis gave the diacid (**3b**), in virtually quantitative yield, which was decarboxylated with $\mathrm{Pb(OAc)_4}$ to give a mixture of predominantly compound (**4**)†, together with compound (**5**) (*ca.* 52% total yield). Treatment of this mixture with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone gave compound (**6**) as pale yellow crystals (32%), m.p. 176—180 °C. The mass spectrum [*m/e* 230·1095 ($\mathrm{C_{18}H_{14}}$ requires 230·1096)] was in accord with the assigned structure, and the ^{1}H n.m.r. [δ 8·27 (s, 2 H, 9- and 10-H), 7·93—8·0 (m, 2 H, 5- and 8-H), 7·35—7·45 (m, 2 H, 6- and 7-H), 3·44—3·49 (m, 4 H), and 3·27—3·31 (m, 4 H)] and ^{13}C n.m.r. (δ 141·3, 138·6, 132·9, 128·5, 127·8, 125·0, 121·4, 29·3, and 29·1 p.p.m.) spectra are similar to those of anthracene. The electronic spectrum shows absorption maxima (hexane) at λ_{max} 228 ($\epsilon \times 10^{-4}$) (2·2), 238 (2·1), 249 (2·9), 255 (5·9), 261 (12·9), 281 (0·28), 337 (0·18), 355 (0·34), 374 (0·52), 390 (0·33), and 395 (0·50) nm. Compound (**6**) is relatively unstable and decomposes

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† Satisfactory high-resolution mass and ^{1}H n.m.r. spectral data were obtained for this compound.

slowly in the solid state, which, in part, may account for the low yield obtained in the dehydrogenation step and may reflect the non-equivalence of the Kekulé structures.

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