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Preliminary communication

The 9-mesityl-9-boraanthracene anion*

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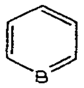
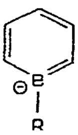
Derivatives of borin (I) with two-coordinate boron have so far evaded synthesis[1]. The anionic analogues (II) with three-coordinate boron (being isosteric with the wellknown borazaro compounds[2]) promised to possess a higher stability and offer a better chance of isolation. Recent investigations in the boranaphthalene series[3] and the successful preparation of the 1-phenylborabenzene anion[4] (II, R = C_6H_5) prompt us to communicate our results with the 9-mesityl-9-boraanthracene anion (III).



(I)



(II)

Reaction of 9-chloro-9,10-dihydro-9-boraanthracene (IV)[1] with mesitylmagnesium bromide in ether yielded 87% 9-mesityl-9,10-dihydro-9-boraanthracene (V)**, m.p. 131–134° after vacuum sublimation at 120°. ^{1}H NMR (CCl_4, internal TMS): δ 4.47 (s, 2H, CH_2); mass spectrum: $(V)^{+}$ *m/e* 296, 50.4%, $[(V)\text{-mesitylene})]^{+}$ *m/e* 176, 100%; UV only end absorption above 320 nm.

When a solution of (V) in benzene was treated with a 100% excess of tert-butyllithium in pentane during 30 to 45 minutes (under nitrogen and in the dark) a deep red colour gradually developed***. The UV spectrum (Fig. 1) can be qualitatively explained by assuming contributions from a diphenylmethyl anion type and an anthracene type chromophoric system ((IIIa), λ max. 4350 Å, and (IIIb), λ max. 3650 Å, respectively)****.

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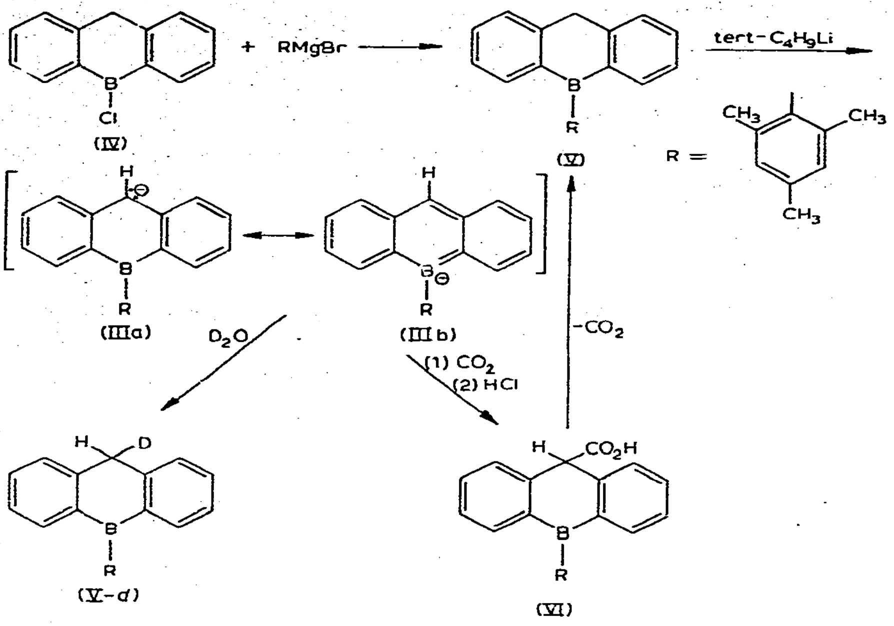
* Presented in part at the International Symposium on the Chemistry of Nonbenzenoid Aromatic Compounds, 24–28 August 1970, Sendai, Japan; Abstracts of Papers, p. 151.

** The compound gave elemental analyses and spectral data in agreement with the proposed structure.

*** A deep red colour was also observed during the preparation of (V), indicating that Grignard compounds and possibly still weaker bases may be sufficient for deprotonation.

**** MO calculations on simple models are being performed by Dr. J. Michl, University of Utah, Salt Lake City; preliminary results show a satisfactory agreement with the observed spectrum. We thank Dr. Michl for this private communication.



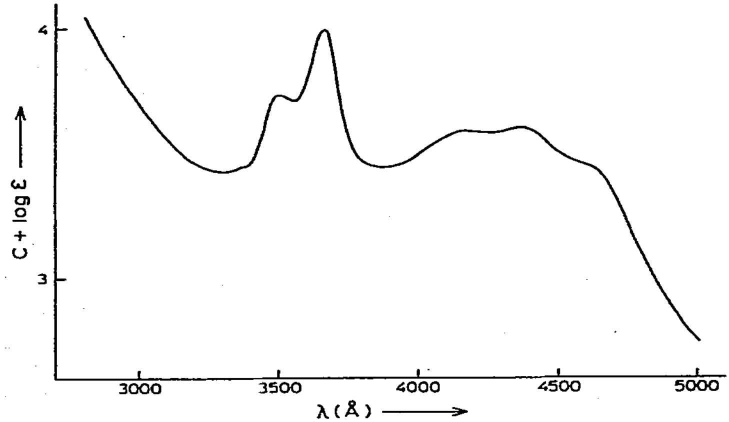


Fig. 1. UV spectrum of III in benzene/pentane. (The value of *C* is unknown).

The presence of the 9-mesityl-9-boraanthracene anion (III) in solution was further substantiated by its reaction with D_2O and CO_2. Reaction with D_2O lead to (V-*d*) (64.5%), m.p. 126–133°. ^1H NMR (CCl_4, internal TMS); δ 4.47 ppm (s, 1H, CHD), IR and mass spectrum $(V\text{-}d)^+$ *m/e* 297, 48.3%; $[(V\text{-}d)\text{-mesitylene}]^+$ *m/e* 177, 100%) were very similar to those of (V) with the expected differences due to the presence of one deuterium. Reaction with CO_2 gave (VI) (66%), m.p. 168–171° (dec.) as the hemihydrate★. (VI) was difficult to purify because of its ready decarboxylation to (V).

★The compound gave elemental analyses and spectral data in agreement with the proposed structure.

Experiments to isolate (VI), or a more stabilized derivative, in pure form are in progress.

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