The Isomerisation of 12-Phenylbenz[*a*]anthracene

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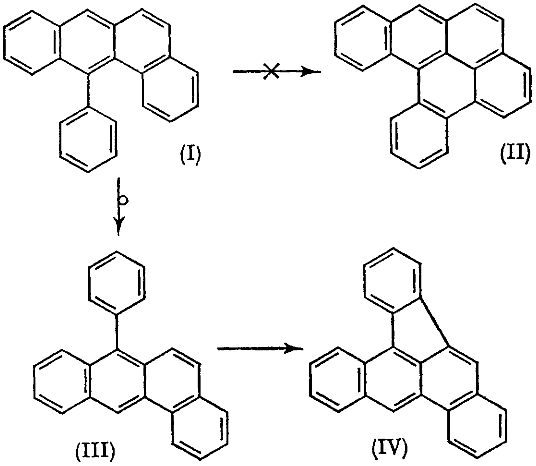
IN contrast to an earlier report that 12-phenylbenz[*a*]anthracene (I) is dehydrogenated with aluminium chloride to dibenzo[*a,l*]pyrene (II),[1] Buu-Hoi and his co-workers[2] reported that the product of this reaction is actually dibenzo[*a,e*]fluoranthene (IV). The first true synthesis of dibenzo[*a,l*]pyrene was published soon after Buu-Hoi's disclosure.[3] Buu-Hoi suggested that compound (IV) is obtained from 7-phenylbenz[*a*]anthracene (III), which itself is formed by a rearrangement of (I).

We now report experimental data which shows that (I) does indeed rearrange to (III).

Both 7- and 12-phenylbenz[*a*]anthracene have been reported previously.[4] Using gas-phase chromatography, it was possible to analyse the products of the reaction of 12-phenylbenz[*a*]anthracene with aluminium chloride.

A mixture of 100 mg. of (I), 300 mg. of $AlCl_3$, and 50 ml. of benzene was heated at the reflux temperature for 10 min. and decomposed with dilute HCl. G.l.c. analysis using a Micro-Tek model 1600 gas chromatograph with a hydrogen flame detector and a 4ft. × $\frac{1}{8}$in. column packed with 2·5% SE 52 on Gas-Chrom Z operated at a column temperature of 225° showed 50% of (I), 30% of (III), 20% of benz[*a*]anthracene, and a very small amount of (IV).



When the above experiment was repeated using toluene in place of benzene, the same results were obtained. This suggests that the rearrangement is intramolecular.

It is likely, as suggested by Buu-Hoi,[2] that not only does 12-phenylbenz[*a*]anthracene rearrange to the 7-isomer, but that the 12-mono- and dimethylphenylbenz[*a*]anthracenes do so also, and those which we have previously reported as methyldibenzo[*a,l*]pyrenes[6] are actually methyldibenzo[*a,e*]fluoranthenes.

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