

Hexaphenyltripentafulvalene¹

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THE triapentafulvalenes (I) are expected to represent a stable system for the same reason as the pentaheptafulvalenes, namely, because of the contribution of such polar structures as (Ia) to the ground state of the molecules. Whilst several derivatives of the system (I) have been described, all of them carry polar substituents; hydrocarbon derivatives have only been reported of benzologues

of (I).²⁻⁵ We now describe a hydrocarbon derived directly from (I), namely the hexaphenyltripentafulvalene (II). The method of its preparation is novel and opens a route to other, similar syntheses, although the yields were low. The lithio-derivative of 1,2,3,4-tetraphenylcyclopentadiene was condensed with 3,3-dichloro-1,2-diphenylcyclopropene, yielding the glistening red

¹ Fulvenes and Thermochromic Ethylenes. Part 40. (Part 39: I. Agranat and E. D. Bergmann, in the press.)

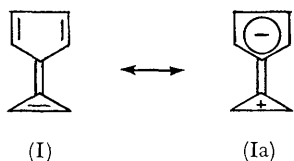
² W. M. Jones and R. S. Pyron, *J. Amer. Chem. Soc.*, 1965, **87**, 1628.

³ A. S. Kende and P. T. Izzo, *J. Amer. Chem. Soc.*, 1965, **87**, 1609.

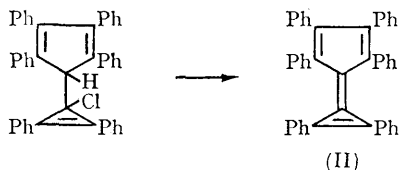
⁴ H. Prinzbach, D. Seip, and U. Fischer, *Angew. Chem., Internat. Edn.*, 1965, **4**, 242.

⁵ H. Prinzbach and U. Fischer, *Angew. Chem., Internat. Edn.*, 1965, **4**, 598.

needles of (II) [from benzene, m.p. 296° (dec.)].



The product (II) probably arises from the intermediate chloro-compound by spontaneous loss of hydrogen chloride:



This synthesis recalls the observation that 1,2,3,4-tetraphenylcyclopentadiene and 1,2,4-triphenyl-

cyclopentadiene condense thermally with diphenyldichloromethane to yield the corresponding phenylated fulvenes.⁶

The infrared spectrum of the hydrocarbon shows the characteristic "molecular vibration" of 3,4-disubstituted triafulvenes⁷ at 1845 cm.⁻¹; the ultraviolet spectrum shows two bands: in cyclohexane 263 (log ϵ 4.54) and 377 m μ (4.47); in acetonitrile 266 (4.55) and 371 m μ (4.51). In benzene, chloroform, and ethanol, the latter maximum lies at 379, 379, and 373 m μ , respectively. The hypsochromic shift, on going from benzene to the highly polar acetonitrile, is in accord with the theoretical expectations for such systems.

The strong contribution of a form of type (Ia) to the ground state of the molecule is best demonstrated by the dipole moment of (II) which is 6.3 ± 0.3 D (benzene, 30°). To the best of our knowledge, this is the highest moment ever reported for a hydrocarbon.

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⁶ W. Dilthey and P. Huchtemann, *J. prakt. Chem.*, 1940, **154**, 238. cf. V. Kaufmann, *Ber.*, 1896, **29**, 73.

⁷ I. Agranat and E. D. Bergmann, in the press.