Tetrahedron Letters No. 34, pp 3153 - 3154.

0040-4039/78/0815-3153$02.00/0

THE SYNTHESIS OF 2,6,7,11-TETRAPHENYLISOBENZOFURAN[b]CYCLOBUTADIENE: A NEW STABLE ANTIAROMATIC COMPOUND

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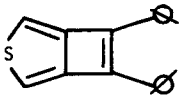
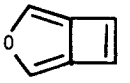
(This paper is dedicated to the founder of Kerman University, A. Afzalipour.)

Recently the synthesis of cyclobutadiene derivatives (I) and (II) with the heteroatom in the ring fused to the cyclobutadiene moiety were reported.[1,2] Compound (I) is quite stable and isolated as red crystals.

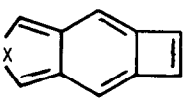


I



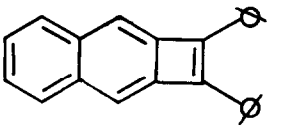
II

The purpose of our investigation was to prepare molecules with structure (III), and compare their stability and chemical reactions with already reported very stable compound (IV).[3,4,8]



III

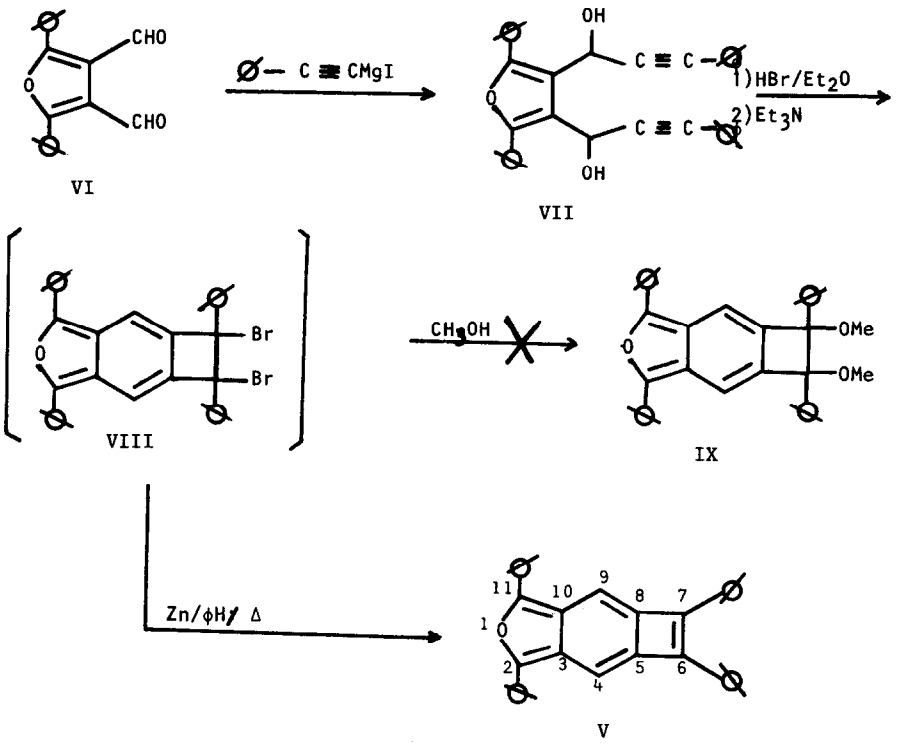
a: x = O
b: x = S
c: x = Se



IV

Now we wish to report the synthesis and isolation of compound (V), starting from dialdehyde (VI) and phenylethynylmagnesiumiodide to afford dipropargylalcohol (VII) in 50% yield as white crystals, m.p. 190-193°; IR (KBr) 3200(s), 1600(m), 1480(s), 1440(s), 1260(m) cm^{-1}; 1Hnmr $\delta^{TMS}_{CDCl_3}$ 4(d,2H), 6.3(d,2H), 7.6-8(m,20H). Hydrogen bromide gas was bubbled through the suspension of diol (VII) in dry ether. After a few minutes a yellow flourescent solution was obtained, which was treated with triethylamine and filtered. The filterate was evaporated and the resulting material was dissolved in benzene and refluxed in the presence of activated zinc dust in 30 minutes. Thin layer chromatography (silica gel, hexane/chloroform, 60/40) of the mixture afforded compound (V) in 10% yield as orange-red stable crystals with an indefinite m.p.; ^{1}Hnmr $\delta^{TMS}_{CDCl_3}$ 6.8(S,2H), close to cis-stilbene, 6.55,[1,3,6] 7.2-7.8(m,20H); m/e 446(M^+), IR (KBr) 1600(s), 1490(s), 1440(m), 840(m), 760(s), 680(s) cm^{-1}; the solution of compound (V) in benzene is photochemically very unstable and will be destroyed in a few minutes under U.V. light.

The attempts made to isolate dibromide (VIII) or its dimethoxy derivative (IX) failed.



The synthesis of compounds ($III_{b,c}$) in this series and investigation of chemical properties of compound (V) are now under way.

Acknowledgements. We are thankful to both the Ministry of Science and Higher Education of Iran for the grant number 600-7-36/1 and Kerman University for the support of this work.

References and Footnotes.

1. P.J. Garratt and K.P.C. Vollhardt, *J. Amer. Chem. Soc.*, 94, 1023 (1972).

2. K.P.C. Vollhardt and R.G. Bergman, *J. Amer. Chem. Soc.*, 94, 8950 (1972).

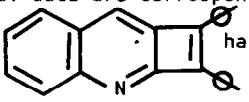
3. M.P. Cava, B. Hwang and J.P. Van Meter, *J. Amer. Chem. Soc.*, 85, 4032 (1963).

4. For a comprehensive review, see M.P. Cava and M.J. Mitchell, "Cyclobutadiene and Related Compounds," *Academic Press*, New York, (1967).

5. *Spectrum No.* 305, Varian Associates, NMR Spectra Catalogue.

6. All yields refer to isolated products.

7. All analytical data are corresponding to the proposed structures.

8. The compound  has also been isolated very recently by A. Af zali and N. Maleki, Chemistry Department, Pahlavi University, Shiraz, Iran, as stable orange-red crystals, mentioned in a private communication, which is now in the process of being published.

(Received in UK 1 June 1978; accepted for publication 22 June 1978)