PHOTOCHEMICAL CONVERSION OF 3,6-DI-tert-BUTYL-o-BENZOQUINONE

V. B. Vol'eva, V. V. Ershov,
I. S. Belostotskaya, and N. L. Komissarova

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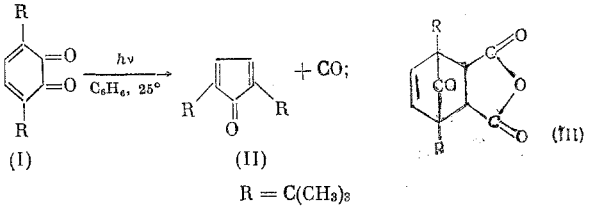
We discovered the unusual, different from the described in [1] for o-quinones, photochemical behavior of 3,6-di-tert-butyl-o-benzoquinone (I), which when irradiated with light ($\lambda \geq 380$ nm) undergoes decarbonylation with the formation of 2,5-di-tert-butylcyclopentadienone (II).



(I) (II) (III)

R = C(CH3)3

After removal of the solvent, the orange crystals of ketone (II) were isolated from the reaction mixture by subliming the residue in vacuo at 20°; mp 59°. Found: C 81.16; H 10.46%. $C_{13}H_{20}O$. Calculated: C 81.17; H 10.48%. NMR spectrum (δ, ppm): 1.06 s (9H) and 6.21 s (1H). Ultraviolet spectrum [λ, nm (ε)]: 217 (3000) and 419 (400). Infrared spectrum: band of CO group at 1720 cm^{-1} and of double bond at 1590 cm^{-1}. When the p otolysis of (I) is run in the presence of maleic anhydride a white crystalline adduct (III) is formed, which is identical with that obtained in the reaction of (II) with maleic anhydride in refluxing benzene; mp 153°. Found: C 70.10; H 7.88%. $C_{17}H_{22}O_4$. Calculated: C 70.34; H 7.64%. NMR spectrum (δ, ppm): 1.00 s (9H), 2.92 s (1H), and 5.34 s (1H).

The stability of the cyclopentadienones depends on the nature and on the number of substituents in the ring, and is assured by a minimum of three substituents [2]. Compound (II) is the first stable cyclopentadienone derivative that contains two alkyl substituents in the ring.

LITERATURE CITED

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2. A. Streitwieser, Jr., Molecular Orbital Theory [Russian translation], Mir (1965), p. 254.

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