## PHOTOCHEMICAL CONVERSION OF

## 3.6-DI-tert-BUTYL-o-BENZOQUINONE

V. B. Vol'eva, V. V. Ershov,

UDC 541.14:547.567

I. S. Belostotskaya, and N. L. Komissarova

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 ( $\lambda \ge 380$  nm) undergoes decarbonylation with the formation of 2,5-di-tert-butyleyclopentadienone (II).

$$\begin{array}{c} R \\ = 0 \\ R \\ = 0 \\ \hline \\ (I) \\ R = C(CH_3)_8 \end{array} + CO; \qquad \begin{array}{c} R \\ = 0 \\ C_0 \\ R \\ = 0 \end{array}$$

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 ( $\delta$ , ppm): 1.06 s (9H) and 6.21 s (1H). Ultraviolet spectrum [ $\lambda$ , nm ( $\epsilon$ )]: 217 (3000) and 419 (400). Infrared spectrum: band of CO group at 1720 cm<sup>-1</sup> and of double bond at 1590 cm<sup>-1</sup>. 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 ( $\delta$ , 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

- 1. N. Turro, Molecular Photochemistry [Russian translation], Mir (1967), p. 231; S. Farid and D. Hess, Chem. Ber., 102, 3747 (1969); H. Bos, J. Polman, and P. Montfort, J. Chem. Soc., Chem. Commun., 188 (1973).
- 2. A. Streitwieser, Jr., Molecular Orbital Theory [Russian translation], Mir (1965), p. 254.

Institute of Chemical Physics, Academy of Sciences of the USSR, Moscow. Translated from Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, No. 3, p. 739, March, 1974. Original article submitted December 7, 1973.

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