Triphenylene-1,4:5,8-diquinones

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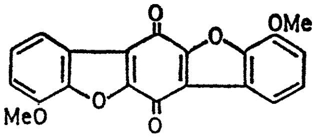
Summary The aluminium chloride-catalysed reaction between benzo-1,4-quinones and either veratrole or 3′,4′-dimethoxyphenylbenzo-1,4-quinones gives derivatives of triphenylene-1,4 : 5,8-diquinone.

ONLY one quinone has been prepared so far in the triphenylene series.[1] We now report a simple method of making compounds which contain the triphenylenediquinone system.

The reaction between benzo-1,4-quinone, veratrole, and anhydrous $AlCl_3$ in CS_2 was originally reported by Pummerer and his co-workers[2] to give a red quinone $C_{18}H_6O_4(OMe)_2$ which was assigned the centrosymmetric structure (I). The substitution pattern in the terminal rings appeared to us to be unlikely and on re-examining the compound we have found that it shows two carbonyl bands in the i.r. (at 1675 and 1650 cm.$^{-1}$) suggesting that the quinonoid system is not symmetrically substituted. It gives a bisleucoacetate

$C_{18}H_6(OMe)_2(OAc)_4$ m.p. 247—249° which has the characteristic u.v. absorption of a triphenylene derivative and, accordingly, we formulate Pummerer's quinone as 10,11-dimethoxytriphenylene-1,4:5,8-diquinone (IIa). Its n.m.r. spectrum [τ 5·92 (S, 6H; methoxy-protons), τ 1·04 (s, 2H; deshielded aromatic protons), AB quartet centred at τ 2·94 and 3·13, J 10 Hz (4H, quinonoid protons)] is in full agreement with this structure. A similar reaction between chlorobenzo-1,4-quinone and veratrole gave both the two symmetrical (IIb) and (IIc) and the unsymmetrical (IId) dichlorotriphenylenediquinones while 2,3-dichlorobenzo-1,4-quinone and veratrole afforded a little of the tetrachloro-analogue (IIe). The last reaction was complicated by the simultaneous oxidation of some of the veratrole by the quinone to 2,3,6,7,10,11-hexamethoxytriphenylene.[3]

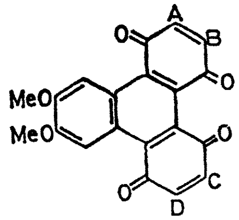


(I)

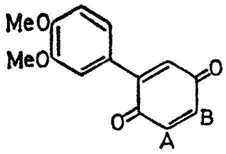
We consider that arylbenzoquinones are intermediates in the formation of these triphenylenediquinones because 3′,4′-dimethoxyphenylbenzo-1,4-quinone (IIIa) reacted with benzo-1,4-quinone and with 2,3-dichlorobenzo-1,4-quinone under the same conditions to give Pummerer's quinone (IIa) and its 2,3-dichloro-analogue (IIf) respectively. A similar reaction between (IIIa) and methylbenzo-1,4-quinone gave an inseparable mixture of the methyl derivatives (IIg) and (IIh). Each of these reactions gave, as an additional product, a mixture of the 3,4-dimethoxyphenyl derivatives (IIi) and (IIj) which results from the self-condensation of two molecules of (IIIa). The latter reaction cannot occur when either 2-chloro- (IIIb) or 2,3-dichloro-5-(3′,4′-dimethoxyphenyl)benzo-1,4-quinone (IIIc) is used and these compounds reacted with benzo-1,4-quinone to give improved yields of the triphenylenediquinones (IIk; 60%) and (IIf; 44%) respectively.

The triphenylenediquinones were isolated by preparative t.l.c., most of them being obtained in yields of *ca.* 10%. They are red solids which decompose on being heated above 200° and do not have well-defined m.ps. Satisfactory mass spectral analytical data have been obtained in each case and the structures of the compounds follow from their u.v. and n.m.r. absorptions and their modes of formation.

(IIa) A = B = C = D = H
(IIb) A = D = H; B = C = Cl
(IIc) A = D = Cl; B = C = H
(IId) A = C = H; B = D = Cl
(IIe) A = B = C = D = Cl
(IIf) A = B = Cl; C = D = H
(IIg) A = Me; B = C = D = H
(IIh) A = C = D = H; B = Me
(IIi) A = C = D = H; B = 3,4-$(MeO)_2C_6H_3$
(IIj) A = 3,4-$(MeO)_2C_6H_3$; B = C = D = H
(IIk) A = C = D = H; B = Cl



(IIIa) A = B = H
(IIIb) A = H; B = Cl
(IIIc) A = B = Cl



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[3] I. M. Matheson, O. C. Musgrave, and C. J. Webster, *Chem. Comm.*, 1965, 278.