H, 9.41. Found: C, 48.94; H, 9.54.

Tri-*n*-butylstannyl ethoxide was prepared by a similar procedure, an ethanolic solution of sodium ethoxide being used. Fractional distillation, 97 °C (1 mm) yielded the product: NMR (CDCl₃) δ 0.65–1.8 (m, 27 H), 1.18 (t, 3 H), 3.78 (q, 2 H).

Solvents benzene, acetonitrile, and methanol were purified and dried by standard procedures.[31]

General Procedure. The typical procedure was to make a stock solution which was 0.1 M in ketone and 0.04 M in internal standard. Similarly, a stock solution which was 0.1 M in tin hydride was made. Equal aliquots of each stock solution were added to a reaction ampule, the mixture was degassed by three freeze–thaw cycles, and then the ampule was sealed under vacuum. The reaction mixture was thermostated in an oil bath at 61 °C for a standard time (16 h) in the dark. The ampule was then opened and the product mixture analyzed by GLPC using either a 5 ft × ¹/₈ in. stainless steel column packed with 10% FFAP on Chromosorb WAW DMCS 60/80 mesh or a 25-m FFAP capillary column. Product peaks were identified by a comparison of their retention times, GLPC–mass spectra, and GLPC–IR with those of authentic samples. Duplicate experiments were run with each ketone to test the effects of inhibition by *m*-dinitrobenzene, initiation by AIBN, structure of the hydride, and polarity of the solvent.

GLPC analyses were carried out with either an HP5840A or a Varian Vista 6000 gas chromatograph. The area ratios were converted to mole ratios for quantitative determinations by using standard calibration curves. ¹H NMR high resolution spectra were obtained on a Brucker WH400 high-field spectrometer. GLPC/IR data were obtained on a Nicolet 7199 FT/IR spectrometer interfaced to a Varian 3700 gas chromatograph.

Competitive Reaction of α,α,α-Trifluoroacetophenone and α-Fluoroacetophenone with Triphenyltin Hydride. A stock solution which was 0.1 M in both α,α,α-trifluoroacetophenone and α-fluoroacetophenone, with a known amount of added internal standard, was made in solvent benzene. Equal aliquots of this solution and a stock solution 0.1 M in triphenyltin hydride, with 4% AIBN added, were added to a reaction ampule. The mixture was degassed and reacted at 61 °C for 3.5 h. The reaction was repeated in solvent acetonitrile. The relative rates of reduction in each solvent were determined from the relative rates of disappearance of the two substrates as found by GLPC analysis.

Reaction of Cyclopropyl Phenyl Ketone with Organotin Hydride in Refluxing Methanol. A solution which was 0.5 M in ketone and 0.5 M in organotin hydride was prepared in methanol. A known amount of *n*-hexadecane, an internal standard, was added. The methanolic solution was heated under total reflux for 4 days. The product solution was analyzed by GLPC on a 25-m 10% FFAP capillary column or a 10 ft × ¹/₆ in. 10 FFAP on Chromosorb WAW stainless steel column. Results are reported in Table III.

Analysis of Noncondensible Gases in the Reduction of α-Fluoroacetophenone. A reaction mixture using the 0.1 M stock solutions in solvent benzene, with 4% AIBN, was added to a reaction vessel fitted with a break seal. The mixture was reacted at 61 °C for 16 h. The vessel was then attached to a vacuum line, the seal broken, and the noncondensible gases transferred, using a Toppler pump, to a bulb of known volume. The temperature and pressure of the gases were measured and the number of moles of product were estimated.

(31) Vogel, A. I. "Textbook of Practical Organic Chemistry", Longman: Birmingham, AL; 1956.

Reactions in the Solid State. 2.[†] The Crystal Structures of the Inclusion Complexes of 1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol with Benzylideneacetophenone and 2,5-Diphenylhydroquinone with Dibenzylideneacetone

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The crystal structures of the inclusion complexes of 1,1,6,6-tetraphenylhexa-2,4-diyne-1,6-diol with benzylideneacetophenone and 2,5-diphenylhydroquinone with dibenzylideneacetone show that in both complexes two molecules of the guest are linked by hydrogen bonds between the carbonyl oxygen atom and the hydroxyl groups of the host. The molecules in both structures are packed with parallel planar guest molecules related by an inversion center with double-bond center-to-center distances ranging from 3.787 to 3.947 Å. Those distances are within the limit for photochemical [2 + 2] cycloaddition in the solid state. Irradiation in the solid state should, in principle, reveal stereoselective cycloadditions to afford the syn head-to-tail dimers.

The courses of certain types of solid-state reactions are determined by the geometry of the reactant lattice. In a long survey by Cohen and Schmidt,[1] the dependence of photochemical reactions in the solid state on the relative geometry of the reactants in the crystal has been discussed.

The postulate that such reactions occur with a minimum amount of atomic or molecular movement implies that the reactions are controlled by the relative fixed distances and orientations, determined by the crystal structure, between potentially reactive centers. The topochemical rules also

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†Part 1: *J. Chem. Soc., Perkin Trans. 2*, **1984**, 757–765.

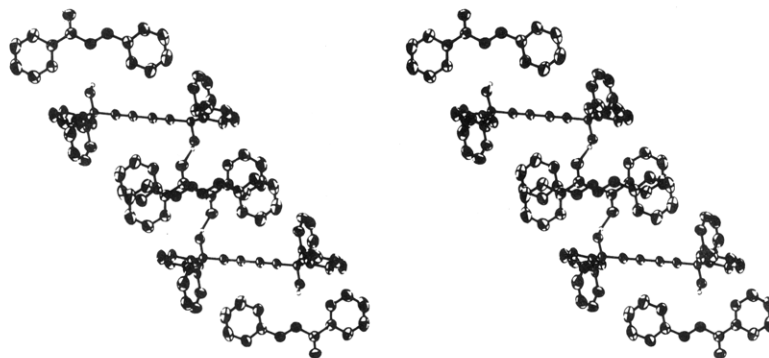(1) Cohen, M. D.; Schmidt, G. M. J. *J. Chem. Soc.* **1964**, 1966.

Figure 1. Stereoscopic view of the two reacting molecules of the host–guest complex (I and II) (the reacting centers are marked by filled circles).

suggest that an upper limit for such distances should exist for each type of reaction to occur.

In intermolecular photodimerization the stereochemistry of the dimer is determined by the contact geometry of the nearest neighbor double bonds, provided that the center-to-center distance is of the order of 4 Å (experimentally observed limits 3.5–4.2 Å)[2] and by the mutual orientation of the reactant molecules. While the knowledge of the factors involved in solid-state reactions has developed dramatically over the years, this cannot be said of the application side. The main problem of crystal engineering which will lead to a desirable product is yet unresolved. An important step forward was achieved by the preparation of inclusion complexes which have the ability to include guest molecules in fixed relative geometries available for photochemical reactions.[3] In many cases the inclusion complexes are formed with guest molecules which may undergo photodimerization which could not occur in the crystals of the pure guest compounds. 1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol (I) or 2,5-diphenylhydro-
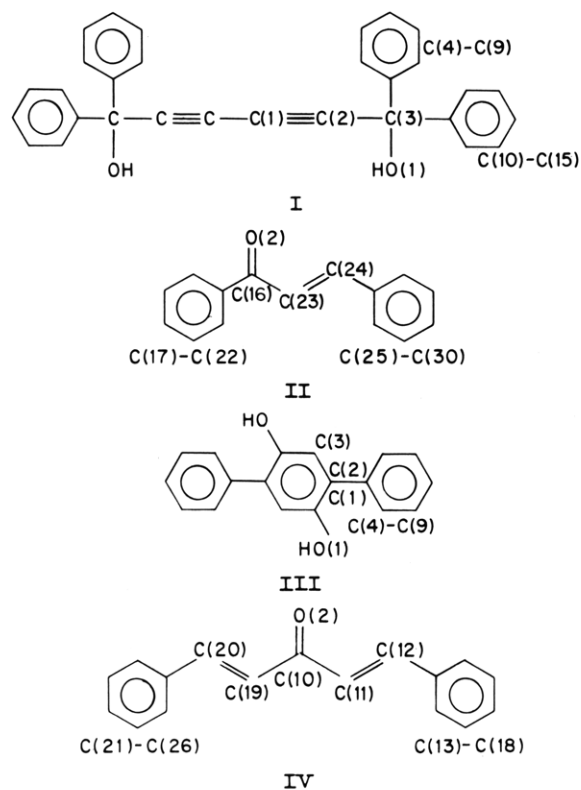
I

II

III

IV

(2) Schmidt, G. M. J. *Pure Appl. Chem.* **1971**, *27*, 647.
(3) Lahav, M.; Leiserowitz, L.; Popovitz-Biro, R.; Tang, C. *J. Am. Chem. Soc.* **1978**, *100*, 2542.

Table I. I and II. Atomic Coordinates for Non-Hydrogen Atoms (×10⁴)[a]

atom	x	y	z	U_{eq}
O(1)	7290 (1)	1679 (2)	2629 (2)	51 (1)
C(1)	9687 (2)	404 (2)	4629 (3)	46 (1)
C(2)	9149 (2)	1108 (2)	3962 (3)	45 (1)
C(3)	8450 (2)	1995 (2)	3211 (3)	41 (1)
C(4)	8590 (2)	3177 (2)	4651 (3)	44 (1)
C(5)	7685 (3)	3797 (3)	5105 (4)	59 (2)
C(6)	7839 (3)	4873 (3)	6406 (4)	76 (2)
C(7)	8894 (4)	5318 (3)	7262 (4)	76 (2)
C(8)	9790 (4)	4714 (3)	6827 (5)	79 (2)
C(9)	9652 (3)	3644 (3)	5533 (4)	63 (2)
C(10)	8762 (2)	2079 (2)	1667 (3)	42 (1)
C(11)	9692 (2)	1528 (2)	1222 (4)	56 (1)
C(12)	9943 (3)	1625 (3)	−176 (4)	73 (2)
C(13)	9243 (4)	2280 (3)	−1167 (4)	80 (2)
C(14)	8319 (3)	2843 (3)	−734 (4)	82 (2)
C(15)	8066 (3)	2744 (3)	662 (4)	64 (2)
O(2)	2847 (2)	480 (2)	−145 (3)	67 (1)
C(16)	3702 (2)	1054 (2)	774 (3)	52 (1)
C(17)	3754 (2)	2246 (2)	704 (3)	54 (1)
C(18)	2865 (3)	2667 (3)	−448 (4)	72 (2)
C(19)	2901 (4)	3759 (4)	−576 (6)	96 (3)
C(20)	3824 (4)	4441 (4)	416 (7)	104 (3)
C(21)	4708 (4)	4044 (3)	1530 (6)	92 (2)
C(22)	4675 (3)	2954 (3)	1689 (5)	72 (2)
C(23)	4660 (2)	578 (2)	1926 (4)	55 (1)
C(24)	4593 (2)	−427 (2)	2180 (3)	55 (1)
C(25)	5489 (2)	−979 (2)	3309 (4)	60 (2)
C(26)	6543 (3)	−487 (3)	4275 (4)	76 (2)
C(27)	7361 (3)	−1028 (4)	5300 (5)	97 (2)
C(28)	7157 (4)	−2076 (4)	5410 (6)	98 (3)
C(29)	6126 (4)	−2587 (4)	4471 (5)	95 (3)
C(30)	5287 (4)	−2043 (3)	3409 (4)	75 (2)

[a] U_{eq} (Å² × 10³) = ¹/₃ trace $\tilde{U}$.

quinone (III) formed crystalline inclusion complexes with a variety of guest molecules in a definite ratio.[4] Many of those inclusion complexes undergo photochemical reactions efficiently and stereoselectively. We chose to study two examples, benzylideneacetophenone (II) (chalcone) and dibenzylideneacetone (IV), in which the pure guest compounds are light-stable in the solid state while the inclusion complexes of those compounds are light-sensitive, leading to stereoselective dimers.

Crystal Structures and Molecular Geometries

1,1,6,6-Tetraphenylhexa-2,4-diyne-1,6-diol–2-Benzylideneacetophenone (Figure 1) shows how two molecules of benzylideneacetophenone (II) and one molecule of the host (I) are linked (atomic coordinates are given in Table I).

(4) Tanaka, K.; Toda, F. *J. Chem. Soc., Chem. Commun.* **593**. (b) Tanaka, K.; Toda, F. *J. Chem. Soc. Jpn.* **1984**, 141.
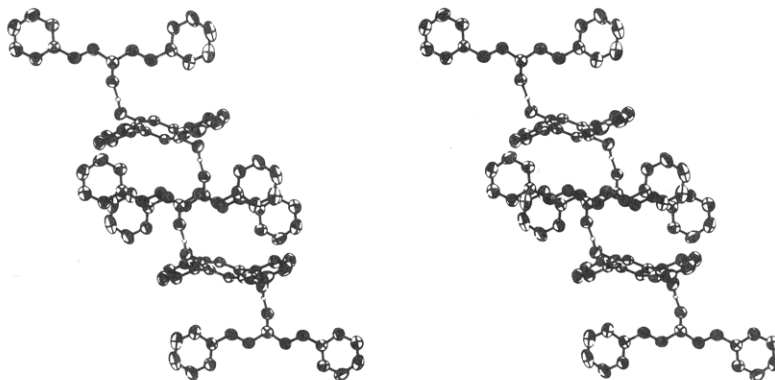
Figure 2. Stereoscopic view of the two reacting molecules of the host–guest complex (III and IV) (the reacting centers are marked by filled circles).

The host molecule occupies a crystallographic inversion center and the two guest molecules which are linked to the host via hydrogen bonds are related by the inversion center. The groups at the hosts sp^3 carbon are staggered, with the hydroxyl groups (including the hydrogens) anti. A similar molecular structure of the host was found in the inclusion complex of I with acetone.[5] The $C^{sp}C^{sp}$ triple bond length of 1.199 (3) Å, the $C^{sp}C^{sp}$ single bond length of 1.367 (3) Å, and the bond angles at those atoms of 176.7 (3)° and 178.3 (3)° are in a good agreement with those observed in similar systems such as in 2,4-hexadiynylenebis(*p*-chlorobenzenesulfonate)[6] (1.187, 1.381 Å, 177.4° and 179.0°, respectively), or in octa-3,5-diyn-1,8-diol[7] (at 120 K) (1.198, 1.376 Å, 178.8° and 179.4°, respectively). Bond lengths and angles in the benzylideneacetophenone (chalcone) molecule are very similar to those observed in the crystal structures of the two polymorphs of pure chalcone.[8] However, the degree of planarity of the molecules is different. The torsion angle of the phenyl ring around the bond C(23)–C(24) is 0.2° in the present work but 9.3° and 0.6° in polymorphs I and II, respectively; the torsion angle around the C(16)–C(23) bond is −8.1° (present work) but 16.9° and 9.7° in polymorphs I and II, respectively; and the other phenyl ring is rotated by −1.5° around C(16)–C(17) (present work) and 4.1° and 21.6° (in polymorphs I and II).

2,5-Diphenylhydroquinone:2Dibenzylideneacetone (Figure 2) shows how two molecules of dibenzylideneacetone (IV) and one molecule of the host (III) are linked (atomic coordinates are given in Table II).

The host molecule occupies a crystallographic inversion center and the guest molecules which are linked to the host through hydrogen bonds are related to each other by the inversion center. The phenyl rings are rotated by 50.5° relative to the hydroquinone ring, similar to that found in the more hindered 2,5-bis(2,4-dimethylphenyl)hydroquinone[9] (62.5°). *p*-Terphenyl has been found to be planar.[10] The rotation of the phenyl rings, in the present work, is attributed to the hindrence of the hydroxyl groups of the central hydroquinone ring.

The crystal structure of dibenzylideneacetone is not known; however, the structures of its complexes with Pd(0) were determined.[11] The conformation of dibenzylidene-

Table II. III and IV. Atomic Coordinates for Non-Hydrogen Atoms (×10⁴)[a]

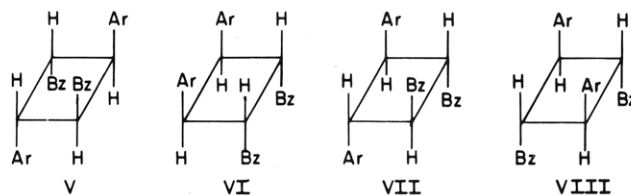| atom	x	y	z	U_{eq}
O(1)	6243 (2)	2214 (2)	4241 (3)	77 (1)
C(1)	5624 (2)	1096 (3)	4606 (4)	56 (2)
C(2)	5959 (2)	867 (3)	6182 (4)	51 (2)
C(3)	5310 (2)	−247 (3)	6548 (4)	53 (2)
C(4)	6956 (2)	1768 (3)	7453 (4)	54 (2)
C(5)	6999 (3)	2379 (4)	9269 (5)	66 (2)
C(6)	7940 (4)	3168 (4)	10450 (6)	76 (3)
C(7)	8840 (3)	3349 (4)	9844 (7)	82 (3)
C(8)	8812 (3)	2756 (4)	8073 (7)	85 (3)
C(9)	7877 (3)	1975 (4)	6876 (6)	68 (2)
O(2)	5427 (2)	3515 (3)	2190 (3)	80 (2)
C(10)	5070 (2)	4568 (4)	2435 (4)	59 (2)
C(11)	5619 (3)	5910 (4)	2244 (4)	61 (2)
C(12)	6543 (3)	6120 (4)	1863 (4)	62 (2)
C(13)	7175 (2)	7403 (3)	1639 (4)	56 (2)
C(14)	6846 (3)	8637 (4)	1823 (5)	76 (2)
C(15)	7455 (4)	9808 (5)	1543 (6)	97 (3)
C(16)	8386 (4)	9751 (5)	1064 (5)	84 (3)
C(17)	8719 (3)	8548 (5)	881 (5)	83 (3)
C(18)	8115 (3)	7387 (5)	1171 (5)	72 (2)
C(19)	4064 (3)	4510 (4)	2921 (4)	62 (2)
C(20)	3485 (3)	3360 (4)	3145 (4)	63 (2)
C(21)	2466 (2)	3184 (4)	3588 (4)	58 (2)
C(22)	1955 (3)	1886 (5)	3716 (5)	76 (2)
C(23)	977 (4)	1678 (7)	4065 (6)	93 (3)
C(24)	502 (4)	2754 (7)	4264 (6)	102 (3)
C(25)	1002 (3)	4065 (6)	4151 (7)	100 (3)
C(26)	1980 (3)	4286 (5)	3829 (5)	76 (3)

[a] U_{eq} (Å² × 10³) = $^1/_3$ trace $\tilde{U}$.

acetone in the complexes is cis and trans with respect to the carbonyl group while both double bonds are cis in the present work. The two phenyl rings are rotated by −1.1° and −1.3° around their bonds to the double bond (present work) while the range of rotation angles is −11.5° to 14.6° in its complexes with Pd.

Discussion

There are four possible structures for the photodimers of benzylideneacetophenone (*trans*-chalcone): syn head-to-tail (V), syn head-to-head (VI), anti head-to-head (VII), and anti head-to-tail (VIII). Irradiation of II in solution

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(6) Mayerle, J. J.; Clarke, T. C. *Acta Crystallogr., Sect. B* **1978**, *B34*, 143.
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(8) (a) Rabinovich, D. *J. Chem. Soc. B* **1970**, 11. (b) Ohkura, K.; Kashino, S.; Haisa, M. *Bull. Chem. Soc. Jpn.* **1973**, *46*, 627.
(9) Toda, F.; Tanaka, K.; Mak, T. C. W. *Chem. Lett.* **1983**, 1697.
(10) Baudour, J. L.; Caillean, H.; Yelon, W. B. *Acta Crystallogr., Sect. B* **1977**, *B33*, 1773.

(11) (a) Mazza, M. C.; Pierpont, C. G. *Inorg. Chem.* **1973**, *12*, 2955. (b) Pierpont, C. G.; Mazza, M. C. *Inorg. Chem.* **1974**, *13*, 1891.

Figure 3. Mutual relation and geometrical parameters of the reacting centers of the guest molecules of benzylideneacetophenone.
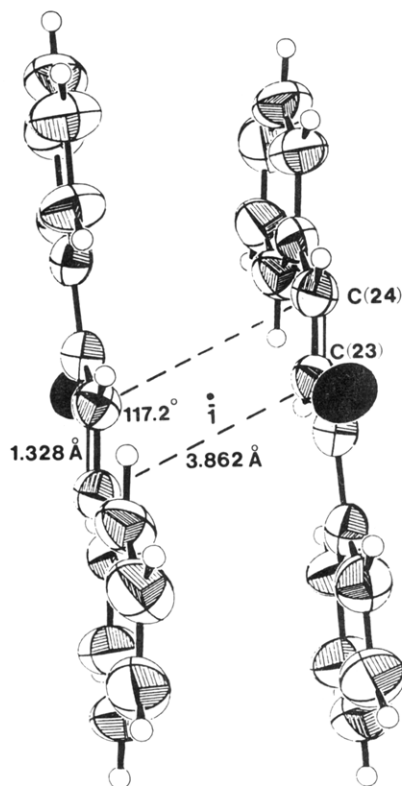

Figure 4. Mutual relation and geometrical parameters of the reacting centers of the guest molecules of dibenzylideneacetone.

gives a mixture of II and its cis isomer[12] or a polymer.[13] Irradiation of II in the solid state gives a complex mixture of stereoisomeric photodimers in low yield.[13] The crystal structures of two polymorphs of II show[8] that although the molecules are packed in parallel manner the distances between the double bonds centers are 5.2 Å in polymorph I and greater than 4.8 Å in polymorph II. Those distances are longer than the limit of 4.2 Å and therefore the two polymorphs are light-stable. The inclusion complex of II (in I) is light-sensitive. Irradiation of crystals of the inclusion complex for 0.5 h gave 24% of the dimer V and 73% of unreacted monomer of chalcone (II). The molecules of the guest are packed in parallel pairs related by an inversion center. As a result, the planes of the double bonds are parallel and the center-to-center distance is 3.862 Å as shown stereoscopically in Figure 1 and in Figure 3. This arrangement enables the photodimerization to give the syn head-to-tail product (V).

Irradiation of a solution of dibenzylideneacetone (IV) affords the *all-trans*-substituted cyclobutane[14] (related to VII), while it is light-stable in the solid state. Irradiation of solid material of the inclusion complex of IV in III for 6 h afforded 70% yield of the syn head-to-tail dimer product (related to V). The guest molecules are packed in a similar way to the inclusion complex of I with II but there are two potentially reactive centers. Pairs of molecules are related by inversion centers, hence, having parallel double bonds with center-to-center distances of 3.787 and 3.947 Å (see stereodiagram in Figure 2 and Figure 4).

Both distances are shorter than the upper limit of 4.2 Å and therefore both pairs may react to afford dimers of the same stereochemistry. The arrangement indicates that
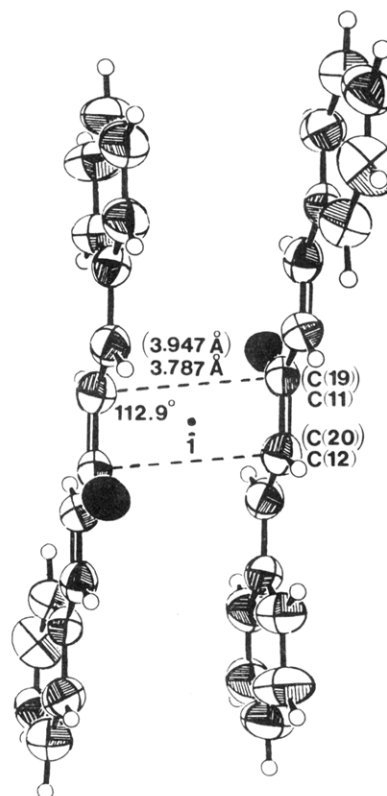
in principle a polymer might be obtained in which all the double bonds are involved in photochemical conversion reaction to cyclobutanes.

Conclusions

It was shown that host molecules may be used as a backbone for various guest molecules which are potentially photochemically reactive. The special packing arrangement of the reactive molecules may lead to efficient and stereoselective cycloaddition reactions.

Experimental Section

The inclusion compounds were obtained according to the procedure given in ref 4.

Crystal data: 1,1,6,6-tetraphenylhexa-2,4-diyne-1,6-diol:2-benzylideneacetophenone [$C_{30}H_{22}O_2$:($C_{15}H_{12}O$)$_2$], triclinic, space group $P\bar{1}$, a = 12.568 (6) Å, b = 12.161 (6) Å, c = 8.532 (4) Å, α = 109.60 (3)°, β = 109.60 (3)°, γ = 82.69 (3)°. The calculated density is 1.192 g/cm^3 for Z = 1.

2,5-Diphenylhydroquinone:2Dibenzylideneacetone [$C_{18}H_{14}O_2$:($C_{17}H_{14}O$)$_2$], triclinic, space group $P\bar{1}$, a = 13.627 (7) Å, β = 10.099 (5) Å, c = 8.056 (4) Å, α = 107.86 (3)°, β = 97.59 (3)°, γ = 103.15 (3)°. The calculated density is 1.210 g/cm^3 for Z = 1.

Intensity data were collected on a PW1100 diffractometer using the θ–2θ scanning technique with graphite-monochromated Mo Kα radiation (λ = 0.71069 Å). Both structures were solved by MULTAN80[15] and refined by SHELX[16] in two separate blocks; the host molecule in one, the guest in the other. At the end of the refinement procedure the final $\sum ||F_o| - |F_c||/\sum |F_c|$ were 0.074 (for

(12) Lutz, R. E.; Jordan, R. H. *J. Am. Chem. Soc.* **1950**, *72*, 4090.
(13) Stobbe, H.; Bremer, K. *J. Prakt. Chem.* **1929**, *123*, 1.
(14) Recktenwald, G. W.; Pitts, J. N.; Letsinger, R. L. *J. Am. Chem. Soc.* **1953**, *75*, 3028.

(15) Main, P.; Fiske, S. J.; Hull, S. E.; Lessinger, L.; Germain, G.; Declercq, S. P.; Woolfson, M. M. MULTAN80, "A System of Computer Programs for the Automatic Solution of Crystal Structures from X-Ray Diffraction Data", Universities of York, England, and Louvain, Belgium.
(16) Sheldrick, G. M. SHELX, Program for Crystal Structure Determination, University of Cambridge, 1976.

3558 measured reflexions) and 0.079 (for 2418 measured reflexions) for the two structures, respectively (see paragraph at end of the paper regarding supplementary material).

Registry No. I-2II, 85429-08-9; III-2IV, 95911-69-6.

Sulfoquinones in the Hydrolysis of Aryl Esters of *o*- and *p*-Hydroxyarenesulfonic Acids in Alkaline Aqueous Solutions of Dioxane[21]

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Received October 25, 1984

The alkaline hydrolysis of *o*- and *p*-hydroxyarenesulfonate esters of acidic phenols proceeds via an E1cB mechanism. Sulfoquinone (IUPAC name thioquinone dioxide) intermediates (e.g., 8) constitute the best hypothesis to account for the observed kinetic results which obey the rate law k_{obsd} (hydrolysis) = $(k_a + k_b [OH^-])/(1 + [H^+]/K_a)$. There is a negligible deuterium oxide solvent isotope effect on k_a and the entropy of activation is slightly positive. Apparent bimolecular rate constants for hydroxide ion attack on the un-ionized hydroxyl esters $(k_a K_a/K_w)$ are many orders of magnitude larger than the bimolecular rate constants for hydroxide ion attack on the corresponding *methoxy* esters which possess the BAc2 mechanism. Amines trap an intermediate to give more amide than is predicted from the second-order rate law for amine attack on the ionized hydroxy ester. The k_b term most likely arises from bimolecular attack of the hydroxide ion on the ionized hydroxy ester. The hydrolysis of *o*-hydroxyarenesulfonate esters undergoes strong competition from the "Smiles" rearrangement.

Zincke and Brüne proposed that a sulfoquinone[1a] intermediate analogous to (1) was formed in the alkaline hydrolysis of 4-hydroxybenzenesulfonyl chlorides.[1b] These authors based their conclusions on the observation of a yellow color which, however, was subsequently shown by Hall[2] to be due to the ionized form of the phenolic group (2). A nitrogen analogue of an *o*-sulfoquinone (3) has been postulated by Burgess[3] to account for transformations of benzothiazete 1,1-dioxides.

(1)   (2)   (3)
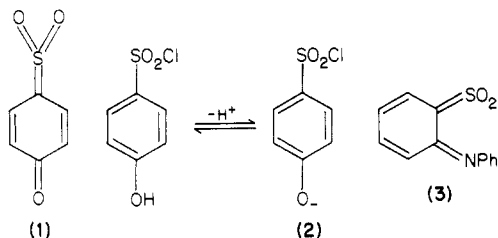
We decided to reinvestigate the possibility of a sulfoquinone intermediate because it would be related to a family of intermediates including sulfene ($R_2C=SO_2$)[4] and sulfonylamine ($RNSO_2$)[5] demonstrated in mechanisms of sulfonyl group transfer. Such a study would extend our knowledge of control of mechanism in acyl group transfer. The best conditions for observing a sulfoquinone in ester hydrolysis would be where the ester has a very good leaving group because the elimination–addition mechanism of ester hydrolysis possesses a large negative sensitivity to the pK of the leaving function. We investigated the hydrolysis and aminolysis of the arene derivatives (4–7) as the quinone analogues of the sulfoquinones from these species are known to be quite stable.[6]

(4)   (5)   (6)

(7)
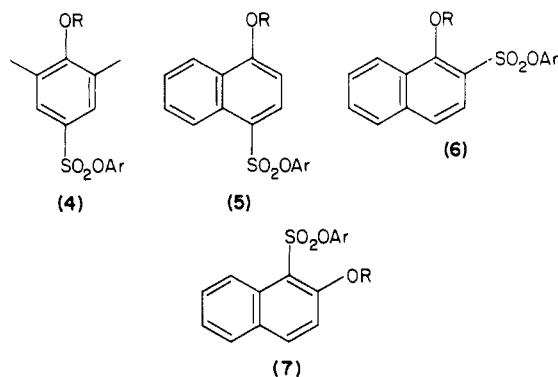
R = H or Me; Ar = C_6H_3-2,4-di-NO_2 or C_6H_3-2-Cl-4-NO_2

The "Smiles" rearrangement competes with the sulfonyl group transfer in the case of the *o*-hydroxyarenesulfonate esters (eq 1)[7] where the leaving phenyl groups are activated

† Istituto di Chimica Organica dell'Università.
‡ University Chemical Laboratory.

(1) (a) We use the original nomenclature[2] although an IUPAC[1c] name for the general species (thioquinone dioxide) might be preferred. (b) Zincke, T.; Brüne, R. *Chem. Ber.* **1980**, *41*, 902. (c) Rigaudy, J.; Klesney, S. P. "IUPAC Nomenclature of Organic Chemistry"; Pergamon Press: Oxford, 1979; Sections A–H.

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