

observed are approximately as expected; the benzene rings are found to be regular hexagons of side 1.39 Å. (to within 0.03 Å.), and the bonds connecting the benzene rings to the cyclobutane ring measure 1.52 Å. At the present stage of the analysis, however, it would be virtually impossible to reconcile the data obtained with a square central ring.

In the second isomer, m.p. 149°, no distortion of the cyclobutane ring is expected to occur, but structure analysis has not so far been carried out for this substance.

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Formulae for Ethylene Oxide and Cyclopropane

DR. A. D. WALSH¹ has misunderstood my criticism², which was not directed against his applications of wave mechanics but against the proposed symbols for ethylene oxide and cyclopropane and also against his statements relating to the reaction types of these substances. His further elaborations are of great intrinsic interest but irrelevant to the issues mentioned.

Dr. Walsh maintains that the hybridization of the three forms of (I) does not give (II):



That can only be justified by attributing to (II) some special significance in regard to the distribution of covalency electrons which is no part of the usual conventional meaning of the symbol. It will accommodate any such distribution of six covalency electrons which fulfils the requirements of symmetry. The formula represents only the mean position in space of the atoms (kernels) and the mode of binding (that is, the structure disclosed by analysis, synthesis, X-ray crystal evidence, etc.).

It is a further step to the space models which again concentrate attention on the atoms rather than on the distribution of valency electrons. We know that the environments of the carbon atoms in cyclopropane derivatives are tetrahedral (not, usually, regular tetrahedral), and this is true whether the valencies are trigonal or not. Incidentally, Dr. Walsh says that the atoms are near-trigonal, but that would appear to mean tetragonal, although of a very distorted type. The formula (II) is, therefore, entirely satisfactory unless we read more into it than was ever intended. On the other hand, (I) is unsatisfactory because its more important implications are lost on hybridization. It suggests that the carbon atom at the business-end of the arrow is negatively charged; this is not true of the hybrid. It suggests that this carbon atom makes no valency-electron contribution to the bond; again this is not true of

the hybrid. It is obvious that any reaction-type implications of (I) are also lost on hybridization. Why should we adopt a formula, each unique feature of which is destroyed by mental reservations, or by the clumsy device of writing three symbols?

Dr. Walsh now finds that the wave-mechanical picture of ethylene oxide allows of some resemblance to acetaldehyde. I can only repeat that the chemical resemblance is very close indeed, that the analogy with ethylene is non-existent, and the parallel with amine-oxides is exiguous. The reaction encountered by Karrer³ is readily explicable by reduction to a tertiary alcohol, a type of process that I mentioned previously². In the presence of an acid catalyst such a substance would suffer dehydration with great facility, especially in these instances where the product is so fully conjugated. This example was naturally not mentioned by me because it is far from representative. If ordinary ethylene oxides were analogous to amine oxides, they should be convertible to ethylenes by mild reducing agents, and that is certainly not the case.

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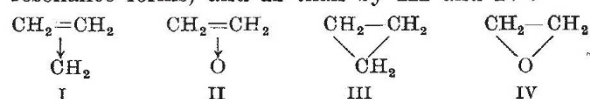
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Structure of Ethylene Oxide and Cyclopropane

A. D. WALSH¹ has suggested that the properties of cyclopropane and ethylene oxide are better accounted for by the formulae I (three equivalent resonance forms) and II than by III and IV:



One consequence of this suggestion is that, in the CH-bonds, the carbon orbitals should be of the sp^3 hybrid type, rather than the sp^2 hybrid suggested by III and IV. In 1945 I obtained the force constants of a number of CH-bonds and found the following: methane, 4.97 (in the usual units); ethane, 4.81; ethylene (sp^2 bonds), 5.1². Fox and Martin² have suggested that in paraffins the CH-force constant is: CH₄, 5.04; CH₃ group, 4.75; CH₂ group, 4.56; CH group, 4.56. The force constant of the CH-link in cyclopropane and ethylene oxide might, therefore, prove valuable in deciding between the above structures.

From the Raman⁴ and infra-red⁵ spectra of cyclopropane it has been decided that the CH-valency vibration frequencies are: A₁', 3,000; E', 3,000; A₂'', 3,050; E'', 3,080 cm.⁻¹. The derived force constants are: 5.04, 5.04, 4.91 and 5.02. The mean is 5.0. (The same values of the fundamental constants have been used as in my previous paper².) The Raman⁴ and infra-red⁵ spectra of ethylene oxide indicate that the CH-valency vibration frequencies are A₁, 3,000; B₁, 3,000; B₂, 3,062; A₂, 3,062 cm.⁻¹. The derived force constants are 5.04, 5.04, 4.95 and 4.95. The mean is again 5.0. Ethylene sulphide is also of interest. Thompson and Dupré, having examined the Raman and infra-red spectra, suggested for the CH-valency vibrations: A₁, 2,990; B₁, 2,990; A₂,