A Reinvestigation of the Structure of Ethylene Oxide by Electron Diffraction

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Recently, Cunningham, Boyd, Gwinn, Myer, and Le Van investigated the structure of ethylene oxide by microwave spectrum,[1] and gave the results different from those of Ackermann and Mayer's earlier electron diffraction study[2] (Table 1). The difference is very large in the C—C distance. Therefore we have reinvestigated the structure by electron diffraction.

Ethylene oxide was prepared from ethylene chlorohydrin and lime. Electron diffraction photographs were obtained by the apparatus with a camera distance of about 9 cm and an electron wave length of about 0.055 Å. The maxima and minima of diffraction halos were measured by the visual method on the photographs; the q values are given in Table 2 and represented by the arrows in Fig. 1 ($q = (40/\lambda)\sin\phi/2$, where λ is the electron wave length and ϕ is the scattering angle).

A the atomic distances are equal to those of Ackermann and others, and in model B they are equal to those of Cunningham and others while in models C and D only the C—C distances are varied from those of B. The theoretical intensity curves (Fig. 1) were calculated by the well-known formula,[3]

$$I = \sum_{ij}(Z_i Z_j / r_{ij}) \exp(-a_i q^2) \sin(\pi q r_{ij}/10)$$

where r_i is the distance between the atoms i and j, and Z_i is the atomic number of the atom i. The value of the coefficient a_i was assumed to be 0.00016 for bonded hydrogen terms, 0.0004 for unbonded hydrogen terms, and zero for all the others. The theoretical values of q and their ratio to the observed values at the maxima and minima are shown in Table 2. It is clear that the models B and C fit better with the observed than the other

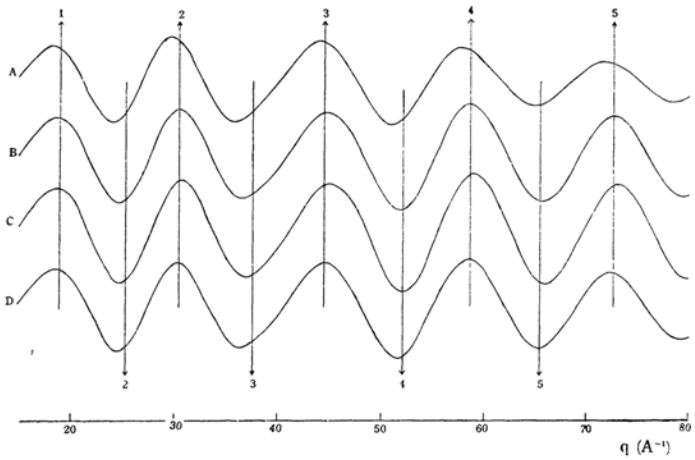

Fig. 1.—Theoretical intensity curves

The molecular models used for the correlation methods are compared in Table 1. In model models. Thus we can conclude that the C—C distance is 1.46±0.03 Å, supporting the results of the microwave spectroscopy.

(1) G. L. Cunningham, A. W. Boyd, W. D. Gwinn, and W. I. Le Van; *J. Chem. Phys.* **17**, 211 (1949); G. L. Cunningham, A. W. Boyd, R. J. Myer, W. D. Gwinn, and W. I. Le Van, ibid. **19**, 676 (1951).

(2) P. C. Ackermann and J. E. Mayer, *J. Chem. Phys.* **4**, 377 (1936).

(3) S. Spurr and V. Schomaker, *J. Am. Chem. Soc.* **64**, 2693 (1942).

Table 1

	(a) Cunningham	(b) Ackermann	(c) Models used for our study			
			A	B	C	D
C—C	1.472A	1.56±0.05A	1.56A	1.47A	1.44A	1.50A
C—O	1.436A	1.45±0.05A	1.45A	1.44A	1.44A	1.44A
C—H	1.082A	1.05±0.07A	1.05A	1.08A	1.08A	1.08A
∠H—C—H	116°41′		109.5°	116°41′	116°41′	116°41′
$\angle H_2$—C—C	159°25′		151°	159°25′	159°25′	159°25′

Table 2

Max.	Min.	q_{obs}	q_{calc} A	q_{calc} B	q_{calc} C	q_{calc} D	q_{calc}/q_{obs} A	q_{calc}/q_{obs} B	q_{calc}/q_{obs} C	q_{calc}/q_{obs} D
1		18.9	18.2	18.6	18.7	18.5	0.962	0.983	0.988	0.978
	2	25.3	24.2	24.8	24.9	24.6	0.965	0.980	9.984	0.972
2		30.45	29.7	30.5	30.7	30.6	**0.975**	**1.002**	**1.008**	**0.998**
	3	37.6	35.8	36.7	37.1	36.5	0.952	0.976	0.987	0.971
3		44.5	44.2	44.6	44.9	44.5	**0.994**	**1.003**	**1.010**	**1.001**
	4	52.1	51.2	51.9	52.2	51.7	0.982	0.996	1.002	0.992
4		58.65	57.8	58.6	59.0	58.4	**0.986**	**0.999**	**1.006**	**0.996**
	5	65.4	65.0	65.8	66.1	65.4	0.994	1.006	1.011	1.000
5		72.6	71.6	72.6	73.2	72.3	0.986	1.000	1.008	0.996
			Average				0.979	0.996	1.002	0.992
			Average deviation				0.012	0.008	0.008	0.009

Values in Gothics were doubly weighted in computing averages.

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