13. On the Molecular Configurations of γ-BHC, δ-and ε-1, 1, 2, 3, 4, 5, 6-Heptachlorocyclohexane

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It has been already reported that by the present authors (Botyu-Kagaku, **15**, 86 (1950)(*)) a new isomer of 1, 1, 2, 3, 4, 5, 6-heptachlorocyclohexane (mp. 55–55.5°; ε-hepta) was obtained from the chlorination product of γ-BHC. At this time δ-1, 1, 2, 3, 4, 5, 6-heptachlorocylohexane (mp. 139–140°; δ-hepta) and ε-hepta were isolated cholorination product of α-BHC with γ-1, 1, 2, 3, 4, 5, 6-heptachlorocyclohexane (mp. from the 85–86°; γ-hepta) and o-1, 1, 2, 2, 3, 4, 5, 6-octachlorocyclohexane by partition chromatography.

The molecular configuration of α-BHC has been already determined as is shown in Table (Botyu-Kagaku, **15**, 32(1950)). The possible isomers of 1, 1, 2, 3, 4, 5, 6-heptachlorocyclohexane (hepta), which can be derived from this, are II, III, and IV. Since II has been assigned to be the molecular configuration of γ-hepta(*), one of the two forms left is of δ-hepta, and the other of ε-hepta. Now, taking into account the fact that the forms III and IV can be also derived from the forms VII and V of 16 possible isomers of BHC respectively, and the experimental results that ε-hepta is also produced by chlorination of γ-BHC, it must be said that one of the two, V or VII, is the molecular configuration of γ-BHC. As has been pointed out by Y. Morino et al. (Botyu-Kagaku, **15**, 181 (1950)), the calcurated values of dipole mements of the two forms are 3.19–2.93 D (V) and 1.88 D (VII), and the experimental value for γ-BHC is 2.80 D. Consequently, V Should be the molecular configuration of γ-BHC. The isomers of hepta which can be derived from V are IV, IV', VI and VI', but among them only IV can be obtained by the chlorination of both α- and γ-BHC. Therefore, the conclusion is that IV is ε-hepta and III is δ-hepta.

Table : The Chlorine Configurations **

I. α-BHC	p, p, e, e, e, e	V. γ-BHC	p, p, p, e, e, e
II. γ-hepta	p, $\widehat{\text{pe}}$, e, e, e, e	IV.'	p, p, p, $\widehat{\text{pe}}$, e, e
III. δ-hepta	p, p, e, $\widehat{\text{pe}}$, e, e	VI.	p, $\widehat{\text{pe}}$, p, e, e, e
IV. ε-hepta	p, p, $\widehat{\text{pe}}$, e, e, e	VI.'	p, p, p, e, $\widehat{\text{pe}}$, e
		VII.	p, p, e, p, e, e

** This is shown by simple notaion of p (polar) and e (equatorial) proposed by C. W. Bekett et al. (J. Am. Chem. Soc., **69**, 2488 (1947)).