

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-heptachlorocyclohexane (mp. 139-140°; δ -hepta) and ϵ -hepta were isolated chlorination product of α -BHC with γ -1, 1, 2, 3, 4, 5, 6-heptachlorocyclohexane (mp. from the 85-86°; γ -hepta) and α -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 calculated values of dipole moments 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, e, e, e, e
II. γ -hepta	p, $\widehat{pe}$, e, e, e, e	IV.'	p, p, p, $\widehat{pe}$, e, e
III. δ -hepta	p, p, e, $\widehat{pe}$, e, e	VI.	p, $\widehat{pe}$, p, e, e, e
IV. ϵ -hepta	p, p, $\widehat{pe}$, e, e, e	VI.'	p, p, p, e, $\widehat{pe}$, e
		VII.	p, p, e, p, e, e

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