CRYSTAL STRUCTURE OF δ-BENZENE HEXACHLORIDE

BY

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(Communicated at the meeting of December 17, 1949)

In continuation of our structure determination of GAMMEXANE, [1]) the γ-isomer of benzene hexachloride, the crystal structure of the δ-isomer has been determined by X-ray analysis.

Rotation diagrams of the δ-isomer around the three axes and zero-layer WEISSENBERG diagrams around [010] and [100].

Cell dimensions: $a = 9{,}64\ A$; $b = 8{,}73\ A$; $c = 14{,}09\ A$; $\beta = 118°$; space group $P\,2_1/c$ from absences, four molecules pro cell.

By systemetical combination of the 10 highest independent PATTERSON maxima of the [100] PATTERSON projection it was possible to determine the rough y and z coordinates of 5 of the six chlorine atoms.

Repeated FOURIER syntheses gave the [100]-FOURIER projection of fig. 1 and satisfactory agreement between calculated and observed intensities.

The model with chair-form of the carbon ring and the $\varepsilon\,\varkappa\,\varkappa\,\varkappa\,\varkappa\,\varkappa$ configuration of the chlorines appears to fit this projection, ε chlorine atom marked A in the figure. [2])

By this projection and the supposed model (fig. 2) there remains as unknown parameter the x of the molecule centre; after the latter had been roughly determined by trial and error, repeated [100] FOURIER syntheses gave fig. 3.

Further refinement of the coordinates is in progress.

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[1]) G. W. v. VLOTEN, CH. A. KRUISSINK, B. STRIJK and J. M. BIJVOET. Nature **162**, 771 (1948). Acta Cryst. in press.

[2]) We owed HASSEL the private communication that by electron diffraction gaseous benzene hexachloride was found by him to be of the $\varepsilon\,\varkappa\,\varkappa\,\varkappa\,\varkappa\,\varkappa$ type. In the meantime all benzene hexachloride isomers have been determined in the gaseous state by HASSEL and coworkers. Research **2**, 248 (1949).

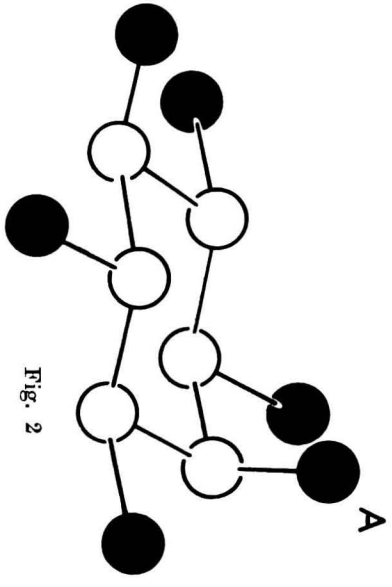

Fig. 2

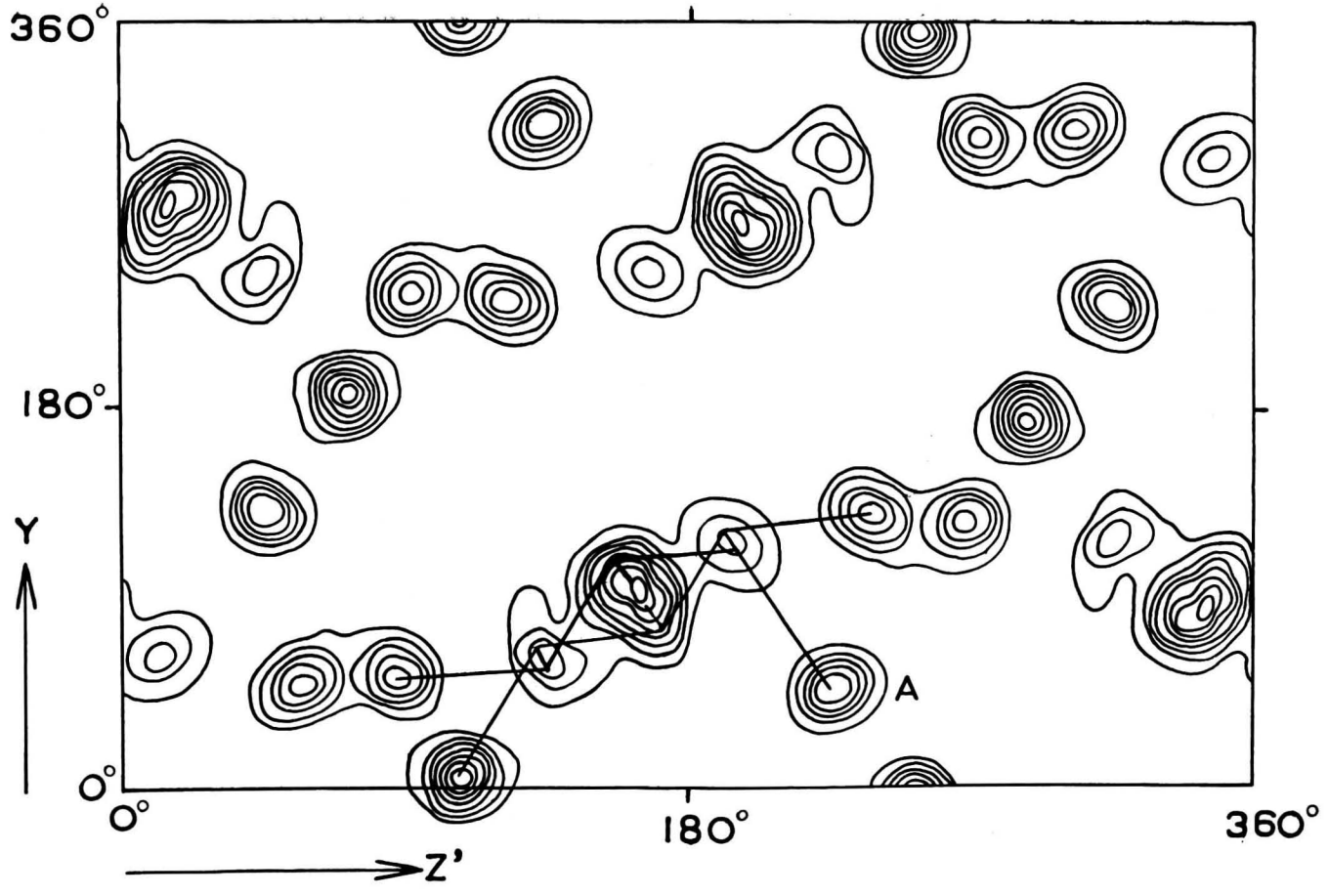

Fig. 1

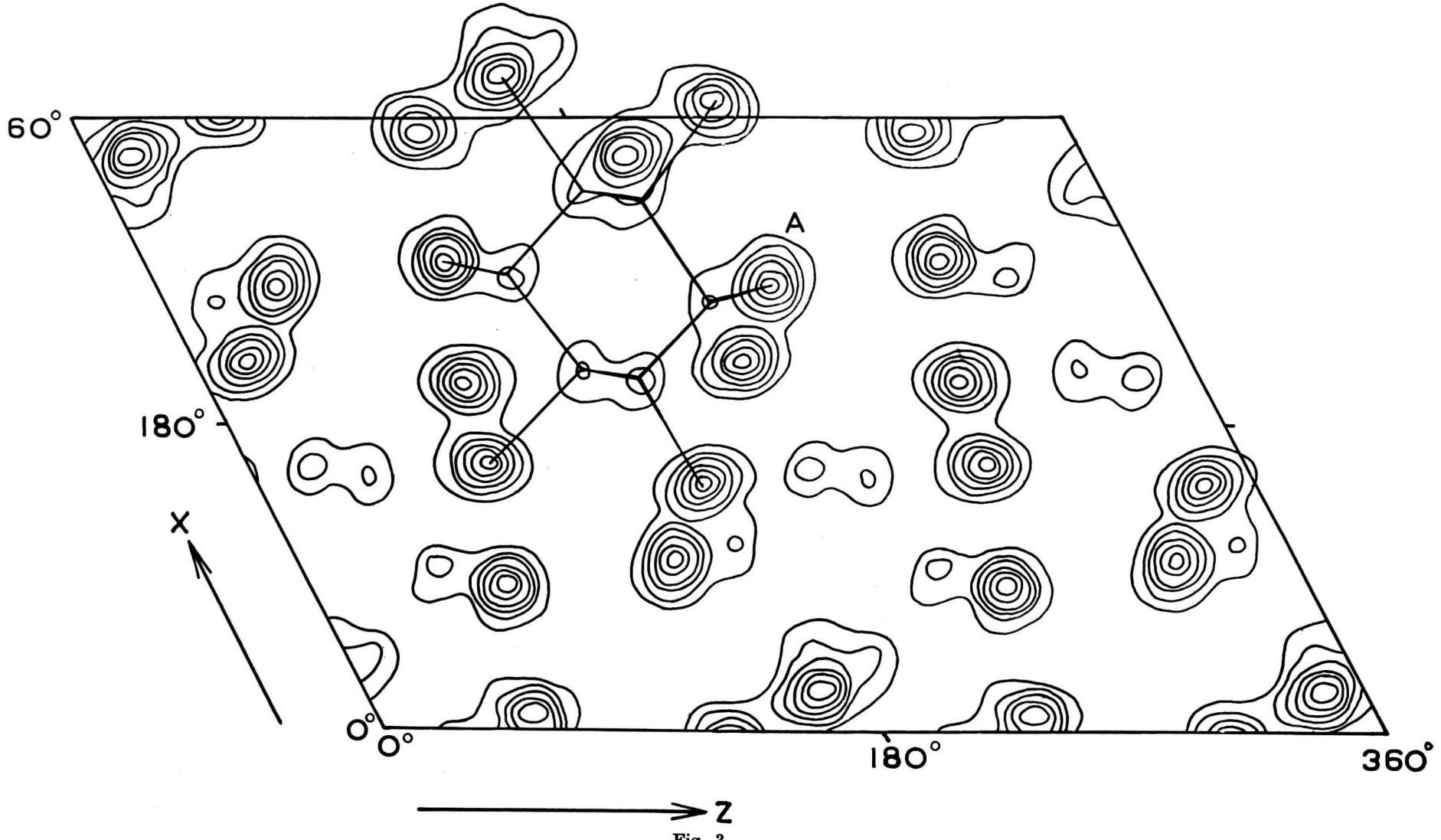

Fig. 3