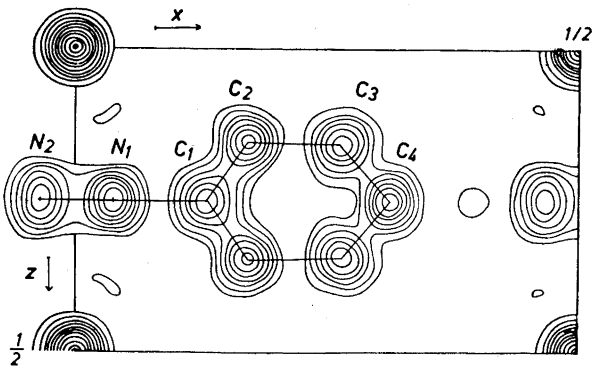

Fig. 1. Electron density projection along the *b* axis. Contour intervals: 2 e.Å^{-2} for chloride ions and 1 e.Å^{-2} for nitrogen and carbon atoms. The first contour is the 2-electron line.

the distance between these atoms is 1.40 Å. The angle between the benzene plane and the plane of projection is about 45°.

The conclusion of this investigation is that solid benzene diazonium chloride has a typical ionic structure, the N-N distance corresponds to that of a normal triple bond, and the N_1-C_1 distance is shortened relative to a single C—N bond by an amount to be expected from similar systems where a multiple bond is conjugated to a benzene ring.

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Charge Transfer Compounds with a Halogen Atom linked to Carbon as the Electron Acceptor

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The crystal structures of several addition compounds have recently been determined in which halogen molecules act as electron acceptors. Structures of compounds in which a halogen atom is linked to carbon in the acceptor molecule have not been investigated, however. Compounds like those formed by iodoform with three molecules of quinoline or S_8 therefore appeared to be of considerable interest. The crystal structure of the former has now been determined and the investigation of the sulphur compound has been started.

The unit cell of the quinoline compound is rhombohedral with the hexagonal axes $a = 22.40$ Å and $c = 4.59$ Å. The rhombohedral unit cell contains *one* molecule of iodoform which is therefore situated on the trigonal axis (the space group is $R3$) whereas the three quinoline molecules occupy general positions. It was not difficult to localize the former, but the lack of symmetry elements others than a threefold axis made the localization of the quinoline molecules more cumbersome.

Fig. 1 shows a difference Fourier map (projection along the trigonal axis) with subtraction of the contribution from iodine atoms. The position of one iodine atom is indicated by an asterisk and the three axes indicated are the projections of the rhombohedral axes into the (111) plane. Already from this projection a linear arrangement N-I-C might be expected. This expectation is confirmed by the analysis. The N-I distance is found equal to 2.99 Å, the C-I distance to 2.12 Å.

These findings also confirm the suggestion that the iodine atoms act as electron acceptors towards the nitrogen atoms and

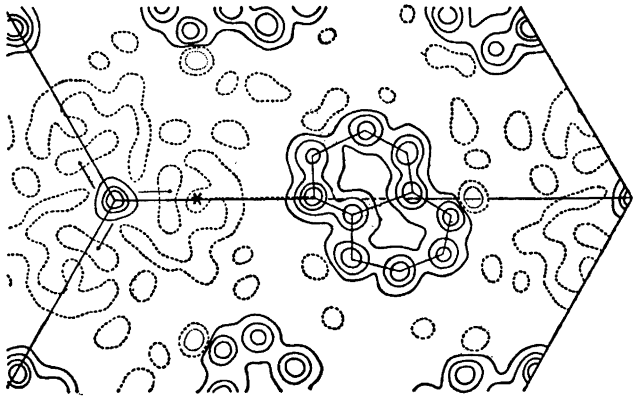

Fig. 1.

makes it appear probable that the iodine atoms have acquired ten electron systems resembling those of the "first" halogen atom in addition compounds formed by halogen molecules.

Apparently, addition compounds in which halogen atoms linked to carbon act as electron acceptors are not numerous. The 1:1 compounds, however, formed by oxalyl halides and dioxan are probably of this kind. X-Ray work on these oxalyl chloride and bromide compounds has therefore been started.

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