A Close Relationship between the Crystal Structure of an Acceptor and That of an Addition Compound

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In particular cases a marked resemblance between crystal structures of electron donor or acceptor substances and their addition compounds with suitable partners may be possible. If we combine, for example, an acceptor molecule with a less bulky donor molecule, it might happen that the mutual arrangement of the acceptor molecules in the solid addition compound will be similar to that present in the crystalline acceptor substance. Let us assume that both donor and acceptor molecule is capable of forming at least *two* charge-transfer bonds and are both centrosymmetrically built. We further consider the case in which the acceptor molecules in the solid acceptor substance are situated in two non-equivalent but centrosymmetrical sets of positions, with one half of the molecules in either set. It then would not be surprising to find the mutual arrangement of the acceptor molecules in the 1:1 addition compound to be very similar to that of one set of acceptor molecules in the acceptor crystal, and the donor molecules in sites corresponding to those of the second set of molecules in the acceptor crystal.

A situation of the kind just outlined has been deduced from X-ray investigations of crystals, choosing tetrabromoethylene and pyrazine as the acceptor resp. the donor molecule. Both crystal species belong to the space group $P2_1/c$ and their lattice constants are:

	Tetrabromoethylene	Addition compound
a	14.193 Å	11.803 Å
b	4.140 Å	4.161 Å
c	12.164 Å	12.094 Å
β	112.0°	113.1°

Photographs of structure models are reproduced in the figure. The endless chains of alternating donor and acceptor molecules in the addition compound crystal are running parallel to the [101] direction. The N···Br bond measures 3.02 Å, the angle between this bond and the plane of the pyrazine molecule is 154°. The parameters of the pyrazine molecule are identical with those derived from earlier X-ray work,[1] the tetrabromoethylene molecules have the same C—Br distance (1.88 Å) in both crystals, but the BrCBr angle is slightly smaller in the addition compound in which the two diagonal Br—Br distances are slightly different.

Full details of the three-dimensional analyses, the R factors of which are both below 0.08 (0.078 and 0.071, respectively) will be given in a forthcoming publication.

1. Wheatley, P. J. *Acta Cryst.* **10** (1957) 182.

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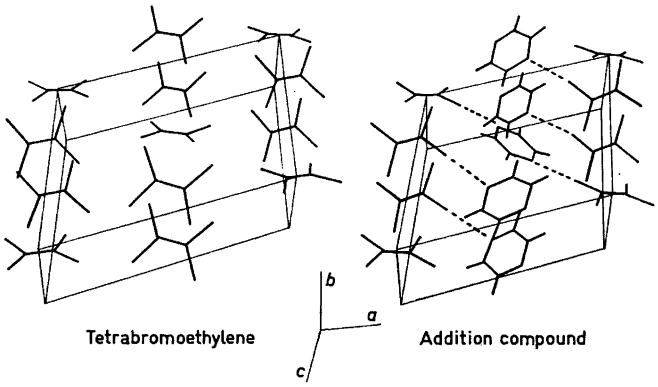

Fig. 1.