

The equations are

$$-0.2577X + 0.0Y + 1.0000Z = 0.0$$

for BD and

$$-0.2547X + 0.0Y + 1.0000Z = 3.238$$

for TCNQ, where X , Y and Z are coordinates in Å with respect to the crystal axes a , b and c . The planes of BD and TCNQ make an angle of 0.2° .

Discussion. BD and TCNQ form solid molecular complexes which contain solvent molecules in the crystal lattice as well as the solvent-free complex. The structure of the BD-TCNQ complex containing dichloromethane has already been reported (Ikemoto, Chikaishi, Yakushi & Kuroda, 1972). In the solvent-free crystal, the relative orientation of the donor and acceptor molecules within a BD-TCNQ column is the same as that in the dichloromethane-containing crystal, but these molecular columns are closely packed without leaving space to accommodate solvent molecules.

In the solvent-containing crystals, there exist two kinds of specific interaction between BD and TCNQ: the charge-transfer interaction and the hydrogen bonding. The former is reflected in the formation of the BD-TCNQ column, and the latter gives the infinite hydrogen-bonded sheet parallel to the (001)

plane. In the solvent-free crystal, however, there is no indication of the hydrogen bonding between BD and TCNQ. Although all molecular planes are parallel to the (10 $\bar{2}$) plane, which is perpendicular to the c axis, the molecular columns lying at $y = \frac{1}{2}$ are shifted by $c/4$ along the c axis, so that the molecules shown by broken lines in Fig. 2 are not on the same plane as those shown by solid lines.

The bond lengths of TCNQ in the solvent-free complex are in good agreement with those in the TCNQ crystal (Long, Sparks & Trueblood, 1965). This implies that TCNQ is in the non-ionic state in this complex.

The computer used in this work was the HITAC 5020E at the Computer Centre, University of Tokyo. The program used were the UNICS program (1967).

References

- IKEMOTO, I., CHIKAISHI, K., YAKUSHI, K. & KURODA, H. (1972). *Acta Cryst.* B28, 3502-3506.
 GRANT, D. F., KILLEAN, R. C. G. & LAWRENCE, J. L. (1969). *Acta Cryst.* B25, 374-376.
 LONG, R. E., SPARKS, R. A. & TRUEBLOOD, K. N. (1965). *Acta Cryst.* 18, 932-939.
 UNICS (1967). *Universal Crystallographic Computation Program System*. Edited by T. SAKURAI. Tokyo: The Crystallographic Society of Japan.

SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

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The crystal and molecular structure of 1-kestose: a correction. By G. A. JEFFREY and YOUNG JA PARK, *Department of Crystallography, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, U.S.A.*

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In Table 1 of Jeffrey & Park [*Acta Cryst.* (1972). B28, 257-267], the C'(3) x coordinate should read -779 instead of -9.

The correction of a typographical error: In the paper on 1-kestose by Jeffrey & Park (1972), Table 1, the C'(3) x coordinate should read -779, instead of -9. All numbers derived using this parameter are correct.

Reference

- JEFFREY, G. A. & PARK, Y. J. (1972). *Acta Cryst.* B28, 257-267.