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The crystal structure of the 1:1 radical cation–radical anion salt of 2,2'bis-I,3-dithiole (TTF) and 7,7,8,8-tetracyanoquinodimethane (TCNQ)

T. J. Kistenmacher, T. E. Phillips and D. O. Cowan

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The Crystal Structure of the 1:1 Radical Cation-Radical Anion Salt of 2,2'-Bis-1,3-dithiole(TTF) and 7,7,8,8-Tetracyanoquinodimethele(TCNQ)*

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Thomas J. Kistenmacher, Terry E. Phillips and Dwaine O. Cowan Department of Chemistry The Johns Hopkins University Baltimore, Maryland 21218 U. S. A. ** ** **

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The salt of the radical cation of 2,2'-bis-1,3-dithiole(TTF) and the radical anion of 7,7,8,8-tetracyanoquinodimethane(TCNQ), $C_{18}H_8N_4S_4$, crystallizes in the monoclinic system, space group $P2_1/c$, with cell constants: $a = 12.298(6)A, b = 3.819(2)A, c = 18.468(8)A, \beta = 104.46(4)^{\circ}, Z = 2,$ $D_m = 1.62(1)$ and $D_c = 1.615$ g cm⁻³. Intensities for 1373 independent reflect. tions were collected on an automated diffractometer. The structure was solved by standard heavy-atom methods and has been refined by full-matrix least squares to an R value of 0.044. The TTF radical cations and the TCNQ radical amions form homologous columnar stacks with interplanar spacings of 3.47A and 3.17A, respectively. The dihedral angle between the least-squares planes of the cations and the amions is 58.5° and is approximately bisected by [010].

TABLE 1 OBSERVED AND CALCULATED STRUCTURE FACTORS

The 8 enclosed sheets should be arranged in the following grid pattern for data retrieval:

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18	2B	3B	4B

The entries in each column contain values, reading from left to right, of <code>l</code>, 10F(obs), and 10/F(colc)/. The reflections designated with an asterisk (*) had negative values for their intensities and were assigned zero weight.

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