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# THE CRYSTAL STRUCTURE OF THE 1:2 COMPLEX OF 1-METHYL-3,3-DIMETHYL-2-(p-N,N-METHYL-β CHLORETYLSTYRYL)INDOLE AND 7,7,8,8-TETRACYANOQUINODIMETHANE, $(C_{22}H_{26}N_2Cl)^+(C_{12}H_4N_4)^-(C_{12}H_4N_4)$

By R.P.Shibaeva, L.O.Atovmyan, and L.P.Rozenberg

Branch of the Institute of Chemical Physics, U.S.S.R.Academy of Sciences, Chernogolovka, Moscow District, U.S.S.R.

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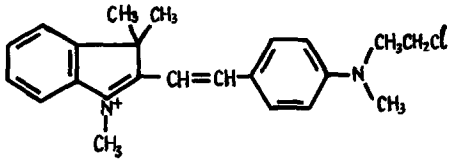
In a programme investigating the conducting complexes of the stable anion-radical 7,7,8,8-tetracyanoquinodimethane ($TCNQ^-$) two classes of complexes have been studied.

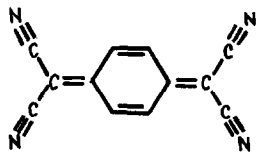
a) complexes of $TCNQ^-$ and paramagnetic cations-arenchromium compounds [1-3];

b) complexes of $TCNQ^-$ and easily polarizable molecules of organic dyes.

This paper deals with the 1:2 complex of the organic dye



and TCNQ



The results of the x-ray analysis of the complex are given below.

Crystal data:

| | |
|---|---|
| a=18.18± 0.03 Å | $C_{46}H_{34}N_{10}Cl$ |
| b= 8.30± 0.02 Å | F (000) = 1588 |
| c=27.03± 0.03 Å | M = 762.3 |
| $\beta$=92± 0.5 ° | $d_{calc.}$ = 1.25 g./cm$^3$ |
| V=4076 Å$^3$ | $\mu$ = 12 cm$^{-1}$ |
| Space group P $2_1/n$ | Z = 4 |

The intensities of ca. 3500 independent non-zero reflections (hol-h71 and okl-3kl layers) were taken with a multiple-film equi-inclination Weissenberg goniometer with unfiltered Cu radiation, and were estimated visually. A spot-size correction was applied [4]. Because of the small size of the crystal the absorption could be ignored.

The crystal structure has been determined by the application of the direct method with the program developed by Dr. V.I.Andrianov[5].

Signs of 452 reflections with $|E| \geq 1.6$ have been calculated from twelve initial reflections $3k + 9a_i$ . From the three dimensional E-map computed with the 452 determined phases all the 57 non-hydrogen atoms have been localized.

Refinement was carried out by means of full matrix least-squares calculation with isotropic temperature factors giving a final R value of 0.15.

The [010] projection of the structure is shown in Figure 1.

Tetrads of TCNQ molecules are essential features of the structure of the complex.They are arranged in a zigzag way along axis a so that the two neighbouring molecules TCNQ 2 and 2'' are not overlapping. There are two modes of overlapping of neighbouring TCNQ molecules within the tetrad (Figure 2a and 2b). The TCNQ planes are parallel and they are approximately parallel to the $(40\bar{6})$ plane. The interplanar spacings of TCNQ molecules in any tetrad are 3.45± 0.04 Å for 1-1' ; 3.22± 0.04 Å for 1-2 and 1' - 2' .

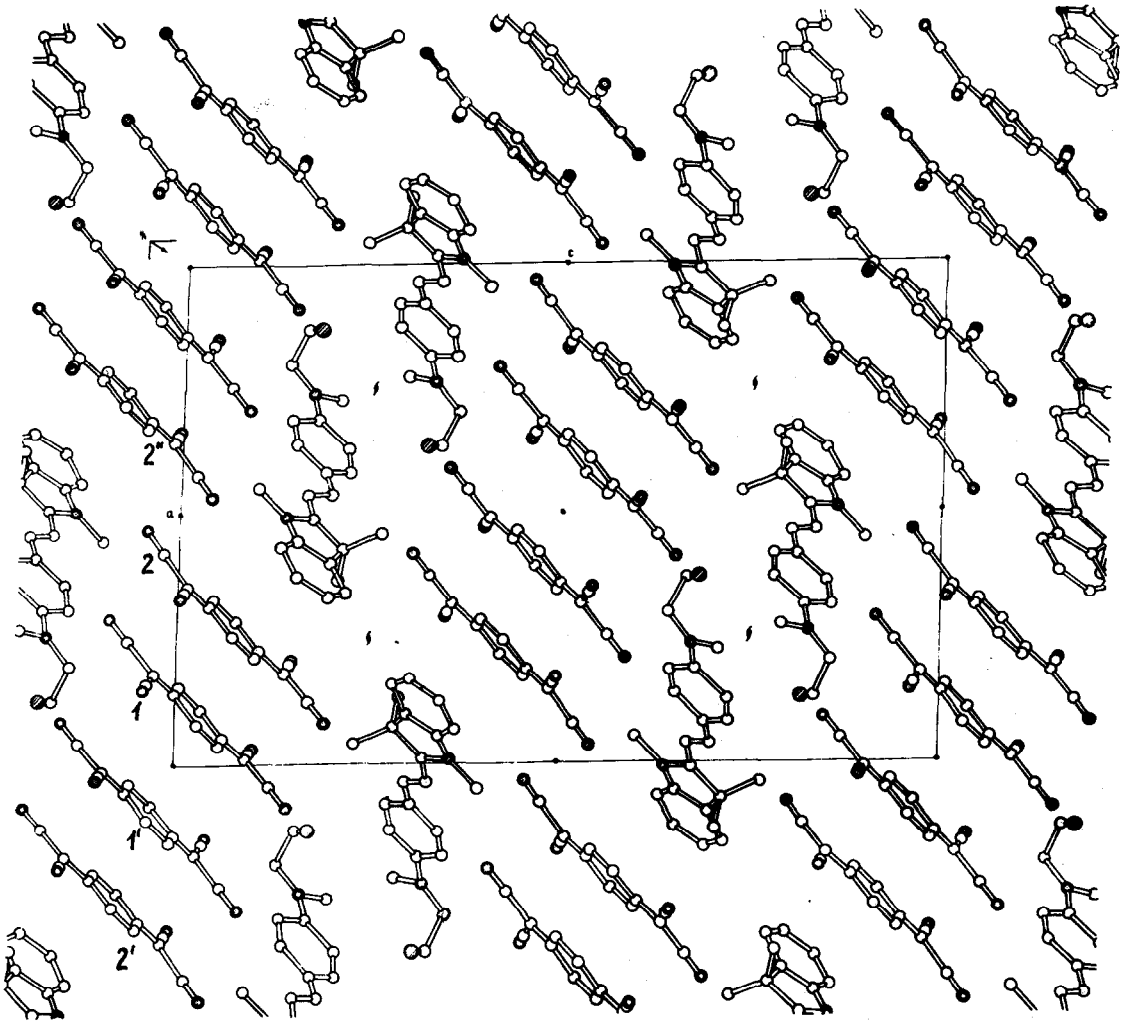



Fig. 1. Projection of the structure on (010).

The molecule of organic dye is almost planar if the methyl groups and chlorethyl group are excluded.

The authors are gratefull to Dr.V.I.Andrianov for his advice on the application of the direct method in computing.We also thank Dr.A.I.Sherle and Prof. A.A.Berlin who performed the synthesis of the complex investigated by us.

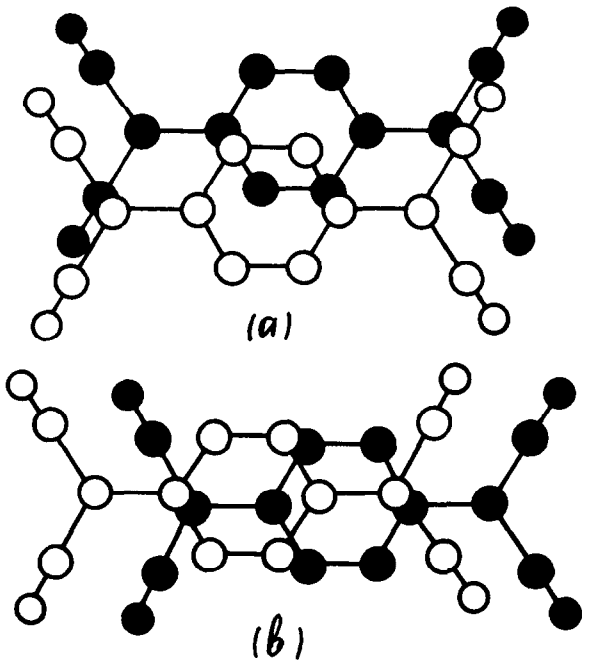



Fig. 2 a) Overlapping of adjacent TCNQ molecules 1-2, and $1' - 2'$.
b) Overlapping of adjacent TCNQ molecules $1 - 1'$.

## References

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