

The Cd(1) atom coordinates three water molecules, O(12), O(14) and O(15), and two oxydiacetate ions, one tridentate and one monodentate; Cd(2) coordinates two water molecules, O(13) and O(16), and two oxydiacetate ions, one tridentate and one bidentate. In both the pentagonal bipyramids the apices are formed by water O atoms. The O(4) atom common to the two bipyramids in a pair is involved in a tridentate chelate with Cd(1) and in a carboxylate chelate with Cd(2), the bite O(4)–O(5) of the latter being 2.203 (19) Å.

An extensive hydrogen-bond system joins the chains to form a three-dimensional network, Fig. 1. The linking occurs *via* the two non-coordinated water molecules, O(11) and O(17), situated between the chains, but also directly between the chains through all the coordinated water molecules. Though no H atoms could be located, it was possible to assign all water H

atoms to definite O atoms from geometrical considerations. The result is shown in Table 7, which also lists the O–O distances in the hydrogen bonds.

A comparison between the three different Cd oxydiacetate structures will be given in the paper dealing with monoclinic cadmium oxydiacetate trihydrate, CDOXY II.

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## The Crystal Structures of Free Radical Salts and Complexes. VIII. The Crystal Structure of and Electrical Anisotropy in [1,4-Di(*N*-quinolinium-methyl)benzene]<sup>2+</sup> (7,7,8,8-Tetracyanoquinodimethane)<sub>3</sub><sup>-</sup>

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The 3:1 complex salt formed between 7,7,8,8-tetracyanoquinodimethane (TCNQ) and 1,4-di(*N*-quinolinium-methyl)benzene<sup>2+</sup> is triclinic, space group *P* $\bar{1}$ , with  $a = 7.50$ ,  $b = 10.07$ ,  $c = 17.75$  Å,  $\alpha = 102.79$ ,  $\beta = 106.17$ ,  $\gamma = 98.91^\circ$ ,  $Z = 1$ . The structure was solved by the Patterson method and refined to  $R = 0.038$  for 2143 reflexions. The TCNQ moieties are stacked plane-to-plane in groups of three along **b** with almost no direct overlap between adjacent triads. The molecular geometries of the two independent TCNQ moieties indicate that the negative charge is delocalized within the triads. Anisotropic conductivities of  $2 \times 10^{-4}$ ,  $1 \times 10^{-4}$  and  $1 \times 10^{-6} \Omega^{-1} \text{cm}^{-1}$  at 300 K were observed along **a**, **b** and **c** respectively. The temperature dependence of conductivity along all three directions is isotropic and varies as  $\exp(-E_a/kT)$  where  $E_a = 0.27 \pm 0.02$  eV.

#### Introduction

The radical anion salts of TCNQ possess interesting electrical and magnetic properties which can be related to their crystal structures. A common feature is a characteristic parallel plane-to-plane stacking of the TCNQ molecules in columns. In a few salts, with favourable overlap and a regular short interplanar separation, metallic behaviour is observed. In the majority, however, different overlaps and intermolecular distances at different points in the stack give rise to

intermediate conductivities. In an attempt to elucidate further this relation, the crystal structure and electrical conductivity of 1,4-di(*N*-quinoliniummethyl)benzene-(TCNQ)<sub>3</sub> have been studied.

#### Experimental

##### Crystal data

(C<sub>26</sub>H<sub>22</sub>N<sub>2</sub>)(C<sub>12</sub>H<sub>4</sub>N<sub>4</sub>)<sub>3</sub>,  $M_r = 975.1$ , triclinic,  $a = 7.50$  (2),  $b = 10.07$  (3),  $c = 17.75$  (4) Å,  $\alpha =$

102.79 (5),  $\beta = 106.17(1)$ ,  $\gamma = 98.91(4)^\circ$ ;  $U = 1221.6 \text{ \AA}^3$ ,  $D_m = 1.31(1)$ ,  $Z = 1$ ,  $D_c = 1.32 \text{ g cm}^{-3}$ ;  $F(000) = 608$ . Mo  $K\alpha$  ( $\lambda = 0.71069 \text{ \AA}$ ),  $\mu = 0.90 \text{ cm}^{-1}$ . Space group  $P\bar{1}$  (assumed).

Black plate-like crystals were deposited when a warm acetonitrile solution (200 ml) of TCNQ (0.2 g) and LiTCNQ (0.2 g) was added to a warm aqueous solution (10 ml) of 1,4-di(*N*-quinoliniummethyl)-benzene dibromide (0.2 g), and allowed to cool. The space group and cell constants were obtained initially from oscillation and Weissenberg photographs. The cell dimensions were subsequently refined on a Hilger & Watts computer-controlled, four-circle diffractometer. Intensities were collected from a crystal  $0.75 \times 0.25 \times 0.1 \text{ mm}$  with a  $\theta/2\theta$  scan, a scintillation counter and Mo  $K\alpha$  radiation. About 4300 reflexions were measured of which 2173 had significant counts [ $I > 3\sigma(I)$ ]. The intensities were corrected for Lorentz and polarization factors but not for absorption.

Table 2. *Final positional and isotropic thermal parameters (all  $\times 10^3$ ) for hydrogen atoms*

The figures in parentheses indicate standard deviations.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i>
H(1)	-309 (3)	37 (3)	-3 (1)	17 (7)
H(2)	253 (3)	63 (2)	125 (1)	12 (6)
H(3)	-189 (3)	426 (3)	95 (1)	17 (7)
H(4)	-172 (3)	320 (2)	-31 (1)	16 (7)
H(5)	403 (3)	340 (2)	69 (1)	14 (7)
H(6)	398 (4)	451 (2)	199 (2)	24 (7)
H(7)	1264 (4)	460 (3)	455 (2)	30 (8)
H(8)	961 (4)	307 (3)	390 (2)	41 (9)
H(9)	556 (3)	316 (3)	464 (2)	25 (8)
H(10)	547 (4)	333 (3)	374 (2)	38 (8)
H(11)	562 (4)	175 (3)	277 (2)	52 (10)
H(12)	572 (5)	-61 (3)	222 (2)	64 (11)
H(13)	670 (4)	-201 (3)	308 (2)	44 (9)
H(14)	774 (4)	-228 (3)	446 (2)	35 (8)
H(15)	833 (5)	-132 (4)	590 (2)	70 (11)
H(16)	814 (4)	94 (3)	639 (2)	41 (9)
H(17)	723 (4)	237 (3)	552 (2)	40 (9)

Table 1. *Final positional and thermal parameters (all  $\times 10^4$ ) for non-hydrogen atoms*

The figures in parentheses indicate standard deviations. Temperature factor:  
 $\text{expl}[-2\pi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hkU_{12}a^*b^* + 2hlU_{13}a^*c^* + 2klU_{23}b^*c^*)]$ .

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>11</sub>	<i>U</i> <sub>22</sub>	<i>U</i> <sub>33</sub>	<i>U</i> <sub>12</sub>	<i>U</i> <sub>13</sub>	<i>U</i> <sub>23</sub>
C(1)	-305 (3)	637 (2)	734 (1)	369 (13)	316 (14)	379 (14)	82 (11)	92 (11)	112 (11)
C(2)	-1800 (3)	244 (3)	-27 (1)	299 (13)	384 (15)	417 (15)	76 (11)	72 (11)	109 (12)
C(3)	1509 (3)	375 (3)	727 (2)	360 (14)	338 (14)	390 (14)	54 (11)	40 (11)	107 (12)
C(4)	-598 (3)	1306 (3)	1462 (1)	343 (13)	369 (14)	406 (15)	83 (11)	67 (11)	112 (12)
C(5)	-2383 (4)	1603 (3)	1477 (2)	469 (16)	450 (16)	402 (15)	104 (13)	136 (13)	137 (13)
C(6)	845 (4)	1709 (3)	2235 (2)	442 (15)	444 (16)	437 (15)	107 (12)	129 (13)	136 (13)
C(7)	1038 (4)	4473 (3)	1620 (2)	551 (17)	291 (14)	524 (17)	134 (12)	205 (13)	129 (13)
C(8)	-629 (4)	4080 (3)	914 (2)	456 (16)	391 (15)	588 (18)	179 (12)	215 (14)	212 (14)
C(9)	-557 (4)	3472 (3)	163 (2)	449 (15)	372 (15)	508 (17)	145 (12)	149 (13)	188 (13)
C(10)	1188 (4)	3191 (3)	57 (2)	450 (15)	331 (14)	442 (15)	112 (12)	131 (12)	154 (12)
C(11)	2853 (4)	3589 (3)	767 (2)	424 (15)	454 (17)	474 (16)	121 (13)	142 (13)	98 (13)
C(12)	2783 (4)	4203 (3)	1510 (2)	482 (16)	446 (17)	472 (17)	107 (13)	130 (14)	73 (14)
C(13)	1020 (4)	5124 (3)	2395 (2)	630 (19)	400 (16)	573 (18)	142 (14)	256 (15)	61 (14)
C(14)	-661 (5)	5458 (3)	2536 (2)	804 (23)	595 (21)	699 (22)	203 (18)	346 (19)	32 (17)
C(15)	2713 (5)	5540 (3)	3076 (2)	739 (21)	459 (18)	525 (18)	62 (15)	295 (16)	-47 (14)
C(16)	1308 (4)	2581 (3)	-699 (2)	460 (15)	409 (16)	434 (16)	88 (12)	125 (13)	142 (13)
C(17)	-274 (4)	2167 (3)	-1431 (2)	601 (18)	424 (16)	495 (17)	107 (13)	185 (14)	167 (14)
C(18)	3077 (4)	2357 (3)	-797 (2)	601 (19)	545 (18)	469 (17)	113 (15)	170 (15)	40 (14)
C(19)	11526 (4)	4770 (3)	4738 (2)	464 (16)	485 (17)	642 (19)	153 (13)	269 (15)	124 (15)
C(20)	9759 (4)	3849 (3)	4370 (2)	532 (17)	456 (17)	648 (19)	141 (14)	220 (15)	65 (15)
C(21)	8222 (4)	4067 (3)	4628 (2)	410 (15)	408 (15)	563 (17)	137 (12)	143 (13)	179 (13)
C(22)	6255 (4)	3101 (3)	4225 (2)	476 (17)	426 (17)	723 (21)	138 (13)	117 (15)	102 (15)
C(23)	5930 (4)	1082 (3)	3126 (2)	497 (17)	712 (21)	416 (17)	93 (15)	109 (13)	90 (15)
C(24)	6054 (5)	-261 (4)	2805 (2)	653 (21)	799 (24)	422 (18)	66 (18)	151 (16)	-19 (16)
C(25)	6607 (4)	-1063 (3)	3306 (2)	542 (18)	457 (18)	697 (21)	24 (14)	241 (16)	-107 (15)
C(26)	7058 (4)	-524 (3)	4152 (2)	364 (14)	418 (16)	594 (18)	41 (12)	192 (13)	49 (14)
C(27)	7629 (4)	-1309 (3)	4705 (2)	531 (18)	496 (19)	898 (24)	138 (15)	235 (17)	268 (17)
C(28)	8000 (4)	-758 (4)	5509 (2)	538 (19)	817 (24)	792 (23)	106 (17)	188 (17)	413 (20)
C(29)	7864 (4)	607 (4)	5811 (2)	603 (20)	932 (26)	414 (17)	41 (18)	134 (15)	171 (17)
C(30)	7343 (4)	1426 (3)	5306 (2)	508 (17)	555 (18)	449 (17)	87 (14)	171 (14)	63 (14)
C(31)	6930 (3)	861 (3)	4469 (2)	315 (13)	445 (16)	449 (16)	65 (12)	103 (12)	84 (13)
N(1)	-3798 (3)	1862 (3)	1512 (2)	529 (15)	849 (19)	683 (17)	272 (14)	254 (13)	287 (15)
N(2)	1960 (4)	2064 (3)	2873 (1)	613 (16)	767 (19)	446 (14)	149 (14)	48 (12)	144 (13)
N(3)	-1998 (5)	5738 (4)	2659 (2)	968 (25)	1122 (28)	1185 (28)	383 (21)	594 (22)	43 (22)
N(4)	-1516 (4)	1829 (3)	-2033 (2)	735 (18)	797 (20)	519 (16)	48 (15)	7 (14)	212 (15)
N(5)	4500 (4)	2175 (3)	-869 (2)	658 (18)	1121 (25)	661 (19)	27 (17)	26 (15)	51 (17)
N(6)	4073 (4)	5871 (3)	3629 (2)	853 (20)	729 (19)	574 (17)	-3 (16)	267 (15)	-103 (14)
N(7)	6359 (3)	1623 (2)	3923 (1)	369 (12)	454 (13)	483 (13)	90 (10)	100 (10)	88 (11)

The structure was solved from a Patterson synthesis and refined by block-diagonal least squares. In the later stages, positional parameters of the H atoms were calculated and confirmed by difference synthesis. Further refinement with anisotropic and isotropic thermal parameters for the non-hydrogen and H atoms respectively, and the weighting scheme  $w = (A/|F_o|)^2$  for  $A > |F_o|$ , otherwise  $w = 1$ , where  $A = 25$  and  $|F_o|$  is on the absolute scale, gave a final  $R = 0.038$ . 30 weak reflexions were omitted from the final stages of refinement. Scattering factors were taken from *International Tables for X-ray Crystallography* (1962). The final positional and thermal parameters are listed in Tables 1 and 2. Least-squares planes were calculated through the cation and TCNQ moieties and are summarized in Table 3.\*

### Discussion of the structure

Fig. 1 shows the structure projected along **a** and **b**. The TCNQ molecules are stacked plane-to-plane in groups of three along **b** with almost no direct overlap between adjacent triads. The cations are stacked along **a** with an interplanar separation of 3.51 Å between partially overlapping quinolinium rings.

\* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32117 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

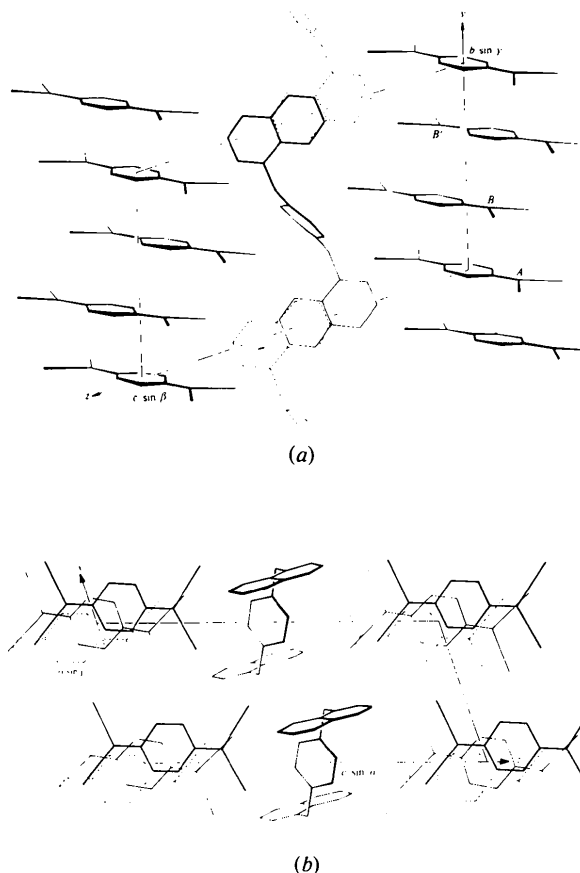


Fig. 1. Projections of the structure of 1,4-di(*N*-quinolinium-methyl)benzene (TCNQ), along (a) the *a* axis and (b) the *b* axis.

Table 3. *Details of molecular planes*

*x, y, z* are fractional atomic coordinates.

#### TCNQ(A)

Equation of the plane:

$$1.4822x + 9.3548y - 7.7374z = 0.$$

Distances from the plane (Å)

C(1)	-0.017	C(5)	0.003
C(2)	-0.018	C(6)	-0.006
C(3)	0.012	N(1)	0.010
C(4)	0.002	N(2)	-0.002

#### Quinolinium group

Equation of the plane:

$$7.0650x + 1.7680y - 4.7773z - 2.8997 = 0.$$

Distances from the plane (Å)

C(23)	-0.012	C(28)	-0.013
C(24)	-0.009	C(29)	-0.013
C(25)	0.001	C(30)	0.006
C(26)	0.010	C(31)	0.014
C(27)	0.011	N(7)	0.006

#### TCNQ(B)

Equation of the plane:

$$0.9950x + 9.5366y - 7.7815z - 3.1476 = 0.$$

Distances from the plane (Å)

C(7)	-0.039	C(16)	-0.012
C(8)	-0.030	C(17)	0.005
C(9)	-0.019	C(18)	0.026
C(10)	-0.031	N(3)	0.057
C(11)	-0.039	N(4)	0.028
C(12)	-0.037	N(5)	0.050
C(13)	-0.022	N(6)	0.033
C(14)	0.019		
C(15)	0.012		

#### Xylyl group (including centrosymmetrically related atoms)

Equation of the plane:

$$1.1173x - 7.6394y + 13.4508z - 4.0230 = 0.$$

Distances from the plane (Å)

C(19)	-0.006	C(21)	0.014
C(20)	0.005	C(22)	-0.010

The type of overlap between adjacent TCNQ's is shown in Fig. 2. The overlap TCNQ(*A*)–TCNQ(*B*) is similar to that found in the majority of TCNQ salts where the quinonoid double bond of one molecule is placed directly above the ring of the second. The dihedral angle and intermolecular separation between TCNQ(*A*) and TCNQ(*B*) are  $3.9^\circ$  ( $2.8^\circ$ ) and  $3.15 \text{ \AA}$  ( $3.12 \text{ \AA}$ ) respectively. The figures in parentheses indicate the values between quinonoid rings. The intermolecular separation is extremely short and only in 1,3-dimethylbenzimidazolium(TCNQ) (Chasseau, Gaultier & Hauw, 1972) and 1,2,3-trimethylbenzimidazolium(TCNQ) (Chasseau, Gaultier, Hauw & Schvoerer, 1972) have shorter distances between TCNQ planes been recorded. Several short inter-TCNQ and TCNQ–cation distances are listed in Table 4.

The dimensions of the two crystallographically independent types of TCNQ moiety are shown in Fig. 3 and the averaged lengths of chemically similar bonds are summarized in Table 5. The averaged lengths for TCNQ(*A*) are indistinguishable from those of TCNQ(*B*) and are intermediate between those found for TCNQ<sup>0</sup> (Long, Sparks & Trueblood, 1965) and the radical anion TCNQ<sup>-</sup>. Where possibly significant differences do arise, for bonds *b* and *c*, the tendency is towards TCNQ(*A*) being negatively charged and TCNQ(*B*) having zero charge. Since this, combined with the stoichiometry of 2(*B*):1(*A*), is inconsistent with the need to have an overall pair of negative charges to neutralize the two positive charges on the cation, it can be concluded that the negative charge is delocalized

with an average  $\frac{2}{3}$  charge on each TCNQ. In this way 1,4-di(*N*-quinoliniummethyl)benzene(TCNQ)<sub>3</sub> differs from other complexes of general formula C<sup>2+</sup>–(TCNQ)<sub>3</sub><sup>2-</sup>. In Cs<sub>2</sub>(TCNQ)<sub>3</sub> (Fritchie & Arthur, 1966), morpholinium<sub>2</sub>(TCNQ)<sub>3</sub> (Sundaresan & Wallwork, 1972*a*) and trimethylammonium<sub>2</sub>(TCNQ)<sub>3</sub> (Kobayashi, Danno & Saito, 1973) the charge is localized. Within the TCNQ columns in these structures the sequence is TCNQ<sup>-</sup> TCNQ<sup>-</sup> TCNQ<sup>0</sup> TCNQ<sup>-</sup> TCNQ<sup>-</sup> TCNQ<sup>0</sup>.

The dimensions of the quinolinium ring and xylol group of the cation are in close agreement with values reported previously for quinolinium(TCNQ)<sub>2</sub> (Kobayashi, Marumo & Saito, 1971) and 1,4-di(*N*-

Table 4. Short intermolecular contacts (Å)

The figures in parentheses indicate standard deviations.

TCNQ( <i>A</i> )–TCNQ( <i>B</i> )	TCNQ( <i>B</i> )–TCNQ( <i>B'</i> )	
C(1 <sup>i</sup> )–C(9 <sup>i</sup> )	C(9 <sup>i</sup> )–C(9 <sup>iv</sup> )	3.281 (4)
C(1 <sup>i</sup> )–C(10 <sup>i</sup> )	C(13 <sup>i</sup> )–N(4 <sup>iv</sup> )	3.257 (4)
C(1 <sup>i</sup> )–C(16 <sup>ii</sup> )	C(14 <sup>i</sup> )–N(4 <sup>iv</sup> )	3.381 (5)
C(1 <sup>i</sup> )–C(17 <sup>ii</sup> )		
C(2 <sup>i</sup> )–C(9 <sup>i</sup> )	TCNQ–cation	
C(2 <sup>i</sup> )–C(10 <sup>i</sup> )	N(1 <sup>i</sup> )–C(23 <sup>v</sup> )	3.184 (5)
C(3 <sup>i</sup> )–C(10 <sup>i</sup> )	N(2 <sup>i</sup> )–C(22 <sup>i</sup> )	3.283 (3)
C(3 <sup>i</sup> )–C(11 <sup>i</sup> )	N(2 <sup>i</sup> )–C(23 <sup>i</sup> )	3.228 (4)
C(3 <sup>i</sup> )–C(16 <sup>ii</sup> )	N(4 <sup>i</sup> )–C(24 <sup>ii</sup> )	3.278 (4)
C(3 <sup>i</sup> )–C(17 <sup>ii</sup> )	N(6 <sup>i</sup> )–C(19 <sup>v</sup> )	3.341 (5)
C(4 <sup>i</sup> )–C(7 <sup>i</sup> )	N(6 <sup>i</sup> )–C(27 <sup>vi</sup> )	3.353 (4)
C(4 <sup>i</sup> )–C(8 <sup>i</sup> )		
C(5 <sup>i</sup> )–C(8 <sup>i</sup> )	Interstack	
C(6 <sup>i</sup> )–C(7 <sup>i</sup> )	C(3 <sup>i</sup> )–N(1 <sup>iii</sup> )	3.361 (3)
C(6 <sup>i</sup> )–C(12 <sup>i</sup> )		
N(2 <sup>i</sup> )–C(15 <sup>i</sup> )		

Superscripts indicate equivalent positions as follows:

- (i)  $\bar{x}, \bar{y}, \bar{z}$ ; (iv)  $\bar{x}, 1-y, \bar{z}$   
 (ii)  $\bar{x}, \bar{y}, \bar{z}$ ; (v)  $x-1, y, z$   
 (iii)  $x+1, y, z$ ; (vi)  $x, y+1, z$

Table 5. Comparison of mean bond lengths (Å) uncorrected for libration

	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>	<i>e</i>
*TCNQ <sup>0</sup>	1.346	1.448	1.374	1.440	1.138
†TCNQ <sup>-</sup>	1.362	1.424	1.413	1.417	1.149
TCNQ( <i>A</i> )	1.354	1.425	1.411	1.420	1.146
TCNQ( <i>B</i> )	1.352	1.433	1.385	1.424	1.146

\* Long, Sparks & Trueblood (1965).

† Chasseau, Gaultier & Hauw (1972); Chasseau, Gaultier, Hauw & Schvoerer (1972); Fritchie (1966); Hanson (1965); Hoekstra, Spoedler & Vos (1972); Kistenmacher, Phillips & Cowan (1974); Konno & Saito (1974); Sundaresan & Wallwork (1972*b,c*).

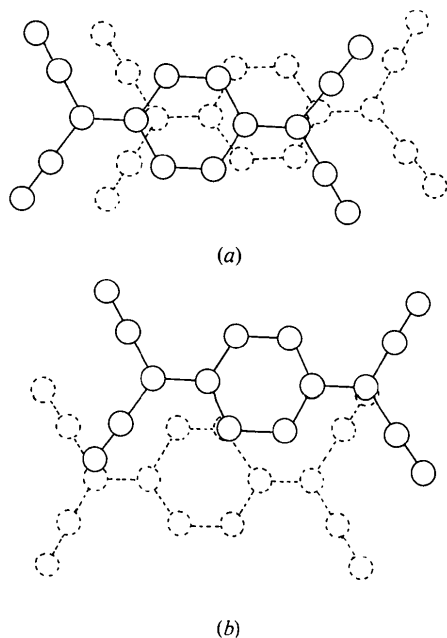


Fig. 2. TCNQ molecular overlap: (a) TCNQ(*A*)–TCNQ(*B*) and (b) TCNQ(*B*)–TCNQ(*B'*).

pyridiniummethyl)benzene(TCNQ)<sub>4</sub> (Ashwell, Wallwork, Baker & Berthier, 1975). The dihedral angle between the xylyl group and quinolinium ring is 87.4°. The angles that these planes make with TCNQ(A) are 38.8 and 60.6° and with TCNQ(B) 36.1 and 64.5° respectively.

### Electrical properties

Anisotropic conductivities of  $2 \times 10^{-4}$ ,  $1 \times 10^{-4}$  and  $1 \times 10^{-6} \Omega^{-1} \text{cm}^{-1}$  at 300 K were observed along the

long, intermediate and short axes respectively of single crystals of 1,4-di(*N*-quinoliniummethyl)benzene-(TCNQ)<sub>3</sub>. These crystal axes correspond to **a**, **b** and **c** of the unit cell respectively. Along **a** and **b**, nearly isotropic conductivities of  $\sim 10^{-4} \Omega^{-1} \text{cm}^{-1}$  reflect the molecular packing within the crystal in which two-dimensional arrays of TCNQ molecules in the (001) plane are separated along **c** by alternate layers of cations. In this direction, the lower conductivity of  $10^{-6} \Omega^{-1} \text{cm}^{-1}$  reflects in part the greater separation between TCNQ's although conduction may well take place *via* the cation.

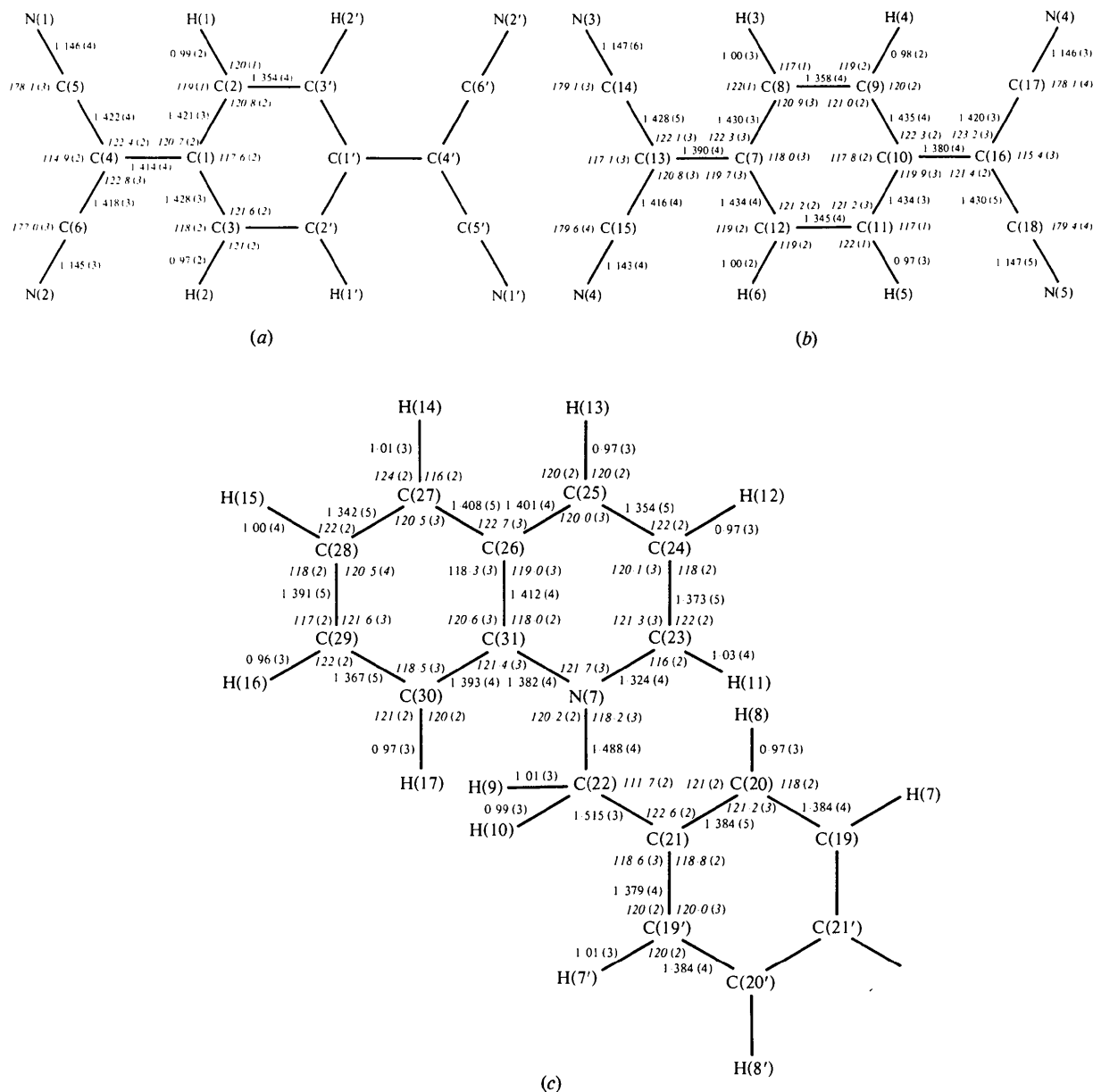


Fig. 3. Bond lengths, angles and their e.s.d.'s of (a) TCNQ(A), (b) TCNQ(B) and (c) the cation.

The temperature dependence of conductivity along all three axes is isotropic and varies as  $\exp(-E_a/kT)$  where  $E_a = 0.27 \pm 0.02$  eV.

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## The Crystal and Molecular Structure of 1-Ethyleneimino-2,4,6-trinitrobenzene

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The structure of 1-ethyleneimino-2,4,6-trinitrobenzene (CB1943) has been determined by a direct method. The crystals are monoclinic,  $a = 4.715$  (4),  $b = 30.48$  (3),  $c = 7.119$  (7) Å,  $\beta = 97.4^\circ$ , space group  $P2_1/c$ ;  $R = 0.067$  for 1815 reflexions. The 2-, 4- and 6-substituted nitro groups are inclined to the plane of the benzene ring by  $40.4$ ,  $12.5$  and  $37.3^\circ$  respectively. The ethyleneimine group is inclined at  $127.5^\circ$ .

#### Introduction

Several derivatives of trinitrobenzene have been investigated for antitumour activity (Ross & Mitchley, 1950), and the crystal structure of the most active derivative, *i.e.* 2,4-dinitro-5-ethyleneiminobenzamide, has been reported (Iball, Scrimgeour & Williams, 1975). The present compound (Fig. 1) has not shown any antitumour activity (Cobb *et al.*, 1969).

#### Experimental

Crystals of 1-ethyleneimino-2,4,6-trinitrobenzene (CB1943) in the form of large yellow prisms were supplied by Professor Ross, Chester Beatty Research Institute, and small pieces were cut from these. Different

crystals were mounted about  $a$  and  $b$ , and data were collected with Cu  $K\alpha$  radiation on a Wooster four-circle diffractometer. The cell dimensions were determined from Weissenberg photographs and refined on the diffractometer. No corrections for absorption were made.

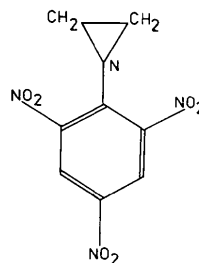


Fig. 1. 1-Ethyleneimino-2,4,6-trinitrobenzene (CB1943).