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1:2 Complexes of (Thio)Morpholinium Derivatives and the Electron Acceptor 7,7,8,8-Tetracyano-*p*-quinodimethane. Part I. *N*-Methyl-*N*-ethylthiomorpholinium Di-7,7,8,8-tetracyano-*p*-quinodimethanide METM(TCNQ)$_2$ and *N*-Methyl-*N*-butylthiomorpholinium Di-7,7,8,8-tetracyano-*p*-quinodimethanide MBTM(TCNQ)$_2$*

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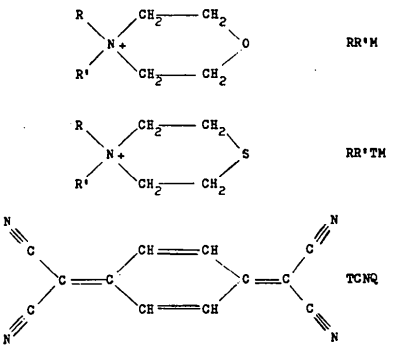
Abstract. METM(TCNQ)$_2$, $C_7H_{16}NS^+.2C_{12}H_4N_4^{1/2-}$, $M_r = 554{\cdot}7$, triclinic, $P\bar{1}$, $a = 15{\cdot}509\ (5)$, $b = 15{\cdot}023\ (6)$, $c = 6{\cdot}513\ (2)$ Å, $\alpha = 90{\cdot}70\ (3)$, $\beta = 101{\cdot}95\ (2)$, $\gamma = 107{\cdot}44\ (2)°$, $V = 1412\ (1)$ Å^3, $Z = 2$, $D_x = 1{\cdot}304$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}156$ mm^{-1}, $F(000) = 578$, $T = 294$ K, $R = 0{\cdot}058$ for 6536 observed reflections. Transformation to conventional cell by $(0,0,-1/0,-1,0/-1,0,0)$. MBTM-(TCNQ)$_2$, $C_9H_{20}NS^+.2C_{12}H_4N_4^{1/2-}$, $M_r = 582{\cdot}7$, triclinic, $P\bar{1}$, $a = 15{\cdot}685\ (2)$, $b = 15{\cdot}573\ (2)$, $c = 6{\cdot}561\ (1)$ Å, $\alpha = 94{\cdot}63\ (1)$, $\beta = 103{\cdot}10\ (1)$, $\gamma = 100{\cdot}62\ (1)°$, $V = 1522\ (1)$ Å^3, $Z = 2$, $D_x = 1{\cdot}272$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}149$ mm^{-1}, $F(000) = 610$, $T = 294$ K, $R = 0{\cdot}123$ for 4816 observed reflections. Transformation to conventional cell by $(0,0,-1/-1,0,-1/0,1,0)$. The packing in the two compounds is very similar: zigzag stacks are connected to form sheets parallel to the *bc* plane. There are two independent molecules *A* and *B* per stack; all overlaps are large and of type I. METM(TCNQ)$_2$ has the shorter N$^+$···TCNQ distance and a significant charge difference $\rho_A^s - \rho_B^s = -0{\cdot}34\ (4)$ e. The charge difference for MBTM-(TCNQ)$_2$, $\rho_A^s - \rho_B^s = 0{\cdot}29\ (19)$ e, has opposite sign.

Introduction. In the course of a systematic study of the charge transfer complexes of substituted (Thio)-morpholinium groups $RR'(\underline{T})M^+$ [(I) R, $R' = —H$ or —alkyl] with the organic acceptor 7,7,8,8-tetracyanoquinodimethane [TCNQ, (II)], a substantial number (*ca* 40) of new members of this class have been prepared. For a selected series of 1:2 complexes, the crystal structures have been determined to find qualitative relationships between packing characteristics and physical properties.



* 1:2 *N*-Ethyl-*N*-methylthiomorpholinium and *N*-Butyl-*N*-methylthiomorpholinium salts with the radical anion of 2,2'-(2,5-cyclohexadiene-1,4-diylidene)bispropanedinitrile.

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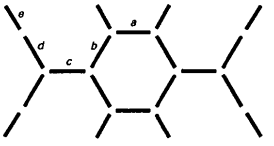
Table 1. *Coordinate system* **L, M, N** *and contents of crystal structure data blocks*

L, M, N axes
Right handed orthonormal inertial axial system for TCNQ quinodimethane carbon skeleton, **L** along longest molecular axis, **M** in (best) plane perpendicular to **L**, and **N** at right angles to the plane.

G, **L, M, N**, *U* block
For quinodimethane carbon skeleton of each independent TCNQ group, relative coordinates of centre of gravity *G* and components of **L, M, N** relative to the cell axes; U = average U_{eq} of quinodimethane C atoms, with $U_{eq} = \sum_i U_{ii}/3$ after diagonalization of the **U** tensor.

Charge block
Charge ρ of each independent TCNQ and bond lengths *a–e*.



a–e calculated by average lengths of bonds, equivalent for adopted TCNQ *mmm* symmetry; ρ obtained from *a–e* according to Flandrois & Chasseau (1977).

Overlap block
Transfer integrals t_{ij}^2 (van Smaalen & Kommandeur, 1985) and components of vectors v_{ij} connecting centres of gravity G_i and G_j of successive TCNQ's *i* and *j*; components given with respect to the **L, M, N** system of *i* and *j* or to the average system $\overline{\mathbf{L}}$, $\overline{\mathbf{M}}$, $\overline{\mathbf{N}}$ for independent groups *i* and *j*.

Standard deviations
For *G*, *U* and *a–e* average values of e.s.d.'s of *individual* quantities from which *G*, *U* and *a–e* are derived.

In the following, *R* and *R'* of (thio)morpholinium derivatives with $R \neq R'$ will be indicated by the first character of the substituents considered, whereas for derivatives with $R = R'$ the substituent character is preceded by a D. Thus, for instance, MEM for *N*-methyl-*N*-ethylmorpholinium, METM for the corresponding thiomorpholinium derivative and DEM for *N*,*N*-diethylmorpholinium.

In the present series of six papers the structure determinations of nine different 1:2 complexes and a brief discussion of the packing will be given. All the structures contain segregated TCNQ stacks, *i.e.* the planar TCNQ molecules are piled face-to-face in linear columns, in the stacking direction. This allows their π electrons to overlap, which accounts for the (semi)metallic behaviour of this group of compounds. Apart from the usual tables of crystallographic interest, the present series of papers will contain for each structure a so-called structure data block, in which the stack characteristics, as outlined in Table 1, are tabulated. The compounds of the intrastack TCNQ–TCNQ vectors v_{ij}, as defined in Table 1, may be compared with v_{ij}'s for the well known overlap types I and II given in Fig. 1. The average angle between the normals to the TCNQ quinodimethane carbon skeletons and the stacking axis will be given as the *inclination* (°) of the stack.

For all compounds of the present series, the unit-cell geometry gives a good indication of the orientation of the TCNQ molecules in the crystals. The basis of our cell choice was, in so far as was permitted by the crystal class, to have *c* along the stacking direction and *a* along the shortest TCNQ distance in or close to the molecular plane.

We remark that there is quite a variation in *R* values in this series of nine structure determinations. This is because we carried out the data collections to $\theta = 30°$ (appreciably beyond the copper sphere), aiming in the first place for high-resolution data and therefore low σ's in atomic parameters. But of course this is at the cost of low *R* values, with the data-sets now having many more weak reflections than if the measurements had been limited to the copper sphere. This is even more significant in cases where the structure is partially disordered.

In a forthcoming paper (Visser, de Boer & Vos, 1990) the characteristic features of the present 1:2 complexes and of further 1:2 complexes, determined by the crystal chemistry group in Groningen, will be summarized and related in a qualitative way to physical properties. Structures of 1:1 complexes encountered in the course of the investigation will be published as a separate series.

Experimental. Dark violet, almost black, crystals were grown by slowly cooling hot solutions of METM or MBTM iodide and neutral TCNQ in acetonitrile. All data were collected with Mo $K\alpha$ radiation on a CAD-4F diffractometer equipped with a graphite monochromator and a beam flattener (Helmholdt & Vos, 1977). $METM(TCNQ)_2$: cell constants from 20 optimized reflections with $0{\cdot}48 < \sin\theta/\lambda < 0{\cdot}62$ Å^{-1}. 8502 reflections measured up to $\theta = 30°$ from a crystal of $0{\cdot}18 \times 0{\cdot}28 \times 0{\cdot}39$ mm, h $-21 \rightarrow 21$, k $0 \rightarrow 21$, l $-9 \rightarrow 9$. Correction for intensity control was within $\pm 1{\cdot}4\%$. Equivalent *h0l*

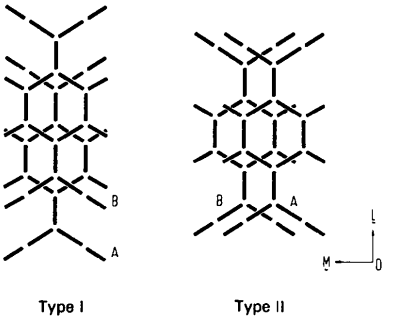


Fig. 1. Favourable overlap modes for TCNQ stacks. I = ring–external bond or type I overlap; II = ring–ring or type II overlap. Idealized displacement vectors (Table 1; **N** component representative for room-temperature structures) are v_{ij}(I) = 2·10**L** + 0·00**M** + 3·25**N**; v_{ij}(II) = 0·00**L** + 1·20**M** + 3·25**N**. Intermolecular shortest C···C ~3·30 Å.

intensities were averaged. 8210 independent reflections among which 760 intensities with $I<0$. MBTM(TCNQ)$_2$: cell constants from 22 reflections with $0{\cdot}21<\sin\theta/\lambda<0{\cdot}34$ Å^{-1}; 8857 reflections measured up to $\theta=30°$, including 2063 with $I<0$, on a crystal of $0{\cdot}04\times0{\cdot}18\times0{\cdot}33$ mm, h $-22\rightarrow22$, k $-21\rightarrow21$, l $0\rightarrow9$. Correction for intensity control was within $\pm1{\cdot}8\%$. For both compounds intensities were corrected for Lorentz and polarization effects, but not for absorption.

In both cases the TCNQ part was found from Patterson syntheses and the cation part from difference Fourier maps after isotropic refinement of the TCNQ molecules. Least-squares blocked-matrix refinement on $|F|$, with blocks for each independent molecule. Scattering factors for non-H atoms were taken from Cromer & Mann (1968) and for H atoms from Stewart, Davidson & Simpson (1965). Anisotropic thermal parameters for non-H and isotropic for H atoms (constrained at 1·08 Å from carbon). Considerable disorder in MBTM(TCNQ)$_2$ methyl and butyl groups has been accounted for by fractional atom refinement for C(40) and C(41) [C(40) being split in two, C(41) in three equal parts] (see Figs. 3 and 5), and enhanced thermal parameters for the remaining atoms. Maximum isotropic extinction correction for METM(TCNQ)$_2$ was 10% in $|F(\bar{1}02)|$, and for MBTM(TCNQ)$_2$ 6% in $|F(\bar{1}\bar{1}2)|$. Refinement criteria for METM(TCNQ)$_2$: weight $w=0$ for $F_o<2\sigma(\text{count};F_o)$, where $\sigma(\text{count};F_o)$ is the standard deviation due to counting statistics, $w=[\sigma^2(\text{count};F_o)+0{\cdot}0007|F_o|^2]^{-1}$ for the remaining reflections. Max. $|\Delta|/\sigma=0{\cdot}51\times10^{-3}$, mean $|\Delta|/\sigma=0{\cdot}73\times10^{-4}$, $R=0{\cdot}058$, $wR=0{\cdot}069$, $S=1{\cdot}64$, $N_o=6536$, $N_v=395$. Residual density $\Delta\rho$ in molecular regions: max. 0·35, min. $-0{\cdot}39$ e Å^{-3}; remote from molecules $|\Delta\rho_{max}|=0{\cdot}20$, $\sigma(\Delta\rho)=0{\cdot}05$ e Å^{-3}. Refinement criteria for MBTM(TCNQ)$_2$: weight $w=0$ for $|F_o|<2{\cdot}2\sigma(\text{count};F_o)$, $w=1$ for remaining reflections; $|\Delta|/\sigma$ max. $=0{\cdot}11\times10^{-1}$, mean $=0{\cdot}20\times10^{-3}$; $R=0{\cdot}123$, $wR=0{\cdot}109$, $S=0{\cdot}46$, $N_o=4816$, $N_v=398$. Residual density predominantly in the neighbourhood of the butyl group, $\Delta\rho_{max}=0{\cdot}61$, $\Delta\rho_{min}=-0{\cdot}41$; $\sigma(\Delta\rho)=0{\cdot}03$ e Å^{-3}. All computations were carried out on a Cyber 170/760 with the

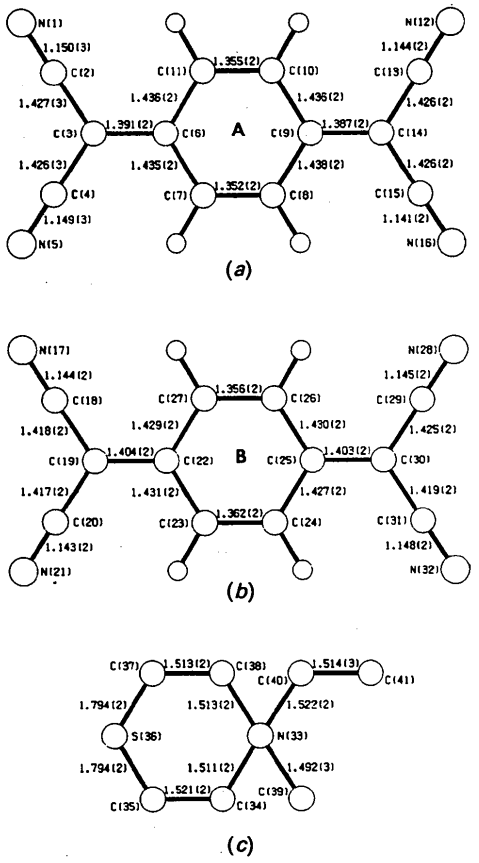


Fig. 2. METM(TCNQ)$_2$: bond lengths (Å) and atomic numbering for the non-H atoms.

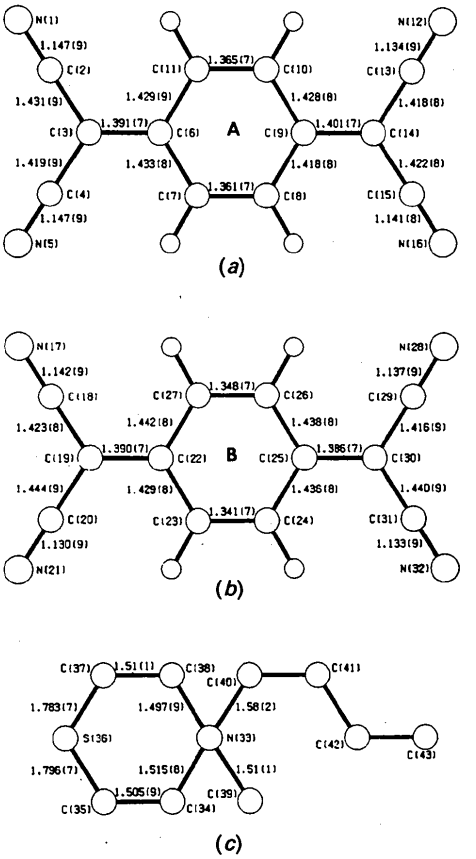


Fig. 3. MBTM(TCNQ)$_2$: bond lengths (Å) and atomic numbering for the non-H atoms. As atoms C(40) and C(41) are disordered, no bond lengths for these atoms are given.

Table 2. *Final fractional coordinates* ($\times 10^{-5}$) *and* U_{eq} *values* ($Å^2 \times 10^{-4}$) *for the non-H atoms of* $METM(TCNQ)_2$, *with e.s.d.'s in parentheses*

	x	y	z	U_{eq}
N(1)	−24862 (11)	−9843 (11)	−33431 (28)	663 (7)
C(2)	−23836 (11)	−1942 (12)	−31900 (26)	478 (6)
C(3)	−22777 (10)	7830 (10)	−30327 (24)	403 (5)
C(4)	−31123 (10)	10307 (11)	−33915 (25)	453 (6)
N(5)	−37840 (10)	12307 (12)	−36723 (26)	603 (6)
C(6)	−14124 (9)	14602 (10)	−25513 (22)	357 (5)
C(7)	−13454 (9)	24339 (10)	−24319 (23)	375 (5)
C(8)	−5107 (9)	31027 (10)	−19737 (23)	363 (5)
C(9)	3366 (9)	28631 (6)	−16031 (20)	320 (4)
C(10)	2692 (9)	18886 (6)	−17097 (21)	342 (5)
C(11)	−5676 (9)	12189 (10)	−21599 (22)	357 (5)
N(12)	27680 (10)	32752 (11)	−4363 (26)	582 (6)
C(13)	20529 (10)	33803 (10)	−7711 (23)	389 (5)
C(14)	11845 (9)	35621 (10)	−11654 (21)	338 (4)
C(15)	12486 (10)	45290 (11)	−10815 (25)	423 (5)
N(16)	13016 (11)	53034 (10)	−10173 (29)	673 (7)
N(17)	−10527 (11)	−862 (11)	25880 (30)	676 (7)
C(18)	−9937 (10)	6918 (11)	26410 (25)	430 (5)
C(19)	−9176 (9)	16569 (10)	27213 (22)	356 (5)
C(20)	−17606 (10)	18776 (11)	22802 (24)	404 (5)
N(21)	−24355 (9)	20656 (12)	19275 (28)	641 (7)
C(22)	−561 (9)	23593 (9)	31885 (21)	328 (4)
C(23)	−3 (9)	33277 (10)	32230 (22)	346 (5)
C(24)	8373 (9)	40072 (10)	36477 (22)	355 (5)
C(25)	16826 (9)	37784 (9)	40544 (21)	332 (4)
C(26)	16217 (9)	28096 (10)	40235 (22)	358 (5)
C(27)	7903 (9)	21297 (10)	36085 (22)	359 (5)
N(28)	40600 (10)	40396 (12)	52592 (26)	609 (6)
C(29)	33875 (10)	42343 (11)	48967 (24)	431 (5)
C(30)	25486 (9)	44726 (10)	44614 (23)	380 (5)
C(31)	26490 (11)	54424 (11)	44290 (26)	471 (6)
N(32)	27533 (12)	62311 (11)	43987 (30)	705 (7)
N(33)	51259 (8)	25203 (9)	5452 (19)	398 (4)
C(34)	43631 (11)	22857 (11)	−14259 (27)	493 (6)
C(35)	34912 (11)	15229 (12)	−12111 (28)	524 (6)
S(36)	36924 (3)	4237 (3)	−6911 (9)	632 (2)
C(37)	46083 (12)	8520 (13)	16065 (32)	607 (7)
C(38)	53965 (11)	16622 (12)	12095 (31)	522 (6)
C(39)	48273 (12)	29252 (14)	22782 (31)	603 (7)
C(40)	59987 (11)	32163 (12)	1196 (31)	537 (6)
C(41)	59256 (15)	41773 (14)	−3699 (37)	725 (9)

Table 3. *Final fractional coordinates* ($\times 10^{-4}$) *and* U_{eq} *values* ($Å^2 \times 10^{-4}$) *for the non-H atoms of* $MBTM(TCNQ)_2$, *with e.s.d.'s in parentheses*

	x	y	z	U_{eq}
N(1)	−2409 (4)	−873 (4)	−3605 (11)	706 (27)
C(2)	−2386 (4)	−130 (4)	−3362 (9)	474 (22)
C(3)	−2350 (4)	799 (4)	−3147 (10)	453 (21)
C(4)	−3190 (4)	1051 (4)	−3434 (10)	495 (22)
N(5)	−3870 (4)	1252 (4)	−3689 (10)	676 (25)
C(6)	−1551 (4)	1422 (4)	−2610 (9)	394 (19)
C(7)	−1549 (4)	2345 (4)	−2466 (9)	403 (20)
C(8)	−769 (3)	2958 (3)	−1937 (8)	346 (17)
C(9)	72 (3)	2708 (3)	−1513 (9)	366 (18)
C(10)	81 (4)	1790 (3)	−1683 (9)	381 (19)
C(11)	−701 (4)	1174 (4)	−2209 (8)	370 (19)
N(12)	2419 (4)	2990 (4)	−134 (11)	690 (26)
C(13)	1721 (4)	3133 (4)	−535 (10)	421 (20)
C(14)	865 (3)	3351 (3)	−1006 (9)	355 (18)
C(15)	878 (4)	4268 (4)	−969 (9)	394 (19)
N(16)	914 (4)	5008 (4)	−931 (10)	610 (23)
N(17)	−1053 (4)	−30 (4)	2449 (11)	703 (27)
C(18)	−1071 (4)	702 (4)	2559 (10)	462 (21)
C(19)	−1083 (4)	1617 (4)	2706 (9)	388 (19)
C(20)	−1954 (4)	1841 (4)	2246 (10)	456 (21)
N(21)	−2637 (3)	2013 (4)	1926 (10)	665 (25)
C(22)	−300 (3)	2261 (3)	3210 (8)	337 (17)
C(23)	−314 (3)	3178 (3)	3311 (8)	363 (18)
C(24)	444 (4)	3795 (4)	3789 (9)	388 (19)
C(25)	1305 (3)	3562 (3)	4279 (8)	359 (18)
C(26)	1325 (4)	2641 (3)	4193 (8)	363 (18)
C(27)	562 (4)	2021 (3)	3661 (9)	404 (20)
N(28)	3631 (4)	3784 (4)	5767 (10)	687 (26)
C(29)	2947 (4)	3964 (4)	5352 (10)	466 (22)
C(30)	2097 (4)	4190 (4)	4824 (9)	409 (19)
C(31)	2101 (4)	5118 (4)	4889 (11)	549 (25)
N(32)	2110 (5)	5848 (4)	4947 (12)	856 (32)
N(33)	4741 (3)	2282 (3)	723 (10)	535 (21)
C(34)	3966 (5)	2009 (5)	−1214 (11)	604 (28)
C(35)	3233 (4)	1287 (4)	−943 (10)	503 (23)
S(36)	3615 (1)	283 (1)	−496 (4)	639 (7)
C(37)	4522 (4)	746 (5)	1724 (13)	636 (30)
C(38)	5163 (4)	1517 (4)	1282 (11)	543 (25)
C(39)	4436 (5)	2664 (5)	2563 (14)	787 (35)
C(401)	5330 (13)	2974 (12)	−439 (34)	773 (48)
C(402)	5567 (11)	2979 (11)	734 (28)	651 (40)
C(411)	6087 (14)	3510 (14)	1113 (34)	560 (49)
C(412)	5412 (17)	3786 (17)	127 (40)	725 (64)
C(413)	5752 (20)	2952 (19)	−1277 (48)	889 (82)
C(42)	6568 (11)	4051 (11)	−654 (25)	1638 (55)
C(43)	6211 (10)	4749 (10)	−1296 (24)	1586 (54)

XRAY system (1976) and local crystallographic programs. Final coordinates of the non-H atoms and U_{eq}'s are given in Tables 2 and 3 for METM- and $MBTM(TCNQ)_2$, respectively. Bond lengths and numbering of non-H atoms of anions and cations are shown in Figs. 2 and 3.*

The relatively high inaccuracy in the parameters of $MBTM(TCNQ)_2$ is caused by an incomplete account of the butyl disorder in the structure model. For comparison of R values in similar cases in this series, see remark in the *Introduction*.

Discussion. Projections of the structures are illustrated in Figs. 4 and 5. The structure data blocks are given in Tables 4 and 5. The packings in METM- and $MBTM(TCNQ)_2$ are very similar. Two independent molecules, *A* and *B*, alternate in the zigzag stacks. All TCNQ molecules are approximately perpendicular to the stacking axis *c*; inclinations for individual molecules vary from 0·5 to 2·0°. The overlaps are large and all of type I. The stacks are connected to form sheets parallel to *bc* by electrostatically favourable $(TCNQ)H^{\delta-}\cdots N^{\delta+}(TCNQ)$ contacts of ~2·7 Å. The packing of the cations around the inversion centre ($\frac{1}{2}$,0,0) is highly analogous in the two compounds. In $MBTM(TCNQ)_2$ the larger butyl groups of the cation push TCNQ molecules of type *B* further away from the N^+ than do the smaller ethyl groups in $METM(TCNQ)_2$. The scaled charges ρ^s_A and ρ^s_B are derived from the charges calculated according to Flandrois & Chasseau (1977), scaled to sum to one, as we assume complete charge transfer from the cation. The scaled charge difference, $\Delta\rho^s = \rho^s_A - \rho^s_B$, is 0·29 (19) e and −0·34 (4) e for MBTM- and $METM(TCNQ)_2$ respectively, and thus differs significantly from zero only in the compound where N^+ is closest to TCNQ.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters, and figures giving bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52302 (56 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 4. *Crystal structure data block for METM(TCNQ)$_2$*

	TCNQ *A*			TCNQ *B*		
G	−0·05405 (9)	0·21641 (10)	−0·20785 (22)	0·08133 (9)	0·30677 (10)	0·36160 (22)
L	0·061743	0·049485	0·033350	0·061460	0·049929	0·030814
M	−0·031462	0·049477	−0·010806	−0·032021	0·049049	−0·015464
N	0·000071	−0·001505	0·153487	0·000137	0·000631	0·153618
U	0·0357 (2)			0·0352 (5)		

Charge (e)	ρ_A = 0·33 (3)	1·353 (2)	1·436 (2)	1·389 (2)	1·429 (2)	1·146 (2)
	ρ_B = 0·67 (3)	1·359 (2)	1·429 (2)	1·403 (2)	1·420 (2)	1·145 (2)

Stack $t^c(A–B)$ = 0·145 eV $\nu(A–B) = 2·074\bar{\mathbf{L}} - 0·228\bar{\mathbf{M}} + 3·255\bar{\mathbf{N}}$
$t^c(B–A^i)$ = 0·144 eV $\nu(B–A^i) = -2·061\bar{\mathbf{L}} + 0·276\bar{\mathbf{M}} + 3·257\bar{\mathbf{N}}$

Symmetry code: (i) $x, y, z + 1$.

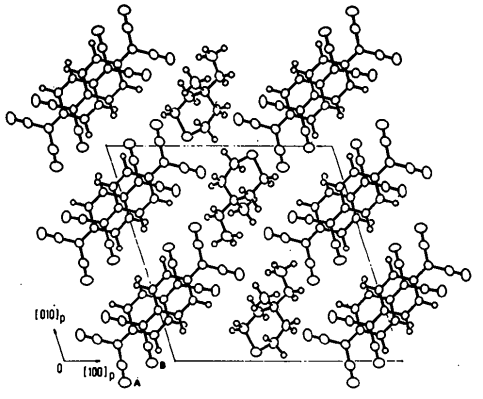
Table 5. *Crystal structure data block for MBTM(TCNQ)$_2$*

	TCNQ *A*			TCNQ *B*		
G	−0·07378 (36)	0·20685 (35)	−0·20714 (86)	0·05044 (35)	0·29081 (35)	0·37465 (86)
L	0·057102	0·045332	0·038187	0·056722	0·045842	0·037750
M	−0·034916	0·047791	−0·010564	−0·035528	0·047261	−0·015184
N	0·000356	−0·000679	0·152730	−0·000505	0·002080	0·152449
U	0·0384 (19)			0·0376 (19)		

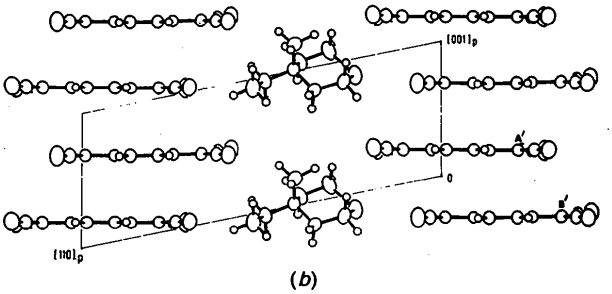
Charge (e)	ρ_A = 0·56 (12)	1·363 (7)	1·427 (8)	1·396 (7)	1·423 (9)	1·142 (9)
	ρ_B = 0·31 (12)	1·344 (7)	1·436 (8)	1·388 (7)	1·431 (9)	1·136 (9)

Stack $t^c(A–B)$ = 0·135 eV $\nu(A–B) = 2·021\bar{\mathbf{L}} - 0·267\bar{\mathbf{M}} + 3·284\bar{\mathbf{N}}$
$t^c(B–A^i)$ = 0·140 eV $\nu(B–A^i) = -2·090\bar{\mathbf{L}} + 0·143\bar{\mathbf{M}} + 3·272\bar{\mathbf{N}}$

Symmetry code: (i) $x, y, z + 1$.



(*a*)



(*b*)

Fig. 4. Projections of the METM(TCNQ)$_2$ structure: (*a*) along [001]; (*b*) along **M** (see Table 1) of one layer of cations and anions, where *A'* and *B'* are related to *A* and *B* by the inversion centre at (0,0,0).

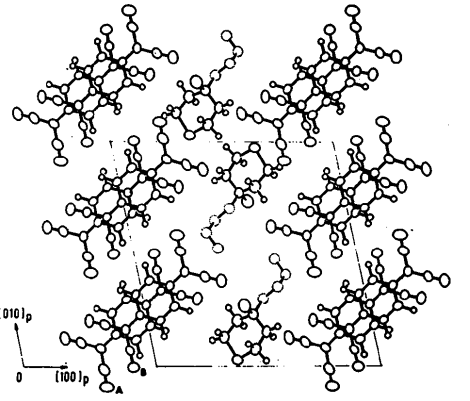


Fig. 5. Projection along [001] of the MBTM(TCNQ)$_2$ structure. The butyl atoms are dashed to illustrate the disorder. Projection along **M** is not given because of the strong similarity with the corresponding projection in Fig. 4.

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