Acta Cryst. (1990). C**46**, 857–860

1:2 Complexes of (Thio)Morpholinium Derivatives and the Electron Acceptor 7,7,8,8-Tetracyano-*p*-quinodimethane. Part II.† *N*-Methyl-*N*-propylmorpholinium Di-7,7,8,8-tetracyano-*p*-quinodimethanide MPM(TCNQ)$_2$ and *N*-Methyl-*N*-butylmorpholinium Di-7,7,8,8-tetracyano-*p*-quinodimethanide MBM(TCNQ)$_2$‡

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(*Received* 1 *September* 1988; *accepted* 1 *June* 1989)

Abstract. MPM(TCNQ)$_2$, $C_8H_{18}NO^+.2C_{12}H_4N_4^{1/2-}$, $M_r = 552{\cdot}6$, triclinic, $P\bar{1}$, $a = 7{\cdot}862\,(1)$, $b = 28{\cdot}518\,(3)$, $c = 6{\cdot}560\,(1)$ Å, $\alpha = 90{\cdot}23\,(1)$, $\beta = 75{\cdot}71\,(1)$, $\gamma = 91{\cdot}44\,(1)°$, $V = 1425\,(1)$ Å^3, $Z = 2$, $D_x = 1{\cdot}29$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}090$ mm^{-1}, $F(000) = 578$, $T = 294$ K, $R = 0{\cdot}074$ for 5701 observed reflections. Transformation to conventional cell by (0,0,−1/−1,0,0/0,1,0). MBM(TCNQ)$_2$, $C_9H_{20}NO^+.2C_{12}H_4N_4^{1/2-}$, $M_r = 566{\cdot}6$, triclinic, $P\bar{1}$, $a = 7{\cdot}944\,(1)$,. $b = 28{\cdot}850\,(2)$, $c = 6{\cdot}584\,(1)$ Å, $\alpha = 95{\cdot}65\,(1)$, $\beta = 77{\cdot}27\,(1)$, $\gamma = 89{\cdot}77\,(1)°$, $V = 1464\,(1)$ Å^3, $Z = 2$, $D_x = 1{\cdot}28$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}090$ mm^{-1}, $F(000) = 594$, $T = 294$ K, $R = 0{\cdot}105$ for 5208 observed reflections. Transformation to conventional cell by (0,0,−1/1,0,0/0,−1,0). The packing in the two compounds is similar. Zigzag TCNQ stacks with type I overlaps are connected to form sheets parallel to the *ac* plane. Within a sheet all TCNQ molecules are equivalent, but sheets at $y = 0$ and $y = \frac{1}{2}$ are independent.

Introduction. A general introduction is given in Part I of this series.

Experimental. Dark violet crystals obtained by slowly cooling hot solutions of MPM or MBM iodide and neutral TCNQ in acetonitrile. MPM(TCNQ)$_2$ crystals always twinned about *c*; a crystal with a small twinning ratio was used for the measurements. All data were collected with Mo radiation on a CAD-4F diffractometer equipped with a graphite monochromator and beam flattener (Helmholdt & Vos, 1977). MPM(TCNQ)$_2$ cell dimensions were from 22 optimized reflections with $0{\cdot}57 < \sin\theta/\lambda < 0{\cdot}64$ Å^{-1}; MBM(TCNQ)$_2$ cell from 22 reflections with $0{\cdot}57 < \sin\theta/\lambda < 0{\cdot}67$ Å^{-1}. Intensity measurements were up to $\theta = 30°$; the short b^* axis was kept as horizontal as possible by use of the modified CAD-4 program developed by de Boer & Duisenberg (1984). For MPM(TCNQ)$_2$ 8268 independent intensities were collected (h −11→11, k −40→40, l 0→9) including 1229 with $I < 0$, ω–2θ scan, crystal $0{\cdot}15 \times 0{\cdot}28 \times 0{\cdot}37$ mm; correction for intensity control was within ±2·2%. In addition to the main series, 1332 $hk1$ reflections were measured for the minor twin individual, including 504 with $I < 0$. Scaling to the main series, according to Hamilton, Rollett & Sparks (1965), gives a twinning ratio of 2·34% and an internal consistency of scaled reflections of $R_{\rm int} = [\sum w(I_{\rm obs} - \bar{I})^2/\sum wI^2]^{1/2} = 0{\cdot}016$; $hk0$ intensities were scaled down by multiplication with $1{\cdot}0234^{-1}$. Collected for MBM(TCNQ)$_2$: 8511 independent intensities (h −11→11, k −40→40, l 0→9) from a crystal of $0{\cdot}17 \times 0{\cdot}22 \times 0{\cdot}34$ mm, including 1523 with $I < 0$, ω scan; intensity control correction was within ±0·8%. Corrections were applied for Lorentz and polarization effects, but not for absorption.

In both cases the TCNQ part of the structure was found from Patterson maps and the cation part from difference Fourier syntheses after isotropic refinement of the TCNQ part. Least-squares blocked-matrix refinement on $|F|$, with blocks for each independent molecule. Scattering factors for non-H atoms from Cromer & Mann (1968) and for H atoms from Stewart, Davidson & Simpson (1965). Anisotropic thermal parameters for non-H atoms and isotropic for H atoms (constrained at 1·08 Å from C atom). Details for MPM(TCNQ)$_2$: largest isotropic extinction correction 7%, in $|F(002)|$. Weight $w = 0$ for $|F_o| < 2{\cdot}5\sigma$(count;F_o), $w = [\sigma^2(\text{count};F_o) + 0{\cdot}0008\ |F_o|^2]^{-1}$ for remaining reflections. Max. $|\Delta|/\sigma = 0{\cdot}006$, mean = 0·0007, $R =$

† Part I: Visser, Bouwmeester, de Boer & Vos (1990).

‡ 1:2 *N*-Methyl-*N*-propylmorpholinium and *N*-butyl-*N*-methylmorpholinium salts with the radical anion of 2,2′-(2,5-cyclohexadiene-1,4-diylidene)bispropanedinitrile.

0108-2701/90/050857-04$03.00

Table 1. *Final fractional coordinates* ($\times 10^{-5}$) *and* U_{eq} *values* ($Å^2 \times 10^{-4}$) *for non-*H *atoms in* $MPM(TCNQ)_2$, *with e.s.d.'s in parentheses*

$U_{eq} = \sum_i U_{ii}/3$ after diagonalization of the U tensor.

	x	y	z	U_{eq}
N(1)	13527 (25)	19618 (6)	−28953 (33)	678 (8)
C(2)	19683 (24)	15985 (6)	−30423 (31)	459 (7)
C(3)	27376 (21)	11497 (6)	−32159 (27)	370 (5)
C(4)	45971 (24)	11442 (7)	−36627 (31)	471 (7)
N(5)	61016 (23)	11455 (7)	−40122 (35)	726 (8)
C(6)	17078 (20)	7345 (5)	−29508 (24)	320 (5)
C(7)	24963 (20)	2840 (6)	−31079 (25)	328 (5)
C(8)	14923 (19)	−1165 (6)	−28581 (24)	319 (5)
C(9)	−3819 (19)	−996 (5)	−24242 (23)	298 (5)
C(10)	−11682 (20)	3512 (5)	−22465 (25)	333 (5)
C(11)	−1635 (20)	7507 (6)	−25061 (26)	341 (5)
N(12)	−47885 (21)	−5057 (6)	−14549 (30)	592 (7)
C(13)	−32931 (21)	−4998 (6)	−17637 (27)	382 (6)
C(14)	−14204 (20)	−5093 (5)	−21829 (25)	321 (5)
C(15)	−7167 (22)	−9637 (6)	−23310 (27)	381 (6)
N(16)	−1995 (23)	−13343 (6)	−24428 (31)	605 (7)
N(17)	52252 (24)	63304 (6)	−26139 (32)	637 (7)
C(18)	57923 (23)	59645 (6)	−26762 (28)	417 (6)
C(19)	65242 (21)	55125 (6)	−27489 (26)	363 (5)
C(20)	83851 (23)	55022 (6)	−30894 (28)	410 (6)
N(21)	98758 (21)	54900 (6)	−33405 (30)	594 (7)
C(22)	55032 (20)	51004 (6)	−25304 (24)	346 (5)
C(23)	62985 (21)	46524 (6)	−26376 (27)	386 (6)
C(24)	53223 (22)	42506 (6)	−24114 (27)	402 (6)
C(25)	34548 (22)	42588 (6)	−20844 (26)	386 (6)
C(26)	26533 (22)	47063 (6)	−19817 (26)	393 (6)
C(27)	36251 (21)	51098 (6)	−21937 (26)	386 (6)
N(28)	−8990 (26)	38359 (8)	−12973 (37)	845 (10)
C(29)	6035 (28)	38379 (8)	−15528 (34)	579 (8)
C(30)	24607 (25)	38407 (7)	−18872 (30)	470 (7)
C(31)	32639 (29)	33961 (8)	−20313 (35)	583 (8)
N(32)	39036 (30)	30403 (7)	−21681 (39)	859 (10)
N(33)	83243 (19)	25415 (5)	31266 (25)	432 (5)
C(34)	77524 (25)	30332 (7)	29700 (36)	602 (9)
C(35)	87570 (28)	33807 (8)	39073 (45)	798 (12)
O(36)	106056 (21)	33556 (6)	29987 (34)	830 (8)
C(37)	112093 (28)	29063 (8)	33384 (39)	760 (11)
C(38)	103161 (26)	25320 (7)	23759 (37)	661 (10)
C(39)	78232 (32)	23604 (10)	53351 (41)	755 (11)
C(40)	75636 (27)	22125 (8)	17735 (36)	606 (9)
C(41)	55990 (30)	21983 (10)	21825 (48)	796 (12)
C(42)	49423 (39)	18383 (12)	8835 (54)	993 (15)

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

$U_{eq} = \sum_i U_{ii}/3$ after diagonalization of the U tensor.

	x	y	z	U_{eq}
N(1)	1211 (5)	1933 (1)	−2018 (7)	74 (2)
C(2)	1833 (5)	1567 (1)	−2333 (6)	52 (1)
C(3)	2624 (4)	1115 (1)	−2708 (6)	43 (1)
C(4)	4463 (5)	1094 (1)	−3153 (6)	52 (1)
N(5)	5936 (5)	1086 (1)	−3487 (7)	78 (2)
C(6)	1653 (4)	713 (1)	−2608 (5)	34 (1)
C(7)	2459 (4)	259 (1)	−2956 (5)	38 (1)
C(8)	1514 (4)	−132 (1)	−2893 (5)	37 (1)
C(9)	−332 (4)	−103 (1)	−2467 (5)	34 (1)
C(10)	−1145 (4)	352 (1)	−2079 (5)	37 (1)
C(11)	−191 (4)	740 (1)	−2164 (5)	38 (1)
N(12)	−4627 (4)	−473 (1)	−1718 (6)	62 (1)
C(13)	−3162 (4)	−480 (1)	−2012 (6)	42 (1)
C(14)	−1313 (4)	−502 (1)	−2413 (5)	36 (1)
C(15)	−572 (5)	−962 (1)	−2787 (6)	43 (1)
N(16)	−20 (5)	−1333 (1)	−3061 (6)	67 (1)
N(17)	4893 (4)	6352 (1)	−2070 (6)	62 (1)
C(18)	5519 (4)	5990 (1)	−2297 (6)	42 (1)
C(19)	6305 (4)	5536 (1)	−2582 (5)	34 (1)
C(20)	8147 (4)	5517 (1)	−2955 (5)	40 (1)
N(21)	9617 (4)	5498 (1)	−3241 (6)	58 (1)
C(22)	5335 (4)	5134 (1)	−2517 (5)	33 (1)
C(23)	6157 (4)	4681 (1)	−2817 (5)	34 (1)
C(24)	5213 (4)	4290 (1)	−2728 (5)	36 (1)
C(25)	3370 (4)	4313 (1)	−2355 (5)	35 (1)
C(26)	2543 (4)	4765 (1)	−2059 (5)	36 (1)
C(27)	3477 (4)	5159 (1)	−2121 (5)	35 (1)
N(28)	−916 (4)	3944 (1)	−1723 (6)	63 (1)
C(29)	559 (5)	3933 (1)	−1973 (6)	46 (1)
C(30)	2397 (4)	3911 (1)	−2303 (5)	40 (1)
C(31)	3175 (5)	3456 (1)	−2596 (6)	50 (1)
N(32)	3779 (5)	3088 (1)	−2842 (7)	74 (2)
N(33)	8624 (5)	2653 (1)	4225 (6)	64 (1)
C(34)	8080 (6)	3160 (2)	4443 (10)	79 (2)
C(35)	9076 (6)	3400 (2)	2649 (12)	103 (3)
O(36)	10854 (4)	3362 (1)	2515 (8)	118 (2)
C(37)	11479 (6)	2901 (2)	2287 (11)	92 (3)
C(38)	10560 (6)	2621 (2)	3948 (12)	114 (3)
C(39)	7891 (21)	2577 (7)	6647 (18)	238 (2)
C(40)	8158 (7)	2362 (2)	2423 (10)	89 (2)
C(41)	6220 (15)	2380 (5)	2751 (26)	224 (8)
C(421)	5606 (15)	2037 (3)	829 (14)	97 (4)
C(422)	6068 (20)	1754 (8)	1761 (29)	92 (8)
C(43)	4552 (15)	1724 (3)	2045 (14)	184 (5)

0·074, $wR = 0·090$, $S = 2·01$, $N_o = 5701$, $N_v = 407$. Residual density $\Delta\rho$ close to molecules $\Delta\rho_{max} = 0·40$, $\Delta\rho_{min} = -0·28$ e Å^{-3}; remote from molecules $|\Delta\rho_{max}| = 0·40$, $\sigma(\Delta\rho) = 0·06$ e Å^{-3}. Details for $MBM(TCNQ)_2$: weight $w = 0$ for $|F_o| < 2·5\sigma(\text{count};F_o)$ and for eight strong low-order reflections with $||F_o| - |F_c|| > 10$, $w = 1$ for remaining reflections. The strongly disordered methyl and butyl groups could not be accounted for by superposition of reasonable models. Where needed, fractional C [C(42) split into C(421) and C(422) with s.o.f.'s of 0·65 and 0·35 respectively] and H atoms refined, initially placed at observed peaks. Max. $|\Delta|/\sigma = 0·38$, mean = 0·008, $R = 0·105$, $wR = 0·088$, $S = 0·92$, $N_o = 5208$, $N_v = 410$. Residual density close to molecules $\Delta\rho_{max} = 0·40$, $\Delta\rho_{min} = -0·44$, $\sigma(\Delta\rho) = 0·06$ e Å^{-3}, the highest peaks are in the vicinity of the disordered substituents. For comparison of R values in similar cases in this series, see remark in the *Introduction* of Part I. All computations were carried out on a Cyber 170/760 with the *XRAY* system (1976) and local crystallographic programs.

Final atomic coordinates and U_{eq} values of non-H atoms are listed in Tables 1 and 2 for $MPM(TCNQ)_2$ and $MBM(TCNQ)_2$ respectively. Bond lengths and atomic numbering are given in Figs. 1 and 2.* The strong disorder of the methyl and butyl groups reduces the accuracy of the $MBM(TCNQ)_2$ parameters, in comparison with $MPM(TCNQ)_2$.

Discussion. The structure data block of $MPM(TCNQ)_2$ is given in Table 3 and the block for $MBM(TCNQ)_2$ in Table 4. Fig. 3 illustrates two projections of $MPM(TCNQ)_2$; corresponding very similar projections of $MBM(TCNQ)_2$ are not given. Both the MPM and MBM cations are extended along [310]. The cell dimensions show that

* 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 52308 (52 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Crystal structure data block for MPM(TCNQ)$_2$*

		TCNQ *A*			TCNQ *B*	
G	0·06625 (20)	0·03181 (6)	−0·26866 (25)	0·44803 (22)	0·46789 (6)	−0·23094 (27)
L	0·073857	0·029469	−0·18430	0·072244	0·029729	−0·015474
M	−0·108334	0·019020	0·024704	−0·108843	0·018598	0·017802
N	−0·006866	0·000452	0·154257	−0·013124	0·000806	0·155528
U	0·0329 (5)			0·0395 (6)		

Charge (e)	ρ_A = 0·60 (3)	1·358 (2)	1·432 (2)	1·399 (2)	1·422 (2)	1·144 (2)
	ρ_B = 0·52 (3)	1·352 (2)	1·433 (2)	1·396 (2)	1·423 (3)	1·143 (3)

Stack

$t^c(A–A^i)$ = 0·127 eV $\nu(A–A^i) = -1·989\mathbf{L} - 0·342\mathbf{M} + 3·300\mathbf{N}$

$t^c(A^i–A^{ii})$ = 0·148 eV $\nu(A^i–A^{ii}) = 2·105\mathbf{L} + 0·006\mathbf{M} + 3·250\mathbf{N}$

$t^c(B–B^{iii})$ = 0·175 eV $\nu(B–B^{iii}) = 2·057\mathbf{L} + 0·028\mathbf{M} + 3·171\mathbf{N}$

$t^c(B^{iii}–B^{ii})$ = 0·101 eV $\nu(B^{iii}–B^{ii}) = -1·834\mathbf{L} - 0·667\mathbf{M} + 3·354\mathbf{N}$

Symmetry code: (i) $\bar{x},\bar{y},\bar{z}$; (ii) $x,y,z+1$; (iii) $\bar{x}+1,\bar{y}+1,\bar{z}$.

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

		TCNQ *A*			TCNQ *B*	
G	0·06583 (40)	0·03049 (11)	−0·25361 (51)	0·43499 (39)	0·47236 (11)	−0·24353 (50)
L	0·070046	0·028758	−0·005276	0·069460	0·028863	−0·005153
M	−0·108380	0·019669	0·032690	−0·108574	0·019489	0·027636
N	−0·003725	0·000419	0·152982	−0·007300	0·001074	0·153979
U	0·0367 (10)			0·0355 (10)		

Charge (e)	ρ_A = 0·43 (6)	1·355 (4)	1·432 (4)	1·392 (4)	1·427 (5)	1·140 (5)
	ρ_B = 0·46 (6)	1·357 (4)	1·435 (4)	1·396 (4)	1·427 (5)	1·142 (5)

Stack

$t^c(A–A^i)$ = 0·134 eV $\nu(A–A^i) = -2·026\mathbf{L} + 0·208\mathbf{M} + 3·290\mathbf{N}$

$t^c(A^i–A^{ii})$ = 0·135 eV $\nu(A^i–A^{ii}) = 2·067\mathbf{L} - 0·008\mathbf{M} + 3·291\mathbf{N}$

$t^c(B–B^{iii})$ = 0·139 eV $\nu(B–B^{iii}) = 1·921\mathbf{L} + 0·188\mathbf{M} + 3·261\mathbf{N}$

$t^c(B^{iii}–B^{ii})$ = 0·120 eV $\nu(B^{iii}–B^{ii}) = -1·883\mathbf{L} + 0·230\mathbf{M} + 3·309\mathbf{N}$

Symmetry code: (i) $\bar{x},\bar{y},\bar{z}$; (ii) $x,y,z,+1$; (iii) $\bar{x}+1,\bar{y}+1,\bar{z}$.

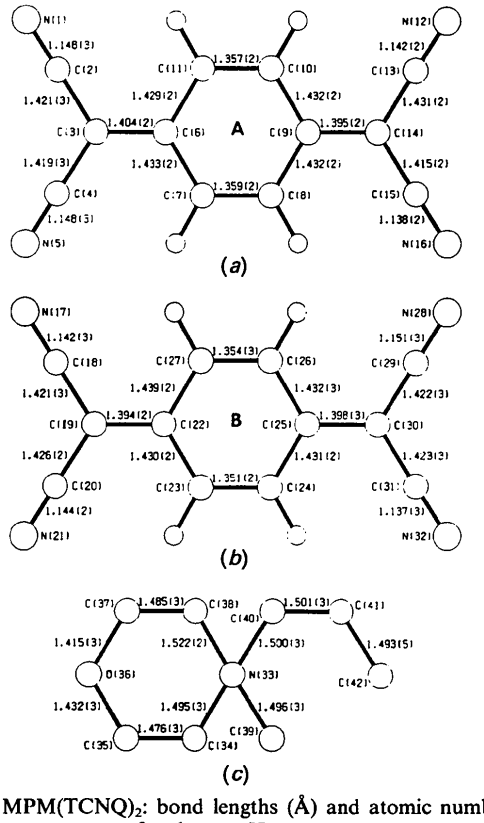

Fig. 1. MPM(TCNQ)$_2$: bond lengths (Å) and atomic numbering for the non-H atoms.

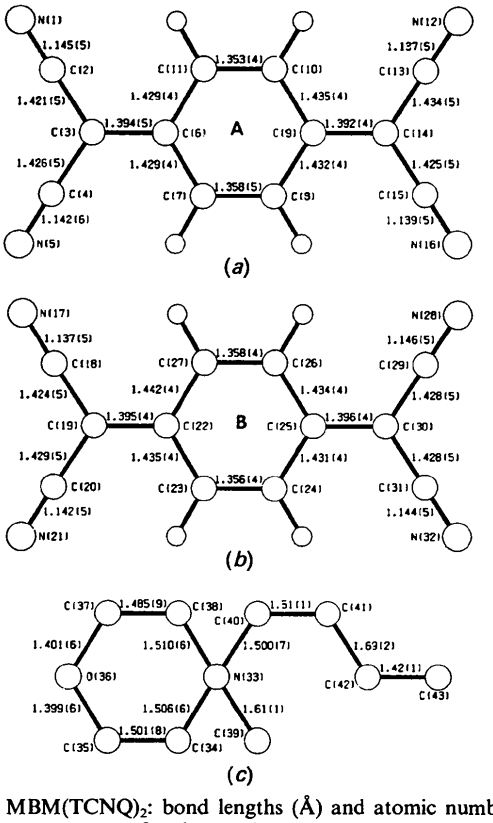

Fig. 2. MBM(TCNQ)$_2$: bond lengths (Å) and atomic numbering for the non-H atoms.

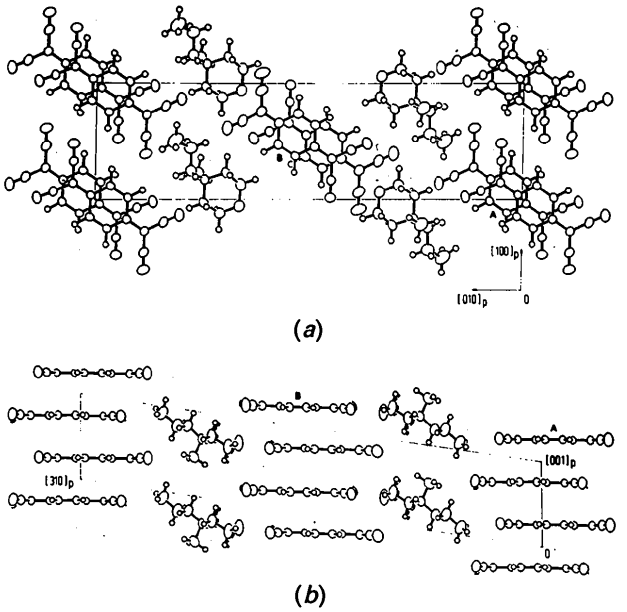

Fig. 3. MPM(TCNQ)$_2$: (*a*) projection along [001]; (*b*) projection along **M** (see Table 1 in Part I) of one layer of cations and anions.

replacement of MPM by MBM makes the diagonal $3a + b$ longer by an increase of a and b and a decrease of γ. The structures contain zigzag stacks along c in which all overlaps have a type I character. The largest deviation from an idealized type I occurs for B^3–B^2 (this is from TCNQ group B at position 3 $= -x+1,-y+1,-z$ to TCNQ group B at position $2 = x,y,z+1$; see Table 3) in MPM(TCNQ)$_2$. Successive stacks along a are connected to form sheets parallel to the ac plane by electrostatically favourable H···N contacts down to 2·65 (1) Å for MPM(TCNQ)$_2$ and 2·71 (1) Å for MBM(TCNQ)$_2$.

Molecules within a sheet are related by inversion centres, but sheets $A(y = 0)$ and $B(y = \frac{1}{2})$ are not equivalent. The TCNQ molecules in successive sheets are approximately parallel with stack inclinations between 1·8 and 5·9°. In both compounds the charges ρ_A and ρ_B are equal within experimental error.

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(*Received* 1 *September* 1988; *accepted* 1 *June* 1989)

Abstract. EBM(TCNQ)$_2$, $C_{10}H_{22}NO^+.2C_{12}H_4N_4^{1/2-}$, $M_r = 580{\cdot}7$, monoclinic, $P2_1/c$, $a = 7{\cdot}965$ (1), $b = 28{\cdot}523$ (2), $c = 15{\cdot}886$ (2) Å, $\beta = 123{\cdot}82$ (1)°, $V = 2998$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}286$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}089$ mm^{-1}, $F(000) = 1220$, $T = 294$ K, $R = 0{\cdot}089$ for 5150 observed reflections. Transformation to conventional cell by (1,0,0/0,1,0/1,0,1). EBTM(TCNQ)$_2$, $C_{10}H_{22}NS^+.2C_{12}H_4N_4^{1/2-}$, $M_r = 596{\cdot}7$ triclinic, $P\bar{1}$, $a = 7{\cdot}725$ (2), $b = 15{\cdot}179$ (3), $c = 14{\cdot}333$ (3) Å, $\alpha = 107{\cdot}79$ (2), $\beta = 96{\cdot}19$ (2), $\gamma = 101{\cdot}79$ (2)°, $V = 1540$ (1) Å^3, $Z = 2$, $D_x = 1{\cdot}287$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu =$

* Part II: Visser, de Boer & Vos (1990).

† 1:2 *N*-Butyl-*N*-ethylmorpholinium and *N*-butyl-*N*-ethylthiomorpholinium salts with the radical anion of 2,2′-(2,5-cyclohexadiene-1,4-diylidene)bispropanedinitrile.

0108-2701/90/050860-05$03.00