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Charge-Transfer Complex from the Reaction Between 10-Methyl-5,10-dihydrophenarsazine (MPA) and 2,2′-(2,3,5,6-Tetrafluoro-2,5-cyclohexadiene-1,4-diylidene)dipropanedinitrile ($TCNQF_4$) in Acetonitrile: $[(C_{13}H_{12}AsNO)_2H]^+[(C_{12}F_4N_4)_2]^-(C_{13}H_{12}AsNO)(CH_3CN)$

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Abstract. $M_r = 1413\cdot88$, monoclinic, $P2_1/a$, $a = 14\cdot305\,(5)$, $b = 25\cdot420\,(9)$, $c = 17\cdot669\,(5)$ Å, $\beta = 106\cdot78\,(2)°$, $V = 6151\cdot53$ Å^3, $Z = 4$, $D_x = 1\cdot526$, $D_m = 1\cdot542$ Mg m^{-3}, $\lambda(\text{Mo}\ K\alpha) = 0\cdot71069$ Å, $\mu = 16\cdot81$ mm^{-1}, $F(000) = 2836$, $T = 293$ K. Final $R = 0\cdot100$ for 3357 unique observed reflections. The complex $[(10\text{-methyl-5,10-dihydrophenarsazine 10-oxide})_2H]^+[(TCNQF_4)_2]^-$(10-methyl-5,10-dihydrophenarsazine 10-oxide)(acetonitrile) can be prepared by reacting neutral MPA with neutral $TCNQF_4$ in acetonitrile. All 10-methyl-5,10-dihydrophenarsazine 10-oxide (MPAO) units are folded around the N–As line by 8(2), 3(2) and 11(2)°, respectively. Also the $C{-}(CN)_2$ groups are not coplanar with the $TCNQF_4$ ring planes. $[(MPAO)_2H]^+$, $[(TCNQF_4)_2]^-$ and $(MPAO)_2$ dimers occur in the lattice with intermolecular overlap between $[(MPAO)_2H]^+$ and adjacent $[(TCNQF_4)_2]^-$ dimers; however, these overlaps are not continued to other unit cells.

Introduction. Charge-transfer complexes containing partially oxidized 10-dialkyl-5,10-dihydrophenazines have found recent interest (Endres, Keller, Moroni & Nöthe, 1980; Soos, Keller, Ludolf, Queckbörner, Wehe & Flandrois, 1981; Keller & Soos, 1984). The intermolecular interactions in these solids should be enhanced by using heterocycles like MPA, with the larger heteroatom arsenic, as donors.

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Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic thermal parameters* ($Å^2 \times 10^3$) *for the non-*H *atoms with e.s.d.'s in parentheses*

	x	*y*	*z*	U_{eq}/U_{iso}
As(2)	9651 (1)	4671 (6)	3350 (8)	49 (1)*
C(1)	7707 (9)	5019 (5)	3159 (6)	40 (4)
C(2)	6983 (10)	5358 (60)	3192 (7)	53 (4)
C(3)	7271 (9)	5824 (6)	3589 (7)	62 (5)
C(4)	8226 (9)	5957 (6)	3888 (6)	49 (4)
C(5)	8981 (9)	5623 (5)	3882 (7)	38 (4)
C(6)	8708 (9)	5121 (5)	3476 (6)	28 (4)
C(7)	12526 (11)	4906 (6)	4673 (7)	71 (5)
C(8)	12477 (11)	5421 (6)	4947 (8)	67 (5)
C(9)	11655 (9)	5665 (6)	4765 (7)	56 (5)
C(10)	10769 (9)	5466 (5)	4325 (7)	44 (4)
C(11)	10767 (9)	4958 (5)	4001 (7)	46 (4)
C(12)	11680 (9)	4687 (6)	4207 (7)	62 (5)
N(13)	9935 (7)	5768 (4)	4194 (5)	34 (3)
O(1)	9672 (7)	4656 (4)	2384 (4)	50 (3)
C(67)	9456 (10)	3957 (6)	3551 (7)	83 (5)
As(3)	2604 (1)	5928 (1)	2476 (1)	59 (1)*
C(15)	2460 (10)	5656 (7)	915 (8)	79 (6)
C(16)	2311 (12)	5724 (7)	118 (10)	90 (6)
C(17)	2020 (11)	6219 (7)	−218 (10)	86 (6)
C(18)	1955 (10)	6634 (6)	284 (8)	65 (5)
C(19)	2131 (10)	6558 (6)	1100 (8)	58 (5)
C(20)	2375 (9)	6050 (6)	1424 (7)	59 (5)
C(21)	2660 (10)	6660 (6)	3686 (8)	72 (5)
C(22)	2524 (11)	7155 (6)	3951 (9)	82 (6)
C(23)	2230 (10)	7572 (7)	3439 (8)	90 (6)
C(24)	2077 (9)	7530 (6)	2645 (7)	70 (5)
C(25)	2202 (10)	7025 (6)	2332 (8)	67 (5)
C(26)	2468 (9)	6602 (5)	2847 (7)	51 (5)
N(27)	2037 (8)	7013 (5)	1524 (7)	62 (4)
O(2)	1735 (6)	5500 (4)	2636 (5)	71 (3)
C(68)	3750 (10)	5580 (6)	2998 (8)	96 (6)
As(1)	−844 (1)	5997 (1)	1388 (1)	53 (1)*
C(29)	−611 (9)	6575 (6)	−754 (7)	54 (5)
C(30)	−654 (9)	6112 (6)	−1200 (8)	60 (5)
C(31)	−742 (9)	5626 (6)	−863 (7)	69 (5)
C(32)	−800 (9)	5595 (6)	−115 (7)	61 (5)
C(33)	−769 (9)	6045 (6)	347 (7)	51 (4)
C(34)	−675 (9)	6544 (5)	50 (8)	46 (4)
C(35)	−460 (9)	7613 (6)	1483 (8)	66 (5)
C(36)	−339 (10)	7728 (6)	2282 (8)	79 (5)
C(37)	−407 (10)	7340 (6)	2761 (8)	67 (5)
C(38)	−509 (10)	6822 (6)	2524 (8)	77 (5)
C(39)	−606 (9)	6699 (5)	1744 (7)	48 (4)
C(40)	−578 (9)	7108 (5)	1210 (7)	43 (4)
N(41)	−649 (7)	7031 (4)	403 (6)	50 (4)
O(3)	−32 (6)	5566 (4)	1933 (5)	68 (3)
C(69)	−2085 (9)	5777 (5)	1462 (8)	73 (5)
C(43)	3044 (9)	3636 (5)	2158 (7)	43 (4)
C(44)	2858 (9)	3413 (5)	2820 (6)	34 (4)
C(45)	2746 (9)	2882 (6)	2927 (7)	42 (4)
C(46)	2828 (9)	2565 (6)	2293 (7)	43 (4)
C(47)	3012 (9)	2759 (5)	1654 (7)	45 (4)
C(48)	3128 (8)	3318 (5)	1524 (7)	28 (4)
C(49)	3320 (9)	3522 (5)	837 (7)	47 (4)
C(50)	3360 (11)	3194 (6)	173 (9)	61 (5)
C(51)	3403 (9)	4062 (6)	695 (7)	57 (4)
C(52)	2576 (9)	2673 (5)	3621 (6)	34 (4)
C(53)	2536 (9)	2138 (5)	3787 (7)	49 (4)
C(54)	2295 (10)	3004 (6)	4178 (8)	66 (5)
N(1)	3365 (9)	2980 (5)	−396 (7)	80 (4)
N(2)	3474 (9)	4505 (6)	568 (7)	84 (5)
N(3)	2538 (8)	1701 (5)	3949 (6)	64 (4)
N(4)	2074 (9)	3255 (5)	4664 (7)	90 (5)
F(1)	3176 (6)	4156 (3)	2127 (4)	70 (4)*
F(2)	2822 (6)	3777 (3)	3383 (4)	75 (5)*
F(3)	3091 (6)	2427 (3)	1087 (4)	67 (4)*
F(4)	2747 (6)	2038 (3)	2341 (4)	69 (6)*
C(55)	5361 (10)	3764 (6)	3116 (8)	39 (4)
C(56)	5191 (9)	3604 (5)	3770 (7)	42 (4)
C(57)	5011 (9)	3076 (6)	3958 (8)	40 (4)
C(58)	5098 (9)	2719 (5)	3360 (7)	36 (4)
C(59)	5264 (9)	2881 (5)	2677 (7)	33 (4)
C(60)	5411 (9)	3406 (5)	2514 (7)	39 (4)
C(61)	5627 (9)	3571 (5)	1795 (7)	42 (4)
C(62)	5690 (9)	3220 (5)	1181 (7)	50 (5)
C(63)	5887 (10)	4100 (6)	1665 (7)	71 (5)
C(64)	4857 (10)	2883 (5)	4657 (7)	56 (5)
C(65)	4822 (9)	2345 (5)	4879 (7)	39 (4)
C(66)	4713 (10)	3232 (6)	5236 (8)	61 (5)
N(6)	5777 (8)	2956 (5)	678 (6)	69 (4)

Table 1 (*cont.*)

	x	*y*	*z*	U_{eq}/U_{iso}
N(7)	4571 (8)	3490 (5)	5731 (6)	77 (4)
N(5)	6116 (9)	4491 (5)	1478 (7)	89 (5)
N(8)	4818 (8)	1911 (5)	5097 (6)	59 (4)
F(5)	5505 (6)	4278 (3)	3027 (4)	69 (4)*
F(6)	5162 (6)	3961 (3)	4336 (4)	72 (4)*
F(7)	5284 (6)	2505 (3)	2128 (4)	59 (4)*
F(8)	4897 (6)	2197 (3)	3414 (4)	60 (4)*
C(70)	4963 (13)	5669 (7)	568 (8)	93 (6)
C(71)	5175 (14)	5920 (9)	1350 (11)	116 (8)
N(9)	5187 (12)	6045 (7)	1896 (10)	118 (7)

* $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}\, a_i^*\, a_j^*\, \mathbf{a}_i.\mathbf{a}_j$.

Experimental. Mixing 1 mmol MPA (preparation: Aeschlimann, 1927) in 15 ml acetonitrile (AN) with 1 mmol $TCNQF_4$ (preparation: Wheland & Martin, 1975) in 65 ml AN (both saturated with dry nitrogen) at room temperature results after slow cooling of the mixture in a refrigerator in an almost quantitative yield of violet platelets of the title complex.

Needle-like crystal, 0·08 × 0·1 × 0·3 mm. D_m measured by flotation. Syntex *R*3 diffractometer (Mo $K\alpha$, θ–2θ scan). Lattice parameters determined by an orientation matrix derived from setting angles of 25 independent reflections. An empirical absorption correction (ψ scan made on five reflections with intensity 0·732–1·000) applied to data. $2\theta_{max} = 39{\cdot}5°$, range of *hkl*: 0,0,−18 to 14,25,18. Intensities of two standard reflections measured after every 100 reflections constant. 3357 unique observed reflections with $I > 0$ included in calculations. Structure solved by direct methods. H atoms in calculated positions and refined with fixed temperature factors. A last six-cycle refinement on *F* (420 parameters) with $(\Delta/\sigma)_{max} = 0{\cdot}864$ for *U* of O(2) yielded $R = 0{\cdot}100$, $R_w = 0{\cdot}058$; $w = 1/\sigma^2(F)$. $\Delta\rho = -0{\cdot}4$–$0{\cdot}5$ e $Å^{-3}$. Atom scattering factors from *International Tables for X-ray Crystallography* (1974). All calculations performed on a NOVA 3 computer with *SHELXTL* (Sheldrick, 1979), plots drawn with *ORTEP* (Johnson, 1965).

Discussion. $[(MPAO)_2H]^+[(TCNQF_4)_2]^-(MPAO)$-(AN) is the first example of a *complex* charge-transfer salt containing $TCNQF_4$ as an acceptor. A projection of nine molecules perpendicular to the *bc* plane is shown in Fig. 1. Atomic coordinates and isotropic temperature factors are listed in Table 1.* Bond distances are given in Table 2 according to the numbering scheme on Figs. 2, 3, and 4.

Molecules *A*, *B*, *C*, *D*, *E* and the AN represent one asymmetric unit. The donors *A*, *B* and *E* are bent

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* Lists of structure factors, anisotropic thermal parameters and bond angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38941 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

around the N–As line by 8 (2), 3 (2) and 11 (2)° respectively. The planes of the overlapping donor molecules *A* and *B* form an angle of 20 (2)° (Fig. 2*a*, *b*). Both molecules are connected over a strong ···O–H–O··· hydrogen bridge [distance O(3)–O(2): 2·39 Å] resulting in an $[\mathrm{MPAO{-}H{-}MPAO}]^+$ cation. *C* and *D* as well as *E* and *E'* form other dimers with the overlaps shown in Figs. 3 and 4. *E* and *E'* are correlated through a center of symmetry. The planes of both parts of the acceptor dimers are nearly parallel (1·3°) (planes through all atoms of the quinoid system). The interplanar distance is 3·18 (3) Å. Because of the twofold axis molecules *A'B'* make an overlap with molecules *CD*. Donor and acceptor molecular planes form an angle of 26·2 (1)°. Fig. 5 shows a projection of adjacent donor and acceptor. This overlap does not continue in any direction. Thus no stack can be found.

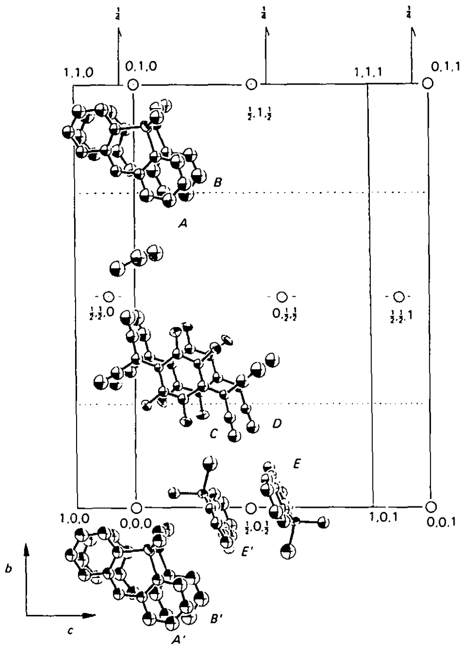

Fig. 1. Projection of nine molecules perpendicular to the *bc* plane. *E* and *E'* lie on a center of symmetry at ½,0,½.

Table 2. *Bond distances* (Å) *with e.s.d.'s in parentheses*

As(2)–O(1)	1·71 (1)	As(2)–C(11)	1·83 (1)
As(2)–C(6)	1·84 (1)	As(2)–C(67)	1·89 (1)
C(1)–C(2)	1·37 (2)	C(1)–C(6)	1·40 (2)
C(2)–C(3)	1·36 (2)	C(3)–C(4)	1·35 (2)
C(4)–C(5)	1·38 (2)	C(5)–N(13)	1·37 (2)
C(5)–C(6)	1·46 (2)	C(7)–C(12)	1·36 (2)
C(7)–C(12)	1·36 (2)	C(7)–C(8)	1·41 (2)
C(8)–C(9)	1·28 (2)	C(9)–C(10)	1·38 (2)
C(10)–C(11)	1·41 (2)	C(11)–C(12)	1·42 (2)
N(13)–C(10)	1·38 (2)		
As(3)–O(2)	1·73 (1)	As(3)–C(20)	1·86 (1)
As(3)–C(26)	1·86 (1)	As(3)–C(68)	1·87 (1)
C(15)–C(16)	1·38 (2)	C(16)–C(17)	1·41 (2)
C(17)–C(18)	1·39 (2)	C(18)–C(19)	1·40 (2)
C(19)–N(27)	1·40 (2)	C(19)–C(20)	1·42 (2)
C(20)–C(15)	1·36 (2)	C(21)–C(22)	1·37 (2)
C(21)–C(26)	1·44 (2)	C(22)–C(23)	1·38 (2)
C(23)–C(24)	1·37 (2)	C(24)–C(25)	1·43 (2)
C(25)–N(27)	1·38 (2)	C(25)–C(26)	1·38 (2)
As(1)–O(3)	1·68 (1)	As(1)–C(33)	1·87 (1)
As(1)–C(39)	1·88 (1)	As(1)–C(69)	1·90 (1)
C(29)–C(30)	1·40 (2)	C(29)–C(34)	1·44 (2)
C(30)–C(31)	1·39 (2)	C(31)–C(32)	1·35 (2)
C(32)–C(33)	1·40 (2)	C(33)–C(34)	1·39 (2)
C(34)–N(41)	1·38 (2)	C(35)–C(40)	1·36 (2)
C(35)–C(36)	1·40 (2)	C(36)–C(37)	1·32 (2)
C(37)–C(38)	1·36 (2)	C(38)–C(39)	1·39 (2)
C(39)–C(40)	1·40 (2)	C(40)–N(41)	1·41 (2)
N(41)–C(34)	1·38 (2)		
C(43)–F(1)	1·33 (2)	C(43)–C(44)	1·39 (2)
C(43)–C(48)	1·41 (2)	C(44)–C(45)	1·36 (2)
C(44)–F(2)	1·37 (2)	C(45)–C(46)	1·41 (2)
C(45)–C(52)	1·43 (2)	C(46)–C(47)	1·31 (2)
C(46)–F(4)	1·36 (2)	C(47)–F(3)	1·33 (2)
C(47)–C(48)	1·45 (2)	C(48)–C(49)	1·41 (2)
C(49)–C(50)	1·44 (2)	C(49)–C(51)	1·40 (2)
C(50)–N(1)	1·14 (2)	C(51)–N(2)	1·16 (2)
C(52)–C(53)	1·40 (2)	C(52)–C(54)	1·43 (2)
C(53)–N(3)	1·13 (2)	C(54)–N(4)	1·19 (2)
C(55)–C(56)	1·31 (2)	C(55)–F(5)	1·33 (2)
C(55)–C(60)	1·41 (2)	C(56)–F(6)	1·36 (2)
C(56)–C(57)	1·42 (2)	C(57)–C(58)	1·40 (2)
C(57)–C(64)	1·41 (2)	C(58)–C(59)	1·35 (2)
C(58)–F(8)	1·39 (1)	C(59)–F(7)	1·36 (1)
C(59)–C(60)	1·38 (2)	C(60)–C(61)	1·46 (2)
C(61)–C(62)	1·42 (2)	C(61)–C(63)	1·43 (2)
C(62)–N(6)	1·14 (2)	C(63)–N(5)	1·12 (2)
C(64)–C(66)	1·41 (2)	C(64)–C(65)	1·43 (2)
C(65)–N(8)	1·17 (2)		

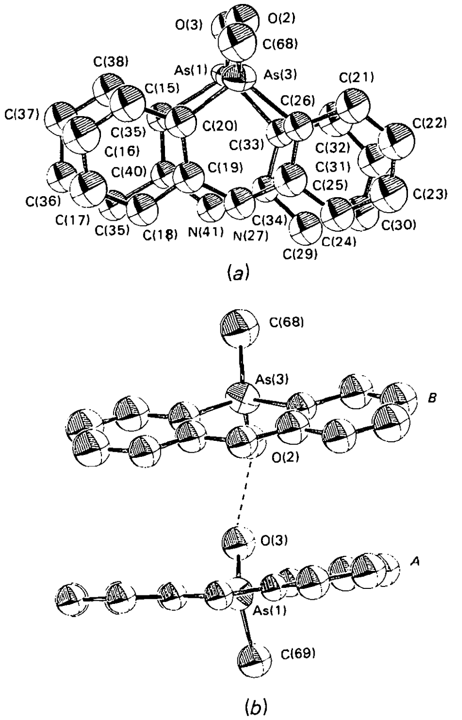

Fig. 2. (*a*) Projection of an $[(\mathrm{MPAO})_2\mathrm{H}]^+$ dimer (*AB*) perpendicular to the ring plane through atoms C(29) to C(34). (*b*) Projection of an $[(\mathrm{MPAO})_2\mathrm{H}]^+$ moiety (*AB*) parallel to the ring plane through atoms C(29) to C(34).

A comparison of the relevant distances (exocyclic 'double' bonds, for example) in neutral $TCNQF_4$ [1·372 (2) Å: Emge, Maxfield, Cowan & Kistenmacher, 1981], in the fully ionic $HMTTF^+.TCNQF_4^-$* [1·412 (6) Å: Torrance, Mayerle, Bechgaard, Silverman & Tomkiewicz, 1980], $HMTSF–TCNQF_4$ [1·405 (5) Å: Emge, Cowan & Kistenmacher, unpublished results] and $DBTTF–TCNQF_4$ (average 1·41 Å: Emge, Bryden, Wiygul, Cowan & Kistenmacher, 1982) strongly suggests an appreciable amount of negative charge on each $TCNQF_4$ unit. Though elucidating ionicity from atomic distances in the *solid* has to be handled with care, the case of $[(MPAO)_2H]^+$-$[(TCNQF_4)_2]^-$(MPAO) (AN) seems to be clear cut: the exocyclic 'double' bonds are stretched relative to the neutral $TCNQF_4$ belonging to the *longest* observed so far for $TCNQF_4$ moieties. Even with taking all precautions in using these bond distance–ionicity relations one has to conclude that the solid contains ionic $TCNQF_4$. The lattice could be described as ionic consisting of dimeric $[(C_{13}H_{12}AsNO)H]^+$ cations and dimeric $[(C_{12}N_4F_4)_2]^-$ anions. The spaces between the huge ions are filled with neutral $(C_{13}H_{12}AsNO)_2$ dimers and one molecule of AN.

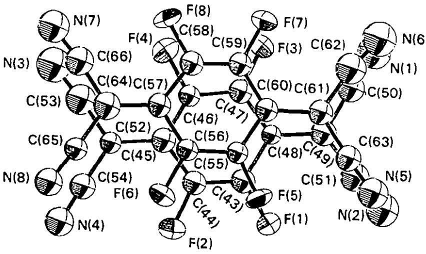

Fig. 3. Projection of a $TCNQF_4$ dimer (*CD*) perpendicular to the benzene ring plane of *C*.

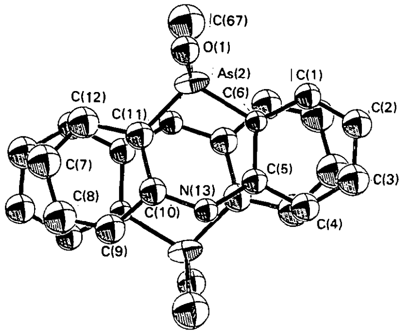

Fig. 4. Projection of an MPAO dimer (*EE'*) perpendicular to the ring plane through atoms C(21) to C(26).

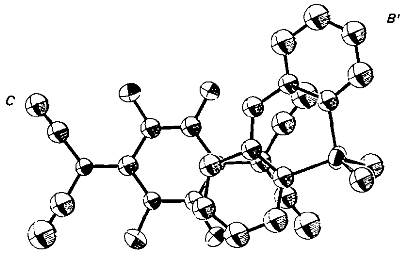

Fig. 5. Projection of adjacent donor and acceptor molecules (*B'*, *C*) perpendicular to the acceptor benzene ring plane.

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* Abbreviations used: HMTTF = hexamethylenetetrathiafulvalene, HMTSF = hexamethylenetetraselenafulvalene, and DBTTF = dibenzotetrathiafulvalene.