Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
C(1)	0.4238 (2)	0.6198 (2)	0.5529 (1)	2.07 (3)
C(2)	0.3881 (2)	0.5536 (2)	0.4125 (1)	2.16 (3)
C(3)	0.7682 (2)	0.5342 (2)	0.6152 (1)	2.12 (3)
C(4)	0.9244 (2)	0.5696 (2)	0.5436 (1)	2.16 (3)
C(5)	0.6550 (2)	0.7705 (2)	0.7278 (1)	2.11 (3)
C(6)	0.8578 (2)	0.8351 (2)	0.7839 (1)	2.19 (3)
C(7)	0.7899 (2)	1.1065 (2)	0.6719 (1)	2.42 (3)
C(8)	0.6319 (2)	1.0863 (2)	0.5416 (1)	2.01 (3)
C(9)	1.1259 (2)	1.0139 (2)	0.7811 (1)	2.30 (3)
C(10)	1.2228 (2)	1.1247 (2)	0.7048 (1)	2.56 (4)
N(1)	0.6303	0.6739 (1)	0.6021	1.69 (2)
N(2)	0.9241 (2)	0.9645 (1)	0.7037 (1)	1.74 (2)
O(1)	0.2195 (2)	0.4875 (1)	0.3639 (1)	2.94 (3)
O(2)	0.5092 (2)	0.5691 (1)	0.3505 (1)	2.75 (3)
O(3)	0.9990 (2)	0.4442 (1)	0.5079 (1)	2.99 (3)
O(4)	0.9671 (2)	0.7109 (1)	0.5267 (1)	2.87 (3)
O(5)	0.5150 (2)	1.2012 (1)	0.5138 (1)	2.76 (3)
O(6)	0.6342 (2)	0.9622 (1)	0.4743 (1)	2.66 (2)
O(7)	1.2129 (2)	1.0526 (2)	0.5808 (1)	3.77 (3)

Table 2. *Geometric parameters* (Å, °)

C(2)—O(1)	1.288 (2)	C(8)—O(5)	1.239 (2)
C(2)—O(2)	1.205 (2)	C(8)—O(6)	1.239 (2)
C(4)—O(3)	1.257 (2)	C(10)—O(7)	1.399 (2)
C(4)—O(4)	1.224 (2)		
C(1)—C(2)—O(1)	115.6 (1)	O(3)—C(4)—O(4)	126.7 (1)
C(1)—C(2)—O(2)	120.8 (2)	C(7)—C(8)—O(5)	114.6 (1)
O(1)—C(2)—O(2)	123.5 (1)	C(7)—C(8)—O(6)	118.3 (1)
C(3)—C(4)—O(3)	113.8 (1)	O(5)—C(8)—O(6)	127.1 (1)
C(3)—C(4)—O(4)	119.5 (1)		
N(1)—C(5)—C(6)—N(2)	68.1 (2)	O(6)—C(8)—C(7)—N(2)	−2.7 (2)
O(2)—C(2)—C(1)—N(1)	−9.6 (2)	N(2)—C(9)—C(10)—O(7)	−52.1 (2)
O(4)—C(4)—C(3)—N(1)	25.1 (2)		

Table 3. *Hydrogen-bond geometry* (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N(1)—H···O(6)	0.90 (2)	1.94 (3)	2.717 (1)	144 (1)
N(2)—H···O(4)	0.85 (2)	2.08 (3)	2.843 (2)	152 (2)
O(1)—H···O(3^{i})	1.21 (2)	1.25 (2)	2.449 (1)	169 (2)
O(7)—H···O(5^{ii})	0.90 (2)	1.84 (3)	2.705 (2)	159 (2)

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

Both positional and thermal parameters were refined for the polar H atoms but for the non-polar H atoms (bonded to C atoms), only the positional parameters were refined; isotropic B values were fixed at 0.5 Å^2 higher than the values of B_{eq} of the associated C atoms. The structure was solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). All remaining calculations were performed using *NRC Crystallographic Programs for the IBM*360 *System* (1973). The refinement used a block-diagonal approximation. The weighting scheme (one of those available in the *NRC* program system) was chosen in order to make $w(\Delta F)^2$ approximately independent of $|F_o|$ and $\sin\theta/\lambda$. The origin was fixed by the x and z coordinates of the atom N(1).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete bond distances have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55922 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: KA1016]

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Structure of the Bis(7,7,8,8-tetracyano-*p*-quinodimethane)–4-(Benzylmethylaminomethyl)-2,2′,5,5′-tetrathiafulvalene Charge-Transfer Complex

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Abstract

The tetrathiafulvalenium (TTF) derivative [4-(benzylmethylaminomethyl)-2-(1,3-dithiol-2-ylidene)-1,3-dithiole cation] sublattice is built from one independent molecule which forms dimerized chains along the [100] direction. Short intra-dimer S···S contacts [3.532 (2) and 3.409 (2) Å] are observed. The anionic tetracyano-*p*-quinodimethane [TCNQ: 2,2′-(2,5-cyclohexadiene-1,4-diylidene)bispropanedinitrile] sublattice is formed by three different molecules (*A*, *B* and *C*) which stack along the [001] direction perpendicular to the TTF chains.

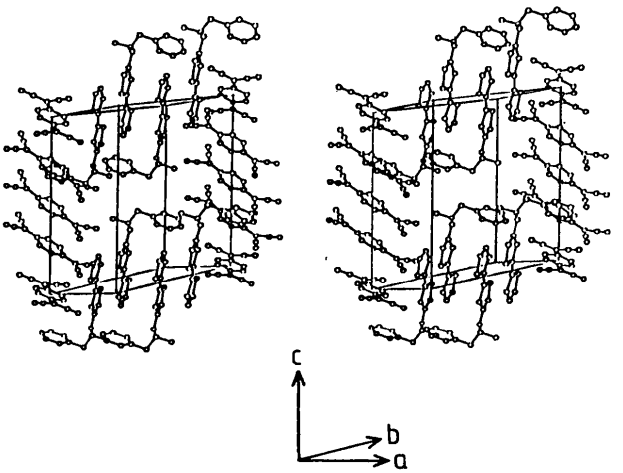

Fig. 1. Stereoscopic view of the crystal structure.

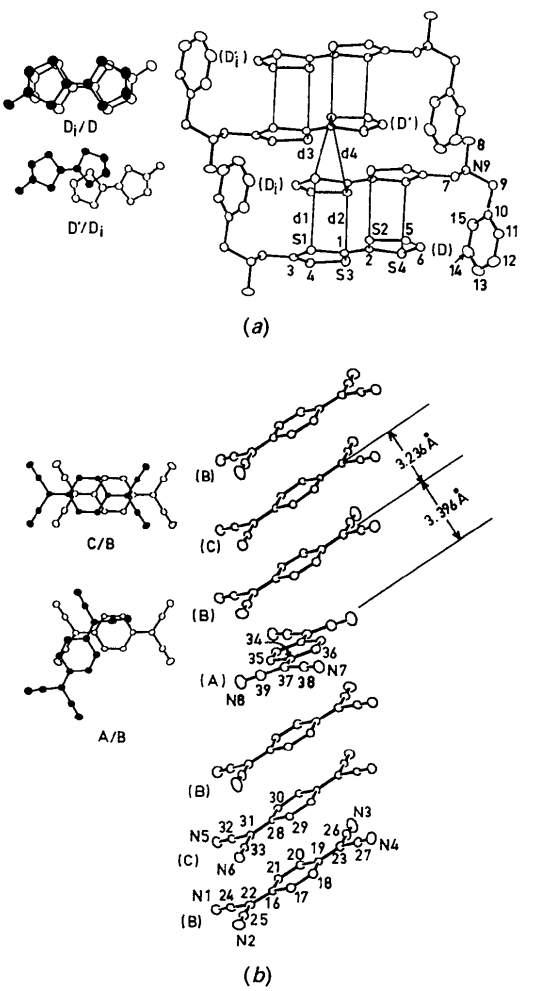

Fig. 2. View of (*a*) the cationic and (*b*) the anionic chains showing atomic numbering and the different overlaps. The shortest intermolecular contacts are also shown: *d*1(S1···S4) = 3.532 (2), *d*2(S2···S3) = 3.409 (2), *d*3(S2···S4) = 3.930 (1), *d*4(S2···S2) = 3.680 (1) Å.

Comment

The crystal structure represented in the stereoscopic view (Fig. 1) is built from three TCNQ molecules (*A*, *B* and *C*) and one molecule of the aminomethyl-TTF derivative (Fabre, Garin & Uriel, 1991, 1992) (Fig. 2). The TTF derivative stacks along the *a* axis and forms dimerized chains, with short intra-dimer S···S contacts [*d*1 = 3.532 (2) and *d*2 = 3.409 (2) Å]. The inter-dimer distances are larger than 3.65 Å (Fig. 2*a*). The anionic sublattice is built from three TCNQ molecules which form chains along the *c* axis. The TCNQ stacks are not regular. They can be described as formed by centrosymmetric trimers (*B*/*C*/*B*) separated by isolated molecules (*A*) (Fig. 2*b*). The intra-trimer overlaps are of the bond-over-ring type (*C*/*B*), whereas the overlap between a trimer and an isolated TCNQ is crisscrossed and shifted (*A*/*B*).

The inter-planar contacts between the *B* and the *C* molecules are 3.236 Å. They are shorter than those observed between the *A* and *B* molecules (3.396 Å) (Fig. 2*b*). Short N···S anion–cation interactions are observed [N2···S2 = 3.079 (3), N1···S3 = 3.228 (4) Å.

Experimental

Crystal data

$C_{15}H_{15}NS_4.2(C_{12}H_4N_4)$
M_r = 745.93
Triclinic
$P\bar{1}$
a = 7.681 (1) Å
b = 14.758 (2) Å
c = 16.377 (4) Å
α = 79.46 (2)°
β = 87.60 (5)°
γ = 79.92 (4)°
V = 1796.8 Å^3
Z = 2
D_x = 1.379 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 7.5–12°
μ = 0.294 mm^{-1}
T = 293 K
Needle
0.5 × 0.2 × 0.1 mm
Black
Crystal source: redox chemical reaction (slow evaporation)

Data collection

Enraf–Nonius CAD-4 diffractometer
θ–2θ scans
Absorption correction: empirical (*DIFABS*; Walker & Stuart, 1983)
T_{min} = 0.713, T_{max} = 1.329
6705 measured reflections
5665 independent reflections
3505 observed reflections [$I \geq 3\sigma$]
R_{int} = 0.018
θ_{max} = 25°
h = 0 → 9
k = −17 → 17
l = −19 → 19
3 standard reflections
frequency: 60 min
intensity variation: <1%

Refinement

Refinement on F
Final R = 0.039
wR = 0.049
S = 1.106
3505 reflections
562 parameters
$\Delta\rho_{max}$ = 0.238 e Å^{-3}
$\Delta\rho_{min}$ = −0.087 e Å^{-3}
Extinction correction: $|F_c|(1+gI_c)^{-1}$
Extinction coefficient: $g = 1.445 \times 10^{-7}$

All H-atom parameters refined
$w = 4F_o^2/[\sigma(I)^2 + (0.07F_o^2)^2]$
$(\Delta/\sigma)_{max} = 0.16$

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = \frac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
S1	0.3565 (1)	0.46133 (5)	0.16443 (5)	3.12 (12)
S2	0.1709 (1)	0.57483 (5)	−0.01252 (5)	3.06 (2)
S3	0.4935 (1)	0.30592 (5)	0.08041 (5)	3.62 (2)
S4	0.3056 (1)	0.41080 (6)	−0.08671 (5)	3.82 (2)
C1	0.3720 (4)	0.4157 (2)	0.0743 (2)	2.83 (7)
C2	0.2900 (4)	0.4630 (2)	−0.0006 (2)	2.79 (7)
C3	0.4878 (4)	0.3647 (2)	0.2219 (2)	3.03 (7)
C4	0.5461 (4)	0.2927 (2)	0.1831 (2)	3.55 (7)
C5	0.1171 (5)	0.5780 (2)	−0.1145 (2)	3.77 (8)
C6	0.1766 (5)	0.5034 (2)	−0.1478 (2)	3.90 (8)
C7	0.5303 (4)	0.3721 (2)	0.3086 (2)	3.53 (7)
C8	0.2467 (5)	0.3840 (3)	0.3794 (3)	5.8 (1)
C9	0.4582 (5)	0.4795 (2)	0.4043 (2)	3.96 (8)
C10	0.5690 (5)	0.5494 (2)	0.3631 (2)	3.49 (7)
C11	0.4895 (6)	0.6288 (3)	0.3103 (2)	5.2 (1)
C12	0.5868 (7)	0.6936 (3)	0.2713 (3)	6.7 (1)
C13	0.7662 (6)	0.6803 (3)	0.2836 (3)	6.5 (1)
C14	0.8481 (6)	0.6031 (3)	0.3358 (3)	6.4 (1)
C15	0.7488 (5)	0.5367 (3)	0.3760 (2)	4.63 (9)
N9	0.3889 (3)	0.4341 (2)	0.3431 (2)	3.51 (6)
N1	0.5600 (4)	0.0819 (2)	0.1409 (2)	4.81 (8)
N2	0.0261 (5)	0.2251 (2)	0.0732 (2)	5.59 (8)
N3	0.1284 (5)	−0.3115 (3)	0.4925 (3)	7.0 (1)
N4	−0.4022 (4)	−0.1542 (3)	0.4303 (2)	6.14 (9)
C16	0.1530 (4)	0.0202 (2)	0.2205 (2)	2.96 (7)
C17	−0.0342 (4)	0.0258 (2)	0.2319 (2)	3.56 (7)
C18	−0.1040 (4)	−0.0359 (2)	0.2893 (2)	3.56 (7)
C19	0.0066 (4)	−0.1109 (2)	0.3409 (2)	3.29 (7)
C20	0.1943 (4)	−0.1180 (2)	0.3277 (2)	3.24 (7)
C21	0.2634 (4)	−0.0551 (2)	0.2709 (2)	3.28 (7)
C22	0.2240 (4)	0.0873 (2)	0.1622 (2)	3.27 (7)
C23	−0.0668 (4)	−0.1728 (2)	0.4027 (2)	3.60 (8)
C24	0.4103 (5)	0.0838 (2)	0.1504 (2)	3.56 (8)
C25	0.1155 (5)	0.1638 (2)	0.1130 (2)	3.73 (8)
C26	0.0414 (5)	−0.2493 (2)	0.4526 (2)	4.44 (9)
C27	−0.2525 (5)	−0.1638 (2)	0.4181 (2)	4.15 (8)
N5	0.4821 (4)	0.1172 (2)	0.3507 (2)	4.91 (8)
N6	−0.0456 (4)	0.2603 (2)	0.2828 (2)	4.82 (8)
C28	0.0750 (4)	0.0630 (2)	0.4382 (2)	2.53 (6)
C29	0.1147 (4)	−0.0725 (2)	0.5488 (2)	2.82 (6)
C30	0.1847 (4)	−0.0129 (2)	0.4899 (2)	2.75 (6)
C31	0.1471 (4)	0.1241 (2)	0.3771 (2)	2.86 (7)
C32	0.3337 (4)	0.1188 (2)	0.3634 (2)	3.24 (7)
C33	0.0384 (4)	0.1994 (2)	0.3254 (2)	3.18 (7)
N7	0.5718 (4)	−0.1600 (3)	0.0737 (2)	6.24 (9)
N8	0.1362 (5)	−0.3030 (3)	0.1574 (3)	7.3 (1)
C34	0.1183 (5)	−0.0778 (2)	0.0402 (2)	3.60 (7)
C35	0.0704 (5)	0.0759 (2)	−0.0467 (2)	3.83 (8)
C36	0.1824 (4)	0.0021 (2)	−0.0080 (2)	3.91 (8)
C37	0.2353 (5)	−0.1537 (2)	0.0781 (2)	4.03 (8)
C38	0.4224 (5)	−0.1561 (3)	0.0750 (2)	4.39 (9)
C39	0.1787 (5)	−0.2363 (3)	0.1228 (3)	5.0 (1)

Table 2. *Geometric parameters* (Å, °)

S1—C1	1.723 (3)	C16—C21	1.424 (4)
S1—C3	1.738 (3)	C16—C22	1.410 (4)
S2—C2	1.722 (3)	C17—C18	1.348 (4)
S2—C5	1.728 (3)	C18—C19	1.431 (4)
S3—C1	1.711 (3)	C19—C20	1.437 (4)
S3—C4	1.715 (3)	C19—C23	1.404 (4)
S4—C2	1.718 (3)	C20—C21	1.351 (4)
S4—C6	1.721 (3)	C22—C24	1.429 (5)
C1—C2	1.408 (4)	C22—C25	1.419 (4)
C3—C4	1.339 (5)	C23—C26	1.422 (4)
C3—C7	1.498 (5)	C23—C27	1.426 (5)
C5—C6	1.318 (5)	N5—C32	1.147 (4)
C7—N9	1.458 (4)	N6—C33	1.148 (4)
C8—N9	1.471 (5)	C28—C29	1.450 (4)
C9—C10	1.500 (5)	C28—C30	1.437 (4)
C9—N9	1.466 (5)	C28—C31	1.385 (4)
C10—C11	1.384 (4)	C29—C30	1.343 (4)
C10—C15	1.381 (5)	C31—C32	1.433 (4)
C11—C12	1.367 (6)	C31—C33	1.427 (4)
C12—C13	1.375 (7)	N7—C38	1.138 (5)
C13—C14	1.365 (5)	N8—C39	1.135 (5)
C14—C15	1.400 (6)	C34—C35	1.445 (5)
N1—C24	1.150 (5)	C34—C36	1.443 (5)
N2—C25	1.149 (4)	C34—C37	1.374 (4)
N3—C26	1.149 (5)	C35—C36	1.340 (4)
N4—C27	1.147 (5)	C37—C38	1.430 (5)
C16—C17	1.432 (4)	C37—C39	1.429 (5)
C1—S1—C3	94.7 (1)	C11—C10—C15	118.9 (3)
C2—S2—C5	94.2 (2)	C10—C11—C12	120.7 (4)
C1—S3—C4	95.5 (2)	C11—C12—C13	120.3 (3)
C2—S4—C6	94.7 (1)	C12—C13—C14	120.3 (4)
S1—C1—S3	115.7 (1)	C13—C14—C15	119.6 (4)
S1—C1—C2	123.8 (2)	C10—C15—C14	120.2 (3)
S3—C1—C2	120.5 (2)	C7—N9—C8	111.4 (3)
S2—C2—S4	115.9 (1)	C7—N9—C9	110.9 (2)
S2—C2—C1	123.3 (2)	C8—N9—C9	111.0 (3)
S4—C2—C1	120.8 (3)	C17—C16—C21	117.2 (3)
S1—C3—C4	116.7 (3)	C17—C16—C22	121.0 (3)
S1—C3—C7	116.7 (2)	C21—C16—C22	121.8 (3)
C4—C3—C7	126.6 (2)	C16—C17—C18	121.7 (3)
S3—C4—C3	117.3 (2)	C17—C18—C19	121.2 (2)
S2—C5—C6	117.8 (3)	C18—C19—C20	117.0 (3)
S4—C6—C5	117.4 (3)	C18—C19—C23	120.9 (3)
C3—C7—N9	110.7 (2)	C20—C19—C23	122.1 (3)
C10—C9—N9	111.1 (3)	C19—C20—C21	121.5 (3)
C16—C22—C24	122.1 (2)	C16—C21—C20	121.4 (2)
C16—C22—C25	122.2 (2)	C28—C31—C32	122.9 (3)
C24—C22—C25	115.7 (2)	C28—C31—C33	121.6 (3)
C19—C23—C26	121.4 (3)	C32—C31—C33	115.5 (3)
C19—C23—C27	122.2 (2)	N5—C32—C31	177.9 (3)
C26—C23—C27	116.4 (3)	N6—C33—C31	178.4 (3)
N1—C24—C22	179.4 (4)	C35—C34—C36	118.4 (3)
N2—C25—C22	179.3 (4)	C35—C34—C37	121.3 (3)
N3—C26—C23	179.4 (5)	C36—C34—C37	120.3 (3)
N4—C27—C23	178.3 (4)	C34—C35—C36	120.5 (3)
C29—C28—C30	117.5 (2)	C34—C36—C35	121.1 (3)
C29—C28—C31	121.0 (3)	C34—C37—C38	122.4 (3)
C30—C28—C31	121.4 (3)	C34—C37—C39	122.3 (3)
C28—C29—C30	121.0 (2)	C38—C37—C39	115.2 (3)
C28—C30—C29	121.4 (2)	N7—C38—C37	178.5 (4)
C9—C10—C11	119.2 (3)	N8—C39—C37	178.5 (4)
C9—C10—C15	121.9 (2)		

The structure was solved by direct methods and successive difference Fourier syntheses. All the H atoms were checked by difference Fourier syntheses. Full-matrix least-squares anisotropic (β_{ij}) refinement was performed on F, except for the H atoms which were refined isotropically. All calculations were performed on a MicroVAX 3100 computer using the *SDP* programs (B. A. Frenz & Associates, Inc., 1985).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55935 (26 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA1030]

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Acta Cryst. (1993). C**49**, 1187–1189

Structures of 3,4-Dimethyl-2,2′,5,5′-tetrathiafulvalene Perrhenate, $(DMTTF)ReO_4$, and 3′,4′-Dimethyl-3,4-tetramethylene-2,5-dithia-2′,5′-diselenafulvalene Hexafluorophosphate, $(CHDTDMDSF)PF_6$

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Abstract

The two compounds $(DMTTF)ReO_4$ (1) [DMTTF = 2-(1,3-dithiol-2-ylidene)-4,5-dimethyl-1,3-dithiole cation] and $(CHDTDMDSF)PF_6$ (2) [CHDTDMDSF = 2-(4,5-dimethyl-1,3-diselenol-2-ylidene)-4,5,6,7-tetrahydro-1,3-benzodithiole cation] contain unsymmetrically substituted tetrathiafulvalene (TTF) derivatives. They present similar crystal structures which are characterized by alternating organic dimers and inorganic pairs of anions. The values of the central C—C bond lengths are 1.39 (1) and 1.40 (1) Å for (1) and (2), respectively. Strong intra-dimer contacts are observed: S1···S2 = 3.379 (2) Å for (1) and Se1···S2 = 3.460 (3) and Se2···S1 = 3.435 (3) Å for (2).

Comment

The single crystals of $(DMTTF)ReO_4$ (1) and $(CHDTDMDSF)PF_6$ (2) were obtained by electro-oxidation, on a platinum electrode, of DMTTF or CHTMDTDSF (10^{-3} M) in a tetrahydrofuran solution containing $(Bu_4N)ReO_4$ or $(Bu_4N)PF_6$ (0.1 M) as supporting electrolytes.

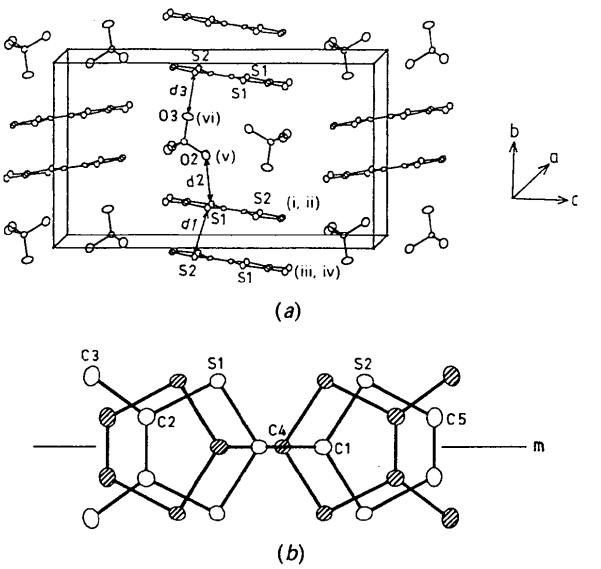

Fig. 1. (*a*) Crystal structure projection of (1) in the (100) plane, showing the alternate packing of the organic dimers and the pairs of inorganic anions, with $d1(S1^{i}\cdots S2^{iii}) = 3.379$ (2), $d2(S1^{i}\cdots O2^{v}) = 3.683$ (9), $d3(S2^{i}\cdots O3^{vi}) = 3.495$ (9), $(S2^{i}\cdots O1^{vii}) = 2.973$ (6) Å [symmetry code: (i) $1+x, y, z$; (ii) $1-x, y, z$; (iii) $1-x, -y, 1-z$; (iv) $1+x, -y, 1-z$; (v) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$; (vi) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$; (vii) $\frac{3}{2}+x, y, \frac{1}{2}-z$]. (*b*) Atomic numbering scheme and intra-dimer overlap.

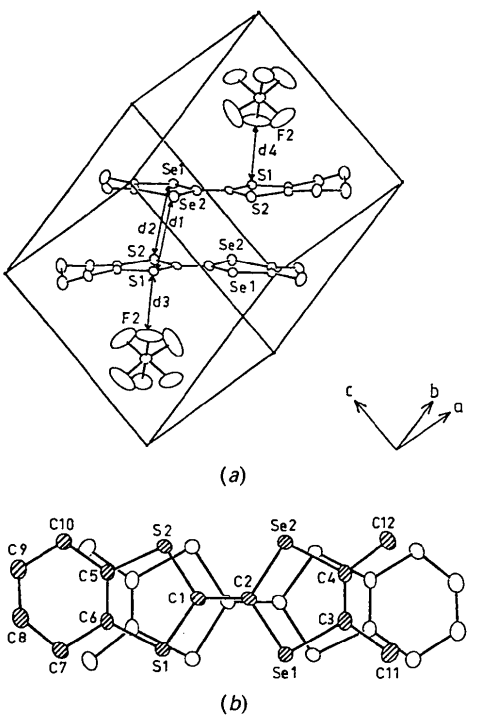

Fig. 2. (*a*) Crystal structure projection of (2) in the (101) plane, showing the alternate packing of the organic dimers and the pairs of inorganic anions, with $d1 = 3.460$ (3), $d2 = 3.435$ (3), $d3 = 3.164$ (8) and $d4 = 3.300$ (11) Å. (*b*) Atomic numbering scheme and intra-dimer overlap.

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