Crystal structure of a new molecular complex of fullerene with tetramethyltetraselenafulvalene: $C_{60} \cdot TMTSF \cdot 2CS_2$

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A new molecular complex of fullerene with tetramethyltetraselenafulvalene (TMTSF), $C_{60} \cdot TMTSF \cdot 2CS_2$, (1) was synthesized. The structure and composition of the complex were established by X-ray diffraction analysis. The crystals of $C_{60} \cdot C_{10}H_{12}Se_4 \cdot 2CS_2$ are monoclinic: $a = 15.407(2)$, $b = 12.934(2)$, $c = 12.026(2)$ Å, $\beta = 108.39(3)°$, $V = 2274.1(6)$ Å^3, space group Cm, $Z = 2$, $d_{calc} = 1.929$ g cm^{-3}, $R = 0.047$. The crystal structure of 1 consists of layers. Layers formed by fullerene and CS_2 molecules alternate with layers of TMTSF molecules. Peculiarities of the crystal structure of 1 are the nonplanar conformation of TMTSF molecules and the absence of shortened C...C contacts between adjacent fullerenes molecules. The energy of intermolecular TMTSF...C_{60} interactions in the crystal was estimated.

Key words: C_{60} fullerene, tetramethyltetraselenafulvalene (TMTSF), synthesis, crystal and molecular structure, X-ray diffraction analysis.

Molecular charge-transfer donor-acceptor complexes based on C_{60} are of great interest as possible starting compounds for doping by alkali metals with the aim of preparing new superconductors based on C_{60}.[1] Complexes of C_{60} with layer structures similar to those of organic conductors and superconductors have attracted particular attention.[2]

It is known that the nature of complexes of C_{60} (charge-transfer complexes or radical-ionic salts) and their stability substantially depend on the type of the donor. Thus, stereochemically flexible molecules that contain heteroatoms and can change conformations to adjust to the spherical shape of C_{60} are favorable for the formation of complexes based on C_{60} with partial charge transfer.[3] We chose tetramethyltetraselenafulvalene (TMTSF) as a donor component. This compound was widely used in 1980s in the synthesis of radical-cationic salts with metallic and superconductor properties.[2] Molecules of TMTSF are planar[4] and form layer structures.[5,6]

As part of our studies, we synthesized new molecular complexes of C_{60}, $C_{60} \cdot TMTSF \cdot 2CS_2$ and $2C_{60} \cdot 2TMTSF \cdot C_6H_6$. In this work, we describe the synthesis and structure of one of them, namely, $C_{60} \cdot TMTSF \cdot 2CS_2$ (1). To our knowledge, 1 is the first complex of C_{60} with the selenium analog of tetrathiafulvalene (TTF) studied by X-ray diffraction analysis. Recently, several charge-transfer complexes of C_{60} with TTF and its principal derivatives have been prepared.[3] However, the data on the complex of C_{60} with tetramethyltetrathiafulvalene (TMTTF) are unavailable.

Experimental

Preparation of crystals of complex 1. Fullerene C_{60} was prepared by evaporation of graphite in an electric arc and was purified according to a procedure reported previously.[7] CS_2 was purified by distillation under argon. A solution of C_{60} (0.02 mol) and TMTSF (Aldrich, 0.02 mol) in CS_2 (30 mL) was stirred under argon at 30 °C for 40 min. The red solution was filtered and slowly evaporated at ~20 °C for 7—10 days. Dark-brown rhombohedron-shaped crystals formed on the bottom of a flask. The crystals had dimensions of up to 2×2×0.3 mm. The crystals were filtered off, washed with anhydrous EtOH, and dried *in vacuo*.

The composition of complex 1 was established by X-ray diffraction analysis. The data of elemental analysis are consistent with the results of X-ray diffraction analysis. Found (%): C, 65.52; H, 1.0. $C_{72}H_{12}S_4Se_4$. Calculated (%): C, 65.47; H, 0.9. According to the data of electron microprobe X-ray analysis, the S : Se ratio was 1 : 1.

X-ray structural analysis. An approximately rhombic-right-prismatic crystal of 1 was chosen for X-ray diffraction analysis. The crystal had dimensions of 0.25×0.25×0.10 mm. Crystals of 1 are monoclinic, $C_{60} \cdot C_{10}H_{12}Se_4 \cdot 2CS_2$, mol. weight 1320.9, $a = 15.407(2)$, $b = 12.934(2)$, $c = 12.026(2)$ Å, $\beta = 108.39(3)°$, $V = 2274.1(6)$ Å^3, space group Cm, $Z = 2$, $d_{calc} = 1.929$ g cm^{-3}, $F(000) = 1288$. The systematic absences indicated the space group $C2/m$, Cm, or $C2$. We failed to solve the structure in the

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space groups *C2/m* and *C2*. The unit cell parameters and 1732 reflections with $I \geq 2\sigma(I)$ were measured on an automated four-circle KM-4 diffractometer (Cu-Kα radiation, λ = 1.5418 Å, graphite monochromator, ω/2θ scanning technique, 3.87° < θ < 79.88°). The structure was solved by the direct method followed by a series of successive Fourier syntheses using the SHELX-86 [8] and SHELXL-93 programs.[9] Hydrogen atoms were not located. All nonhydrogen atoms of the structure were refined anisotropically by the full-matrix least-squares method to R = 0.047. Absorption was ignored; μ(Cu-Kα) = 77.8 cm^{-1}.

Table 1. Coordinates of nonhydrogen atoms (×10^4) and equivalent isotropic thermal parameters (U_{eq}) in the crystal of **1**

Atom	x	y	z	$U_{eq} \cdot 10^3$/Å^2
		TMTSF		
Se(1)	−7990(1)	1321(1)	−5474(1)	45(1)
Se(2)	−9713(1)	1347(1)	−4609(1)	53(1)
C(1)	−8865(4)	521(3)	−5050(6)	38(1)
C(2)	−8177(4)	2498(4)	−4642(5)	41(1)
C(3)	−8914(5)	2523(4)	−4285(5)	50(2)
C(4)	−7453(5)	3351(5)	−4493(6)	62(2)
C(5)	−9197(5)	3373(6)	−3618(6)	67(2)
		CS_2		
S(1)	−7255(2)	5000	−1155(3)	71(1)
S(2)	−5580(2)	5000	−2014(3)	81(1)
S(3)	−1511(2)	0	2771(3)	75(1)
S(4)	106(2)	0	1802(2)	57(1)
C(6)	−704(5)	0	2327(8)	46(2)
C(7)	−6431(5)	5000	−1559(8)	48(2)
		C_{60}		
C(8)	−4863(4)	2020(4)	2330(5)	46(2)
C(9)	−4427(3)	2023(4)	1444(6)	49(2)
C(10)	−3832(4)	1100(5)	1617(6)	50(2)
C(11)	−3921(3)	539(5)	2602(5)	48(2)
C(12)	−4562(4)	1108(5)	3063(6)	50(2)
C(13)	−3745(3)	560(4)	660(5)	44(1)
C(14)	−4247(3)	908(5)	−517(6)	51(2)
C(15)	−4572(5)	0	−1271(7)	43(2)
C(16)	−5436(5)	0	−2135(7)	40(2)
C(17)	−5998(3)	914(4)	−2290(5)	40(1)
C(18)	−5685(4)	1770(4)	−1590(5)	45(1)
C(19)	−4793(4)	1763(4)	−682(6)	46(1)
C(20)	−4883(4)	2339(4)	311(5)	45(1)
C(21)	−6930(4)	566(4)	−2556(5)	45(2)
C(22)	−7542(4)	1111(4)	−2105(5)	46(2)
C(23)	−7215(4)	2012(4)	−1393(5)	45(2)
C(24)	−6329(4)	2344(4)	−1131(6)	47(2)
C(25)	−5814(4)	2682(3)	54(6)	44(1)
C(26)	−6249(4)	2672(3)	892(5)	42(2)
C(27)	−7191(4)	2330(4)	613(6)	49(2)
C(28)	−7664(4)	1998(4)	−502(6)	48(2)
C(29)	−8167(3)	532(4)	−1670(5)	44(1)
C(30)	−8239(3)	1098(4)	−642(6)	44(1)
C(31)	−8321(3)	563(4)	310(5)	41(1)
C(32)	−7832(3)	893(4)	1474(5)	42(1)
C(33)	−7271(3)	1776(4)	1632(5)	44(1)
C(34)	−5775(4)	2345(3)	2060(5)	45(2)
C(35)	−5134(4)	575(5)	3490(5)	47(2)
C(36)	−6078(4)	927(5)	3243(5)	47(1)
C(37)	−6403(4)	1770(4)	2516(5)	44(1)
C(38)	−6650(6)	0	3070(7)	48(2)
C(39)	−7496(5)	0	2219(7)	40(2)

Atomic coordinates in the structure of **1** are given in Table 1. The bond lengths and bond angles are given in Tables 2 and 3, respectively.

Results and Discussion

In the crystals of **1** (Fig. 1), molecules of C_{60}, TMTSF, and CS_2 are packed in layers of two types: homomolecular layers consisting of TMTSF molecules and heteromolecular layers formed by C_{60} and CS_2 molecules. Both types of layers are parallel to the *ab* plane and uniformly alternate along the *c* axis. In the heteromolecular layer, each C_{60} molecule is surrounded by four fullerene molecules, which form a quasi-square, and eight CS_2 molecules, which form a quasi-square prism inscribed in the "fullerene square". The distances between the center of the C_{60} molecule and the centers of the four adjacent fullerene molecules are equal (10.06(7) Å), which is typical of molecular complexes of C_{60}[10–14] in which these distances are in the range of 10.01–10.12 Å.

It is remarkable that there are no shortened contacts between the C_{60} molecules in the structure of **1** (the

Table 2. Bond lengths (d) in complex **1**

Bond	d/Å	Bond	d/Å
Se(1)—C(1)	1.894(6)	Se(1)—C(2)	1.893(6)
Se(2)—C(1)	1.888(6)	Se(2)—C(3)	1.919(6)
C(1)—C(1a)	1.347(8)	C(2)—C(3)	1.334(9)
C(2)—C(4)	1.539(9)	C(3)—C(5)	1.507(9)
S(1)—C(6)	1.497(9)	S(2)—C(6)	1.572(9)
S(3)—C(7)	1.500(9)	S(4)—C(7)	1.565(9)
C(8)—C(9)	1.428(9)	C(8)—C(12)	1.458(8)
C(8)—C(34)	1.402(9)	C(9)—C(10)	1.480(8)
C(9)—C(20)	1.383(8)	C(10)—C(11)	1.433(9)
C(10)—C(13)	1.388(9)	C(11)—C(11a)	1.395(9)
C(11)—C(12)	1.472(9)	C(12)—C(35)	1.342(9)
C(13)—C(13a)	1.448(9)	C(13)—C(14)	1.454(8)
C(14)—C(15)	1.471(8)	C(14)—C(19)	1.366(8)
C(15)—C(16)	1.407(9)	C(16)—C(17)	1.442(7)
C(17)—C(18)	1.382(8)	C(17)—C(21)	1.441(8)
C(18)—C(19)	1.462(8)	C(18)—C(24)	1.478(9)
C(19)—C(20)	1.451(9)	C(20)—C(25)	1.439(8)
C(21)—C(22)	1.415(9)	C(22)—C(23)	1.440(8)
C(22)—C(29)	1.442(9)	C(23)—C(24)	1.369(9)
C(23)—C(28)	1.447(9)	C(24)—C(25)	1.462(9)
C(25)—C(26)	1.375(9)	C(26)—C(27)	1.452(8)
C(26)—C(34)	1.428(8)	C(27)—C(28)	1.377(9)
C(27)—C(33)	1.459(9)	C(28)—C(30)	1.439(8)
C(29)—C(29a)	1.376(9)	C(29)—C(30)	1.471(9)
C(30)—C(31)	1.377(9)	C(31)—C(31a)	1.456(9)
C(31)—C(32)	1.430(8)	C(32)—C(33)	1.408(8)
C(32)—C(39)	1.454(7)	C(33)—C(37)	1.422(8)
C(34)—C(37)	1.458(9)	C(35)—C(35a)	1.487(9)
C(35)—C(36)	1.463(9)	C(36)—C(37)	1.388(8)
C(36)—C(38)	1.464(8)	C(38)—C(39)	1.380(9)

Note. The symmetry operation for generation of the equivalent atoms (a) x, $-y$, z.

Table 3. Bond angles (ω) in complex **1**

Angle	ω/deg
C(1)—Se(1)—C(2)	93.2(2)
Se(2)—C(1)—C(1a)	124.5(2)
Se(1)—C(1)—Se(2)	112.4(2)
Se(1)—C(2)—C(3)	118.5(4)
C(2)—C(3)—C(5)	127.6(6)
Se(2)—C(3)—C(5)	114.2(5)
S(1)—C(6)—S(2)	178.7(7)
C(9)—C(8)—C(34)	119.9(5)
C(9)—C(8)—C(12)	108.5(5)
C(10)—C(9)—C(20)	118.4(6)
C(11)—C(10)—C(12)	119.4(5)
C(9)—C(10)—C(11)	107.9(6)
C(12)—C(11)—C(11a)	120.0(3)
C(8)—C(12)—C(35)	121.6(6)
C(8)—C(12)—C(11)	107.5(6)
C(10)—C(13)—C(14)	119.4(5)
C(13)—C(14)—C(19)	120.4(6)
C(13)—C(14)—C(15)	109.0(5)
C(16)—C(15)—C(14a)	121.0(4)
C(15)—C(16)—C(17a)	119.0(4)
C(17)—C(16)—C(17a)	110.1(6)
C(16)—C(17)—C(18)	119.9(5)
C(17)—C(18)—C(19)	121.0(5)
C(19)—C(18)—C(24)	108.0(5)
C(14)—C(19)—C(18)	120.3(5)
C(9)—C(20)—C(25)	117.7(6)
C(19)—C(20)—C(25)	109.2(5)
C(22)—C(21)—C(21a)	119.9(3)
C(21)—C(22)—C(23)	118.8(5)
C(23)—C(22)—C(29)	110.7(6)
C(24)—C(23)—C(28)	120.6(5)
C(23)—C(24)—C(25)	120.9(6)
C(18)—C(24)—C(25)	107.0(5)
C(24)—C(25)—C(26)	118.1(5)
C(25)—C(26)—C(34)	120.5(5)
C(27)—C(26)—C(34)	107.5(6)
C(28)—C(27)—C(33)	120.4(5)
C(27)—C(28)—C(30)	118.9(6)
C(23)—C(28)—C(30)	110.1(5)
C(30)—C(29)—C(29a)	119.9(3)
C(28)—C(30)—C(31)	121.6(6)
C(29)—C(30)—C(28)	107.1(5)
C(30)—C(31)—C(31a)	120.2(3)
C(31)—C(32)—C(33)	119.1(5)
C(31)—C(32)—C(39)	109.9(5)
C(27)—C(33)—C(32)	119.7(5)
C(8)—C(34)—C(26)	118.8(6)
C(26)—C(34)—C(37)	109.1(5)
C(12)—C(35)—C(35a)	120.9(4)
C(35)—C(36)—C(37)	120.7(6)
C(35)—C(36)—C(38)	106.8(5)
C(34)—C(37)—C(36)	119.2(5)
C(36)—C(38)—C(39)	119.4(4)
C(36)—C(38)—C(36a)	110.0(7)
C(32)—C(39)—C(38)	121.8(4)
C(1)—Se(2)—C(3)	92.8(3)
Se(1)—C(1)—C(1a)	123.1(2)
C(3)—C(2)—C(4)	127.1(6)
Se(1)—C(2)—C(4)	114.3(5)
Se(2)—C(3)—C(2)	118.2(4)
S(3)—C(7)—S(4)	177.3(6)
C(12)—C(8)—C(34)	119.2(6)
C(8)—C(9)—C(20)	121.6(5)
C(8)—C(9)—C(10)	108.0(5)
C(9)—C(10)—C(13)	120.5(6)
C(10)—C(11)—C(11a)	120.4(4)
C(10)—C(11)—C(12)	108.0(5)
C(11)—C(12)—C(35)	119.1(6)
C(10)—C(13)—C(13a)	120.2(3)
C(13a)—C(13)—C(14)	108.0(3)
C(15)—C(14)—C(19)	118.8(5)
C(14)—C(15)—C(16)	121.0(4)
C(14)—C(15)—C(14a)	105.9(7)
C(15)—C(16)—C(17)	119.0(4)
C(18)—C(17)—C(21)	121.1(5)
C(16)—C(17)—C(21)	106.7(5)
C(17)—C(18)—C(24)	118.9(5)
C(14)—C(19)—C(20)	120.7(5)
C(18)—C(19)—C(20)	107.5(5)
C(9)—C(20)—C(19)	120.6(5)
C(17)—C(21)—C(22)	119.8(5)
C(17)—C(21)—C(21a)	108.2(3)
C(21)—C(22)—C(29)	118.8(5)
C(22)—C(23)—C(24)	121.7(6)
C(22)—C(23)—C(28)	105.7(5)
C(18)—C(24)—C(23)	119.7(5)
C(20)—C(25)—C(26)	121.5(5)
C(20)—C(25)—C(24)	108.4(5)
C(25)—C(26)—C(27)	121.1(5)
C(26)—C(27)—C(28)	120.3(6)
C(26)—C(27)—C(33)	107.1(5)
C(23)—C(28)—C(27)	119.1(5)
C(22)—C(29)—C(29a)	121.3(3)
C(22)—C(29)—C(30)	106.4(5)
C(29)—C(30)—C(31)	119.9(5)
C(32)—C(31)—C(30)	120.3(5)
C(32)—C(31)—C(31a)	107.4(3)
C(33)—C(32)—C(39)	118.5(5)
C(32)—C(33)—C(37)	119.3(5)
C(27)—C(33)—C(37)	108.7(5)
C(8)—C(34)—C(37)	119.7(5)
C(12)—C(35)—C(36)	119.6(6)
C(36)—C(35)—C(35a)	108.1(3)
C(37)—C(36)—C(38)	118.2(5)
C(33)—C(37)—C(36)	122.8(5)
C(33)—C(37)—C(34)	107.2(5)
C(39)—C(38)—C(36a)	119.4(4)
C(38)—C(39)—C(32a)	121.8(4)
C(32)—C(39)—C(32a)	105.3(7)

Note. The symmetry operation for generation of the equivalent atoms (a) *x*, −*y*, *z*.

of the van der Waals radii of carbon atoms is 3.40 Å).[15] This situation is unlike that of fullerene complexes studied previously,[10–14] which have at least one shortened contact. Note that there are no shortened intermolecular contacts in the homomolecular or in the heteromolecular layers. Shortened contacts occur only between molecules of C_{60} and TMTSF molecules of adjacent layers. In this case, each TMTSF molecule links two C_{60} molecules from adjacent layers (Fig. 2). Both molecules of fullerene are bonded to the TMTSF molecule through C atoms at double C=C bonds (C(21)...Se(1) and C(22)...C(3) are 3.509(7) and 3.343(8) Å, respectively, and C(38) [*x*, *y*, *z* − 1]...Se(1) and C(39) [*x*, *y*, *z* − 1]...Se(1) are 3.540(7) and 3.539(7) Å, respectively). As a result of these intermolecular interactions, the stack of layers is cross-linked by zigzag chains along the *c* axis:

The C_{60} fullerene molecule has the molecular symmetry *m*. The symmetry plane passes through the C(15), C(16), C(38), and C(39) atoms. The molecule has an approximately spherical shape. The minimum and maximum distances from the atoms to the center of the molecule are 3.522(9) and 3.559(9) Å, respectively. The average value of the radius of the sphere is 3.54(2) Å. In the five-membered rings, the lengths of the 30 C—C bonds of the type d_{56} are in the range of 1.422(8)—1.487(8) Å; the average d_{56} bond length is 1.45(3) Å. In the six-membered rings, the lengths of the 15 C=C bonds of the type d_{66} vary from 1.342(9) to 1.415(9) Å; the average d_{66} bond length is 1.38(4) Å. In spite of the

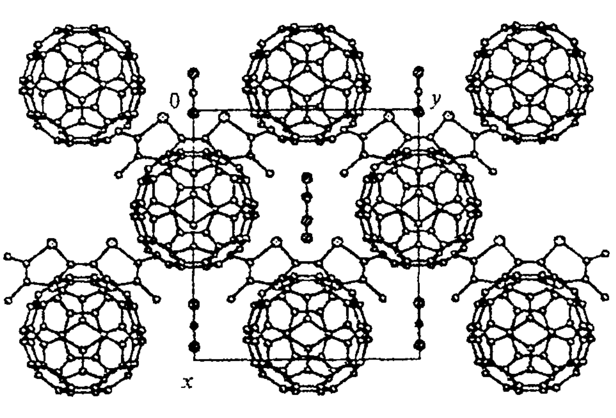

Fig. 1. Projection of the crystal structure of complex **1** onto the *xy*0 plane.

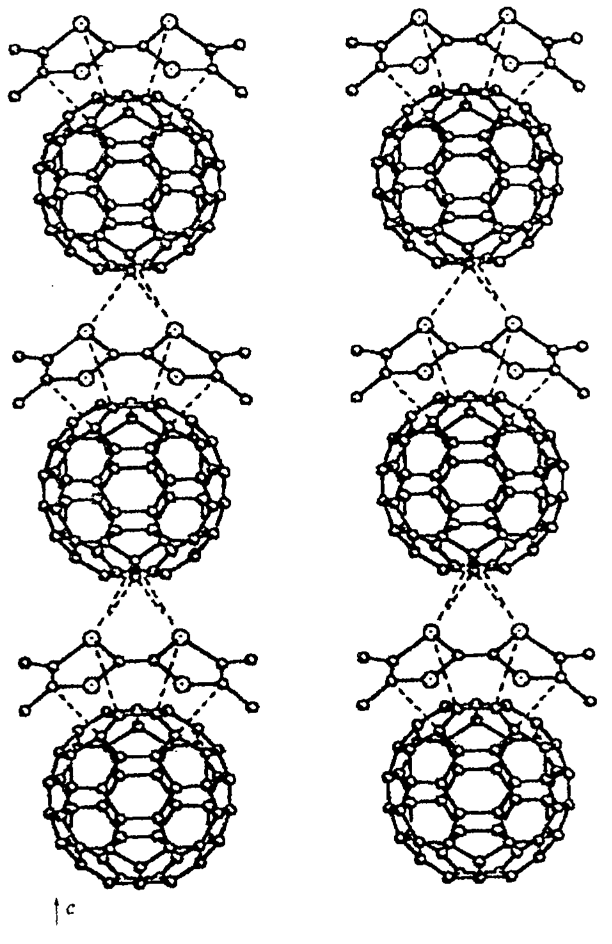

Fig. 2. Zigzag chains formed by TMTSF and C_{60} molecules in the crystal of **1** (CS_2 molecules are omitted for clarity).

substantial variation in the bond lengths, the average values of the d_{56} and d_{66} bond lengths (1.45(3) and 1.38(4) Å, respectively) are indicative of a substantial alternation of the bond lengths in fullerene. The C—C—C bond angles in the five-membered rings vary from 105.3(6) to 110.0(7)°. The bond angles in the six-membered rings are in the range of 117.7(6)—122.8(5)°.

Like the C_{60} molecule, the TMTSF molecule has a crystallographic symmetry plane. The plane *m* passes perpendicular to the C(1)—C(1a) bond through its midpoint (Fig. 3). The bond lengths and bond angles in the TMTSF molecule in complex **1** agree with the data[4] obtained for crystals of TMTSF (**2**). In both structures, the equivalent bonds (Se(1)—C(1) and Se(2)—C(1); and Se(1)—C(2) and Se(2)—C(3)) are equal within the experimental error in spite of the fact that in complex **1**, the Se(1) atom is involved in nonbonded interactions with two C_{60} molecules. Unlike the TMTSF molecule in the crystal of **2**, the TMTSF molecule in the crystal of **1** is nonplanar and adopts a boat conformation. To our knowledge, this is the first example of a nonplanar conformation of the TMTSF molecule in a crystal. In the crystal of **2**, the TMTSF molecule is virtually planar. The maximum deviation of the atoms from the mean plane of the molecule is under 0.005 Å. In the crystal of **1**, only the C(1), C(1a), Se(1), Se(2), Se(1a), and Se(2a) atoms of the TMTSF molecule are in a single plane. The molecule is folded along the Se(1)...Se(2) line. The dihedral angle between the plane through the C(1), C(1a), Se(1), Se(2), Se(1a), and Se(2a) atoms (C_2Se_4) and the plane through the Se(1), Se(2), C(2), C(3), C(4), and C(5) atoms (C_4Se_4) is 23.8°. Apparently, two factors favor the occurrence of a boat conformation of the TMTSF molecule in the crystal of **1**. First, it is known that selenium atoms are involved in π conjugation to only a small extent[16] and, therefore, no substantial expenditure of energy is necessary for distortion of the structure. Second, the C(3) atom is involved in nonbonded interactions with the fullerene molecule.

Figure 3 shows the TMTSF molecule and the fragments of the C_{60} molecule of complex **1** involved in nonbonded TMTSF...C_{60} interactions. It is readily seen that these interactions are different. In the first case (see Fig. 3, *a*), atoms of one of the six-membered rings of the fullerene molecule are involved in the interaction. The angle between the mean plane of the six-membered C(21)C(22)C(29)C(29a)C(22a)C(21a) ring of the C_{60} molecule and the C_2Se_4 fragment of the TMTSF molecule is 5.9°. The distance between these planes is 3.507(9) Å. This suggests that the TMTSF...C_{60} interaction occurs through the π orbitals of the molecules. Apparently, the TMTSF molecule acts as a donor, *i.e.*, this is a π(TMTSF)...π^*(C_{60}) type bond. In the second case (see Fig. 3, *b*), the atoms of the six-membered ring belonging to the d_{66} bond are involved in nonbonded TMTSF...C_{60} [*x*, *y*, *z* − 1] interactions. The angle between the mean plane of the C_2Se_4 fragment of the TMTSF molecule and the planes of the six-membered C(38a)C(39a)C(32b)C(33b)C(37b)C(36b) and C(38a)C(39a)C(32a)C(33a)C(37a)C(36a) rings is 65.2°, which excludes π—π interaction. Presently, we cannot

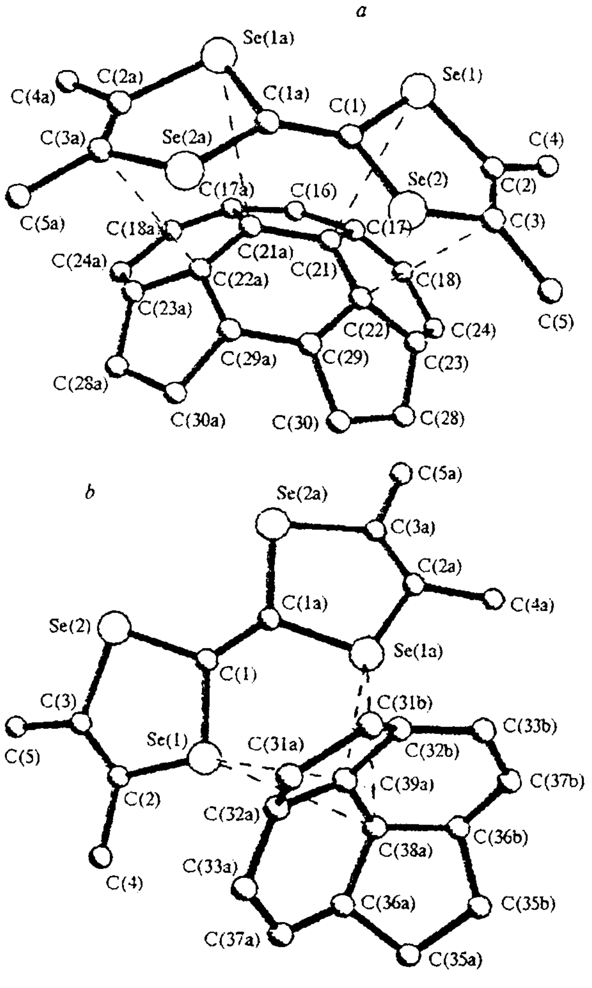

Fig. 3. Fragments of the C_{60} molecule and the TMTSF molecule involved in nonbonded TMTSF...C_{60} interactions in **1**: (*a*) TMTSF...C_{60}; and (*b*) TMTSF...C_{60}[*x*, *y*, *z* − 1].

unambiguously assign the TMTSF...C_{60}[*x*, *y*, *z* − 1] contacts to any particular type, but it is apparent that the TMTSF and C_{60} molecules in the chains are linked to each other in various fashions.

The energy of the TMTSF...C_{60} bond was estimated by a method we suggested previously.[17] According to this method, the energy of intermolecular X...fullerene interactions (W) is equal to the difference between the energy of the conformer of the molecule X (W_c) that is observed in the crystal, and the energetically most favorable conformer of the molecule X (W_f): $W = W_c - W_f$. With the aim of estimating the energies of the conformers of the TMTSF molecule, we calculated the energy of the planar molecule, which is the energetically most favorable conformation, (W_f) and the energy of a boat conformation of the molecule (W_c), which is observed in the crystal of **1**, by the quantum-chemical PM3 method. The planar molecule was calculated with full optimization of geometry. The bond lengths, bond angles, and torsion angles of the TMTSF molecule determined by X-ray diffraction analysis[4] were used as starting values. Calculations of a boat-like conformation of the molecule were carried out with optimization of the bond lengths and bond angles. The values of the C=C—Se—C torsion angles, which determine the conformation of the molecule, were taken from X-ray diffraction data on the TMTSF molecule in the crystal of **1** and were fixed in the calculations. Other torsion angles were optimized. Calculations demonstrated that the difference in the energies of the conformers of the TMTSF molecule is 3.3 kcal mol^{-1}. This value corresponds to the energy of a weak hydrogen bond[18] and seems reasonable.

The CS_2 molecules are in symmetry plane *m* and are almost collinear with each other. Both molecules are approximately linear. The S(1)C(6)S(2) and S(3)C(7)S(4) bond angles are 178.7(6) and 177.3(7)°, respectively. The C=S bond lengths are in the range of 1.497(9)—1.572(9) Å, which is consistent with that observed in other molecular complexes containing the CS_2 fragment[19—22] (1.46(2)—1.57(2) Å). The average C=S bond length (1.534 Å) is close to the bond length in the CS_2 molecule (1.554(5) Å) in the gas phase determined by microwave spectroscopy.[23]

Therefore, in this work, the molecular and crystal structure of the new complex of C_{60} fullerene was determined. A nonplanar conformation of the TMTSF molecule in the complex was observed for the first time. This conformation is to a large extent determined by intermolecular interactions with C_{60}. The existence of a second equilibrium conformation of the TMTSF molecule and the value of the energy (3.3 kcal mol^{-1}) required (according to the data of quantum-chemical calculations) for the transition from the major (planar) conformation to a boat conformation correspond to the definition of stereochemically flexible molecules and, therefore, confirm the tendency of C_{60} fullerene to form stable complexes with conformationally flexible molecules. Taking into account the fact that C_{60} fullerene forms[12] a complex with bis(ethylenedithio)tetrathiafulvalene (BEDT—TTF or ET), which is another well known donor in the class of organic conductors and superconductors, it can be suggested that stereochemical flexibility is a rather important structural criterion for choosing new donors for conducting systems. As a whole, the structure of complex **1** exhibits all the necessary structural characteristics (a layer structure, the absence of shortened intermolecular contacts between the CS_2 solvate molecule and the C_{60} and TMTSF molecules) that make it possible to continue studies (removal of the solvate, doping by alkali metals) with the aim of obtaining a conducting fullerene complex based on **1**.

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