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A Mesogenic Perfluorinated Compound

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Abstract

The structure of 4-(2,2,3,3,4,4,4-heptafluorobutyloxycarbonyl)]phenyl 4-undecyloxybenzoate, $C_{29}H_{33}F_7O_5$, adopts a slightly bent conformation. Molecules are aligned in the same direction and orientation as in an S_A smectic-like molecular arrangement. It is, therefore, a precursor of a ferroelectric phase.

Comment

Liquid crystals play an important role in a wide variety of electro-optical display devices and their development is currently of great interest (Kaneko, 1987). Recently, liquid crystals incorporating F atoms have shown very interesting results for such displays (Schad & Kelly, 1985; Goto, Ogawa, Sawada & Sugimori, 1991). There are numerous ways to introduce fluorine into liquid crystals; one is discussed in a recent paper regarding the 4-cyanophenyl 4-perfluoroheptylbenzoate with a cyano group on one side and a perfluoroheptyl chain on the

©1995 International Union of Crystallography Printed in Great Britain – all rights reserved other (Kromm, Bideau, Cotrait, Destrade & Nguyen, 1994), which gives an S_{A_2} -like arrangement. For the present compound, structural characterization shows that the material has a monolayer S_A phase. In order to clarify the precise relationship between the S_A structure and the molecular interactions, we solved the crystal structure of the present compound (1).



The molecule can be analysed as consisting of three parts, the alkoxy chain, the central core and the semiperfluorinated chain. The title compound crystallizes in the P1 space group with two independent molecules in the cell, (I) and (II). The atom labelling, along with the molecular conformations, are given in a SNOOPI drawing (Davies, 1983) (Fig. 1). Both alkoxy chains (O30-C41) for (I) and (O80-C91) for (II) are planar with torsion angles differing by less than 5° from 180°. Both semi-perfluorinated chains O18-C22 for (I) and O68-C72 for (II) are fully extended. The only conformational differences between molecules (I) and (II) are relative to the central core: C1-O18 and C51-O68 for (I) and (II), respectively. The torsion angles which differentiate molecules are as follows: C3-C4-C7-O9 -10.3 (12), C53-C54-C57-O59 -167.2 (7), C7-O9-C10-C11 -121.0 (9) and C57-O59-C60-C61 -71.1 (11)°.

Both molecules are bent at the homologous C16 and C66 level: $C(22) \cdots C(16) \cdots C(41)$ and $C(72) \cdots C(66) \cdots C(91)$ are 131.7 and 127.8°, respectively. The two phenyl rings of the cores make angles of 52.5 and



Fig. 1. View of $C_{29}H_{33}F_7O_5$ showing the labelling of the non-H atoms. Displacement ellipsoids are shown at 50% probability levels (the projection of the structure is along the z axis).

58.5° for (I) and (II), respectively. The distances and angles in the core are in agreement with those found in similar structures (Bideau, Bravic, Cotrait, Nguyen & Destrade, 1991). The semi-perfluorinated chains are characterized by an average C—F distance of 1.33 Å and F—C—F and C—C—F angles of 107.1 and 108.5°, respectively. These values are in full agreement with those found in the 4-cyanophenyl 4-perfluoroheptylbenzoate. The lengths of molecules (I) and (II) are 30.8 and 30.7 Å, respectively. This is in agreement with the Xray measurement on the mesophase of 28.86 Å for the S_C phase and 29.78 Å for the S_A phase.

Molecules form monomolecular sheets almost parallel to the y0z plane. The thickness of the layers is close to the value of the *a* parameter. The interactions between the end of the alkoxy chain of one molecule and the end of the perfluorinated chain of another are very weak. The interactions between neighbouring molecules in a layer are also very weak, particularly in the vicinity of the perfluorinated chains. Because of the absence of centres of symmetry (space group P1), the two independent molecules are slightly different and approximately parallel (see the torsion angles given above). Such compounds may eventually give rise to ferroelectric properties which will be studied later.

Experimental

Crystal data		C32
		C33
$C_{29}H_{33}F_7O_5$	Mo $K\alpha$ radiation	C34
$M_r = 594.60$	$\lambda = 0.71069 \text{ Å}$	C35
Triclinic	Cell parameters from 17	C36
P1	reflections	C37
a = 30.012(7) Å	$A = 12 \cdot 10^{\circ}$	C30
a = 50.912(7) A	0 = 12 - 19	C40
b = 7.719(2) A	$\mu = 0.114 \text{ mm}^{-1}$	C40
c = 6.184(6) A	T = 293 K	F201
$\alpha = 95.40 (7)^{\circ}$	Prism	F202
$\beta = 87.16 (7)^{\circ}$	$0.50 \times 0.25 \times 0.10$ mm	F211
$\gamma = 94.85(2)^{\circ}$	Colourless	F212
$V = 1462(2) Å^3$	Crystal source: crystallized	F221
7 = 1402(2) A	from toluono	F222
Z = Z	fioni toluene	F223
$D_x = 1.350 \text{ Mg m}^{-3}$		C51 C52
		C52
Data collection		C54
Enraf-Nonius CAD-4	$R_{i-1} = 0.016$	C55
diffractometer	$A = 22^{\circ}$	C56
	$v_{\rm max} = 22$	C57
$\omega/2\theta$ scans	$h = -32 \rightarrow 32$	O58
Absorption correction:	$k = -8 \rightarrow 8$	059
none	$l = 0 \rightarrow 6$	C60
5100 measured reflections	3 standard reflections	C61
3169 independent reflections	frequency: 120 min	C62
2386 observed reflections	intensity decay: none	C63
[I > 2-(D)]	intensity decay: none	C65
$[I > 5\sigma(I)]$		C66
P.C. I		067
Refinement		O68
Refinement on F	$(\Delta/\sigma)_{\rm max} = 0.30$	C69
R = 0.0452	$\Delta q_{max} = 0.20 \text{ e} \text{ Å}^{-3}$	C70
N = 0.0452	$\Delta_{a} = 0.20 \text{ cm}^{3}$	C71
$W_{\rm A} = 0.0439$	$\Delta \rho_{\rm min} = -0.20 \ {\rm e} \ {\rm A}$	C72
S = 1.229	Extinction correction: none	O80

2387 reflections	Atomic scattering factors
739 parameters	from International Tables
H-atom parameters not	for X-ray Crystallography
refined	(1974, Vol. IV, Table
$w=1/\sigma^2(F)$	2.3.1)

 Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

 $B_{\rm eq} = (4/3) \sum_i \sum_j \beta_{ij} \mathbf{a}_i . \mathbf{a}_j.$

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		x	У	Z	Beq
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Cl	1.2494 (3)	0.8429 (10)	0.3677 (13)	4.2 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C2	1.2114 (3)	0.7824 (10)	0.4770 (13)	4.3 (4)
$\begin{array}{ccccc} C4 & 1.700 (3) & 0.8941 (10) & 0.2077 (12) & 4.0 (4) \\ C5 & 1.2078 (3) & 0.9233 (11) & 0.1088 (13) & 5.2 (4) \\ C6 & 1.2470 (3) & 0.9293 (11) & 0.1088 (13) & 5.1 (4) \\ 08 & 1.1250 (2) & 1.0106 (9) & -0.0353 (11) & 7.7 (4) \\ 09 & 1.0940 (2) & 0.8314 (8) & 0.2039 (9) & 5.2 (3) \\ C10 & 1.0526 (3) & 0.8361 (11) & 0.1157 (14) & 4.9 (4) \\ C11 & 1.0209 (3) & 0.9000 (13) & 0.2558 (14) & 5.5 (5) \\ C12 & 0.9793 (3) & 0.8961 (13) & 0.1832 (15) & 6.0 (5) \\ C13 & 0.9708 (3) & 0.8351 (11) & -0.0296 (14) & 5.0 (4) \\ C14 & 1.0035 (3) & 0.7686 (13) & -0.1677 (14) & 5.8 (5) \\ C15 & 1.0454 (3) & 0.7697 (13) & -0.0933 (14) & 5.5 (5) \\ C16 & 0.9274 (3) & 0.8331 (13) & -0.1198 (15) & 5.8 (5) \\ C17 & 0.9184 (2) & 0.7886 (10) & -0.3045 (11) & 7.9 (6) \\ O18 & 0.8974 (2) & 0.8897 (9) & 0.0347 (10) & 6.8 (6) \\ C20 & 0.8253 (3) & 0.7855 (12) & 0.0994 (15) & 5.3 (5) \\ C21 & 0.7773 (3) & 0.7919 (13) & 0.0526 (14) & 5.6 (5) \\ C22 & 0.7431 (3) & 0.6905 (14) & 0.1867 (17) & 7.0 (6) \\ O30 & 1.2905 (2) & 0.8260 (7) & 0.4235 (8) & 5.0 (7) \\ C31 & 1.2979 (3) & 0.7475 (13) & 0.6895 (17) & 6.2 (5) \\ C33 & 1.3618 (3) & 0.7093 (12) & 0.8453 (14) & 5.7 (5) \\ C34 & 1.4110 (3) & 0.6797 (14) & 1.2770 (16) & 6.6 (7) \\ C33 & 1.3618 (3) & 0.7093 (12) & 0.8453 (14) & 5.7 (5) \\ C34 & 1.4110 (3) & 0.6747 (15) & 1.4766 (17) & 7.3 (6) \\ C40 & 1.6123 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (6) \\ C40 & 1.6123 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (6) \\ C40 & 1.6123 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (7) \\ C41 & 1.6337 (4) & 0.615 (2) & 1.1270 (16) & 6.6 (7) \\ C52 & 0.2203 (3) & 0.4524 (7) & 0.3145 (8) & 6.8 (3) \\ F212 & 0.7716 (2) & 0.9609 (8) & 0.0892 (11) & 8.3 (6) \\ F221 & 0.7716 (2) & 0.5234 (10) & 0.1614 (15) & 12.4 (6) \\ C52 & 0.2203 (3) & 0.4524 (1) & 0.7737 (9) & 8.4 (7) \\ C53 & 0.2203 (3) & 0.4534 (11) & 0.9848 (13) & 4.8 (7) \\ C54 & 0.2034 (2) & 0.3748 (10) & 0.3899 (10) & 1.02 (2) \\ C55 & 0.2281 (3) & 0.3671 (10) & 0.730 (12) & 4.4 (7) \\ C55 & 0.2281 (3) & 0.3671 (10) & 0.773 (9) & 8.4 (7) \\ C64 & 0.0552 (3) & 0.3041 (12) & 0.4585 (13) & 0.573$	C3	1.1714 (3)	0.8095 (11)	0.3970 (13)	4.8 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C4	1.1700 (3)	0.8941 (10)	0.20//(12)	4.0 (4)
$\begin{array}{cccccc} C6 & 1.2470 (3) & 0.9293 (11) & 0.189 (13) & 4.5 (4) \\ C7 & 1.1285 (3) & 0.9234 (11) & 0.1081 (14) & 5.1 (4) \\ O9 & 1.0940 (2) & 0.8314 (8) & 0.2039 (9) & 5.2 (3) \\ C10 & 1.0526 (3) & 0.8361 (11) & 0.1157 (14) & 4.9 (4) \\ C11 & 1.0209 (3) & 0.9000 (13) & 0.2558 (14) & 5.5 (5) \\ C12 & 0.9793 (3) & 0.8961 (13) & 0.1832 (15) & 6.0 (6) \\ C14 & 1.0035 (3) & 0.7686 (13) & -0.1677 (14) & 5.8 (6) \\ C15 & 1.0454 (3) & 0.7697 (13) & -0.0933 (14) & 5.5 (5) \\ C16 & 0.9274 (3) & 0.8331 (13) & -0.1198 (15) & 5.8 (5) \\ O17 & 0.9184 (2) & 0.7886 (10) & -0.3045 (11) & 7.9 (6) \\ C18 & 0.8974 (2) & 0.8897 (9) & 0.0347 (10) & 6.8 (6) \\ C20 & 0.8253 (3) & 0.7855 (12) & 0.0994 (15) & 5.3 (5) \\ C21 & 0.7773 (3) & 0.7919 (13) & 0.0526 (14) & 5.6 (5) \\ C22 & 0.7431 (3) & 0.6905 (14) & 0.1867 (17) & 7.0 (6) \\ C33 & 1.2905 (2) & 0.8260 (7) & 0.4235 (8) & 5.0 (7) \\ C31 & 1.2979 (3) & 0.7475 (11) & 0.6188 (13) & 5.1 (6) \\ C33 & 1.3618 (3) & 0.7093 (12) & 0.8453 (14) & 5.7 (5) \\ C34 & 1.4110 (3) & 0.7475 (13) & 0.8895 (17) & 6.2 (7) \\ C35 & 1.4293 (3) & 0.6826 (13) & 1.0627 (15) & 6.2 (7) \\ C36 & 1.4776 (3) & 0.7221 (13) & 1.0813 (16) & 6.1 (7) \\ C37 & 1.4971 (3) & 0.6572 (14) & 1.2724 (16) & 6.9 (7) \\ C38 & 1.5447 (3) & 0.6999 (14) & 1.2874 (16) & 6.9 (7) \\ C39 & 1.5656 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (6) \\ C39 & 1.5656 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (7) \\ C40 & 1.6123 (3) & 0.6745 (17) & 1.4911 (19) & 8.7 (7) \\ C41 & 1.6337 (4) & 0.615 (2) & 1.672 (2) & 1.12 (6) \\ F201 & 0.8297 (2) & 0.8248 (7) & 0.3145 (8) & 6.8 (7) \\ C42 & 1.61337 (4) & 0.6178 (7) & 0.0610 (9) & 6.9 (7) \\ F212 & 0.7498 (2) & 0.5234 (10) & 0.1614 (15) & 12.4 (7) \\ F222 & 0.7498 (2) & 0.5234 (10) & 0.1614 (15) & 12.4 (7) \\ C55 & 0.2281 (3) & 0.3076 (8) & 0.8392 (11) & 8.3 (7) \\ C56 & 0.2081 (3) & 0.3255 (12) & 0.3136 (13) & 4.5 (7) \\ C66 & 0.0058 (3) & 0.3323 (12) & 0.5436 (14) & 5.7 (7) \\ C66 & 0.0058 (3) & 0.3323 (12) & 0.5436 (14) & 5.7 (7) \\ C66 & 0.0058 (3) & 0.3323 (12) & 0.5436 (14) & 5.7 (7) \\ C66 & -0.0321 (2) & 0.3746 (10) & 0.4615 (10) $	C5	1.2078 (3)	0.9521 (12)	0.1018 (13)	5.2 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C6	1.2470 (3)	0.9293 (11)	0.1809 (13)	4.5 (4)
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	C7	1.1285 (3)	0.9234 (11)	0.1081 (14)	5.1 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	08	1.1250 (2)	1.0106 (9)	-0.0353 (11)	7.7 (4) 5.2 (2)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	09	1.0940 (2)	0.8314 (8)	0.2039 (9)	5.2 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Clu	1.0526 (3)	0.8301 (11)	0.1157 (14)	4.9 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1.0209 (3)	0.9000 (13)	0.2558 (14)	5.5 (5)
	C12 C12	0.9793 (3)	0.8961 (13)	0.1852(13)	5 O (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$		1.0025 (2)	0.8551 (11)	-0.0290(14)	58(5)
$\begin{array}{cccc} C16 & 0.9274 (3) & 0.8331 (13) & -0.1198 (15) & 5.8 (5) \\ O17 & 0.9184 (2) & 0.7886 (10) & -0.3045 (11) & 7.9 (4) \\ O18 & 0.8974 (2) & 0.8897 (9) & 0.0347 (10) & 6.8 (4) \\ C19 & 0.8546 (3) & 0.8999 (14) & -0.0319 (17) & 6.8 (6) \\ C20 & 0.8253 (3) & 0.7855 (12) & 0.0994 (15) & 5.3 (5) \\ C21 & 0.7773 (3) & 0.7919 (13) & 0.0526 (14) & 5.6 (5) \\ C22 & 0.7431 (3) & 0.6905 (14) & 0.1867 (17) & 7.0 (6) \\ O30 & 1.2905 (2) & 0.8260 (7) & 0.4235 (8) & 5.0 (5) \\ C31 & 1.2979 (3) & 0.7475 (11) & 0.6188 (13) & 5.1 (6) \\ C32 & 1.3461 (3) & 0.7815 (13) & 0.6495 (16) & 6.3 (6) \\ C33 & 1.3618 (3) & 0.7093 (12) & 0.8453 (14) & 5.7 (5) \\ C34 & 1.4110 (3) & 0.7475 (13) & 0.8695 (17) & 6.2 (5) \\ C35 & 1.4293 (3) & 0.6826 (13) & 1.0627 (15) & 6.2 (5) \\ C36 & 1.4776 (3) & 0.7221 (13) & 1.0813 (16) & 6.1 (6) \\ C37 & 1.4971 (3) & 0.6572 (14) & 1.2720 (16) & 6.6 (5) \\ C38 & 1.5447 (3) & 0.6969 (14) & 1.2874 (16) & 6.9 (6) \\ C39 & 1.5656 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (6) \\ C40 & 1.6123 (3) & 0.6745 (17) & 1.4911 (19) & 8.7 (7) \\ C41 & 1.6337 (4) & 0.615 (2) & 1.672 (2) & 11.2 (6) \\ F201 & 0.8297 (2) & 0.8248 (7) & 0.3145 (8) & 6.8 (7) \\ F212 & 0.7716 (2) & 0.7419 (9) & -0.1573 (9) & 8.4 (7) \\ F222 & 0.7498 (2) & 0.5234 (10) & 0.1614 (15) & 12.4 (7) \\ F223 & 0.7047 (2) & 0.7049 (10) & 0.1208 (12) & 12.0 (7) \\ C53 & 0.2203 (3) & 0.4211 (10) & 1.0500 (13) & 4.2 (7) \\ C54 & 0.2034 (3) & 0.3761 (10) & 0.7920 (12) & 3.7 (7) \\ C55 & 0.2281 (3) & 0.2294 (11) & 0.7725 (12) & 4.4 (7) \\ C57 & 0.1592 (3) & 0.4152 (10) & 0.7401 (12) & 4.4 (7) \\ C58 & 0.1397 (2) & 0.5298 (8) & 0.8276 (9) & 5.5 (12) \\ C51 & 0.2834 (2) & 0.3037 (8) & 0.5730 (8) & 5.3 (14) & 5.4 (13) \\ C54 & 0.2034 (3) & 0.3761 (10) & 0.7920 (12) & 3.7 (7) \\ C55 & 0.2281 (3) & 0.2494 (11) & 0.7255 (12) & 4.5 (2) \\ C51 & 0.0253 (13) & 0.3455 (12) & 0.5136 (14) & 5.7 (16) \\ C53 & 0.1397 (2) & 0.5298 (8) & 0.8276 (9) & 5.5 (12) \\ C54 & 0.0255 (3) & 0.3041 (12) & 0.5486 (14) & 5.7 (16) \\ C55 & 0.0968 (3) & 0.3325 (12) & 0.5138 (13) & 5.5 (14) \\ C66 & -0.0232 (3) & 0.3380 (1$	C14 C15	1.0055(3)	0.7697 (13)	-0.0933(14)	55(5)
$\begin{array}{cccc} 0&0.927(2)&0.7886(10)&-0.3045(11)&7.9(2)\\ 018&0.8974(2)&0.7886(10)&-0.3045(11)&7.9(2)\\ 018&0.8974(2)&0.7885(10)&-0.3045(11)&7.9(2)\\ 018&0.8974(2)&0.7885(12)&0.0994(15)&5.3(2)\\ 020&0.8253(3)&0.7855(12)&0.0994(15)&5.3(2)\\ 021&0.7773(3)&0.7919(13)&0.0526(14)&5.6(2)\\ 022&0.7431(3)&0.6905(14)&0.1867(17)&7.0(1)\\ 030&1.2905(2)&0.8260(7)&0.4235(8)&5.0(2)\\ 031&1.2979(3)&0.7475(11)&0.6188(13)&5.1(2)\\ 032&1.3461(3)&0.7915(13)&0.6495(16)&6.3(2)\\ 033&1.3618(3)&0.7993(12)&0.8453(14)&5.7(2)\\ 034&1.4110(3)&0.7475(13)&0.8695(17)&6.2(2)\\ 035&1.4293(3)&0.6826(13)&1.0627(15)&6.2(2)\\ 036&1.4776(3)&0.7221(13)&1.0813(16)&6.1(2)\\ 037&1.4971(3)&0.6572(14)&1.2720(16)&6.6(2)\\ 038&1.5447(3)&0.6969(14)&1.2874(16)&6.9(2)\\ 039&1.5556(3)&0.6347(15)&1.4766(17)&7.3(2)\\ 040&1.6123(3)&0.6745(17)&1.4911(19)&8.7(2)\\ 041&1.6337(4)&0.615(2)&1.672(2)&11.2(2)\\ F201&0.8297(2)&0.8248(7)&0.3145(8)&6.8(2)\\ F201&0.8297(2)&0.8248(7)&0.3145(8)&6.8(2)\\ F201&0.8297(2)&0.8248(7)&0.3145(8)&6.8(2)\\ F211&0.7679(2)&0.9609(8)&0.0892(11)&8.3(2)\\ F221&0.7716(2)&0.7419(9)&-0.1573(9)&8.4(2)\\ F221&0.7716(2)&0.7419(12)&0.3389(10)&1.20(2)\\ F222&0.7498(2)&0.5234(10)&0.1614(15)&12.4(2)\\ C53&0.2203(3)&0.4534(11)&0.9848(13)&4.8(2)\\ C54&0.2034(3)&0.3761(10)&0.7920(12)&3.7(2)\\ C55&0.2281(3)&0.2609(10)&0.6665(12)&4.3(2)\\ C55&0.2281(3)&0.2609(10)&0.6665(12)&4.3(2)\\ C56&0.2681(3)&0.2244(11)&0.7275(12)&4.4(2)\\ C57&0.1592(3)&0.4532(11)&0.3849(12)&4.2(2)\\ C61&0.0670(3)&0.2305(13)&0.6464(14)&5.7(2)\\ C64&0.0552(3)&0.3041(12)&0.5383(14)&5.4(2)\\ C65&0.0268(3)&0.3325(12)&0.5136(14)&5.2(2)\\ C65&0.0268(3)&0.3325(12)&0.5136(14)&5.2(2)\\ C65&0.0252(3)&0.3041(12)&0.338(13)&5.5(0)\\ C66&0.0032(3)&0.4534(11)&0.9848(13)&4.8(2)\\ C64&0.0552(3)&0.3041(12)&0.5383(14)&5.4(2)\\ C65&0.0268(3)&0.3325(12)&0.5136(14)&5.2(2)\\ C65&0.0258(3)&0.3041(12)&0.5486(14)&5.7(0)\\ C66&0.0057(3)&0.3380(13)&0.3052(15)&6.0(0)\\ 067&-0.0311(2)&0.4088(12)&0.1251(11)&9.3(0)\\ 068&-0.0542(2)&0.3746(10)&0.4615(10)&7.7(0)\\ C69&-0.0522(3)&0.3019(12)&0.5486(14)&5.8(0)\\ C71&-0.1747(3)&0.3391(12)&0.5149(15)&6.0(0)\\ C72&-0.2100(3$	C15	0.0274(3)	0.8331 (13)	-0.1198(15)	5.8 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	017	0.9274(3)	0.0331 (13)	-0.3045(11)	79(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	018	0.9104(2)	0.8807 (0)	0.0045(11) 0.0347(10)	68(4)
$\begin{array}{cccccc} C19 & 0.8036 (3) & 0.7855 (12) & 0.0914 (15) & 5.3 (2) \\ C21 & 0.7773 (3) & 0.7919 (13) & 0.0526 (14) & 5.6 (2) \\ C22 & 0.7431 (3) & 0.6905 (14) & 0.1867 (17) & 7.0 (0) \\ O30 & 1.2905 (2) & 0.8260 (7) & 0.4235 (8) & 5.0 (2) \\ C31 & 1.2979 (3) & 0.7475 (11) & 0.6188 (13) & 5.1 (4) \\ C32 & 1.3461 (3) & 0.7815 (13) & 0.6495 (16) & 6.3 (2) \\ C33 & 1.3618 (3) & 0.7903 (12) & 0.8453 (14) & 5.7 (2) \\ C34 & 1.4110 (3) & 0.7475 (13) & 0.8695 (17) & 6.2 (2) \\ C35 & 1.4293 (3) & 0.6826 (13) & 1.0627 (15) & 6.2 (2) \\ C36 & 1.4776 (3) & 0.7221 (13) & 1.0813 (16) & 6.1 (2) \\ C37 & 1.4971 (3) & 0.6572 (14) & 1.2720 (16) & 6.6 (2) \\ C38 & 1.5447 (3) & 0.6969 (14) & 1.2874 (16) & 6.9 (2) \\ C40 & 1.6123 (3) & 0.6745 (17) & 1.4911 (19) & 8.7 (2) \\ C41 & 1.6337 (4) & 0.615 (2) & 1.6726 (2) & 11.2 (6) \\ F201 & 0.8297 (2) & 0.8248 (7) & 0.3145 (8) & 6.8 (2) \\ F202 & 0.8347 (2) & 0.6178 (7) & 0.0610 (9) & 6.9 (2) \\ F211 & 0.7679 (2) & 0.9609 (8) & 0.0892 (11) & 8.3 (6) \\ F221 & 0.7716 (2) & 0.7419 (9) & -0.1573 (9) & 8.4 (2) \\ F222 & 0.7498 (2) & 0.5234 (10) & 0.1614 (15) & 12.4 (6) \\ F223 & 0.7047 (2) & 0.7049 (10) & 0.1208 (12) & 10.2 (6) \\ C53 & 0.2203 (3) & 0.4534 (11) & 0.9848 (13) & 4.2 (6) \\ C54 & 0.2034 (3) & 0.3761 (10) & 0.7920 (12) & 3.7 (6) \\ C55 & 0.2281 (3) & 0.2609 (10) & 0.6665 (12) & 4.3 (6) \\ C56 & 0.2681 (3) & 0.2244 (11) & 0.7275 (12) & 4.4 (6) \\ C57 & 0.1592 (3) & 0.4152 (10) & 0.7401 (12) & 4.3 (6) \\ C53 & 0.1397 (2) & 0.5298 (8) & 0.8276 (9) & 5.5 (7) \\ C60 & 0.1011 (3) & 0.3255 (12) & 0.5136 (14) & 5.2 (7) \\ C64 & 0.0552 (3) & 0.3037 (8) & 0.5730 (8) & 5.3 (2) \\ C66 & -0.0232 (3) & 0.3451 (11) & 0.9848 (13) & 4.2 (6) \\ C64 & 0.0552 (3) & 0.3041 (12) & 0.5853 (14) & 5.4 (7) \\ C64 & 0.0552 (3) & 0.3041 (12) & 0.5853 (14) & 5.4 (7) \\ C66 & -0.0232 (3) & 0.3376 (8) & 0.3730 (8) & 5.3 (7) \\ C66 & -0.0232 (3) & 0.33615 (11) & 0.3849 (12) & 4.4 (7) \\ C66 & -0.0232 (3) & 0.3361 (13) & 0.3052 (15) & 6.0 (7) \\ C70 & -0.1273 (3) & 0.3199 (12) & 0.5486 (14) & 5.8 (7) \\ C71 & -0.1747 (3) & 0.3391 (12) & 0.5149 $	C19	0.8546(3)	0.8000 (14)	-0.0319(17)	68(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C19	0.8340 (3)	0.7855 (12)	0.0994(15)	53(5)
$\begin{array}{ccccc} C22 & 0.7431 (3) & 0.6905 (14) & 0.1867 (17) & 7.0 (0) \\ O30 & 1.2905 (2) & 0.8260 (7) & 0.4235 (8) & 5.0 (7) \\ C31 & 1.2979 (3) & 0.7475 (11) & 0.6188 (13) & 5.1 (6) \\ C32 & 1.3461 (3) & 0.7815 (13) & 0.6495 (16) & 6.3 (7) \\ C33 & 1.3618 (3) & 0.7933 (12) & 0.8453 (14) & 5.7 (7) \\ C34 & 1.4110 (3) & 0.7475 (13) & 0.8695 (17) & 6.2 (7) \\ C35 & 1.4293 (3) & 0.6826 (13) & 1.0627 (15) & 6.2 (7) \\ C36 & 1.4776 (3) & 0.7221 (13) & 1.0813 (16) & 6.1 (7) \\ C37 & 1.4971 (3) & 0.6572 (14) & 1.2720 (16) & 6.6 (7) \\ C38 & 1.5447 (3) & 0.6969 (14) & 1.2874 (16) & 6.9 (7) \\ C39 & 1.5656 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (7) \\ C40 & 1.6123 (3) & 0.6745 (17) & 1.4911 (19) & 8.7 (7) \\ C41 & 1.6337 (4) & 0.615 (2) & 1.672 (2) & 11.2 (9) \\ F201 & 0.8297 (2) & 0.8248 (7) & 0.3145 (8) & 6.8 (7) \\ F202 & 0.8347 (2) & 0.6178 (7) & 0.0610 (9) & 6.9 (7) \\ F211 & 0.7679 (2) & 0.9609 (8) & 0.0892 (11) & 8.3 (6) \\ F222 & 0.7498 (2) & 0.5234 (10) & 0.1614 (15) & 12.4 (7) \\ F223 & 0.7047 (2) & 0.7049 (10) & 0.1208 (12) & 10.2 (7) \\ C53 & 0.2203 (3) & 0.4534 (11) & 0.9848 (13) & 4.8 (7) \\ C54 & 0.2034 (2) & 0.3040 (10) & 0.9244 (12) & 4.0 (7) \\ C52 & 0.2602 (3) & 0.4211 (10) & 1.0500 (13) & 4.2 (7) \\ C53 & 0.2203 (3) & 0.4534 (11) & 0.7730 (8) & 4.3 (7) \\ C54 & 0.2034 (3) & 0.3761 (10) & 0.7920 (12) & 3.7 (7) \\ C55 & 0.2281 (3) & 0.2298 (8) & 0.8276 (9) & 5.5 (7) \\ O59 & 0.1438 (2) & 0.3037 (8) & 0.5730 (8) & 5.3 (7) \\ C60 & 0.1011 (3) & 0.3255 (12) & 0.5136 (14) & 5.2 (7) \\ C61 & 0.0670 (3) & 0.2805 (13) & 0.6464 (14) & 5.7 (7) \\ C62 & 0.0255 (3) & 0.3041 (12) & 0.5853 (14) & 5.4 (7) \\ C64 & 0.0552 (3) & 0.3041 (12) & 0.5853 (14) & 5.4 (7) \\ C66 & -0.0522 (3) & 0.3041 (12) & 0.5853 (14) & 5.4 (7) \\ C66 & -0.0522 (3) & 0.3037 (8) & 0.5730 (8) & 5.3 (7) \\ C66 & -0.0542 (2) & 0.3746 (10) & 0.4205 (13) & 0.6464 (14) & 5.7 (7) \\ C66 & -0.0522 (3) & 0.3080 (13) & 0.3052 (15) & 6.0 (7) \\ C70 & -0.1273 (3) & 0.3199 (12) & 0.5486 (14) & 5.8 (7) \\ C71 & -0.1747 (3) & 0.3391 (12) & 0.5149 (15) & 6.0 (7) \\ C72 & -0.2100 (3) & 0.2480 (13$	C20	0.8233(3)	0.7855 (12)	0.0576(13)	56(5)
$\begin{array}{ccccc} 0.1751 (2) & 0.030 (17) & 0.1235 (8) & 5.0 (17) \\ 0.300 (1.2905 (2) & 0.8260 (7) & 0.4235 (8) & 5.0 (7) \\ 0.31 & 1.2979 (3) & 0.7475 (11) & 0.6188 (13) & 5.1 (4) \\ 0.32 & 1.3461 (3) & 0.7815 (13) & 0.6495 (16) & 6.3 (5) \\ 0.33 & 1.3618 (3) & 0.7093 (12) & 0.8453 (14) & 5.7 (5) \\ 0.34 & 1.4110 (3) & 0.7475 (13) & 0.8695 (17) & 6.2 (5) \\ 0.35 & 1.4293 (3) & 0.6826 (13) & 1.0627 (15) & 6.2 (5) \\ 0.36 & 1.4776 (3) & 0.7221 (13) & 1.0813 (16) & 6.1 (5) \\ 0.37 & 1.4971 (3) & 0.6572 (14) & 1.2720 (16) & 6.6 (5) \\ 0.38 & 1.5447 (3) & 0.6969 (14) & 1.2874 (16) & 6.9 (6) \\ 0.39 & 1.5656 (3) & 0.6347 (15) & 1.4766 (17) & 7.3 (6) \\ 0.40 & 1.6123 (3) & 0.6745 (17) & 1.4911 (19) & 8.7 (7) \\ 0.41 & 1.6337 (4) & 0.615 (2) & 1.672 (2) & 11.2 (6) \\ F201 & 0.8297 (2) & 0.8248 (7) & 0.3145 (8) & 6.8 (6) \\ F202 & 0.8347 (2) & 0.6178 (7) & 0.0610 (9) & 6.9 (6) \\ F211 & 0.7679 (2) & 0.9609 (8) & 0.0892 (11) & 8.3 (6) \\ F212 & 0.7716 (2) & 0.7419 (12) & 0.3899 (10) & 12.0 (7) \\ F223 & 0.7047 (2) & 0.7049 (10) & 0.1208 (12) & 10.2 (7) \\ F223 & 0.7047 (2) & 0.7049 (10) & 0.1208 (12) & 10.2 (7) \\ C55 & 0.2281 (3) & 0.2534 (11) & 0.9244 (12) & 4.0 (7) \\ C52 & 0.2602 (3) & 0.4211 (10) & 1.0500 (13) & 4.2 (7) \\ C53 & 0.2203 (3) & 0.4534 (11) & 0.9248 (13) & 4.8 (7) \\ C54 & 0.2034 (3) & 0.3761 (10) & 0.7920 (12) & 3.7 (7) \\ C55 & 0.2281 (3) & 0.2298 (8) & 0.8276 (9) & 5.5 (7) \\ 0.59 & 0.1438 (2) & 0.3037 (8) & 0.5730 (8) & 5.3 (7) \\ C64 & 0.0552 (3) & 0.4015 (11) & 0.3849 (12) & 4.4 (7) \\ C55 & 0.0298 (3) & 0.3615 (11) & 0.3849 (12) & 4.4 (7) \\ C64 & 0.0552 (3) & 0.3041 (12) & 0.5833 (14) & 5.4 (7) \\ C64 & 0.0552 (3) & 0.3041 (12) & 0.5833 (14) & 5.5 (7) \\ C65 & 0.0968 (3) & 0.3823 (12) & 0.3138 (13) & 5.5 (7) \\ C66 & -0.0311 (2) & 0.4088 (12) & 0.1251 (11) & 9.3 (7) \\ C66 & -0.0542 (2) & 0.3746 (10) & 0.4615 (10) & 7.7 (7) \\ C66 & -0.0522 (3) & 0.3190 (12) & 0.5486 (14) & 5.8 (7) \\ C70 & -0.1273 (3) & 0.3199 (12) & 0.5486 (14) & 5.8 (7) \\ C71 & -0.1747 (3) & 0.3391 (12) & 0.5149 (15) & 6.3 (7) \\ C72 & -0.2100 (3) & 0.2480 (13) & $	C21	0.773(3)	0.6905 (14)	0.0320(14) 0.1867(17)	70(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	030	1 2005 (2)	0.8260 (7)	0.4235 (8)	50(3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C31	1 2070 (3)	0.3200(1)	0.4233(0)	5.1 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C32	1 3461 (3)	0.7815(13)	0.6495 (16)	6.3 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C33	1 3618 (3)	0.7093 (12)	0.8453 (14)	5.7 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C34	1 4110 (3)	0.7475 (13)	0.8695 (17)	6.2 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C35	1 4293 (3)	0.6826 (13)	1.0627 (15)	6.2 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C36	1 4776 (3)	0.0020(10)	1.0813 (16)	6.1 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C37	1 4971 (3)	0.6572(14)	1.2720 (16)	6.6 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C38	1 5447 (3)	0.6969 (14)	1.2874 (16)	6.9 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C39	1.5656 (3)	0.6347 (15)	1.4766 (17)	7.3 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C40	1.6123 (3)	0.6745 (17)	1.4911 (19)	8.7 (7)
F201 0.8297 (2) 0.8248 (7) 0.3145 (8) 6.8 (2)F202 0.8347 (2) 0.6178 (7) 0.0610 (9) 6.9 (2)F211 0.7679 (2) 0.9609 (8) 0.0892 (11) 8.3 (1)F212 0.7716 (2) 0.7419 (9) -0.1573 (9) 8.4 (1)F212 0.77437 (2) 0.7419 (9) -0.1573 (9) 8.4 (1)F221 0.7437 (2) 0.7419 (9) -0.1573 (9) 8.4 (1)F222 0.7437 (2) 0.7449 (10) 0.1614 (15) 12.0 (1)F223 0.7047 (2) 0.7049 (10) 0.1208 (12) 10.2 (10)C51 0.2834 (2) 0.3040 (10) 0.9244 (12) 4.0 (1)C52 0.2602 (3) 0.4211 (10) 1.0500 (13) 4.2 (1)C53 0.2203 (3) 0.4534 (11) 0.9848 (13) 4.8 (1)C54 0.2034 (3) 0.3761 (10) 0.7920 (12) 3.7 (1)C55 0.2281 (3) 0.2244 (11) 0.7275 (12) 4.4 (1)C56 0.2681 (3) 0.2244 (11) 0.7275 (12) 4.4 (1)C57 0.1592 (3) 0.4152 (10) 0.7401 (12) 4.4 (1)C58 0.1397 (2) 0.5298 (8) 0.8276 (9) 5.5 (1)C56 0.0968 (3) 0.3615 (11) 0.3849 (12) 4.4 (1)C61 0.0670 (3) 0.2805 (13) 0.6464 (14) 5.7 (1)C62 0.0255 (3) 0.3041 (12) 0.5853 (14) 5.4 (1)C64 0.0552 (3) 0.30860 (13) <td>C41</td> <td>1.6337 (4)</td> <td>0.615 (2)</td> <td>1.672 (2)</td> <td>11.2 (9)</td>	C41	1.6337 (4)	0.615 (2)	1.672 (2)	11.2 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F201	0.8297 (2)	0.8248 (7)	0.3145 (8)	6.8 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F202	0.8347 (2)	0.6178 (7)	0.0610 (9)	6.9 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F211	0.7679 (2)	0.9609 (8)	0.0892 (11)	8.3 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F212	0.7716 (2)	0.7419 (9)	-0.1573 (9)	8.4 (3)
F222 0.7498 (2) 0.5234 (10) 0.1614 (15) 12.4 (2)F223 0.7047 (2) 0.7049 (10) 0.1208 (12) 10.2 (2)C51 0.2834 (2) 0.3040 (10) 0.9244 (12) 4.0 (2)C52 0.2602 (3) 0.4211 (10) 1.0500 (13) 4.2 (2)C53 0.2203 (3) 0.4534 (11) 0.9848 (13) 4.8 (2)C54 0.2034 (3) 0.3761 (10) 0.7920 (12) 3.7 (2)C55 0.2281 (3) 0.2609 (10) 0.6665 (12) 4.3 (2)C56 0.2681 (3) 0.2244 (11) 0.7275 (12) 4.4 (2)C57 0.1592 (3) 0.4152 (10) 0.7401 (12) 4.4 (2)C58 0.1397 (2) 0.5298 (8) 0.8276 (9) 5.5 (2)C59 0.1438 (2) 0.3037 (8) 0.5730 (8) 5.3 (2)C60 0.1011 (3) 0.3255 (12) 0.5136 (14) 5.2 (2)C61 0.0670 (3) 0.2805 (13) 0.6464 (14) 5.7 (2)C62 0.0255 (3) 0.3041 (12) 0.2500 (14) 5.9 (2)C64 0.0552 (3) 0.3041 (12) 0.2500 (14) 5.9 (2)C66 -0.0232 (3) 0.3860 (13) 0.3052 (15) 6.0 (10)C66 -0.0542 (2) 0.3746 (10) 0.4615 (10) 7.7 (2)C66 -0.0542 (2) 0.3746 (10) 0.4615 (10) 7.7 (2)C66 -0.0542 (2) 0.3746 (10) 0.4615 (10) 7.7 (2)C70 -0.1273 (3) 0.3109 (12)<	F221	0.7437 (2)	0.7419 (12)	0.3899 (10)	12.0 (5)
F223 0.7047 (2) 0.7049 (10) 0.1208 (12) 10.2 (2C51 0.2834 (2) 0.3040 (10) 0.9244 (12) 4.0 (2C52 0.2602 (3) 0.4211 (10) 1.0500 (13) 4.2 (2C53 0.2203 (3) 0.4534 (11) 0.9848 (13) 4.8 (2C54 0.2034 (3) 0.3761 (10) 0.7920 (12) 3.7 (2C55 0.2281 (3) 0.2609 (10) 0.6665 (12) 4.3 (2C56 0.2681 (3) 0.2244 (11) 0.7775 (12) 4.4 (2C57 0.1592 (3) 0.4152 (10) 0.7401 (12) 4.4 (2C58 0.1397 (2) 0.5298 (8) 0.8276 (9) 5.5 (2C60 0.1011 (3) 0.3255 (12) 0.5136 (14) 5.2 (2C61 0.0670 (3) 0.2805 (13) 0.6464 (14) 5.7 (2C62 0.0255 (3) 0.3041 (12) 0.5853 (14) 5.4 (2C63 0.0198 (3) 0.3615 (11) 0.3849 (12) 4.4 (2C64 0.0552 (3) 0.4019 (12) 0.2500 (14) 5.9 (2C65 0.0968 (3) 0.3823 (12) 0.3138 (13) 5.5 (2C66 -0.0232 (3) 0.3860 (13) 0.3052 (15) 6.0 (2C66 -0.0542 (2) 0.3746 (10) 0.4615 (10) 7.7 (2C66 -0.0542 (2) 0.3746 (10) 0.4615 (10) 7.7 (2C66 -0.0572 (4) 0.4051 (16) 0.4035 (17) 7.9 (2C70 -0.1273 (3) 0.3109 (12) 0.5486 (14	F222	0.7498 (2)	0.5234 (10)	0.1614 (15)	12.4 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	F223	0.7047 (2)	0.7049 (10)	0.1208 (12)	10.2 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C51	0.2834 (2)	0.3040 (10)	0.9244 (12)	4.0 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C52	0.2602 (3)	0.4211 (10)	1.0500 (13)	4.2 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C53	0.2203 (3)	0.4534 (11)	0.9848 (13)	4.8 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C54	0.2034 (3)	0.3761 (10)	0.7920 (12)	3.7 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C55	0.2281 (3)	0.2609 (10)	0.6665 (12)	4.3 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C56	0.2681 (3)	0.2244 (11)	0.7275(12)	4.4 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C57	0.1592 (3)	0.4152(10)	0.7401 (12)	4.4 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	058	0.1397 (2)	0.5298 (8)	0.8276 (9)	5.5 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	059	0.1438 (2)	0.3037(8)	0.5/30(8)	5.5 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C60	0.1011 (3)	0.3255 (12)	0.5130(14)	5.2 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C61	0.0670(3)	0.2805(13)	0.0404 (14)	5.7 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C62	0.0255 (3)	0.3041(12)	0.3633(14) 0.2840(12)	J.4 (J)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C03	0.0198(3)	0.3013(11)	0.3649(12) 0.2500(14)	50(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C04	0.0332 (3)	0.4019 (12)	0.2300 (14)	5.7(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C03	-0.0708(3)	0.3623 (12)	0.3136(13)	60(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	067	-0.0232(3) -0.0311(2)	0.3800 (13)	0.3052(13) 0.1251(11)	93(5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	069	-0.0511(2) -0.0542(2)	0.7000 (12)	0.4615 (10)	77(A)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C60	-0.0342(2) -0.0072(4)	0.0740(10)	0.4035 (17)	79(6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C70	-0.0772(4) -0.1273(2)	0.3109(17)	0.5486 (14)	58(5)
C72 = -0.2100 (3) = 0.2480 (13) = 0.6470 (15) = 6.3 (0.00 = 0.325 (2) = 0.2480 (13) = 0.6470 (15) = 6.3 (0.00 = 0.325 (2) = 0.2511 (7) = 0.9705 (8) = 4.9 (15) = 0.051 (15) (15) = 0.051 (15) (15) (15) (15) (15) (15) (15) (1	C71	-0.1273(3) -0.1747(3)	0 3301 (12)	0.5149 (15)	60(5)
$O_{20} = 0.2100(3) = 0.2100(13) = 0.010($	C72	-0.2100 (3)	0.3371(12) 0.2480(13)	0.6470 (15)	6.3 (5)
	080	0.3225 (2)	0.2511 (7)	0.9795 (8)	4.9 (3)

(1)

C81	0.3376 (3)	0.3075 (11)	1.1906 (14)	4.8 (4)
C82	0.3766 (3)	0.2064 (12)	1.2252 (15)	5.7 (5)
C83	0.3989 (3)	0.2674 (12)	1.4347 (15)	5.5 (5)
C84	0.4392 (3)	0.1745 (13)	1.4587 (15)	5.8 (5)
C85	0.4642 (3)	0.2386 (13)	1.6568 (16)	6.1 (5)
C86	0.5060 (3)	0.1479 (14)	1.6710 (16)	6.5 (5)
C87	0.5317 (3)	0.2089 (15)	1.8709 (17)	7.2 (6)
C88	0.5738 (3)	0.1251 (15)	1.8775 (19)	7.6 (6)
C89	0.6005 (4)	0.1918 (16)	2.071 (2)	8.8 (7)
C90	0.6422 (4)	0.1078 (18)	2.077 (3)	11.2 (9)
C91	0.6675 (5)	0.171 (3)	2.257 (4)	17.6 (16)
F701	-0.1202 (2)	0.3562 (9)	0.7611 (8)	8.6 (4)
F702	-0.1233 (2)	0.1382 (8)	0.5182 (12)	9.3 (4)
F711	-0.1794 (2)	0.5111 (7)	0.5503 (9)	7.1 (3)
F712	-0.1824 (2)	0.2918 (8)	0.3016 (8)	7.5 (3)
F721	-0.2049 (2)	0.2821 (9)	0.8554 (9)	9.0 (4)
F722	-0.2109 (2)	0.0771 (8)	0.6051 (11)	9.7 (4)
F723	-0.2487 (2)	0.2931 (11)	0.6044 (12)	10.9 (5)

Table 2. Selected geometric parameters (Å, °)

C1C2	1.39 (1)	C51-C52	1.36 (1)
C1C6	1.39(1)	C51-C56	1.39(1)
C1-030	1.35 (1)	C51-080	1.38 (1)
C2-C3	1.40(1)	C52C53	1.36(1)
C3C4	1.39(1)	C53	1.39(1)
C4C5	1 37 (1)	C54-C55	1 38 (1)
C4C7	1.49(1)	C54-C57	1.68 (1)
C5 C6	1.49 (1)	C55_C56	1.40(1)
CJ_C0	1.30(1)	C57 058	1.10(1)
C7_00	1.10(1)	C57_O50	1.19(1)
00 010	1.37(1)	050 060	1.30(1)
	1.42(1)	039-000	1.42(1)
	1.37(1)		1.34(1)
	1.37(1)	C60-C65	1.36(1)
C11-C12	1.38(1)	C61C62	1.39(1)
C12C13	1.39(1)	C62—C63	1.38 (1)
C13—C14	1.39 (1)	C63—C64	1.37 (1)
C13-C16	1.48 (1)	C63—C66	1.47 (1)
C14-C15	1.40 (1)	C64—C65	1.39 (1)
C16-017	1.20(1)	C66—O67	1.18(1)
C16-018	1.37 (1)	C66—O68	1.33(1)
O18C19	1.42 (1)	O68-C69	1.44 (1)
C19-C20	1.48 (1)	C69-C70	1.46 (2)
C20-C21	1.53 (1)	C70-C71	1.53 (1)
C20 E20	1.35 (1)	C70_F701	1.35(1)
C20 1201	1.33(1)	C70_F702	1.33(1)
$C_{20} - 1_{202}$	1.57(1)	C71 - C72	1.54(1)
C21-C22	1.32(1)	C71 E711	1.30(1)
C21—F211	1.30(1)	C71 F711	1.34(1)
C21F212	1.34 (1)	C/I—F/I2	1.30(1)
C22—F221	1.28 (1)	C/2—F/21	1.31(1)
C22—F222	1.32(1)	C/2—F/22	1.32(1)
C22—F223	1.29(1)	C72—F723	1.32(1)
O30—C31	1.44 (1)	O80—C81	1.43 (1)
C31C32	1.51 (1)	C81C82	1.53 (1)
C32C33	1.50(1)	C82—C83	1.52 (1)
C33C34	1.54 (1)	C83—C84	1.51 (1)
C34—C35	1.49(1)	C84—C85	1.50(1)
C35C36	1.51 (1)	C85—C86	1.53 (1)
C36—C37	1.50(1)	C86—C87	1.52 (2)
C37—C38	1.48 (2)	C87C88	1.51 (2)
C38-C39	1.50 (2)	C88-C89	1.52 (2)
C39-C40	1.46 (2)	C89—C90	1.49 (2)
C40-C41	1.46 (2)	C90-C91	1.42 (3)
C2 C1 C6	110.0 (9)	C52 C51 C54	121 5 (9)
$C_2 - C_1 - C_0$	119.9 (8)	C32-C31-C30	121.5 (8)
C2C1O30	126.3 (8)	C52-C51-080	124.0(7)
C6-C1-O30	113.8 (7)	C56-C51-080	114.5 (7)
C1C2C3	118.9 (8)	C51-C52-C53	118.4 (8)
C2C3C4	119.8 (8)	C52—C53—C54	122.4 (8)
C3-C4-C5	120.3 (8)	C53—C54—C55	117.7 (8)
C3C4C7	123.0 (8)	C53-C54-C57	118.1 (7)
C5C4C7	116.7 (8)	C55-C54-C57	124.1 (8)
C4C5C6	120.4 (8)	C54—C55—C56	121.4 (8)
C1-C6-C5	120.5 (8)	C51-C56-C55	118.5 (8)
C4—C7—O8	125.9 (9)	C54—C57—O58	125.4 (8)
C4-C7-09	110.8 (7)	C54—C57—O59	110.9 (7)
08	123.3 (9)	O58-C57-O59	123.7 (8)
C7-09-C10	117.5 (7)	C57-059-C60	115.6 (7)
			(-)

09-C10-C11	116.0 (8)	O59-C60-C61	120.0 (8)
09-C10-C15	120.4 (8)	O59—C60—C65	116.8 (8)
C11-C10-C15	123.5 (9)	C61-C60-C65	123.1 (9)
C10-C11-C12	118.3 (9)	C60—C61—C62	119.0 (9)
C11-C12-C13	120.1 (9)	C61-C62-C63	119.6 (9)
C12-C13-C14	120.3 (9)	C62-C63-C64	120.2 (8)
C12-C13-C16	122.8 (9)	C62-C63-C66	123.1 (8)
C14-C13-C16	116.9 (8)	C64-C63-C66	116.7 (8)
C13-C14-C15	119.5 (9)	C63—C64—C65	120.0 (9)
C10-C15-C14	118.2 (9)	C60C65C64	118.1 (9)
C13-C16-017	126.0 (9)	C63-C66-O67	127 (1)
C13-C16-018	111.5 (8)	C63—C66—O68	111.7 (8)
017-C16-018	122.6 (9)	O67C66O68	122 (1)
C16-018-C19	117.2 (8)	C66—O68—C69	116.3 (8)
O18-C19-C20	107.3 (8)	O68-C69-C70	106.5 (9)
C19C20C21	112.9 (8)	C69—C70—C71	112.6 (9)
F201-C20-F202	105.2 (7)	F701-C70-F702	105.7 (8)
C20-C21-C22	119.0 (8)	C70-C71-C72	119.6 (9)
F211-C21-F212	107.6 (8)	F711-C71-F712	107.0 (8)
F221-C22-F222	108.6 (9)	F721-C72-F722	107.1 (9)
F221-C22-F223	108.5 (9)	F721-C72-F723	108.0 (9)
F222-C22-F223	106.9 (9)	F722-C72-F723	106.6 (9)
C1-030-C31	119.8 (7)	C51-080-C81	118.1 (6)
O30-C31-C32	104.7 (7)	O80-C81-C82	107.3 (7)
C31—C32—C33	114.4 (8)	C81C82C83	112.9 (8)
C32—C33—C34	112.7 (8)	C82C83C84	112.4 (8)
C33-C34-C35	116.4 (9)	C83	114.3 (8)
C34-C35-C36	114.8 (9)	C84—C85—C86	113.0 (9)
C35-C36-C37	116.1 (9)	C85-C86-C87	114.3 (9)
C36-C37-C38	115.2 (9)	C86—C87—C88	113.8 (9)
C37C38C39	117.0 (9)	C87C88C89	114 (1)
C38-C39-C40	117 (1)	C88C89C90	114 (1)
C39-C40-C41	118(1)	C89-C90-C91	114 (1)

H atoms were introduced at theoretical positions (Lehman, Koetzel & Hamilton, 1972).

Data collection: CAD-4 Software (Enraf-Nonius, 1977). Cell refinement: CAD-4 Software. Data reduction: SDP (B. A. Frenz & Associates, Inc., 1982). Program(s) used to solve structure: SHELXS86 (Sheldrick, 1985). Program(s) used to refine structure: CRISAF (local program). Molecular graphics: SNOOPI (Davies, 1983); private communication.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: PA1138). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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