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Crystal Structures of Several Fluoro-Mesogens

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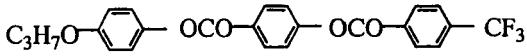
Crystal structures of 4-propyloxyphenyl 4-(4-trifluoromethylbenzoyloxy)benzoate (**I**), *p*-phenylene 4-methoxy-benzoate 4-trifluoromethylbenzoate (**II**), ethyl 4-[2-(perfluorooctyl)ethoxy]benzoate (**III**), and 3-[2-(perfluorooctyl)ethoxy]nitrobenzene (**IV**) have been determined. All the crystals have smectic-like layer structures. In a layer, molecules are arranged in an antiparallel way in **I** and **II**, where CF_3 groups are sorrounded by alkyl groups. In **III** and **IV**, head-to-head arrangements result in the segregation of perfluorochains and the other moieties in bimolecular layers.

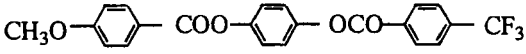
Keywords: crystal structure; fluoro-mesogen; trifluoromethyl group; perfluorooctyl chain; fluorophilic interaction

INTRODUCTION

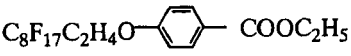
A lot of fluorinated mesogens have been synthesized in order to improve physical properties and chemical stabilities and to modify phase sequencies. In order to elucidate the influence of F atoms on the packing modes of molecules, crystal structures have been determined for following compounds. It is noteworthy that S_A appears for **I** in spite of the relatively short chain length [1] and a mesophase, although monotropic, appears for uni-ring molecules (**III** and **IV**) [2].

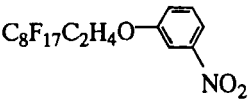
I 

Cryst - 130 - (S_B - 123) - S_A - 215 - iso. (in °C)

II 

Cryst - 231 - N - 233 - iso.

III  Cryst - 80 - (S_A-70) - iso.

IV  Cryst - 55 - (S_A-41) - iso.

EXPERIMENTAL

The synthesis of the compound was described elsewhere [1,2]. Plate-shape single crystals were obtained by slow evaporation from ethyl acetate/ethanol (**I**), dichloromethane/ethanol (**II** and **III**), and ethanol (**IV**).

Cell parameters and reflection intensities were measured on an AFC-7R four-circle diffractometer using CuKα radiation monochromated by graphite (λ= 1.54184 Å). The 2θ-ω mode was applied. Three standard reflections were measured after every 150 reflections. No significant change was observed. For **III** and **IV**, reflection data were collected at 200 K, because data collected at room temperature could not be solved due to the high disorder of perfluoro-chains.. All the reflection data were corrected for Lorentz and polarization factors. Absorption correction was made based on the Ψ-scan for **III** (Tmin/Tmax=0.811 (**I**), 0.908 (**II**), 0.628 (**III**), and 0.927 (**IV**)).

The structures were solved by applying SHELXS86 [3] and refined by full-matrix least-squares method on F^2 by using SHELXL93 [4]. All the non-hydrogen atoms were refined anisotropically. Hydrogen atoms, calculated geometrically were included in structure-factor calculations but not refined. The atomic scattering factors were taken from International Tables for Crystallography [5]. Crystal data and final results of refinements are summarized in TABLE 1. For **II**, systematic absences showed the space group of $P2_1$. However, crystallographically independent two molecules were highly symmetric and reflections h=2n+1 for h0l were relatively weak (about 1/10 of h=2n, on average). Therefore, regarding the structure to be suffered from a pseudo-symmetry, the space group of $P2_1/a$ was applied. The

TABLE 1. Crystal data and experimental details.

	I	II	III	IV
formula	$C_{24}H_{19}O_5F_3$	$C_{22}H_{15}O_5F_3$	$C_{19}H_{13}O_3F_{17}$	$C_{16}H_8O_3F_{17}N$
F. W.	444.39	416.34	612.26	585.23
crystal size	0.2,0.2,0.01	0.2,0.2,0.02	0.2,0.2,0.02	0.3,0.3,0.1
T/K	293	293	200	200
crystal system	monoclinic	monoclinic	triclinic	monoclinic
space group	$P2_1$	$P2_1/a$	P-1	$P2_1/c$
a/Å	7.454(4)	43.658(8)	6.335(11)	20.664(3)
b/Å	5.771(6)	5.609(8)	30.21(3)	8.8851(13)
c/Å	24.234(3)	7.685(7)	5.992(7)	11.297(2)
α/°	90	90	90.29(9)	90
β/°	95.90(3)	91.27(6)	102.56(11)	100.84(2)
γ/°	90	90	91.63(12)	90
V/Å^3	1037.0(12)	1882(3)	1119(3)	2037.1(6)
Z	2	4	2	4
dx/g cm^{-3}	1.423	1.470	1.817	1.908
μ/mm^{-1}	1.000	1.063	1.983	2.159
total refl.	1875	4740	3657	4293
independent refl.	1726	3289	3308	3022
R(int)	0.0447	0.0792	0.0522	0.0418
obs. refl. (>2σ(I))	1358	2068	2108	2520
R1 for obs. refl.	0.0775	0.1308	0.0976	0.0687
Rw2 for obs. refl.	0.2237	0.2664	0.2247	0.2154
S	1.042	1.158	1.209	1.084
Δ/σ	0.285	0.228	0.018	0.028
Δρ/e Å^{-3}	0.412,-0.266	0.272,-0.303	0.361,-0.420	0.980,-0.434

resultant R value was high due to the pseudo-symmetry as well as the disorder of the CF_3 group. For **IV**, the final Fourier difference map gave several peaks of 0.5-1.0 e $Å^{-3}$ around the perfluoro-chain, indicating the chain is still slightly disordered. However, we ignored the disorder because of the small occupancies of the disordered atoms estimated to be only 0.1. Final atomic coordinates and related data have been deposited at the CCDC, Cambridge CB2 1EZ, UK.

RESULTS AND DISCUSSION

Figure 1 shows molecular structures of **I-IV**. Each ester linkage is coplanar with the benzene ring to which the C atom of the linkage is attached in **I** and **II**. The trifluoromethy group in **II** has two disordered conformations. Both of the C-C-C-C backbones of perfluorochains in **III** and **IV** have torsion angles of the same sign: 164-170° (**III**) and 161-173° (**IV**), resulting in the twist of the chains of about 90°. On the other hand, the torsion angles of the roots of the chains, $C(F_2)$-$C(H_2)$-$C(H_2$-O- moieties, are 70.0(10)° (**III**) and 174.9(3)° (**IV**).

Crystal packings are shown in Figs. 2 and 3. All the crystals have smectic-like layer structures: mono- (**I** and **II**) and bimolecular (**III** and **IV**) ones. In **I** and **II**, molecules in a layer are arranged in an anti-parallel way, in which CF_3 groups are srrounded by alkyl groups. In spite of the different direction of the ester linkages in the alkoxy sides, two crystal structures are similar with closely arranged ester linkages (O(2)(x, y, z)...O(4)(-x, -0.5+y, 1-z), 3.17 Å for **I** and O(2)(x, y, z)...

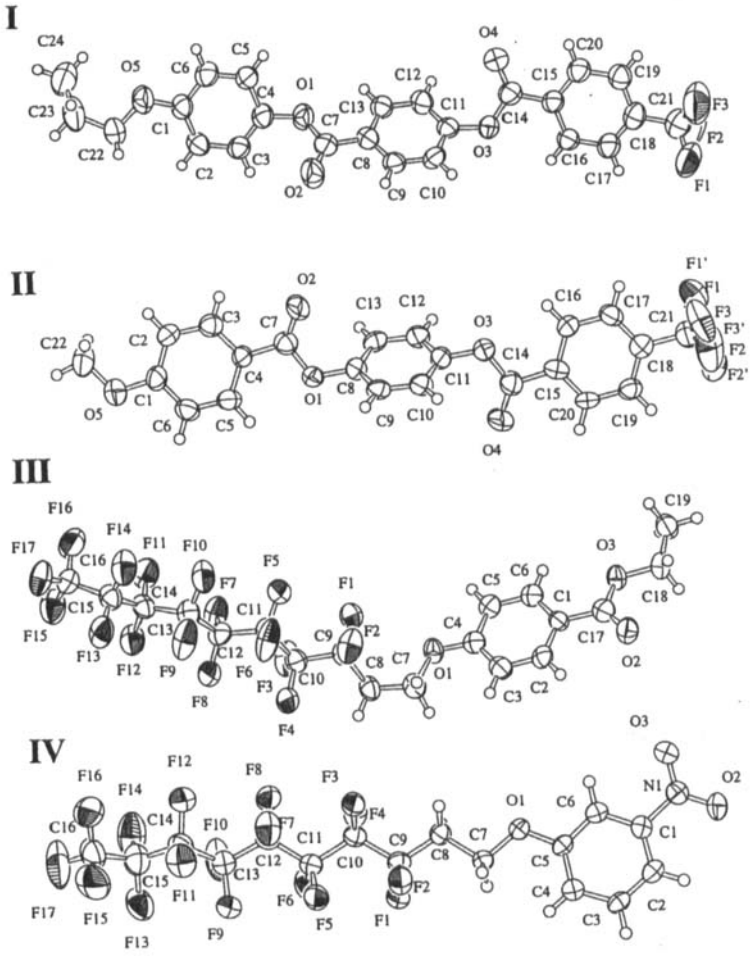


Fig. 1. Molecular structures with numbering schemes. Atoms are shown with 50% probability thermal ellipsoids.

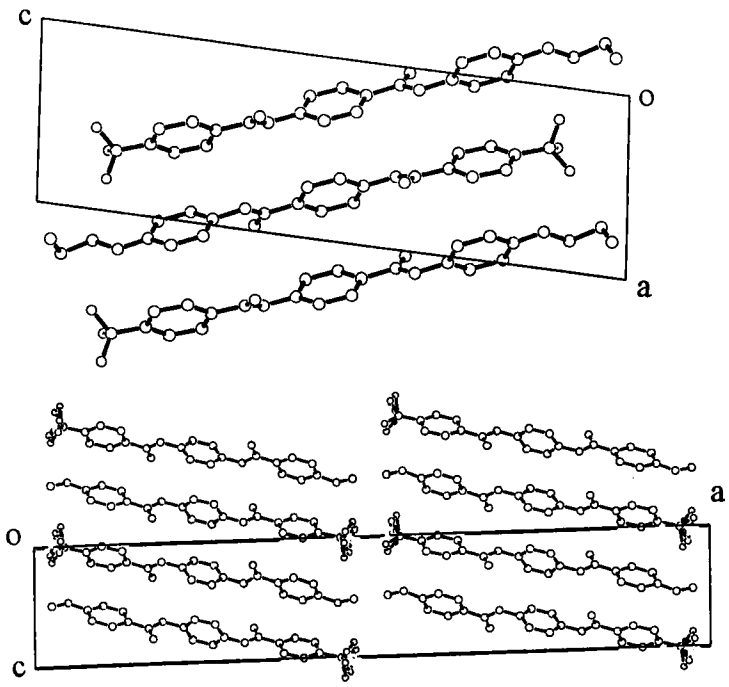


Fig. 2. Crystal structures of I (upper) and II (lower) viwed along the b axes..

O(3)(0.5-x, 0.5+y, -z), 3.18 Å and O(1)(x, y, z)...O(4)(0.5-x, -0.5+y, 1-z), 3.29 Å for **II**).

In **III** and **IV**, head-to-head arrangements result in the segregation of perfluorochains and the other moieties. In **IV**, O atoms of NO_2 group are close to O atoms of adjacent molecules; 3.18 Å for O(3)(x, y, z)...O(3)(1-x, 1-y, 3-z), 3.32 Å for O(1)(x, y, z)...O(2)(1-x,

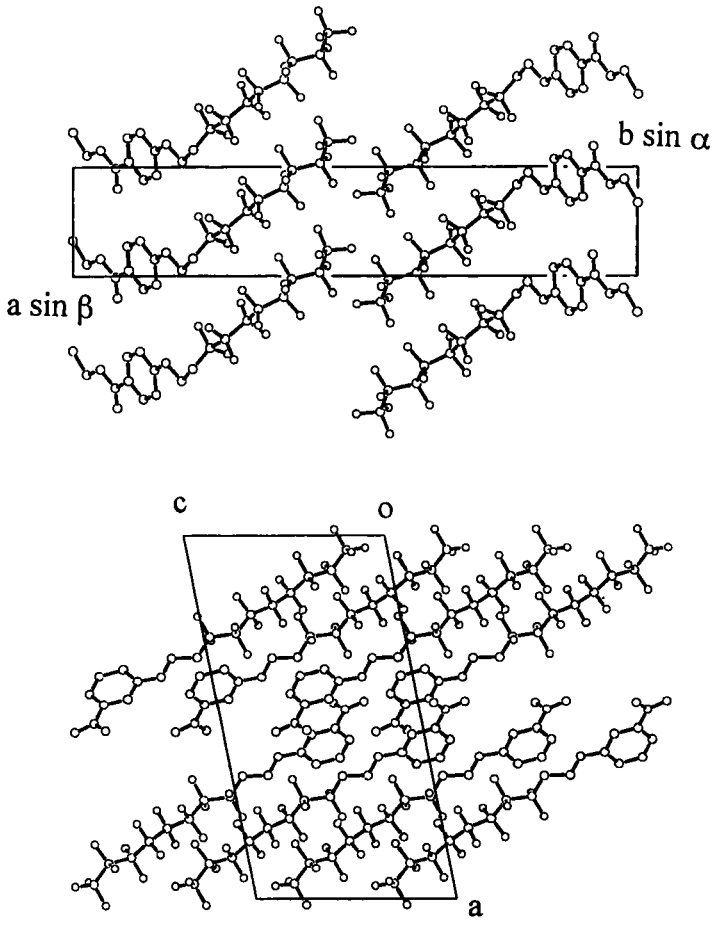


Fig. 3. Crystal structures of **III** (upper) and **IV** (lower) viwed along the c and b axes, respectively.

y, 3-z), and 3.48 Å for O(1)(x, y, z)...O(2)(x, 0.5-y, -0.5+z), suggesting strong intermolecular interactions. On the other hand, ethyl groups face each other in the interface of layers in **III**. In spite of the difference of the end groups, both compounds crystallize in similar packing modes, showing that the crystals are governed by fluorophilic interaction. A similar arrangement was observed in 4-cyanophenyl 4-perfluoroheptylbenzoate [5].

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Table I-1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for I. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	6713(13)	-1007(16)	8808(3)	154(3)
F(2)	8228(9)	1852(23)	8824(2)	193(5)
F(3)	5561(11)	2003(21)	9021(2)	164(4)
O(1)	1150(7)	1874(10)	3548(2)	70(2)
O(2)	309(11)	-1736(13)	3718(2)	114(3)
O(3)	3987(7)	1145(9)	6092(2)	63(1)
O(4)	3713(13)	4966(12)	6236(3)	110(3)
O(5)	-2013(7)	2808(12)	1398(2)	78(2)
C(24)	-1913(17)	4425(25)	247(4)	120(4)
C(23)	-2642(13)	2147(26)	424(4)	102(4)
C(22)	-1709(13)	1182(20)	959(3)	86(3)
C(1)	-1198(9)	2415(15)	1916(3)	61(2)
C(2)	-178(10)	442(15)	2076(3)	65(2)
C(3)	549(10)	205(15)	2623(3)	62(2)
C(4)	330(9)	1903(15)	3001(3)	62(2)
C(5)	-651(9)	3924(14)	2843(3)	60(2)
C(6)	-1386(9)	4122(17)	2306(3)	68(2)
C(7)	1018(11)	78(15)	3878(3)	66(2)
C(8)	1797(9)	478(13)	4449(3)	56(2)
C(9)	1574(9)	-1178(15)	4849(3)	62(2)
C(10)	2278(9)	-884(14)	5390(3)	61(2)
C(11)	3252(9)	1103(13)	5540(3)	56(2)
C(12)	3509(9)	2797(15)	5147(3)	62(2)
C(13)	2778(9)	2507(14)	4605(3)	59(2)
C(14)	4129(10)	3044(16)	6406(3)	64(2)
C(15)	4806(9)	2552(13)	6980(3)	56(2)
C(16)	5700(9)	511(13)	7134(3)	60(2)
C(17)	6301(10)	97(16)	7678(3)	69(2)
C(18)	6017(10)	1669(16)	8082(3)	67(2)
C(19)	5118(10)	3767(16)	7938(3)	68(2)
C(20)	4531(9)	4172(16)	7385(3)	67(2)
C(21)	6649(12)	1184(22)	8674(4)	82(3)

Table I-2. Bond lengths [A] and angles [deg] for I.

F(1)-C(21)	1.306(14)	F(2)-C(21)	1.256(10)
F(3)-C(21)	1.316(12)	O(1)-C(7)	1.320(10)
O(1)-C(4)	1.402(8)	O(2)-C(7)	1.218(10)
O(3)-C(14)	1.332(10)	O(3)-C(11)	1.392(8)
O(4)-C(14)	1.213(11)	O(5)-C(1)	1.356(8)
O(5)-C(22)	1.453(11)	C(24)-C(23)	1.50(2)
C(23)-C(22)	1.514(13)	C(1)-C(6)	1.382(11)
C(1)-C(2)	1.402(11)	C(2)-C(3)	1.386(10)
C(3)-C(4)	1.362(11)	C(4)-C(5)	1.408(11)
C(5)-C(6)	1.363(10)	C(7)-C(8)	1.463(10)
C(8)-C(9)	1.383(11)	C(8)-C(13)	1.411(10)
C(9)-C(10)	1.370(10)	C(10)-C(11)	1.386(11)
C(11)-C(12)	1.392(11)	C(12)-C(13)	1.378(10)
C(14)-C(15)	1.459(10)	C(15)-C(20)	1.386(10)
C(15)-C(16)	1.386(10)	C(16)-C(17)	1.369(10)
C(17)-C(18)	1.367(12)	C(18)-C(19)	1.410(12)
C(18)-C(21)	1.490(12)	C(19)-C(20)	1.385(10)

C(7)-O(1)-C(4)	122.1(6)	C(14)-O(3)-C(11)	124.3(6)
C(1)-O(5)-C(22)	118.7(7)	C(24)-C(23)-C(22)	114.8(10)
O(5)-C(22)-C(23)	107.3(9)	O(5)-C(1)-C(6)	116.5(7)
O(5)-C(1)-C(2)	124.8(7)	C(6)-C(1)-C(2)	118.7(6)
C(3)-C(2)-C(1)	119.5(7)	C(4)-C(3)-C(2)	120.6(8)
C(3)-C(4)-O(1)	123.8(7)	C(3)-C(4)-C(5)	120.5(6)
O(1)-C(4)-C(5)	115.5(7)	C(6)-C(5)-C(4)	118.3(8)
C(5)-C(6)-C(1)	122.3(8)	O(2)-C(7)-O(1)	122.5(7)
O(2)-C(7)-C(8)	123.7(8)	O(1)-C(7)-C(8)	113.8(7)
C(9)-C(8)-C(13)	118.8(7)	C(9)-C(8)-C(7)	119.3(7)
C(13)-C(8)-C(7)	121.9(7)	C(10)-C(9)-C(8)	121.5(7)
C(9)-C(10)-C(11)	119.5(7)	O(3)-C(11)-C(10)	114.3(7)
O(3)-C(11)-C(12)	125.2(7)	C(10)-C(11)-C(12)	120.4(6)
C(13)-C(12)-C(11)	119.9(7)	C(12)-C(13)-C(8)	119.9(7)
O(4)-C(14)-O(3)	123.8(7)	O(4)-C(14)-C(15)	123.6(8)
O(3)-C(14)-C(15)	112.6(7)	C(20)-C(15)-C(16)	119.0(7)
C(20)-C(15)-C(14)	118.9(7)	C(16)-C(15)-C(14)	122.1(7)
C(17)-C(16)-C(15)	120.5(7)	C(18)-C(17)-C(16)	121.0(8)
C(17)-C(18)-C(19)	119.8(7)	C(17)-C(18)-C(21)	120.5(8)
C(19)-C(18)-C(21)	119.7(8)	C(20)-C(19)-C(18)	118.6(8)
C(15)-C(20)-C(19)	121.1(8)	F(2)-C(21)-F(1)	102.4(11)
F(2)-C(21)-F(3)	109.0(10)	F(1)-C(21)-F(3)	101.4(10)
F(2)-C(21)-C(18)	114.5(8)	F(1)-C(21)-C(18)	115.0(9)
F(3)-C(21)-C(18)	113.2(8)		

Table I-3. Anisotropic displacement parameters (A^2 x 10^3) for I.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	240(9)	126(6)	85(4)	38(5)	-35(4)	-24(6)
F(2)	121(5)	344(15)	99(4)	85(7)	-55(3)	-115(7)
F(3)	181(7)	233(11)	77(4)	-1(6)	7(4)	69(8)
O(1)	73(3)	72(4)	61(3)	2(3)	-11(2)	-10(3)
O(2)	186(7)	84(5)	67(4)	6(4)	-12(4)	-52(5)
O(3)	64(3)	61(3)	60(3)	0(3)	-14(2)	4(3)
O(4)	188(8)	64(4)	74(4)	-1(4)	-16(4)	19(5)

O(5)	78(3)	92(4)	59(3)	-6(3)	-14(2)	9(3)
C(24)	146(10)	122(11)	87(6)	22(7)	-8(6)	-2(9)
C(23)	91(6)	146(11)	64(5)	-19(7)	-12(4)	6(7)
C(22)	101(6)	90(7)	64(5)	-13(5)	-15(4)	4(6)
C(1)	52(4)	68(5)	60(4)	-2(4)	-4(3)	-2(4)
C(2)	58(4)	68(6)	67(4)	-15(4)	1(3)	6(4)
C(3)	56(4)	59(5)	69(4)	1(4)	-6(3)	4(4)
C(4)	53(4)	67(5)	62(4)	0(4)	-8(3)	-3(4)
C(5)	57(4)	57(4)	66(4)	3(4)	-1(3)	-6(4)
C(6)	55(4)	73(5)	74(5)	4(5)	-9(3)	5(4)
C(7)	74(5)	57(5)	66(5)	-1(5)	-2(4)	-5(4)
C(8)	41(3)	61(5)	64(4)	-7(4)	-2(3)	4(3)
C(9)	58(4)	53(5)	71(4)	-5(4)	-6(3)	1(4)
C(10)	61(4)	53(4)	67(4)	13(4)	-4(3)	-4(4)
C(11)	49(4)	53(4)	65(4)	-5(4)	-5(3)	11(4)
C(12)	51(4)	64(5)	67(4)	-7(4)	-4(3)	-2(4)
C(13)	55(4)	57(5)	64(4)	-1(4)	1(3)	2(4)
C(14)	60(4)	61(5)	69(5)	0(5)	-4(3)	9(4)
C(15)	50(4)	53(5)	63(4)	1(4)	-5(3)	1(3)
C(16)	55(4)	57(5)	65(4)	-5(4)	-6(3)	6(3)
C(17)	63(4)	71(5)	68(4)	3(5)	-10(4)	2(4)
C(18)	55(4)	80(6)	65(4)	11(5)	-3(3)	-9(4)
C(19)	65(5)	71(6)	67(4)	-1(4)	2(3)	-6(4)
C(20)	61(4)	68(5)	70(4)	3(5)	-5(3)	4(4)
C(21)	64(5)	97(8)	84(6)	9(6)	-5(4)	-10(5)

Table I-4. Hydrogen coordinates (x 10^{-4}) and isotropic displacement parameters (A^{-2} x 10^{-3}) for 1.

	x	y	z	U(eq)
H(24A)	-2583(17)	4919(25)	-92(4)	180
H(24B)	-665(17)	4249(25)	189(4)	180
H(24C)	-2025(17)	5562(25)	530(4)	180
H(23A)	-2541(13)	1023(26)	131(4)	122
H(23B)	-3913(13)	2334(26)	466(4)	122
H(22A)	-2201(13)	-325(20)	1037(3)	104
H(22B)	-427(13)	1011(20)	931(3)	104
H(2)	10(10)	-700(15)	1817(3)	78
H(3)	1193(10)	-1125(15)	2733(3)	75
H(5)	-793(9)	5095(14)	3098(3)	73
H(6)	-2037(9)	5450(17)	2199(3)	82
H(9)	932(9)	-2522(15)	4749(3)	74
H(10)	2103(9)	-2010(14)	5653(3)	73
H(12)	4172(9)	4121(15)	5249(3)	74
H(13)	2932(9)	3646(14)	4343(3)	71
H(16)	5895(9)	-587(13)	6866(3)	72
H(17)	6911(10)	-1273(16)	7774(3)	82
H(19)	4923(10)	4856(16)	8208(3)	82
H(20)	3944(9)	5553(16)	7285(3)	80

Table II-1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for II. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	363(10)	5288(70)	320(69)	146(23)
F(1')	400(11)	5315(75)	-415(107)	214(30)
F(2')	260(5)	2797(67)	1251(36)	107(10)
F(2)	231(6)	1692(70)	606(65)	161(19)
F(3)	392(8)	3084(76)	-1687(51)	126(15)
F(3')	323(8)	1803(93)	-1272(59)	142(17)
O(1)	3103(1)	1460(10)	3480(7)	52(2)
O(2)	3245(2)	4747(16)	2052(11)	100(3)
O(3)	1887(1)	2464(10)	1514(8)	52(2)
O(4)	1745(2)	-969(15)	2750(12)	104(3)
O(5)	4507(2)	1015(14)	5343(10)	82(2)
C(1)	4224(2)	1597(17)	4685(12)	56(2)
C(2)	4158(2)	3676(17)	3760(12)	55(2)
C(3)	3856(2)	4060(17)	3196(12)	58(2)
C(4)	3624(2)	2484(16)	3557(10)	45(2)
C(5)	3699(2)	392(16)	4473(11)	54(2)
C(6)	3992(2)	-24(17)	5013(12)	60(3)
C(7)	3313(2)	3061(18)	2934(12)	56(2)
C(8)	2796(2)	1754(15)	2950(10)	44(2)
C(9)	2665(2)	52(15)	1917(11)	50(2)
C(10)	2361(2)	212(16)	1448(11)	51(2)
C(11)	2194(2)	2135(16)	2027(11)	48(2)
C(12)	2324(2)	3873(16)	3073(11)	52(2)
C(13)	2629(2)	3709(15)	3534(11)	50(2)
C(14)	1681(2)	801(20)	1966(12)	60(3)
C(15)	1364(2)	1446(15)	1394(10)	47(2)
C(16)	1298(2)	3549(16)	506(12)	54(2)
C(17)	997(2)	4082(17)	26(12)	56(2)
C(18)	767(2)	2543(17)	453(11)	53(2)
C(19)	829(2)	446(16)	1354(12)	56(2)
C(20)	1131(2)	-111(15)	1784(12)	55(2)
C(21)	442(3)	3130(23)	-2(18)	71(3)
C(22)	4746(2)	2658(24)	5092(18)	101(4)

Table II-2. Bond lengths [A] and angles [deg] for II.

F(1)-C(21)	1.28(3)	F(1')-C(21)	1.28(4)
F(2')-C(21)	1.27(2)	F(2)-C(21)	1.32(3)
F(3)-C(21)	1.31(4)	F(3')-C(21)	1.32(4)
O(1)-C(7)	1.356(10)	O(1)-C(8)	1.402(10)
O(2)-C(7)	1.197(11)	O(3)-C(14)	1.346(11)
O(3)-C(11)	1.401(10)	O(4)-C(14)	1.191(11)
O(5)-C(1)	1.361(10)	O(5)-C(22)	1.409(12)
C(1)-C(6)	1.388(12)	C(1)-C(2)	1.393(13)
C(2)-C(3)	1.393(12)	C(3)-C(4)	1.379(12)
C(4)-C(5)	1.403(12)	C(4)-C(7)	1.467(12)
C(5)-C(6)	1.359(12)	C(8)-C(9)	1.359(11)
C(8)-C(13)	1.396(12)	C(9)-C(10)	1.369(12)
C(10)-C(11)	1.383(12)	C(11)-C(12)	1.379(12)
C(12)-C(13)	1.373(12)	C(14)-C(15)	1.488(12)
C(15)-C(20)	1.377(12)	C(15)-C(16)	1.390(12)
C(16)-C(17)	1.391(12)	C(17)-C(18)	1.370(12)
C(18)-C(19)	1.389(13)	C(18)-C(21)	1.492(13)
C(19)-C(20)	1.387(12)		

C(7)-O(1)-C(8)	118.7(7)	C(14)-O(3)-C(11)	118.4(7)
C(1)-O(5)-C(22)	117.4(9)	O(5)-C(1)-C(6)	115.7(9)
O(5)-C(1)-C(2)	124.6(9)	C(6)-C(1)-C(2)	119.8(9)
C(3)-C(2)-C(1)	118.3(9)	C(4)-C(3)-C(2)	122.1(9)
C(3)-C(4)-C(5)	118.3(8)	C(3)-C(4)-C(7)	118.2(8)
C(5)-C(4)-C(7)	123.5(8)	C(6)-C(5)-C(4)	120.3(9)
C(5)-C(6)-C(1)	121.3(9)	O(2)-C(7)-O(1)	122.5(9)
O(2)-C(7)-C(4)	125.2(9)	O(1)-C(7)-C(4)	112.3(8)
C(9)-C(8)-C(13)	121.6(8)	C(9)-C(8)-O(1)	118.3(8)
C(13)-C(8)-O(1)	120.1(7)	C(8)-C(9)-C(10)	120.0(8)
C(9)-C(10)-C(11)	118.9(8)	C(12)-C(11)-C(10)	121.6(8)
C(12)-C(11)-O(3)	116.8(8)	C(10)-C(11)-O(3)	121.5(8)
C(13)-C(12)-C(11)	119.3(9)	C(12)-C(13)-C(8)	118.6(8)
O(4)-C(14)-O(3)	124.0(9)	O(4)-C(14)-C(15)	123.8(9)
O(3)-C(14)-C(15)	112.2(8)	C(20)-C(15)-C(16)	120.0(9)
C(20)-C(15)-C(14)	117.9(8)	C(16)-C(15)-C(14)	122.1(8)
C(15)-C(16)-C(17)	119.7(9)	C(18)-C(17)-C(16)	119.7(9)
C(17)-C(18)-C(19)	121.1(9)	C(17)-C(18)-C(21)	120.3(10)
C(19)-C(18)-C(21)	118.6(9)	C(18)-C(19)-C(20)	119.0(9)
C(15)-C(20)-C(19)	120.4(8)	F(2')-C(21)-F(3')	104(2)
F(1)-C(21)-F(3)	100(3)	F(1)-C(21)-F(2)	109(3)
F(3)-C(21)-F(2)	104(2)	F(2')-C(21)-F(1')	104(3)
F(3')-C(21)-F(1')	108(3)	F(1)-C(21)-C(18)	115(2)
F(2')-C(21)-C(18)	113(2)	F(3')-C(21)-C(18)	114(2)
F(3)-C(21)-C(18)	111(2)	F(2)-C(21)-C(18)	117(2)
F(1')-C(21)-C(18)	114(2)		

Table II-3. Anisotropic displacement parameters (A^2 x 10^3) for II.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	70(18)	109(33)	257(38)	-103(35)	-42(21)	30(19)
F(1')	78(19)	107(33)	457(82)	99(38)	-16(35)	28(20)

F(2)	36(9)	175(34)	111(14)	3(16)	20(9)	2(12)
F(2')	87(15)	118(23)	274(57)	59(25)	-72(23)	-36(15)
F(3)	86(19)	189(43)	102(16)	0(22)	-23(13)	57(23)
F(3')	96(18)	194(39)	132(31)	-97(28)	-52(20)	16(21)
O(1)	52(4)	46(3)	58(4)	10(3)	-11(3)	-4(3)
O(2)	59(5)	109(7)	131(7)	76(6)	-8(4)	-1(5)
O(3)	51(4)	44(3)	60(4)	-1(3)	-4(3)	-1(3)
O(4)	67(5)	94(6)	152(8)	81(6)	-2(5)	2(4)
O(5)	62(5)	75(5)	107(6)	9(5)	-23(4)	-3(4)
C(1)	49(6)	56(6)	61(6)	-9(5)	-11(4)	-6(5)
C(2)	52(6)	51(6)	64(6)	5(5)	6(4)	-8(5)
C(3)	62(6)	54(6)	57(6)	-1(5)	0(5)	-1(5)
C(4)	44(5)	47(5)	43(5)	2(4)	-2(4)	-2(4)
C(5)	67(6)	42(5)	55(5)	5(4)	-5(5)	-5(5)
C(6)	68(7)	42(5)	68(6)	1(5)	-8(5)	5(5)
C(7)	58(6)	58(6)	51(6)	8(5)	6(5)	2(5)
C(8)	50(5)	44(5)	39(4)	-6(4)	-5(4)	0(4)
C(9)	66(6)	31(4)	54(5)	-9(4)	-3(4)	-1(4)
C(10)	62(6)	41(5)	49(5)	-7(4)	-12(4)	-2(4)
C(11)	48(5)	53(5)	43(5)	7(4)	-4(4)	-4(4)
C(12)	56(6)	44(5)	55(5)	-8(4)	-1(4)	2(4)
C(13)	64(6)	39(5)	48(5)	-7(4)	0(4)	-12(4)
C(14)	52(6)	71(7)	56(6)	14(5)	0(4)	0(5)
C(15)	68(6)	38(5)	37(4)	0(4)	2(4)	6(4)
C(16)	50(5)	45(5)	67(6)	-3(5)	-4(4)	-8(4)
C(17)	62(6)	49(6)	56(6)	8(5)	-7(4)	6(5)
C(18)	58(6)	51(5)	49(5)	-9(4)	3(4)	-1(5)
C(19)	59(6)	43(5)	65(6)	-3(5)	3(5)	-4(5)
C(20)	62(6)	34(5)	70(6)	18(5)	1(5)	-5(4)
C(21)	59(7)	68(8)	85(9)	-1(7)	-10(7)	3(6)
C(22)	56(7)	96(10)	151(12)	1(9)	-23(7)	-11(7)

Table II-4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for II.

	x	y	z	U(eq)
H(2)	4310(2)	4778(17)	3525(12)	67
H(3)	3810(2)	5425(17)	2554(12)	69
H(5)	3547(2)	-715(16)	4711(11)	65
H(6)	4039(2)	-1422(17)	5614(12)	72
H(9)	2782(2)	-1221(15)	1530(11)	60
H(10)	2270(2)	-953(16)	752(11)	61
H(12)	2207(2)	5143(16)	3461(11)	62
H(13)	2723(2)	4877(15)	4221(11)	60
H(16)	1455(2)	4597(16)	234(12)	65
H(17)	952(2)	5476(17)	-583(12)	67
H(19)	671(2)	-570(16)	1664(12)	67
H(20)	1177(2)	-1545(15)	2340(12)	66
H(22A)	4932(2)	2047(24)	5611(18)	152
H(22B)	4695(2)	4149(24)	5627(18)	152
H(22C)	4773(2)	2895(24)	3869(18)	152

Table III-1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for III. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	-5044(11)	2225(2)	4543(10)	79(2)
F(2)	-3718(10)	2741(2)	7000(12)	85(2)
F(3)	-9038(9)	2415(2)	4654(12)	82(2)
F(4)	-8020(12)	2859(2)	7555(11)	97(2)
F(5)	-6406(10)	2972(2)	2418(11)	85(2)
F(6)	-6243(11)	3422(2)	5246(13)	102(3)
F(7)	-10579(10)	2992(2)	1234(11)	76(2)
F(8)	-10885(10)	3285(2)	4457(11)	82(2)
F(9)	-9111(12)	4038(2)	3584(12)	102(3)
F(10)	-8010(10)	3753(2)	708(13)	92(2)
F(11)	-11912(11)	3644(2)	-1705(10)	82(2)
F(12)	-13369(9)	3764(2)	1173(12)	82(2)
F(13)	-12077(12)	4604(2)	1483(11)	88(2)
F(14)	-10004(10)	4503(2)	-919(13)	93(2)
F(15)	-15579(11)	4353(3)	-1936(13)	101(2)
F(16)	-13489(13)	4332(3)	-4260(12)	103(2)
F(17)	-13751(11)	4936(2)	-2463(12)	92(2)
O(1)	-2607(10)	1648(2)	7849(11)	53(2)
O(2)	6554(11)	809(2)	11908(12)	62(2)
O(3)	5600(9)	501(2)	8387(10)	51(2)
C(1)	3195(13)	999(3)	9470(15)	44(2)
C(2)	2567(15)	1255(3)	11132(16)	50(2)
C(3)	658(15)	1480(3)	10652(17)	56(2)
C(4)	-660(15)	1451(3)	8490(16)	51(2)
C(5)	-66(15)	1194(3)	6802(16)	50(2)
C(6)	1865(15)	971(3)	7277(16)	49(2)
C(7)	-3252(15)	1942(3)	9446(17)	55(2)
C(8)	-5404(14)	2125(3)	8351(17)	55(2)
C(9)	-5361(15)	2445(3)	6443(17)	52(2)
C(10)	-7456(16)	2697(3)	5686(17)	57(2)
C(11)	-7386(16)	3093(3)	4043(17)	56(2)
C(12)	-9644(16)	3275(3)	2951(17)	54(2)
C(13)	-9579(16)	3734(3)	1861(19)	62(3)
C(14)	-11711(15)	3879(3)	265(18)	56(2)
C(15)	-11832(17)	4365(3)	-326(19)	63(3)
C(16)	-13730(19)	4496(4)	-2287(19)	69(3)
C(17)	5283(16)	771(3)	10072(17)	51(2)
C(18)	7583(14)	252(3)	8853(16)	54(2)
C(19)	7703(16)	3(4)	6721(17)	62(3)

Table III-2. Bond lengths [A] and angles [deg] for III.

F(1)-C(9)	1.370(11)	F(2)-C(9)	1.337(11)
F(3)-C(10)	1.339(11)	F(4)-C(10)	1.342(11)
F(5)-C(11)	1.319(11)	F(6)-C(11)	1.324(11)
F(7)-C(12)	1.356(11)	F(8)-C(12)	1.320(11)
F(9)-C(13)	1.358(12)	F(10)-C(13)	1.328(12)
F(11)-C(14)	1.355(11)	F(12)-C(14)	1.323(10)
F(13)-C(15)	1.339(12)	F(14)-C(15)	1.340(12)
F(15)-C(16)	1.297(13)	F(16)-C(16)	1.321(12)
F(17)-C(16)	1.335(12)	O(1)-C(4)	1.364(11)
O(1)-C(7)	1.434(11)	O(2)-C(17)	1.217(11)
O(3)-C(17)	1.347(11)	O(3)-C(18)	1.458(10)
C(1)-C(2)	1.390(12)	C(1)-C(6)	1.399(12)
C(1)-C(17)	1.484(13)	C(2)-C(3)	1.380(13)
C(3)-C(4)	1.381(13)	C(4)-C(5)	1.394(12)
C(5)-C(6)	1.388(13)	C(7)-C(8)	1.500(13)
C(8)-C(9)	1.505(13)	C(9)-C(10)	1.532(13)
C(10)-C(11)	1.559(14)	C(11)-C(12)	1.555(14)
C(12)-C(13)	1.537(13)	C(13)-C(14)	1.552(14)
C(14)-C(15)	1.511(14)	C(15)-C(16)	1.55(2)
C(18)-C(19)	1.496(13)		

C(4)-O(1)-C(7)	118.2(7)	C(17)-O(3)-C(18)	116.6(7)
C(2)-C(1)-C(6)	119.1(8)	C(2)-C(1)-C(17)	118.7(8)
C(6)-C(1)-C(17)	122.1(8)	C(3)-C(2)-C(1)	121.1(9)
C(2)-C(3)-C(4)	119.8(9)	O(1)-C(4)-C(3)	124.7(8)
O(1)-C(4)-C(5)	115.2(8)	C(3)-C(4)-C(5)	120.0(9)
C(6)-C(5)-C(4)	120.2(9)	C(5)-C(6)-C(1)	119.7(8)
O(1)-C(7)-C(8)	108.6(8)	C(7)-C(8)-C(9)	115.0(8)
F(2)-C(9)-F(1)	105.9(8)	F(2)-C(9)-C(8)	111.6(8)
F(1)-C(9)-C(8)	110.4(7)	F(2)-C(9)-C(10)	108.2(8)
F(1)-C(9)-C(10)	106.4(8)	C(8)-C(9)-C(10)	113.9(8)
F(3)-C(10)-F(4)	107.6(9)	F(3)-C(10)-C(9)	109.1(8)
F(4)-C(10)-C(9)	108.4(8)	F(3)-C(10)-C(11)	107.6(8)
F(4)-C(10)-C(11)	107.1(8)	C(9)-C(10)-C(11)	116.6(8)
F(5)-C(11)-F(6)	108.8(9)	F(5)-C(11)-C(12)	109.6(8)
F(6)-C(11)-C(12)	107.1(8)	F(5)-C(11)-C(10)	109.1(8)
F(6)-C(11)-C(10)	107.8(8)	C(12)-C(11)-C(10)	114.2(8)
F(8)-C(12)-F(7)	108.3(8)	F(8)-C(12)-C(13)	109.4(8)
F(7)-C(12)-C(13)	106.2(8)	F(8)-C(12)-C(11)	110.9(8)
F(7)-C(12)-C(11)	107.1(8)	C(13)-C(12)-C(11)	114.6(8)
F(10)-C(13)-F(9)	108.3(9)	F(10)-C(13)-C(12)	109.7(8)
F(9)-C(13)-C(12)	107.5(9)	F(10)-C(13)-C(14)	108.7(9)
F(9)-C(13)-C(14)	106.1(8)	C(12)-C(13)-C(14)	116.3(8)
F(12)-C(14)-F(11)	107.5(8)	F(12)-C(14)-C(15)	109.2(8)
F(11)-C(14)-C(15)	108.0(9)	F(12)-C(14)-C(13)	109.4(8)
F(11)-C(14)-C(13)	106.2(8)	C(15)-C(14)-C(13)	116.2(9)
F(13)-C(15)-F(14)	108.5(9)	F(13)-C(15)-C(14)	110.1(9)
F(14)-C(15)-C(14)	109.9(8)	F(13)-C(15)-C(16)	104.8(8)
F(14)-C(15)-C(16)	106.8(9)	C(14)-C(15)-C(16)	116.3(9)
F(15)-C(16)-F(16)	108.3(11)	F(15)-C(16)-F(17)	109.1(9)
F(16)-C(16)-F(17)	107.6(9)	F(15)-C(16)-C(15)	111.6(9)
F(16)-C(16)-C(15)	110.6(9)	F(17)-C(16)-C(15)	109.5(10)
O(2)-C(17)-O(3)	122.9(9)	O(2)-C(17)-C(1)	124.3(9)
O(3)-C(17)-C(1)	112.7(8)	O(3)-C(18)-C(19)	108.0(7)

Table III-3. Anisotropic displacement parameters (A^2 x 10^3) for III.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
F(1)	107(5)	62(4)	77(4)	7(3)	32(4)	37(3)
F(2)	69(4)	60(4)	113(5)	22(4)	-6(3)	-15(3)
F(3)	63(4)	47(3)	127(5)	23(3)	1(4)	-11(3)
F(4)	134(6)	93(5)	74(4)	17(4)	37(4)	68(5)
F(5)	83(4)	98(5)	85(4)	30(4)	39(4)	33(4)
F(6)	101(5)	42(3)	129(6)	9(4)	-46(4)	-7(3)
F(7)	89(4)	39(3)	88(4)	-2(3)	-8(3)	1(3)
F(8)	91(5)	80(4)	84(4)	33(3)	37(4)	32(4)
F(9)	127(6)	44(3)	104(5)	-19(3)	-41(4)	13(4)
F(10)	59(4)	82(5)	141(6)	53(4)	36(4)	13(3)
F(11)	104(5)	62(4)	71(4)	-10(3)	2(3)	16(3)
F(12)	62(4)	72(4)	114(5)	33(4)	24(4)	4(3)
F(13)	125(6)	52(4)	81(4)	-6(3)	4(4)	30(4)
F(14)	67(4)	71(4)	139(6)	37(4)	18(4)	-3(3)
F(15)	62(4)	105(6)	131(6)	34(5)	9(4)	8(4)
F(16)	140(6)	95(5)	72(5)	13(4)	13(4)	40(5)
F(17)	101(5)	58(4)	108(5)	27(4)	3(4)	22(3)
O(1)	56(4)	39(3)	62(4)	-7(3)	7(3)	11(3)
O(2)	61(4)	60(4)	61(4)	-2(3)	2(4)	10(3)
O(3)	51(4)	40(3)	60(4)	-1(3)	7(3)	9(3)
C(1)	47(5)	42(5)	48(5)	3(4)	18(4)	6(4)
C(2)	59(6)	34(5)	56(6)	8(4)	13(5)	2(4)
C(3)	56(6)	53(6)	61(6)	1(5)	19(5)	4(5)
C(4)	56(6)	45(5)	52(6)	1(4)	13(5)	-1(4)
C(5)	58(6)	36(5)	53(6)	-2(4)	8(4)	-1(4)
C(6)	59(6)	34(5)	55(6)	1(4)	15(5)	-2(4)
C(7)	58(6)	40(5)	71(7)	5(5)	20(5)	0(4)
C(8)	50(6)	45(5)	73(7)	7(5)	21(5)	6(4)
C(9)	55(6)	34(5)	68(6)	7(5)	16(5)	3(4)
C(10)	66(6)	45(6)	61(6)	-3(5)	17(5)	9(5)
C(11)	60(6)	47(6)	57(6)	-2(5)	6(5)	7(5)
C(12)	70(6)	36(5)	56(6)	7(4)	19(5)	-2(5)
C(13)	58(6)	47(6)	79(7)	4(5)	11(5)	0(5)
C(14)	49(6)	49(6)	74(7)	8(5)	22(5)	2(4)
C(15)	64(7)	49(6)	79(7)	5(5)	21(6)	6(5)
C(16)	77(8)	69(8)	62(7)	16(6)	18(6)	20(6)
C(17)	61(6)	35(5)	61(6)	3(5)	18(5)	0(4)
C(18)	49(5)	43(5)	64(6)	1(5)	1(5)	7(4)
C(19)	54(6)	68(7)	64(6)	-5(5)	12(5)	12(5)

Table III-4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for III.

	x	y	z	U(eq)
H(2)	3466(15)	1275(3)	12623(16)	60
H(3)	252(15)	1654(3)	11806(17)	67
H(5)	-984(15)	1171(3)	5322(16)	60
H(6)	2281(15)	800(3)	6117(16)	59
H(7A)	-2162(15)	2187(3)	9872(17)	66
H(7B)	-3364(15)	1781(3)	10851(17)	66
H(8A)	-5989(14)	2277(3)	9545(17)	66
H(8B)	-6412(14)	1875(3)	7745(17)	66
H(18A)	7571(14)	43(3)	10118(16)	64
H(18B)	8856(14)	456(3)	9305(16)	64
H(19A)	9026(16)	-167(4)	6994(17)	93
H(19B)	7721(16)	213(4)	5483(17)	93
H(19C)	6440(16)	-199(4)	6291(17)	93

Table IV-1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for IV. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
F(1)	2895(2)	-1505(3)	9677(3)	63(1)
F(2)	2235(1)	241(4)	10103(2)	65(1)
F(3)	2527(1)	2025(3)	8382(2)	55(1)
F(4)	3280(1)	507(4)	8017(2)	59(1)
F(5)	1676(2)	-657(5)	7978(3)	82(1)
F(6)	2475(2)	-1588(3)	7187(3)	76(1)
F(7)	1497(2)	1600(4)	6513(3)	71(1)
F(8)	2420(1)	1254(4)	5927(3)	67(1)
F(9)	1212(2)	-1477(4)	5675(3)	99(1)
F(10)	2045(2)	-1156(5)	4780(3)	93(1)
F(11)	560(2)	710(4)	4565(3)	83(1)
F(12)	1398(2)	1683(4)	3995(3)	77(1)
F(13)	827(2)	-1952(4)	3280(4)	91(1)
F(14)	1503(2)	-494(6)	2512(3)	107(2)
F(15)	-171(2)	-115(6)	2459(5)	119(2)
F(16)	459(2)	1472(5)	1826(4)	100(1)
F(17)	342(3)	-737(7)	1097(4)	145(2)
O(1)	3902(1)	1151(3)	12520(2)	43(1)
O(2)	5420(2)	2249(4)	17349(3)	53(1)
O(3)	5380(2)	3676(4)	15792(3)	70(1)
N(1)	5190(2)	2597(4)	16300(3)	45(1)
C(1)	4666(2)	1648(4)	15627(4)	37(1)
C(2)	4363(2)	600(5)	16235(4)	41(1)
C(3)	3874(2)	-279(5)	15578(4)	43(1)
C(4)	3698(2)	-118(5)	14329(4)	42(1)
C(5)	4019(2)	932(5)	13747(3)	36(1)
C(6)	4505(2)	1846(5)	14387(4)	38(1)
C(7)	3388(2)	282(5)	11823(4)	42(1)
C(8)	3367(2)	745(5)	10521(4)	41(1)
C(9)	2803(2)	9(5)	9699(4)	45(1)
C(10)	2700(2)	566(5)	8392(4)	42(1)
C(11)	2180(2)	-297(5)	7465(4)	49(1)
C(12)	1923(2)	544(5)	6274(4)	48(1)
C(13)	1573(2)	-439(6)	5234(4)	55(1)
C(14)	1135(2)	369(6)	4186(5)	55(1)
C(15)	967(3)	-511(7)	3024(6)	74(2)
C(16)	402(3)	36(8)	2059(6)	85(2)

Table IV-2. Bond lengths [A] and angles [deg] for IV.

F(1)-C(9)	1.360(5)	F(2)-C(9)	1.352(5)
F(3)-C(10)	1.344(5)	F(4)-C(10)	1.345(5)
F(5)-C(11)	1.323(5)	F(6)-C(11)	1.363(6)
F(7)-C(12)	1.349(5)	F(8)-C(12)	1.326(5)
F(9)-C(13)	1.339(6)	F(10)-C(13)	1.345(6)
F(11)-C(14)	1.370(6)	F(12)-C(14)	1.322(6)
F(13)-C(15)	1.355(8)	F(14)-C(15)	1.342(7)
F(15)-C(16)	1.351(9)	F(16)-C(16)	1.312(8)
F(17)-C(16)	1.272(8)	O(1)-C(5)	1.376(5)
O(1)-C(7)	1.425(5)	O(2)-N(1)	1.230(5)
O(3)-N(1)	1.220(5)	N(1)-C(1)	1.467(6)
C(1)-C(2)	1.375(6)	C(1)-C(6)	1.389(6)
C(2)-C(3)	1.380(6)	C(3)-C(4)	1.397(6)
C(4)-C(5)	1.382(6)	C(5)-C(6)	1.384(6)
C(7)-C(8)	1.520(6)	C(8)-C(9)	1.497(6)
C(9)-C(10)	1.534(6)	C(10)-C(11)	1.554(6)
C(11)-C(12)	1.543(7)	C(12)-C(13)	1.531(7)
C(13)-C(14)	1.528(7)	C(14)-C(15)	1.511(8)
C(15)-C(16)	1.520(8)		

C(5)-O(1)-C(7)	116.8(3)	O(3)-N(1)-O(2)	123.5(4)
O(3)-N(1)-C(1)	118.7(4)	O(2)-N(1)-C(1)	117.9(4)
C(2)-C(1)-C(6)	123.0(4)	C(2)-C(1)-N(1)	119.4(4)
C(6)-C(1)-N(1)	117.6(4)	C(1)-C(2)-C(3)	118.1(4)
C(2)-C(3)-C(4)	120.7(4)	C(5)-C(4)-C(3)	119.5(4)
O(1)-C(5)-C(4)	124.5(4)	O(1)-C(5)-C(6)	114.6(3)
C(4)-C(5)-C(6)	120.9(4)	C(5)-C(6)-C(1)	117.7(4)
O(1)-C(7)-C(8)	105.7(3)	C(9)-C(8)-C(7)	111.1(3)
F(2)-C(9)-F(1)	106.9(4)	F(2)-C(9)-C(8)	110.3(3)
F(1)-C(9)-C(8)	110.3(4)	F(2)-C(9)-C(10)	107.7(4)
F(1)-C(9)-C(10)	107.3(3)	C(8)-C(9)-C(10)	114.0(4)
F(3)-C(10)-F(4)	106.7(3)	F(3)-C(10)-C(9)	107.9(3)
F(4)-C(10)-C(9)	108.6(3)	F(3)-C(10)-C(11)	108.8(4)
F(4)-C(10)-C(11)	108.2(3)	C(9)-C(10)-C(11)	116.3(4)
F(5)-C(11)-F(6)	108.7(4)	F(5)-C(11)-C(12)	109.2(4)
F(6)-C(11)-C(12)	107.6(4)	F(5)-C(11)-C(10)	109.0(4)
F(6)-C(11)-C(10)	106.7(4)	C(12)-C(11)-C(10)	115.4(4)
F(8)-C(12)-F(7)	107.4(4)	F(8)-C(12)-C(13)	109.0(4)
F(7)-C(12)-C(13)	108.6(4)	F(8)-C(12)-C(11)	109.2(4)
F(7)-C(12)-C(11)	107.0(4)	C(13)-C(12)-C(11)	115.3(4)
F(9)-C(13)-F(10)	108.1(5)	F(9)-C(13)-C(14)	108.7(4)
F(10)-C(13)-C(14)	107.1(4)	F(9)-C(13)-C(12)	108.8(4)
F(10)-C(13)-C(12)	106.9(4)	C(14)-C(13)-C(12)	116.8(4)
F(12)-C(14)-F(11)	105.2(4)	F(12)-C(14)-C(15)	110.5(5)
F(11)-C(14)-C(15)	108.4(4)	F(12)-C(14)-C(13)	109.8(4)
F(11)-C(14)-C(13)	106.5(4)	C(15)-C(14)-C(13)	115.8(5)
F(14)-C(15)-F(13)	109.2(5)	F(14)-C(15)-C(14)	107.2(5)
F(13)-C(15)-C(14)	109.1(5)	F(14)-C(15)-C(16)	105.8(6)
F(13)-C(15)-C(16)	106.8(5)	C(14)-C(15)-C(16)	118.5(5)
F(17)-C(16)-F(16)	110.6(7)	F(17)-C(16)-F(15)	106.4(6)
F(16)-C(16)-F(15)	106.3(6)	F(17)-C(16)-C(15)	112.2(6)
F(16)-C(16)-C(15)	111.7(5)	F(15)-C(16)-C(15)	109.4(6)

Table IV-3. Anisotropic displacement parameters (A^2 x 10^3) for IV.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

U11	U22	U33	U23	U13	U12

F(1)	83(2)	43(2)	57(2)	1(1)	-2(1)	-12(1)
F(2)	44(2)	103(2)	50(2)	-1(2)	17(1)	-14(2)
F(3)	68(2)	44(2)	51(2)	-2(1)	5(1)	-1(1)
F(4)	45(1)	89(2)	47(1)	-3(1)	16(1)	-2(1)
F(5)	66(2)	122(3)	57(2)	11(2)	7(1)	-49(2)
F(6)	101(2)	49(2)	65(2)	-10(1)	-16(2)	10(2)
F(7)	75(2)	71(2)	63(2)	-15(2)	7(2)	23(2)
F(8)	57(2)	85(2)	57(2)	13(2)	9(1)	-17(2)
F(9)	125(3)	82(2)	73(2)	24(2)	-26(2)	-55(2)
F(10)	87(2)	106(3)	75(2)	-33(2)	-13(2)	47(2)
F(11)	52(2)	108(3)	89(2)	-6(2)	16(2)	10(2)
F(12)	83(2)	67(2)	73(2)	14(2)	-2(2)	-17(2)
F(13)	109(3)	57(2)	91(2)	-10(2)	-24(2)	6(2)
F(14)	83(2)	170(4)	69(2)	-17(2)	14(2)	27(3)
F(15)	67(2)	124(4)	148(4)	20(3)	-26(2)	-10(2)
F(16)	90(3)	90(3)	105(3)	33(2)	-17(2)	-3(2)
F(17)	182(5)	140(4)	82(3)	-29(3)	-56(3)	36(4)
O(1)	50(2)	46(2)	34(1)	1(1)	10(1)	-9(1)
O(2)	58(2)	61(2)	38(2)	-8(1)	4(1)	5(2)
O(3)	86(3)	61(2)	59(2)	3(2)	1(2)	-29(2)
N(1)	50(2)	43(2)	45(2)	-6(2)	12(2)	3(2)
C(1)	39(2)	36(2)	38(2)	-6(2)	12(2)	7(2)
C(2)	48(2)	40(2)	37(2)	2(2)	16(2)	10(2)
C(3)	50(2)	45(2)	37(2)	6(2)	19(2)	5(2)
C(4)	42(2)	41(2)	45(2)	1(2)	11(2)	1(2)
C(5)	40(2)	38(2)	34(2)	3(2)	14(2)	7(2)
C(6)	40(2)	36(2)	39(2)	1(2)	15(2)	3(2)
C(7)	44(2)	43(2)	39(2)	0(2)	10(2)	-5(2)
C(8)	43(2)	43(2)	39(2)	-2(2)	13(2)	-3(2)
C(9)	45(2)	45(2)	48(2)	-1(2)	16(2)	-3(2)
C(10)	41(2)	41(2)	47(2)	-3(2)	16(2)	-3(2)
C(11)	52(3)	46(3)	49(2)	-1(2)	10(2)	-7(2)
C(12)	40(2)	48(3)	58(3)	-1(2)	15(2)	-3(2)
C(13)	57(3)	56(3)	53(3)	0(2)	7(2)	-2(2)
C(14)	43(2)	54(3)	65(3)	4(2)	5(2)	-5(2)
C(15)	76(4)	74(4)	67(4)	-7(3)	-2(3)	12(3)
C(16)	74(4)	84(4)	83(4)	-1(4)	-22(3)	-4(4)

Table IV-4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for IV.

	x	y	z	U(eq)
H(2)	4488(2)	485(5)	17084(4)	49
H(3)	3654(2)	-1002(5)	15980(4)	51
H(4)	3360(2)	-727(5)	13883(4)	51
H(6)	4720(2)	2584(5)	13992(4)	45
H(7A)	2961(2)	498(5)	12067(4)	50
H(7B)	3483(2)	-807(5)	11931(4)	50
H(8A)	3321(2)	1852(5)	10450(4)	49
H(8B)	3785(2)	456(5)	10277(4)	49