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− Supporting Information −

Synthesis, Characterization and Applications of Fluorous Resorcin[4]arenes

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I. Experimental Procedures and Spectroscopic Data for Compounds **1a-c**

General Remarks: Chemicals and solvents were purchased from commercial suppliers and used as received. Flash column chromatography was performed with 230–400 mesh silica gel purchased from Sorbent Technologies as the stationary phase. Proton (^{1}H), carbon (^{13}C) and fluorine (^{19}F) nuclear magnetic resonance spectra were measured on a Bruker Avance 300 instrument at 300 MHz, 75 MHz and 282 MHz respectively. The chemical shifts in spectra were measured in parts per million (ppm) on the delta (δ) scale relative to the resonance of the solvent peak (MeOD signal as reference, ^{1}H = 3.31 ppm, ^{13}C = 49.0 ppm). ^{19}F chemical shifts are given relative to $CFCl_3$ (^{19}F = 0 ppm). NMR spectra were recorded in MeOD at 300 K. The following abbreviations were used to describe coupling: s = singlet; d = doublet; t = triplet; q = quartet; br = broad; m = multiplet.

Experimental Procedures:

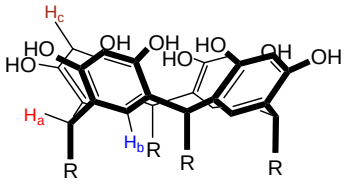
Fluorous resorcin[4]arene 1a: Resorcinol (0.11 g, 1.0 mmol) and *2H,2H,3H,3H*-Perfluoroheptan-1-al (0.28 g, 1.0 mmol) were dissolved in ethanol (5.0 mL). Concentrated hydrochloric acid (0.3 mL) was added under argon. After refluxing for 72 h, the reaction mixture was concentrated. The residue was purified on a column of silica gel with hexane/EtOAc/ (4:7). The fluorous resorcin[4]arene **1a** (0.25 g, 0.17 mmol, 68%) was isolated as a white solid. ^{1}H NMR (300 MHz, MeOD) δ = 7.06 (s, 4H), 6.32 (s, 4H), 4.50 (t, 4H), 2.30 (m, 8H), 2.05 (m, 8 H); partial ^{13}C NMR (75 MHz, MeOD) δ = 153.3, 124.5, 123.0, 119.5 (m), 115.5 (m), 103.2, 33.8, 30.0, 25.5 ppm; ^{19}F NMR (282 MHz, MeOD) δ = -82.4 (s, 12F), -115.5 (s, 8F), -125.8 (s, 8F), -127.9 (s, 8F) ppm.

Fluorous resorcin[4]arene 1b: Resorcinol (0.11 g, 1.0 mmol) and *2H,2H,3H,3H*-Perfluorononan-1-al (0.38 g, 1.0 mmol) were dissolved in ethanol (5.0 mL). Concentrated hydrochloric acid (0.3 mL) was added under argon. After refluxing for 72 h, the reaction mixture was concentrated. The residue was purified on a column of silica gel with hexane/EtOAc (1:3). The fluorous resorcin[4]arene **1b** (0.34 g, 0.18 mmol, 72%) was isolated as a white solid. ^{1}H NMR (300 MHz, MeOD) δ = 7.09 (s, 4H), 6.33 (s, 4H), 4.50 (t, 4H), 2.32 (m, 8H), 2.06 (m, 8 H); partial ^{13}C NMR (75 MHz, MeOD) δ = 153.4, 124.3, 123.0, 119.5 (m), 115.5 (m), 111.8 (m), 103.4, 33.5, 30.0, 25.5 ppm; ^{19}F NMR (282 MHz, MeOD) δ = -82.3 (s, 13F), -115.1 (s, 8F), -123.6 (s, 8F), -124.4 (s, 8F), -124.6 (s, 8F), -128.0 (s, 8F) ppm.

Fluorous resorcin[4]arene 1c: Resorcinol (0.11 g, 1.0 mmol) and *2H,2H,3H,3H*-Perfluoroundecan-1-al (0.48 g, 1.0 mmol) were dissolved in ethanol (5.0 mL). Concentrated hydrochloric acid (0.3 mL) was added under argon. After refluxing for 72 h, the reaction mixture was concentrated. The residue was purified on a column of silica gel with hexane/EtOAc (1:3). The fluorous resorcin[4]arene **1c** (0.43 g, 0.19 mmol, 76%) was isolated as a white solid. ^{1}H NMR (300 MHz, MeOD) δ = 7.12 (s, 4H), 6.33 (s, 4H), 4.49 (t, 4H), 2.36 (m, 8H), 2.07 (m, 8 H); partial ^{13}C NMR (75 MHz, MeOD) δ = 153.5, 123.8, 123.0, 119.5 (m), 115.5 (m), 111.8 (m), 108.0 (m), 103.7, 33.3, 30.0, 25.5 ppm; ^{19}F NMR (282 MHz, MeOD) δ = -82.2 (s, 12F), -115.0 (s, 8F), -125.6 (s, 24F), -124.1 (s, 8F), -124.7 (s, 8F), -128.2 (s, 8F) ppm.

II. Comparison of ^{1}H, ^{13}C and ^{19}F NMR Spectra

In order to bind its guest(s) and form a molecular assembly, a host needs to exhibit both electronic and steric complementarity to the guest(s). Therefore, it is necessary to measure the effects of electron-withdrawing fluorous tag on the resorcin[4]arenes. The compound **2** and **1a-c** were dissolved in the same deuterated solvent (MeOD) to determine the effects by both ^{1}H and ^{13}C NMR. A comparison of ^{1}H and ^{13}C NMR of resorcin[4]arenes **1a-c** and **2** are shown in Figure 1. Among them, compound **2** and **1c** have tags with similar length. While the protons on the bridging sp^3 C (H_a) shifted downfield for 0.16 ppm from **2** to **1c**, the chemical shifts of two protons on the aromatic rings shifted -0.11 ppm for H_b on the lower rim and 0.06 ppm for H_c on the upper rim, respectively. Meanwhile, the ^{13}C chemical shifts of the aromatic carbons of **1c** were changed only by about 1 ppm comparing to those of **2**. Thus, although the strong electron withdrawing effects of fluorous alkyl chains have not been completely insulated, they are mostly reduced by the sp^3 C spacers.



1: R = $-CH_2CH_2(CF_2)_nF$, (**1a**, n = 4; **1b**, n = 6; **1c**, n = 8), **2**: R = $-C_{11}H_{23}$

Scheme 2. Fluorous Resorcin[4]arenes **1a-c** and their organic variant **2**.

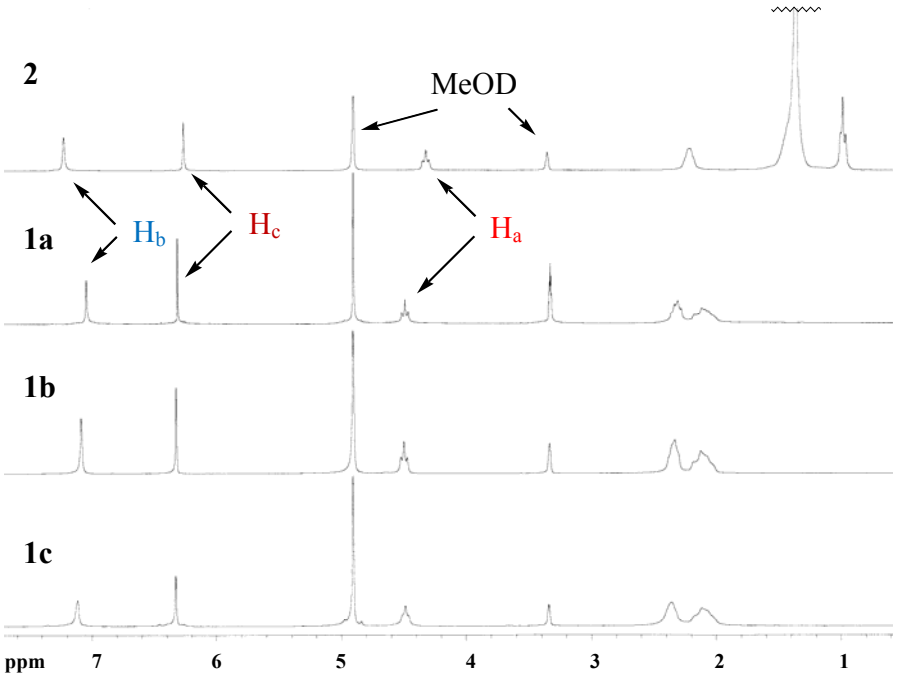


Figure 1. Comparison of ^{1}H NMR of compounds **2** and **1a-c**.

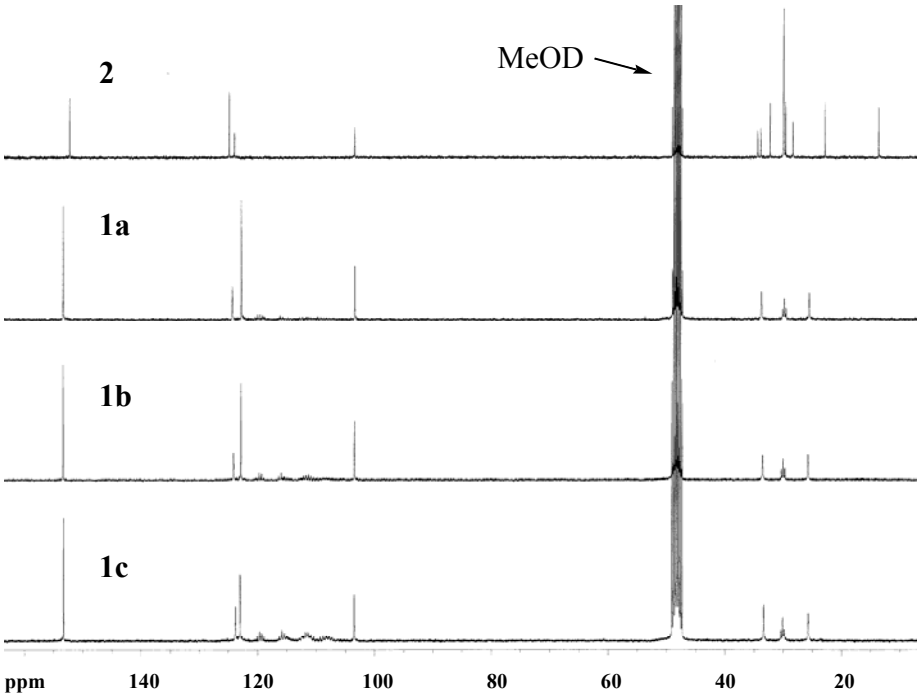


Figure 2. Comparison of ^{13}C NMR of compounds **2** and **1a-c**.

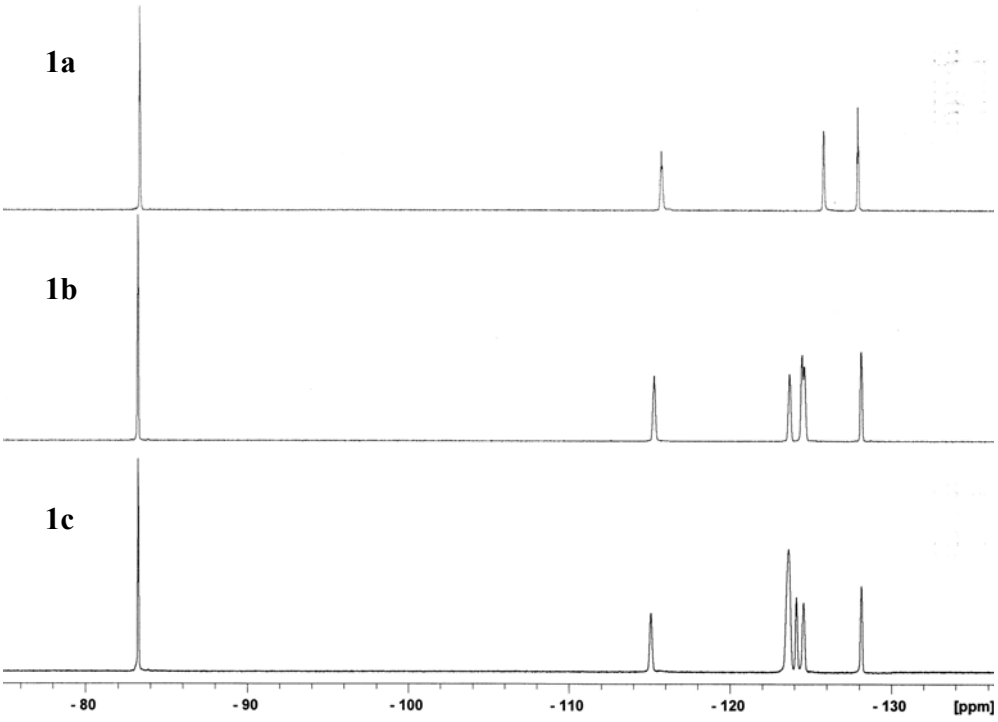


Figure 3. Comparison of ^{19}F NMR of compounds **1a-c**.

III. X-ray Data of **1b**

Table 1. Crystal data and structure refinement for rcc129s.

Identification code	rcc129s	
Empirical formula	C80 H64 F52 O12	
Formula weight	2205.31	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.6231(15) Å	α= 72.853(3)°.
	b = 18.888(3) Å	β= 86.220(3)°.
	c = 24.412(3) Å	γ = 76.854(3)°.
Volume	4557.9(11) $Å^3$	
Z	2	
Density (calculated)	1.607 Mg/m^3	
Absorption coefficient	0.177 mm^{-1}	
F(000)	2216	
Crystal size	0.25 x 0.12 x 0.12 mm^3	
Theta range for data collection	1.64 to 25.00°.	
Index ranges	-12<=h<=12, -22<=k<=22, -29<=l<=29	
Reflections collected	36782	
Independent reflections	16051 [R(int) = 0.0798]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	multi-scan (SADABS)	
Max. and min. transmission	0.9791 and 0.9571	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16051 / 0 / 1262	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.1221, wR2 = 0.3201	
R indices (all data)	R1 = 0.2157, wR2 = 0.3713	
Largest diff. peak and hole	1.749 and -0.814 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for rcc129s. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9548(6)	12682(4)	8129(3)	29(2)
F(1)	9846(7)	11089(3)	6551(2)	82(2)
O(1)	11050(5)	13779(3)	8798(2)	38(1)
C(2)	9764(6)	13315(4)	8244(3)	32(2)
F(2)	7846(6)	11207(4)	6804(3)	102(2)
O(2)	11934(4)	11154(3)	9048(2)	33(1)
C(3)	10748(6)	13199(4)	8635(3)	30(2)
F(3)	10159(6)	9531(3)	6977(3)	83(2)
O(3)	10991(4)	9913(3)	9099(2)	34(1)
C(4)	11472(6)	12484(4)	8881(3)	30(2)
F(4)	8136(7)	9689(4)	7163(3)	106(2)
O(4)	6828(4)	9737(3)	9967(2)	31(1)
C(5)	11206(6)	11860(4)	8761(3)	28(2)
O(5)	5567(5)	10976(3)	10366(2)	37(1)
F(5)	9370(30)	10397(12)	5859(4)	369(17)
C(6)	10240(6)	11939(4)	8381(3)	29(2)
O(6)	4530(5)	13644(3)	10041(2)	38(1)
F(6)	7620(14)	10410(7)	6066(5)	236(9)
C(7)	9980(7)	11254(4)	8247(3)	30(2)
O(7)	4914(5)	15076(3)	9410(2)	45(1)
F(7)	10088(14)	9420(30)	5945(9)	650(40)
C(8)	9145(6)	10853(4)	8713(3)	23(1)
O(8)	9155(5)	15086(3)	8624(3)	49(1)
F(8)	8833(15)	8734(5)	6490(3)	205(7)
C(9)	9670(6)	10181(4)	9126(3)	24(2)
O(9)	822(6)	4135(4)	613(4)	84(2)
F(9)	8416(8)	9949(4)	5072(2)	104(2)
C(10)	8929(6)	9805(4)	9543(3)	29(2)
O(10)	8493(5)	1482(3)	183(2)	43(1)
F(10)	6984(10)	9317(9)	5620(13)	450(20)
C(11)	7623(6)	10096(4)	9552(3)	25(2)

O(11)	4228(6)	3043(3)	1237(2)	59(2)
F(11)	10054(13)	8800(10)	5307(11)	350(15)
C(12)	7024(6)	10766(4)	9149(3)	26(2)
O(12)	6001(6)	2823(3)	7536(2)	55(2)
F(12)	8239(13)	8694(7)	4829(4)	181(5)
C(13)	7814(6)	11126(4)	8743(3)	27(2)
F(13)	8585(9)	8041(5)	5713(4)	133(3)
C(14)	5574(6)	11089(4)	9157(3)	27(2)
F(14)	5100(5)	10982(3)	7440(2)	54(1)
C(15)	5281(6)	11783(4)	9382(3)	26(2)
F(15)	3244(4)	10901(3)	7848(2)	55(1)
C(16)	5282(6)	11682(4)	9968(3)	32(2)
F(16)	5844(5)	9429(3)	7769(3)	70(2)
C(17)	5022(7)	12293(4)	10187(3)	35(2)
F(17)	3984(6)	9361(3)	8166(2)	81(2)
C(18)	4766(6)	13028(4)	9822(3)	32(2)
F(18)	4709(12)	10171(5)	6768(3)	161(5)
C(19)	4759(6)	13163(4)	9228(3)	28(2)
F(19)	2902(9)	10191(7)	7123(5)	222(7)
C(20)	5016(6)	12527(4)	9027(3)	27(2)
F(20)	4918(9)	8534(5)	7315(5)	177(5)
C(21)	4515(7)	13969(4)	8841(3)	32(2)
F(21)	3006(12)	8855(6)	7387(4)	182(5)
C(22)	5734(7)	14294(4)	8777(3)	30(2)
F(22)	4754(9)	9140(7)	6117(5)	192(5)
C(23)	5874(7)	14794(4)	9073(3)	34(2)
F(23)	2776(7)	9673(4)	6233(3)	97(2)
C(24)	7023(7)	15059(4)	9023(3)	39(2)
F(24)	4316(9)	7786(4)	6611(4)	144(4)
C(25)	7997(7)	14836(4)	8670(3)	33(2)
F(25)	3149(8)	8422(5)	5876(3)	128(3)
C(26)	7886(6)	14351(4)	8362(3)	29(2)
F(26)	2241(11)	8370(8)	6703(7)	260(8)
C(27)	6758(6)	14077(4)	8426(3)	27(2)
F(27)	3624(5)	14721(3)	7036(2)	58(1)
C(28)	8976(7)	14115(4)	7967(3)	36(2)

F(28)	1755(4)	14787(3)	7446(2)	62(1)
C(29)	9408(7)	11419(4)	7644(3)	33(2)
F(29)	3554(5)	16185(3)	6926(2)	71(2)
C(30)	9400(8)	10673(4)	7524(3)	39(2)
F(30)	1805(6)	16284(3)	7422(2)	81(2)
C(31)	9036(7)	10761(5)	6924(3)	42(2)
F(31)	1543(6)	16957(3)	6309(3)	87(2)
C(32)	9018(8)	10004(5)	6809(4)	51(2)
F(32)	445(5)	16085(4)	6664(2)	76(2)
F(33)	3361(5)	15771(3)	5964(2)	73(2)
C(33)	8744(12)	9991(7)	6207(4)	74(3)
F(34)	1811(6)	15168(3)	6169(2)	75(2)
C(34)	8763(12)	9280(9)	6084(6)	89(4)
F(35)	1954(6)	16924(4)	5224(2)	90(2)
C(35)	8442(17)	9247(10)	5491(8)	136(6)
F(36)	189(5)	16549(4)	5509(2)	84(2)
C(36)	8410(40)	8691(13)	5259(7)	290(20)
C(37)	4958(6)	11226(4)	8568(3)	26(2)
F(37)	1159(7)	16379(4)	4477(3)	109(2)
C(38)	5071(7)	10472(4)	8439(3)	34(2)
F(38)	988(10)	15352(5)	5117(3)	136(3)
C(39)	4511(6)	10545(4)	7876(3)	30(2)
F(39)	2838(8)	15618(5)	4916(3)	128(3)
C(40)	4597(7)	9790(4)	7750(3)	38(2)
F(40)	6417(5)	14891(3)	6529(2)	73(2)
C(41)	4057(8)	9804(5)	7183(4)	49(2)
F(41)	8315(5)	14923(3)	6154(2)	71(2)
C(42)	4107(10)	9072(6)	7058(4)	61(3)
F(42)	5946(4)	16339(3)	6461(2)	56(1)
C(43)	3648(12)	9062(7)	6484(5)	81(3)
F(43)	7901(5)	16430(3)	6213(2)	55(1)
C(44)	3405(15)	8371(9)	6348(7)	106(4)
F(44)	5906(5)	15803(3)	5479(2)	62(1)
C(45)	3935(7)	14066(4)	8256(3)	30(2)
F(45)	7688(5)	16166(3)	5244(2)	70(2)
C(46)	3477(8)	14905(4)	7950(3)	44(2)

F(46)	4583(5)	17114(3)	5477(2)	67(2)
C(47)	2849(7)	15068(4)	7376(3)	39(2)
F(47)	6246(6)	17567(3)	5496(2)	68(2)
C(48)	2461(9)	15926(5)	7061(4)	55(2)
F(48)	5626(7)	16838(3)	4427(2)	83(2)
C(49)	1649(8)	16198(5)	6501(4)	55(2)
F(49)	6923(7)	17539(4)	4456(2)	97(2)
C(50)	2076(8)	15853(5)	6027(4)	48(2)
F(50)	3561(7)	17947(4)	4464(3)	104(2)
C(51)	1446(9)	16324(6)	5430(4)	63(3)
F(51)	4873(7)	18337(3)	3817(2)	90(2)
C(52)	1620(14)	15897(8)	4991(5)	86(4)
F(52)	4839(7)	18645(4)	4592(3)	101(2)
C(53)	8483(7)	14218(4)	7372(3)	35(2)
C(54)	7977(8)	15057(4)	7076(3)	40(2)
C(55)	7442(8)	15231(4)	6491(3)	41(2)
C(56)	6968(7)	16072(4)	6183(3)	38(2)
C(57)	6599(7)	16284(4)	5543(3)	41(2)
C(58)	5840(9)	17093(5)	5289(4)	51(2)
C(59)	5738(9)	17381(5)	4639(4)	56(2)
C(60)	4778(13)	18101(7)	4367(5)	84(4)
C(61)	-1415(10)	4167(6)	556(5)	82(3)
C(62)	6(8)	3836(5)	525(4)	59(2)
C(63)	293(6)	3207(4)	397(3)	25(2)
C(64)	1650(8)	2845(6)	325(5)	69(3)
C(65)	1747(9)	2030(5)	443(4)	65(3)
C(66)	8161(7)	2760(4)	-378(3)	44(2)
C(67)	8155(7)	2148(4)	174(4)	40(2)
C(68)	7768(5)	2385(3)	615(2)	14(1)
C(69)	7655(9)	1819(5)	1161(4)	63(3)
C(70)	8848(10)	1604(7)	1471(4)	88(4)
C(71)	5491(12)	3414(6)	1828(5)	89(4)
C(72)	4343(9)	3167(4)	1681(4)	54(2)
C(73)	3538(7)	3083(4)	2101(3)	31(2)
C(74)	2485(14)	2829(7)	2023(5)	111(5)
C(75)	1475(17)	2871(11)	2491(8)	177(9)

C(76)	6710(9)	3105(5)	6562(4)	57(2)
C(77)	5723(9)	2955(4)	7039(4)	47(2)
C(78)	4579(6)	3008(3)	6849(3)	16(1)
C(79)	3586(8)	2877(5)	7267(4)	51(2)
C(80)	2352(10)	2941(7)	6943(4)	86(4)

Table 3. Bond lengths [Å] and angles [°] for rcc129s.

C(1)-C(2)	1.375(9)
C(1)-C(6)	1.405(9)
C(1)-H(1A)	0.9500
F(1)-C(31)	1.327(9)
O(1)-C(3)	1.375(8)
C(2)-C(3)	1.400(9)
C(2)-C(28)	1.530(10)
F(2)-C(31)	1.347(9)
O(2)-C(5)	1.384(8)
C(3)-C(4)	1.373(9)
F(3)-C(32)	1.339(10)
O(3)-C(9)	1.383(7)
C(4)-C(5)	1.387(10)
C(4)-H(4A)	0.9500
F(4)-C(32)	1.350(10)
O(4)-C(11)	1.394(7)
C(5)-C(6)	1.382(9)
O(5)-C(16)	1.380(8)
F(5)-C(33)	1.237(14)
C(6)-C(7)	1.511(10)
O(6)-C(18)	1.384(8)
F(6)-C(33)	1.278(14)
C(7)-C(8)	1.523(9)
C(7)-C(29)	1.547(9)
C(7)-H(7A)	1.0000
O(7)-C(23)	1.379(9)
F(7)-C(34)	1.49(2)
F(7)-C(33)	1.79(4)
C(8)-C(9)	1.392(9)
C(8)-C(13)	1.395(9)
O(8)-C(25)	1.401(8)
F(8)-C(34)	1.193(15)
C(9)-C(10)	1.372(9)
O(9)-C(62)	1.198(10)

F(9)-C(35)	1.411(18)
C(10)-C(11)	1.372(9)
C(10)-H(10A)	0.9500
O(10)-C(67)	1.221(9)
F(10)-C(35)	1.54(2)
C(11)-C(12)	1.399(9)
O(11)-C(72)	1.196(10)
F(11)-C(36)	1.82(4)
F(11)-C(35)	1.82(2)
C(12)-C(13)	1.380(9)
C(12)-C(14)	1.524(9)
O(12)-C(77)	1.206(9)
F(12)-C(36)	1.074(17)
C(13)-H(13A)	0.9500
F(13)-C(36)	1.37(2)
C(14)-C(15)	1.529(9)
C(14)-C(37)	1.546(9)
C(14)-H(14A)	1.0000
F(14)-C(39)	1.356(8)
C(15)-C(16)	1.386(9)
C(15)-C(20)	1.392(9)
F(15)-C(39)	1.357(8)
C(16)-C(17)	1.376(10)
F(16)-C(40)	1.341(8)
C(17)-C(18)	1.388(10)
C(17)-H(17A)	0.9500
F(17)-C(40)	1.334(8)
C(18)-C(19)	1.396(9)
F(18)-C(41)	1.303(11)
C(19)-C(20)	1.392(9)
C(19)-C(21)	1.511(9)
F(19)-C(41)	1.270(10)
C(20)-H(20A)	0.9500
F(20)-C(42)	1.212(11)
C(21)-C(22)	1.536(10)
C(21)-C(45)	1.537(9)

C(21)-H(21A)	1.0000
F(21)-C(42)	1.443(13)
C(22)-C(23)	1.383(10)
C(22)-C(27)	1.403(9)
F(22)-C(43)	1.438(13)
C(23)-C(24)	1.406(10)
F(23)-C(43)	1.318(12)
C(24)-C(25)	1.376(10)
C(24)-H(24A)	0.9500
F(24)-C(44)	1.321(16)
C(25)-C(26)	1.372(10)
F(25)-C(44)	1.173(15)
C(26)-C(27)	1.392(9)
C(26)-C(28)	1.530(10)
F(26)-C(44)	1.462(17)
C(27)-H(27A)	0.9500
F(27)-C(47)	1.335(9)
C(28)-C(53)	1.520(10)
C(28)-H(28A)	1.0000
F(28)-C(47)	1.364(8)
C(29)-C(30)	1.524(10)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
F(29)-C(48)	1.344(10)
C(30)-C(31)	1.491(10)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
F(30)-C(48)	1.332(10)
C(31)-C(32)	1.542(12)
F(31)-C(49)	1.350(10)
C(32)-C(33)	1.525(13)
F(32)-C(49)	1.360(10)
F(33)-C(50)	1.343(9)
C(33)-C(34)	1.456(15)
F(34)-C(50)	1.327(9)
C(34)-C(35)	1.53(2)

F(35)-C(51)	1.317(11)
C(35)-C(36)	1.34(2)
F(36)-C(51)	1.325(10)
C(37)-C(38)	1.524(9)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
F(37)-C(52)	1.361(12)
C(38)-C(39)	1.490(10)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
F(38)-C(52)	1.306(14)
C(39)-C(40)	1.528(10)
F(39)-C(52)	1.304(14)
C(40)-C(41)	1.525(11)
F(40)-C(55)	1.370(9)
C(41)-C(42)	1.490(12)
F(41)-C(55)	1.345(9)
C(42)-C(43)	1.520(14)
F(42)-C(56)	1.323(8)
C(43)-C(44)	1.516(18)
F(43)-C(56)	1.337(8)
F(44)-C(57)	1.339(9)
C(45)-C(46)	1.519(10)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
F(45)-C(57)	1.338(9)
C(46)-C(47)	1.510(10)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
F(46)-C(58)	1.379(10)
C(47)-C(48)	1.547(11)
F(47)-C(58)	1.309(10)
C(48)-C(49)	1.554(12)
F(48)-C(59)	1.307(10)
C(49)-C(50)	1.487(13)
F(49)-C(59)	1.376(11)

C(50)-C(51)	1.567(12)
F(50)-C(60)	1.379(14)
C(51)-C(52)	1.499(16)
F(51)-C(60)	1.288(12)
F(52)-C(60)	1.316(13)
C(53)-C(54)	1.520(10)
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-C(55)	1.489(10)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)	1.524(10)
C(56)-C(57)	1.547(11)
C(57)-C(58)	1.522(11)
C(58)-C(59)	1.521(12)
C(59)-C(60)	1.502(14)
C(61)-C(62)	1.503(13)
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-C(63)	1.283(11)
C(63)-C(64)	1.471(11)
C(63)-H(63A)	0.9500
C(64)-C(65)	1.461(13)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(66)-C(67)	1.496(10)
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800
C(67)-C(68)	1.291(10)
C(68)-C(69)	1.460(10)
C(68)-H(68A)	0.9500

C(69)-C(70)	1.434(13)
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(71)-C(72)	1.499(13)
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-C(73)	1.286(12)
C(73)-C(74)	1.357(16)
C(73)-H(73A)	0.9500
C(74)-C(75)	1.522(16)
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(75)-H(75A)	0.9800
C(75)-H(75B)	0.9800
C(75)-H(75C)	0.9800
C(76)-C(77)	1.522(12)
C(76)-H(76A)	0.9800
C(76)-H(76B)	0.9800
C(76)-H(76C)	0.9800
C(77)-C(78)	1.302(10)
C(78)-C(79)	1.429(10)
C(78)-H(78A)	0.9500
C(79)-C(80)	1.538(13)
C(79)-H(79A)	0.9900
C(79)-H(79B)	0.9900
C(80)-H(80A)	0.9800
C(80)-H(80B)	0.9800
C(80)-H(80C)	0.9800

C(2)-C(1)-C(6)	124.2(6)
C(2)-C(1)-H(1A)	117.9
C(6)-C(1)-H(1A)	117.9

C(1)-C(2)-C(3)	117.0(6)
C(1)-C(2)-C(28)	122.7(6)
C(3)-C(2)-C(28)	120.3(6)
C(4)-C(3)-O(1)	116.2(6)
C(4)-C(3)-C(2)	120.7(7)
O(1)-C(3)-C(2)	123.1(6)
C(3)-C(4)-C(5)	120.4(6)
C(3)-C(4)-H(4A)	119.8
C(5)-C(4)-H(4A)	119.8
C(6)-C(5)-O(2)	121.6(6)
C(6)-C(5)-C(4)	121.4(6)
O(2)-C(5)-C(4)	117.0(6)
C(5)-C(6)-C(1)	116.2(6)
C(5)-C(6)-C(7)	120.7(6)
C(1)-C(6)-C(7)	123.0(6)
C(6)-C(7)-C(8)	110.2(5)
C(6)-C(7)-C(29)	114.7(5)
C(8)-C(7)-C(29)	111.4(6)
C(6)-C(7)-H(7A)	106.7
C(8)-C(7)-H(7A)	106.7
C(29)-C(7)-H(7A)	106.7
C(34)-F(7)-C(33)	51.8(9)
C(9)-C(8)-C(13)	116.3(6)
C(9)-C(8)-C(7)	121.5(6)
C(13)-C(8)-C(7)	122.2(6)
C(10)-C(9)-O(3)	121.3(6)
C(10)-C(9)-C(8)	122.3(6)
O(3)-C(9)-C(8)	116.4(5)
C(11)-C(10)-C(9)	119.1(6)
C(11)-C(10)-H(10A)	120.5
C(9)-C(10)-H(10A)	120.5
C(10)-C(11)-O(4)	121.4(6)
C(10)-C(11)-C(12)	122.0(6)
O(4)-C(11)-C(12)	116.6(5)
C(36)-F(11)-C(35)	43.2(9)
C(13)-C(12)-C(11)	116.6(6)

C(13)-C(12)-C(14)	121.3(6)
C(11)-C(12)-C(14)	122.1(6)
C(12)-C(13)-C(8)	123.7(6)
C(12)-C(13)-H(13A)	118.1
C(8)-C(13)-H(13A)	118.1
C(12)-C(14)-C(15)	111.0(5)
C(12)-C(14)-C(37)	111.0(5)
C(15)-C(14)-C(37)	114.2(5)
C(12)-C(14)-H(14A)	106.7
C(15)-C(14)-H(14A)	106.7
C(37)-C(14)-H(14A)	106.7
C(16)-C(15)-C(20)	117.2(6)
C(16)-C(15)-C(14)	119.4(6)
C(20)-C(15)-C(14)	123.4(6)
C(17)-C(16)-O(5)	115.7(6)
C(17)-C(16)-C(15)	121.1(6)
O(5)-C(16)-C(15)	123.1(6)
C(16)-C(17)-C(18)	120.4(7)
C(16)-C(17)-H(17A)	119.8
C(18)-C(17)-H(17A)	119.8
O(6)-C(18)-C(17)	120.5(6)
O(6)-C(18)-C(19)	118.6(6)
C(17)-C(18)-C(19)	120.9(7)
C(20)-C(19)-C(18)	116.7(6)
C(20)-C(19)-C(21)	123.6(6)
C(18)-C(19)-C(21)	119.7(6)
C(19)-C(20)-C(15)	123.8(6)
C(19)-C(20)-H(20A)	118.1
C(15)-C(20)-H(20A)	118.1
C(19)-C(21)-C(22)	111.2(5)
C(19)-C(21)-C(45)	113.7(6)
C(22)-C(21)-C(45)	111.9(6)
C(19)-C(21)-H(21A)	106.5
C(22)-C(21)-H(21A)	106.5
C(45)-C(21)-H(21A)	106.5
C(23)-C(22)-C(27)	117.9(7)

C(23)-C(22)-C(21)	121.4(6)
C(27)-C(22)-C(21)	120.7(6)
O(7)-C(23)-C(22)	123.3(7)
O(7)-C(23)-C(24)	116.7(6)
C(22)-C(23)-C(24)	120.0(7)
C(25)-C(24)-C(23)	120.0(7)
C(25)-C(24)-H(24A)	120.0
C(23)-C(24)-H(24A)	120.0
C(26)-C(25)-C(24)	121.6(7)
C(26)-C(25)-O(8)	117.8(6)
C(24)-C(25)-O(8)	120.5(6)
C(25)-C(26)-C(27)	117.8(6)
C(25)-C(26)-C(28)	120.8(6)
C(27)-C(26)-C(28)	121.3(6)
C(26)-C(27)-C(22)	122.5(6)
C(26)-C(27)-H(27A)	118.7
C(22)-C(27)-H(27A)	118.7
C(53)-C(28)-C(2)	113.2(6)
C(53)-C(28)-C(26)	112.0(6)
C(2)-C(28)-C(26)	111.2(6)
C(53)-C(28)-H(28A)	106.7
C(2)-C(28)-H(28A)	106.7
C(26)-C(28)-H(28A)	106.7
C(30)-C(29)-C(7)	109.4(6)
C(30)-C(29)-H(29A)	109.8
C(7)-C(29)-H(29A)	109.8
C(30)-C(29)-H(29B)	109.8
C(7)-C(29)-H(29B)	109.8
H(29A)-C(29)-H(29B)	108.2
C(31)-C(30)-C(29)	113.9(6)
C(31)-C(30)-H(30A)	108.8
C(29)-C(30)-H(30A)	108.8
C(31)-C(30)-H(30B)	108.8
C(29)-C(30)-H(30B)	108.8
H(30A)-C(30)-H(30B)	107.7
F(1)-C(31)-F(2)	107.3(7)

F(1)-C(31)-C(30)	111.0(7)
F(2)-C(31)-C(30)	110.0(7)
F(1)-C(31)-C(32)	107.4(6)
F(2)-C(31)-C(32)	107.2(7)
C(30)-C(31)-C(32)	113.6(7)
F(3)-C(32)-F(4)	105.4(8)
F(3)-C(32)-C(33)	107.8(8)
F(4)-C(32)-C(33)	107.3(8)
F(3)-C(32)-C(31)	107.6(6)
F(4)-C(32)-C(31)	107.7(7)
C(33)-C(32)-C(31)	120.1(8)
F(5)-C(33)-F(6)	97.8(17)
F(5)-C(33)-C(34)	113.2(12)
F(6)-C(33)-C(34)	106.4(11)
F(5)-C(33)-C(32)	108.7(10)
F(6)-C(33)-C(32)	107.0(9)
C(34)-C(33)-C(32)	120.9(11)
F(5)-C(33)-F(7)	69.5(16)
F(6)-C(33)-F(7)	142.4(11)
C(34)-C(33)-F(7)	53.5(16)
C(32)-C(33)-F(7)	110.6(11)
F(8)-C(34)-C(33)	115.9(10)
F(8)-C(34)-F(7)	108.4(18)
C(33)-C(34)-F(7)	75(2)
F(8)-C(34)-C(35)	120.5(12)
C(33)-C(34)-C(35)	122.4(14)
F(7)-C(34)-C(35)	97.0(15)
C(36)-C(35)-F(9)	112.3(16)
C(36)-C(35)-C(34)	135.1(18)
F(9)-C(35)-C(34)	111.3(14)
C(36)-C(35)-F(10)	89(2)
F(9)-C(35)-F(10)	100.2(13)
C(34)-C(35)-F(10)	93.7(17)
C(36)-C(35)-F(11)	68(2)
F(9)-C(35)-F(11)	95.0(11)
C(34)-C(35)-F(11)	97.7(14)

F(10)-C(35)-F(11)	156.2(17)
F(12)-C(36)-C(35)	132(2)
F(12)-C(36)-F(13)	122.6(15)
C(35)-C(36)-F(13)	104.9(15)
F(12)-C(36)-F(11)	109(2)
C(35)-C(36)-F(11)	68.4(15)
F(13)-C(36)-F(11)	93(2)
C(38)-C(37)-C(14)	110.0(5)
C(38)-C(37)-H(37A)	109.7
C(14)-C(37)-H(37A)	109.7
C(38)-C(37)-H(37B)	109.7
C(14)-C(37)-H(37B)	109.7
H(37A)-C(37)-H(37B)	108.2
C(39)-C(38)-C(37)	114.1(6)
C(39)-C(38)-H(38A)	108.7
C(37)-C(38)-H(38A)	108.7
C(39)-C(38)-H(38B)	108.7
C(37)-C(38)-H(38B)	108.7
H(38A)-C(38)-H(38B)	107.6
F(14)-C(39)-F(15)	106.0(6)
F(14)-C(39)-C(38)	110.9(6)
F(15)-C(39)-C(38)	110.4(6)
F(14)-C(39)-C(40)	107.6(6)
F(15)-C(39)-C(40)	107.3(5)
C(38)-C(39)-C(40)	114.3(6)
F(17)-C(40)-F(16)	107.5(7)
F(17)-C(40)-C(41)	107.0(6)
F(16)-C(40)-C(41)	106.7(6)
F(17)-C(40)-C(39)	108.4(6)
F(16)-C(40)-C(39)	108.5(6)
C(41)-C(40)-C(39)	118.3(7)
F(19)-C(41)-F(18)	105.7(11)
F(19)-C(41)-C(42)	109.1(8)
F(18)-C(41)-C(42)	104.5(8)
F(19)-C(41)-C(40)	109.3(7)
F(18)-C(41)-C(40)	108.3(7)

C(42)-C(41)-C(40)	119.1(8)
F(20)-C(42)-F(21)	97.1(10)
F(20)-C(42)-C(41)	116.2(8)
F(21)-C(42)-C(41)	99.5(8)
F(20)-C(42)-C(43)	117.7(9)
F(21)-C(42)-C(43)	96.6(9)
C(41)-C(42)-C(43)	120.8(9)
F(23)-C(43)-F(22)	102.7(10)
F(23)-C(43)-C(44)	110.6(11)
F(22)-C(43)-C(44)	96.2(10)
F(23)-C(43)-C(42)	113.4(9)
F(22)-C(43)-C(42)	103.9(10)
C(44)-C(43)-C(42)	125.4(11)
F(25)-C(44)-F(24)	117.2(14)
F(25)-C(44)-F(26)	110.0(15)
F(24)-C(44)-F(26)	108.4(13)
F(25)-C(44)-C(43)	119.0(14)
F(24)-C(44)-C(43)	107.0(12)
F(26)-C(44)-C(43)	92.1(12)
C(46)-C(45)-C(21)	109.6(6)
C(46)-C(45)-H(45A)	109.7
C(21)-C(45)-H(45A)	109.7
C(46)-C(45)-H(45B)	109.7
C(21)-C(45)-H(45B)	109.7
H(45A)-C(45)-H(45B)	108.2
C(47)-C(46)-C(45)	114.2(6)
C(47)-C(46)-H(46A)	108.7
C(45)-C(46)-H(46A)	108.7
C(47)-C(46)-H(46B)	108.7
C(45)-C(46)-H(46B)	108.7
H(46A)-C(46)-H(46B)	107.6
F(27)-C(47)-F(28)	106.2(6)
F(27)-C(47)-C(46)	111.1(6)
F(28)-C(47)-C(46)	110.0(6)
F(27)-C(47)-C(48)	108.8(6)
F(28)-C(47)-C(48)	107.5(6)

C(46)-C(47)-C(48)	112.9(7)
F(30)-C(48)-F(29)	107.0(8)
F(30)-C(48)-C(47)	108.7(7)
F(29)-C(48)-C(47)	107.7(7)
F(30)-C(48)-C(49)	106.7(7)
F(29)-C(48)-C(49)	106.5(7)
C(47)-C(48)-C(49)	119.5(8)
F(31)-C(49)-F(32)	106.6(7)
F(31)-C(49)-C(50)	110.0(8)
F(32)-C(49)-C(50)	108.1(7)
F(31)-C(49)-C(48)	105.6(7)
F(32)-C(49)-C(48)	106.0(7)
C(50)-C(49)-C(48)	119.8(8)
F(34)-C(50)-F(33)	108.1(7)
F(34)-C(50)-C(49)	108.6(7)
F(33)-C(50)-C(49)	109.1(7)
F(34)-C(50)-C(51)	108.8(7)
F(33)-C(50)-C(51)	107.3(7)
C(49)-C(50)-C(51)	114.8(8)
F(35)-C(51)-F(36)	109.2(9)
F(35)-C(51)-C(52)	108.0(9)
F(36)-C(51)-C(52)	108.1(9)
F(35)-C(51)-C(50)	108.9(8)
F(36)-C(51)-C(50)	108.1(7)
C(52)-C(51)-C(50)	114.5(9)
F(39)-C(52)-F(38)	109.3(13)
F(39)-C(52)-F(37)	106.7(10)
F(38)-C(52)-F(37)	106.6(11)
F(39)-C(52)-C(51)	111.5(11)
F(38)-C(52)-C(51)	112.9(10)
F(37)-C(52)-C(51)	109.5(10)
C(28)-C(53)-C(54)	109.8(6)
C(28)-C(53)-H(53A)	109.7
C(54)-C(53)-H(53A)	109.7
C(28)-C(53)-H(53B)	109.7
C(54)-C(53)-H(53B)	109.7

H(53A)-C(53)-H(53B)	108.2
C(55)-C(54)-C(53)	114.9(7)
C(55)-C(54)-H(54A)	108.5
C(53)-C(54)-H(54A)	108.5
C(55)-C(54)-H(54B)	108.5
C(53)-C(54)-H(54B)	108.5
H(54A)-C(54)-H(54B)	107.5
F(41)-C(55)-F(40)	105.7(7)
F(41)-C(55)-C(54)	110.7(6)
F(40)-C(55)-C(54)	108.7(6)
F(41)-C(55)-C(56)	108.4(6)
F(40)-C(55)-C(56)	107.4(6)
C(54)-C(55)-C(56)	115.4(7)
F(42)-C(56)-F(43)	108.2(6)
F(42)-C(56)-C(55)	108.0(6)
F(43)-C(56)-C(55)	108.1(6)
F(42)-C(56)-C(57)	108.1(6)
F(43)-C(56)-C(57)	107.2(6)
C(55)-C(56)-C(57)	117.0(7)
F(45)-C(57)-F(44)	106.4(7)
F(45)-C(57)-C(58)	109.3(6)
F(44)-C(57)-C(58)	108.7(6)
F(45)-C(57)-C(56)	108.0(6)
F(44)-C(57)-C(56)	108.7(6)
C(58)-C(57)-C(56)	115.3(7)
F(47)-C(58)-F(46)	105.4(7)
F(47)-C(58)-C(59)	111.2(7)
F(46)-C(58)-C(59)	104.8(7)
F(47)-C(58)-C(57)	110.9(7)
F(46)-C(58)-C(57)	106.9(6)
C(59)-C(58)-C(57)	116.7(8)
F(48)-C(59)-F(49)	105.4(8)
F(48)-C(59)-C(60)	110.7(8)
F(49)-C(59)-C(60)	104.7(8)
F(48)-C(59)-C(58)	110.6(7)
F(49)-C(59)-C(58)	105.0(7)

C(60)-C(59)-C(58)	119.1(9)
F(51)-C(60)-F(52)	109.9(9)
F(51)-C(60)-F(50)	104.9(9)
F(52)-C(60)-F(50)	108.6(11)
F(51)-C(60)-C(59)	113.8(11)
F(52)-C(60)-C(59)	111.6(9)
F(50)-C(60)-C(59)	107.6(9)
C(62)-C(61)-H(61A)	109.5
C(62)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(62)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
O(9)-C(62)-C(63)	121.8(9)
O(9)-C(62)-C(61)	122.8(9)
C(63)-C(62)-C(61)	115.4(8)
C(62)-C(63)-C(64)	120.6(7)
C(62)-C(63)-H(63A)	119.7
C(64)-C(63)-H(63A)	119.7
C(65)-C(64)-C(63)	108.3(7)
C(65)-C(64)-H(64A)	110.0
C(63)-C(64)-H(64A)	110.0
C(65)-C(64)-H(64B)	110.0
C(63)-C(64)-H(64B)	110.0
H(64A)-C(64)-H(64B)	108.4
C(64)-C(65)-H(65A)	109.5
C(64)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(64)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(67)-C(66)-H(66A)	109.5
C(67)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(67)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5

H(66B)-C(66)-H(66C)	109.5
O(10)-C(67)-C(68)	125.0(7)
O(10)-C(67)-C(66)	120.0(8)
C(68)-C(67)-C(66)	115.0(7)
C(67)-C(68)-C(69)	117.9(7)
C(67)-C(68)-H(68A)	121.0
C(69)-C(68)-H(68A)	121.0
C(70)-C(69)-C(68)	109.5(8)
C(70)-C(69)-H(69A)	109.8
C(68)-C(69)-H(69A)	109.8
C(70)-C(69)-H(69B)	109.8
C(68)-C(69)-H(69B)	109.8
H(69A)-C(69)-H(69B)	108.2
C(69)-C(70)-H(70A)	109.5
C(69)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(69)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(72)-C(71)-H(71A)	109.5
C(72)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(72)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
O(11)-C(72)-C(73)	125.2(9)
O(11)-C(72)-C(71)	123.5(10)
C(73)-C(72)-C(71)	111.3(9)
C(72)-C(73)-C(74)	116.3(8)
C(72)-C(73)-H(73A)	121.9
C(74)-C(73)-H(73A)	121.9
C(73)-C(74)-C(75)	113.0(13)
C(73)-C(74)-H(74A)	109.0
C(75)-C(74)-H(74A)	109.0
C(73)-C(74)-H(74B)	109.0
C(75)-C(74)-H(74B)	109.0

H(74A)-C(74)-H(74B)	107.8
C(74)-C(75)-H(75A)	109.5
C(74)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
C(74)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
C(77)-C(76)-H(76A)	109.5
C(77)-C(76)-H(76B)	109.5
H(76A)-C(76)-H(76B)	109.5
C(77)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5
O(12)-C(77)-C(78)	125.3(8)
O(12)-C(77)-C(76)	121.8(8)
C(78)-C(77)-C(76)	112.9(7)
C(77)-C(78)-C(79)	116.9(7)
C(77)-C(78)-H(78A)	121.5
C(79)-C(78)-H(78A)	121.5
C(78)-C(79)-C(80)	107.3(7)
C(78)-C(79)-H(79A)	110.3
C(80)-C(79)-H(79A)	110.3
C(78)-C(79)-H(79B)	110.3
C(80)-C(79)-H(79B)	110.3
H(79A)-C(79)-H(79B)	108.5
C(79)-C(80)-H(80A)	109.5
C(79)-C(80)-H(80B)	109.5
H(80A)-C(80)-H(80B)	109.5
C(79)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5
H(80B)-C(80)-H(80C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for rcc129s. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(4)	37(4)	28(4)	-8(3)	-5(3)	-11(3)
F(1)	139(5)	86(4)	41(3)	-21(3)	29(3)	-66(4)
O(1)	31(3)	37(3)	47(3)	-11(2)	-9(2)	-10(2)
C(2)	19(4)	33(4)	32(4)	7(3)	-3(3)	-7(3)
F(2)	91(5)	104(5)	111(5)	-67(4)	-61(4)	41(4)
O(2)	21(2)	33(3)	34(3)	4(2)	-9(2)	2(2)
C(3)	24(4)	31(4)	36(4)	-7(3)	-3(3)	-10(3)
F(3)	84(4)	80(4)	94(4)	-52(4)	-26(3)	9(3)
O(3)	22(3)	33(3)	37(3)	0(2)	-2(2)	-2(2)
C(4)	23(4)	43(4)	21(4)	-4(3)	-3(3)	-8(3)
F(4)	142(6)	136(6)	96(5)	-73(4)	65(4)	-106(5)
O(4)	25(2)	38(3)	27(3)	-2(2)	3(2)	-12(2)
C(5)	21(4)	29(4)	27(4)	0(3)	5(3)	-2(3)
O(5)	42(3)	39(3)	23(3)	4(2)	-3(2)	-12(2)
F(5)	830(40)	430(20)	66(6)	-115(10)	129(14)	-540(30)
C(6)	19(3)	35(4)	25(4)	-1(3)	3(3)	-3(3)
O(6)	47(3)	36(3)	30(3)	-12(2)	5(2)	-5(2)
F(6)	291(14)	200(12)	191(11)	-147(10)	-177(11)	167(11)
C(7)	24(4)	35(4)	24(4)	3(3)	1(3)	-5(3)
O(7)	47(3)	49(3)	45(3)	-26(3)	7(3)	-6(3)
F(7)	76(9)	1420(110)	220(20)	10(40)	32(11)	-70(30)
C(8)	22(3)	24(4)	22(3)	-4(3)	-3(3)	-7(3)
O(8)	35(3)	40(3)	75(4)	-16(3)	-10(3)	-13(3)
F(8)	500(20)	95(6)	73(5)	-45(5)	46(8)	-162(10)
C(9)	16(3)	26(4)	30(4)	-11(3)	0(3)	-2(3)
O(9)	54(4)	86(5)	138(7)	-72(5)	-17(4)	-12(4)
F(9)	181(7)	95(5)	47(3)	-20(3)	-5(4)	-47(5)
C(10)	32(4)	24(4)	27(4)	-4(3)	-3(3)	-3(3)
O(10)	43(3)	36(3)	39(3)	3(2)	-2(2)	-3(3)
F(10)	76(7)	224(14)	870(50)	70(20)	182(16)	-12(8)
C(11)	20(3)	28(4)	30(4)	-10(3)	-3(3)	-9(3)

O(11)	88(5)	59(4)	36(3)	-21(3)	8(3)	-21(3)
F(11)	132(11)	247(15)	460(30)	168(18)	105(15)	-7(10)
C(12)	30(4)	27(4)	18(3)	-1(3)	-1(3)	-7(3)
O(12)	62(4)	69(4)	33(3)	-12(3)	-6(3)	-12(3)
F(12)	292(14)	217(11)	95(6)	-82(7)	16(7)	-133(10)
C(13)	23(4)	32(4)	26(4)	-7(3)	-3(3)	-8(3)
F(13)	179(8)	115(6)	129(7)	-39(6)	-23(6)	-70(6)
C(14)	27(4)	30(4)	22(4)	-3(3)	3(3)	-9(3)
F(14)	85(4)	51(3)	31(2)	-8(2)	9(2)	-36(3)
C(15)	20(3)	26(4)	30(4)	-2(3)	-2(3)	-8(3)
F(15)	36(3)	70(3)	61(3)	-30(3)	-17(2)	1(2)
C(16)	19(4)	38(4)	34(4)	-1(3)	0(3)	-9(3)
F(16)	46(3)	67(4)	107(4)	-50(3)	-27(3)	7(3)
C(17)	27(4)	47(5)	26(4)	-5(4)	3(3)	-10(3)
F(17)	138(5)	81(4)	49(3)	-20(3)	26(3)	-81(4)
C(18)	20(4)	40(4)	36(4)	-13(4)	6(3)	-5(3)
F(18)	344(14)	122(6)	56(4)	-6(4)	-12(6)	-155(9)
C(19)	21(4)	36(4)	33(4)	-16(3)	3(3)	-12(3)
F(19)	123(7)	301(13)	293(13)	-270(12)	-150(8)	136(8)
C(20)	20(3)	41(4)	23(4)	-6(3)	-4(3)	-14(3)
F(20)	175(8)	107(6)	271(11)	-135(7)	-180(9)	86(6)
C(21)	31(4)	33(4)	30(4)	-8(3)	2(3)	-7(3)
F(21)	261(13)	208(11)	125(7)	-51(7)	70(8)	-160(10)
C(22)	36(4)	23(4)	28(4)	-6(3)	-8(3)	2(3)
F(22)	118(7)	273(13)	180(10)	-47(9)	77(7)	-77(8)
C(23)	41(4)	31(4)	31(4)	-12(3)	-5(3)	-4(3)
F(23)	124(6)	77(4)	91(4)	-39(4)	-55(4)	11(4)
C(24)	47(5)	32(4)	43(5)	-15(4)	-14(4)	-8(4)
F(24)	193(9)	87(5)	153(7)	-68(5)	-78(7)	32(5)
C(25)	28(4)	24(4)	46(5)	-10(3)	-3(3)	-3(3)
F(25)	136(6)	171(8)	109(6)	-101(6)	-42(5)	-6(5)
C(26)	27(4)	25(4)	29(4)	-1(3)	-5(3)	-3(3)
F(26)	128(9)	247(14)	327(18)	16(13)	104(11)	-42(9)
C(27)	29(4)	24(4)	27(4)	-8(3)	-5(3)	-1(3)
F(27)	55(3)	62(3)	42(3)	-4(2)	-3(2)	0(3)
C(28)	30(4)	33(4)	46(5)	-8(4)	-7(3)	-11(3)

F(28)	43(3)	81(4)	54(3)	6(3)	-13(2)	-29(3)
C(29)	37(4)	34(4)	24(4)	0(3)	1(3)	-9(3)
F(29)	65(4)	57(3)	83(4)	6(3)	-26(3)	-26(3)
C(30)	41(5)	40(4)	30(4)	-2(3)	6(3)	-8(4)
F(30)	96(4)	63(4)	69(4)	-26(3)	-28(3)	29(3)
C(31)	35(5)	52(5)	35(4)	-12(4)	0(4)	-1(4)
F(31)	120(5)	43(3)	81(4)	0(3)	-43(4)	4(3)
C(32)	29(5)	70(6)	60(6)	-26(5)	4(4)	-11(4)
F(32)	36(3)	119(5)	57(3)	-14(3)	-9(2)	3(3)
F(33)	38(3)	108(5)	57(3)	-11(3)	0(2)	-1(3)
C(33)	94(9)	91(8)	51(6)	-36(6)	4(6)	-29(7)
F(34)	119(5)	59(3)	49(3)	-1(3)	-20(3)	-35(3)
C(34)	92(9)	124(11)	94(9)	-77(9)	13(7)	-53(8)
F(35)	101(5)	91(4)	64(4)	21(3)	-22(3)	-42(4)
F(36)	43(3)	133(5)	57(3)	-5(3)	-15(3)	-4(3)
C(36)	750(70)	190(20)	63(10)	-74(12)	80(20)	-330(30)
C(37)	16(3)	35(4)	21(3)	1(3)	-2(3)	-4(3)
F(37)	125(6)	144(6)	49(4)	-14(4)	-15(4)	-25(5)
C(38)	37(4)	30(4)	33(4)	-5(3)	-8(3)	-8(3)
F(38)	215(10)	129(7)	79(5)	-18(5)	-30(5)	-76(7)
C(39)	20(4)	36(4)	31(4)	-3(3)	0(3)	-6(3)
F(39)	115(6)	169(8)	79(5)	-46(5)	8(5)	20(6)
C(40)	29(4)	43(5)	41(4)	-6(4)	1(3)	-12(4)
F(40)	62(3)	55(3)	90(4)	15(3)	-36(3)	-27(3)
C(41)	48(5)	54(6)	49(5)	-18(4)	1(4)	-16(4)
F(41)	87(4)	61(3)	40(3)	-7(3)	-7(3)	23(3)
C(42)	74(7)	68(7)	53(6)	-29(5)	-1(5)	-21(6)
F(42)	47(3)	58(3)	43(3)	-2(2)	1(2)	12(2)
F(43)	55(3)	46(3)	55(3)	9(2)	-18(2)	-18(2)
F(44)	72(3)	51(3)	57(3)	-1(2)	-23(3)	-16(3)
C(45)	28(4)	28(4)	33(4)	-7(3)	0(3)	-8(3)
F(45)	53(3)	88(4)	42(3)	4(3)	0(2)	8(3)
C(46)	41(5)	39(5)	45(5)	-9(4)	-15(4)	2(4)
F(46)	53(3)	64(3)	70(4)	-2(3)	-11(3)	-5(3)
C(47)	22(4)	45(5)	44(5)	-6(4)	0(3)	-4(3)
F(47)	97(4)	47(3)	54(3)	4(2)	-29(3)	-20(3)

C(48)	58(6)	45(5)	55(6)	-8(5)	-13(5)	-4(5)
F(48)	140(6)	56(4)	45(3)	-8(3)	-36(3)	-6(3)
C(49)	41(5)	55(6)	61(6)	-5(5)	-14(4)	-6(4)
F(49)	93(5)	111(5)	61(4)	17(4)	6(3)	-28(4)
C(50)	39(5)	57(6)	53(5)	-16(4)	3(4)	-21(4)
F(50)	81(5)	108(5)	99(5)	16(4)	-34(4)	-20(4)
C(51)	45(6)	84(7)	46(6)	4(5)	-2(4)	-17(5)
F(51)	131(6)	75(4)	40(3)	21(3)	-27(3)	-16(4)
C(52)	97(10)	99(10)	46(7)	-2(7)	-7(6)	-14(8)
F(52)	149(7)	61(4)	81(4)	-12(3)	-54(4)	2(4)
C(53)	35(4)	23(4)	40(4)	-3(3)	-5(3)	-3(3)
C(54)	39(4)	33(4)	41(5)	0(4)	-8(4)	-6(4)
C(55)	43(5)	37(4)	34(4)	5(4)	-9(4)	-5(4)
C(56)	29(4)	39(5)	43(5)	-9(4)	-2(4)	-6(4)
C(57)	34(4)	43(5)	39(5)	-2(4)	-4(4)	-8(4)
C(58)	54(6)	47(5)	47(5)	2(4)	-15(4)	-15(4)
C(59)	61(6)	52(6)	46(5)	0(5)	-11(5)	-9(5)
C(60)	105(10)	60(7)	72(8)	3(6)	-35(7)	-5(7)
C(61)	69(7)	78(8)	108(9)	-36(7)	1(7)	-19(6)
C(62)	34(5)	60(6)	81(7)	-10(5)	-3(5)	-21(5)
C(64)	33(5)	112(9)	84(7)	-60(7)	17(5)	-25(5)
C(65)	52(6)	64(7)	82(7)	-23(5)	8(5)	-20(5)
C(66)	30(4)	37(4)	48(5)	12(4)	-5(4)	-8(3)
C(67)	21(4)	26(4)	63(5)	10(4)	-16(4)	-8(3)
C(69)	67(6)	63(6)	41(5)	5(5)	3(5)	-9(5)
C(70)	68(7)	131(11)	59(7)	-9(7)	0(6)	-31(7)
C(71)	114(10)	51(6)	105(9)	-11(6)	-32(8)	-33(6)
C(72)	65(6)	29(5)	66(6)	-13(4)	-19(5)	-1(4)
C(74)	134(12)	95(9)	52(7)	8(6)	35(7)	28(8)
C(75)	138(15)	185(18)	174(18)	-26(14)	94(14)	-28(13)
C(76)	52(6)	69(6)	50(5)	-18(5)	-3(4)	-14(5)
C(77)	71(6)	27(4)	40(5)	-9(4)	4(4)	-6(4)
C(79)	66(6)	39(5)	49(5)	-13(4)	-17(4)	-6(4)
C(80)	58(7)	128(10)	59(7)	-7(7)	-5(5)	-19(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for rcc129s.

	x	y	z	U(eq)
H(1A)	8887	12753	7862	34
H(4A)	12159	12417	9134	36
H(7A)	10833	10891	8260	36
H(10A)	9315	9350	9822	35
H(13A)	7431	11585	8467	32
H(14A)	5190	10690	9437	32
H(17A)	5019	12211	10590	41
H(20A)	5011	12605	8625	32
H(21A)	3857	14279	9039	38
H(24A)	7126	15393	9233	47
H(27A)	6677	13730	8224	32
H(28A)	9575	14468	7919	43
H(29A)	8516	11729	7624	40
H(29B)	9935	11710	7351	40
H(30A)	10271	10338	7606	47
H(30B)	8785	10419	7790	47
H(37A)	4035	11483	8570	31
H(37B)	5401	11559	8265	31
H(38A)	5996	10216	8447	41
H(38B)	4629	10143	8746	41
H(45A)	4595	13827	8021	35
H(45B)	3199	13811	8312	35
H(46A)	2851	15139	8199	52
H(46B)	4226	15149	7893	52
H(53A)	7782	13941	7402	42
H(53B)	9193	14006	7143	42
H(54A)	7293	15263	7318	48
H(54B)	8690	15324	7050	48
H(61A)	-1538	4644	655	123
H(61B)	-1817	3808	849	123

H(61C)	-1817	4263	183	123
H(63A)	-377	2972	348	30
H(64A)	1939	3059	-71	83
H(64B)	2208	2940	593	83
H(65A)	2647	1779	401	97
H(65B)	1201	1941	173	97
H(65C)	1457	1823	836	97
H(66A)	7882	3257	-308	65
H(66B)	7567	2713	-650	65
H(66C)	9036	2709	-538	65
H(68A)	7563	2912	584	17
H(69A)	6944	2031	1389	75
H(69B)	7450	1367	1091	75
H(70A)	8789	1202	1827	132
H(70B)	9015	2046	1563	132
H(70C)	9555	1418	1235	132
H(71A)	5376	3487	2210	133
H(71B)	5573	3893	1545	133
H(71C)	6274	3024	1823	133
H(73A)	3673	3193	2445	38
H(74A)	2764	2296	2013	133
H(74B)	2087	3135	1648	133
H(75A)	758	2660	2424	265
H(75B)	1149	3402	2486	265
H(75C)	1867	2579	2865	265
H(76A)	7551	3057	6728	85
H(76B)	6427	3619	6304	85
H(76C)	6787	2735	6345	85
H(78A)	4411	3129	6451	20
H(79A)	3438	3259	7482	62
H(79B)	3839	2366	7542	62
H(80A)	1646	2860	7218	129
H(80B)	2507	2557	6737	129
H(80C)	2117	3448	6670	129