Supporting Information for "On the Negligible Impact of Ruffling on the Electronic Spectra of Porphine, Tetramethylporphyrin, and Perfluoroalkylporphyrins"

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Instrumentation and Materials. Manipulations of air- and water-sensitive reagents were carried out either in a glovebox (Innovative Technologies Labmaster 150) or in standard Schlenk-style glassware. Solvents used in the glovebox were degassed at least three times by successive freeze/pump/thaw cycles. THF, diethyl ether, and benzene were distilled from sodium/benzophenone prior to use. Deuterated benzene was dried over $LiAlH_4$ and distilled prior to use. CH_2Cl_2 ane pyrrole were distilled from CaH_2. $NaBH_4$ was recrystallized from diglyme and stored in the glovebox. The remaining reagents were obtained from Aldrich, Fisher, or Cambridge Isotope Laboratories and used as received. Optical spectra were performed using an OLIS-14 modification of a Carey-14 UV-Vis-NIR spectrophotometer equipped with a variable-temperature cell holder and a circulating VT bath (Laude RC3). NMR spectra were obtained in the instrumentation center at the University of Nebraska-Lincoln using 360 or 500 MHz spectrometers. Proton NMR spectra were collected in the solvents indicated, using the residual protons in the solvents as a chemical shift references. ^{19}F NMR was conducted at 470 MHz, and chemical shifts are given with reference to an added internal standard, hexafluorobenzene. The data sets for the crystal structure analyses were collected at the University of Illinois crystallography facility. Mass spectra were collected at the University of Nebraska Center for Mass Spectroscopy.

5,5' Bis(2,2,3,3,4,4,4 heptafluoro-1-butanol) -2,2'-dipyrryl methane, 1. In a 500 mL flask under N_2, a stirred solution of 2,2'-dipyrrylmethane[1] (1.300 g, 8.9 mmol), THF (300 mL) and triethylamine (3.0 mL, 21.4 mmol) was chilled to 0° C and heptafluorobutyryl chloride (2.1 g, 8.9 mmol) was added slowly by syringe. Upon completion of the addition, the mixture was warmed to RT, stirred for 45 min, filtered by suction, and the amine salt was washed with 3 (50 mL) portions of dry ethyl ether. The filtrate was collected and the solvents were removed by rotary evaporation leaving a dark brown solid. The solid was immediately dissolved in 250 mL of methanol, transferred to a 1 L Erlenmeyer flask, and treated with saturated sodium bicarbonate (20 mL) and distilled water (150 mL). Sodium borohydride (4 g) was slowly added to the stirred solution. After 3 h an additional portion of sodium borohydride (4 g) was added and the solution was allowed to stir for 2 h. The methanol was removed by rotary evaporation, and the remainder was extracted with three portions of diethyl ether (100 mL), evaporated. Final purification involved separating the desired product from black residue with hot hexane. Several hot hexane fractions were added and decanted, the fractions were combined and dried by rotary evaporation leaving a mixture of diastereomeric products isolated as a light brown solid (4.419 g, 91.6%). An analytical sample was crystallized from benzene/ethyl acetate (1:1) leaving a white solid, mp 96-98°C. ^{1}H NMR ($CDCl_3$, 360 MHz): δ 8.87 (br s, 1 H), 8.80 (br s, 1 H), 6.19 (m, 2 H), 6.02 (m, 2 H), 4.97 (dd, 2 H, J_1=7.0Hz, J_2=20 Hz), 3.98 (s, 1 H), 3.96 (s, 1 H), 2.26 (br s, 1 H), 2.16 (br s, 1 H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -81.5 (m, 6 F), -118.0 (s, 1 F), -118.6 (s, 1 F), -126.6 (m, 6 F). HREI MS [*m/z* (rel inten)]: 543.07117 (M + 1, 9.46), 542.06720 (M^+, 45.60). Anal. Calcd for $C_{17}H_{12}N_2O_2F_{14}$: C, 37.65; H, 2.23; N, 5.17. Found: C, 37.58; H, 2.09; N, 5.44.

2,2,3,3,4,4,4-Heptafluoro-1-(2-pyrrolyl)-1-butanol, 2.[2] Under N_2, a stirred cooled (0°C) solution of pyrrole (7.46 mL, 0.108 mol), triethylamine (18.1 mL, 0.129 mol), and THF (500 mL) was treated with heptafluorobutyryl chloride (25 g, 0.108 mol). A thick white precipitate formed immediately, and swirling was required to free the stir bar. After the addition the mixture was stirred for 4 h at 25 °C, filtered under suction, and the amine salt was washed with 3 (100 mL) portions of dry diethyl ether. The filtrate was collected, and the solvents were removed by rotary evaporation leaving a brown oil. The oil was dissolved in 50% aqueous methanol (300 mL), and the resulting solution was treated with $NaHCO_3$ (1 g) and $NaBH_4$ (8.2 g). The mixture was stirred at 25 °C for 10 h, and an additional portion of $NaBH_4$ (2 g) was added. After 2 h approximately half of the solvent was removed by rotary evaporation, water (250 mL) was added, and the mixture was extracted twice with 200 mL of diethyl ether. The combined organic layers were dried over $NaSO_4$ and the solvents were evaporated leaving **2** isolated as a light brown solid. This material was recrystallized from toluene yielding a colorless crystalline solid (23.5 g, 82%). ^{1}H NMR ($CDCl_3$, 360 MHz): δ 8.55 (br s, 1H), 6.87 (dt, 1H, J_1=2.7 Hz, J_2=1.51 Hz), 6.32 (m, 1H), 6.22 (dt, 1H, J_1=2.7 Hz, J_2=3.5 Hz), 5.26 (dd, 1H, J_1=7.8 Hz, J_2=16.7 Hz), 2.42 (br s, 1H).

1,1-Bis(2-pyrrolyl)-2,2,3,3,4,4,4-heptafluorobutane. 3. In a two-necked 500 mL round bottom flask, benzene (350 mL) and TSA were dried for 1 h using a Dean-Stark apparatus with 4 A molecular sieves in the sidearm. Pyrrole (6.25 mL, 90 mmol) and **2** (1.200g, 4.5mmol) were added, and heating at reflux was continued. An additional 150

mg of TSA was added to the mixture after 2 h, heating was terminated 15 minutes thereafter. The reaction mixture was allowed to cool, 100 mL of aq. $NaHCO_3$ (sat.) was added, and the organic layer separated, dried over $MgSO_4$, filtered, and evaporated. The crude product was purified by column chromatography (chloroform:hexane, 1:1) to yield colorless crystals (1.095 g, 77.5%). An analytical sample was further purified by vacuum sublimation, mp 57 °C. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.12 (br s, 2 H), 6.76 (m, 2 H), 6.24 (s, 2 H), 6.19 (dd, 2 H, J_1=2.8 Hz, J_2=3.2 Hz), 4.93 (t, 1 H, J=16.9). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -81.18 (m, 3F), -113.58 (s, 2F), -125.48 (m, 2F). HREI MS [*m/z* (rel inten)]: 315.06878 (M + 1, 6.35), 314.06545 (M^+, 43.57). Anal. Calcd for $C_{12}H_9N_2F_7$: C, 45.87; H, 2.89; N, 8.92. Found: C, 46.09; H, 2.69; N, 8.68.

5,10,15-Tris(heptafluoropropyl)porphyrin, $(R_f)_3P$. Reagent grade benzene (1600 mL) and *p*-toluenesulfonic acid (314 mg) were placed in a 2 L two-necked round bottom flask equipped with a recycling Dean-Stark trap (4 Å sieves) , condenser and magnetic stirring bar and heated at reflux for 2 h. Compound **1** (1.061 g) and compound **3** (0.614 g) were dissolved in dry benzene and added to the refluxing solution. After 50 min of strong heating the reaction was quenched with DDQ (1.200 g), heated for 55 min, treated with pyridine (10 mL) and cooled to RT over the course of 1 h. The benzene was removed by rotary evaporation and the remaining black solid was dissolved in 100 ml of warm hexane, loaded onto a hexane packed silica gel column (4 x 14 cm), and eluted with carried out with 10% chloroform/hexane solution. The dark purple band was collected and the solvent was evaporated. The resulting light brown solid was crystallized from hot hexane to yield purple-red needles (73 mg, 4.5 %). An analytic sample was

recrystallized from chloroform (mp 211 °C). ^{1}H NMR ($CDCl_3$, 360 MHz): δ 10.33 (s, 1 H), 9.63 (br s, 4 H), 9.56 (br s, 2 H), 9.44 (d, 2 H, J = 5.0 Hz), -2.77 (br s, 2 H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -75.28 (d, 2 F, J = 8.28 Hz), -79.40 (t, 6 F, J = 10.4 Hz), -79.47 (t, 3 F, J = 10.4 Hz), -82.31 (br s, 4F), -118.00 (s, 2F), -119.74 (s, 4F). UV-vis (CH_2Cl_2): 401 (92.6), 506 (10.0), 539 (8.82), 583 (5.94), 636 (9.04). HRFAB MS: 815.070282 (M + 1), 814.062286 (M^+). Anal. Calcd for $C_{29}H_{11}N_4F_{21}$: C, 42.77; H, 1.36; N, 6.88. Found: C, 42.94; H, 1.49; N, 6.72.

5,15,-Bis(heptafluoropropyl)porphyrin, $(R_f)_2P$. The general procedure, up to the chromatographic work up, was the same as for $(R_f)_3P$ except that TSA (150 mg), compound **1** (407 mg), and 2,2' dipyrrylmethane (110 mg) were used and the initial reaction time was 30 min. The benzene solution was evaporated and the remaining black solid was dissolved in hot $CHCl_3$ (125 mL) and chromatographed on silica gel ($CHCl_3$). The dark purple band was collected and was dried by rotary evaporation. The resulting solid was crystallized from hot chloroform to yield purple needles (26.7 mg, 5.6%). Analytical samples required no further purification (mp >300 °C, subl. ~260 °C). ^{1}H NMR ($CDCl_3$, 360 MHz): δ 10.49 (s, 2 H), 9.67 (m, 4 H), 9.54 (d, 4 H, J = 5.2 Hz), -2.58 (br s, 2 H). ^{19}F NMR ($CDCl_3$, 500 MHz): δ -79.38 (t, 6 F, J = 11.1 Hz), -84.93 (m, 4 F), -120.75 (dd, 4 F, J_1 = 11.9 Hz, J_2 = 11.1 Hz). UV-vis (CH_2Cl_2): 394 (752), 500 (33.7), 538 (70.1), 576 (18.8), 628 (72.0). HRFAB MS: 647.092310 (M + 1), 646.083436 (M^+). Anal. Calcd for $C_{26}H_{12}N_4F_{14}$: C, 48.31; H, 1.87; N, 8.67. Found: C, 47.71; H, 1.75; N, 8.43.

Calculations. All calculations were performed using the Gaussian 98W suite of programs[3] and a 500 MHz PC. No symmetry constraints were used in any of the calculations. The results of the modeling calculations (B3LYP/3-21G*) are summarized in the following table. All energies are reported in Hartrees.

Compd	Calc. Type	HOMO-1	HOMO	LUMO	LUMO+1	Energy
Porphine	Optimized	-0.200306	-0.191162	-0.083929	-0.083803	-984.090917799
$(R_f)_1P$	Optimized	-0.208692	-0.204253	-0.098494	-0.091212	-1555.79599176
$(R_f)_2P$	Optimized	-0.216986	-0.215882	-0.112187	-0.098742	-2127.50019965
$(R_f)_3P$	Optimized	-0.226514	-0.222560	-0.117855	-0.111531	-2699.19725398
$(R_f)_4P$	Optimized	-0.236047	-0.228920	-0.125344	-0.122254	-3270.89874064

References for Supporting Information

(1) Chong, R. Clezy, P. S.; Liepa, A. J.; Nichol, A. W. *Aust. J. Chem.* **1969**, *22*, 229.

(2) DiMagno, S. G.; Williams, R. A.; Therien, M. J. *J. Org. Chem.* **1994**, *59*, 6943-6948.

(3) Frisch, M. J. et al. *Gaussian 98W*, Gaussian, Pittsburgh, 1998.

Crystal Structure Determination of $(C_3F_7)_3P$.

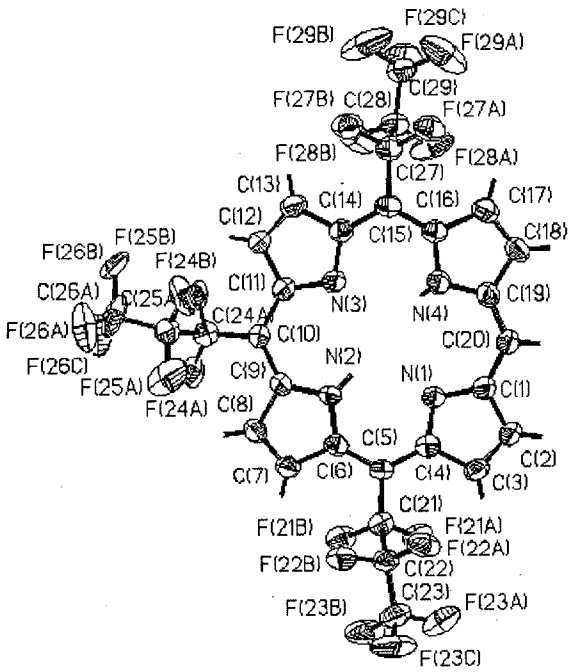

Table 1. Data collection.

Identification code	sdc3
Empirical formula	$C_{29}H_{11}F_{21}N_4$
Formula weight	814.42
Temperature	198(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 17.4086(6) Å b = 18.4656(6) Å c = 9.1527(3) Å β = 95.4050(10) deg.
Volume, Z	2929.15(17) $Å^3$, 4
Density (calculated)	1.847 g/cm^3
Absorption coefficient	0.205 mm^{-1}
F(000)	1608
Crystal size	0.60 x 0.14 x 0.12 mm
Theta range for data collection	1.17 to 25.04 °
Limiting indices	-20<=h<=20, -14<=k<=21, -10<=l<=10
Reflections collected	14793
Independent reflections	5157 [R_{int} = 0.0720]
Absorption correction	Integration
Max. and min. transmission	0.9758 and 0.8869
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5157 / 62 / 577
Goodness-of-fit on F^2	1.170
Final R indices [I>2σ(I)]	R_1 = 0.0665, wR_2 = 0.1678
R indices (all data)	R_1 = 0.1133, wR_2 = 0.1992
Largest diff. peak and hole	0.591 and -0.350 $e/Å^3$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for sdc3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	2661(2)	3270(2)	954(3)	39(1)
N(2)	3002(2)	1823(2)	415(3)	39(1)
N(3)	1692(2)	1375(2)	2225(4)	41(1)
N(4)	1360(2)	2820(2)	2836(4)	40(1)
C(1)	2386(2)	3925(2)	1386(5)	46(1)
C(2)	2840(2)	4497(2)	840(5)	53(1)
C(3)	3378(3)	4197(2)	109(5)	49(1)
C(4)	3267(2)	3415(2)	164(4)	39(1)
C(5)	3711(2)	2872(2)	-443(4)	37(1)
C(6)	3593(2)	2127(2)	-264(4)	36(1)
C(7)	4062(2)	1540(2)	-720(4)	45(1)
C(8)	3760(2)	924(2)	-305(5)	47(1)
C(9)	3075(2)	1085(2)	400(5)	49(1)
C(10)	2577(3)	573(2)	946(6)	80(2)
C(11)	1920(2)	713(2)	1727(5)	50(1)
C(12)	1388(2)	169(2)	2145(5)	50(1)
C(13)	864(3)	493(2)	2863(5)	51(1)
C(14)	1042(2)	1254(2)	2951(4)	38(1)
C(15)	644(2)	1793(2)	3660(4)	38(1)
C(16)	786(2)	2534(2)	3594(4)	39(1)
C(17)	381(2)	3138(2)	4174(5)	48(1)
C(18)	708(2)	3748(2)	3732(5)	51(1)
C(19)	1324(2)	3554(2)	2903(5)	45(1)
C(20)	1789(2)	4044(2)	2234(5)	51(1)
C(21)	4376(2)	3112(2)	-1251(4)	42(1)
F(21A)	4215(2)	3738(1)	-2016(3)	58(1)
F(21B)	4558(1)	2632(1)	-2287(2)	56(1)
C(22)	5143(2)	3263(2)	-284(4)	47(1)
F(22A)	4992(1)	3662(2)	890(3)	61(1)
F(22B)	5427(1)	2624(2)	227(3)	58(1)
C(23)	5784(3)	3642(3)	-1004(6)	65(1)
F(23A)	5592(2)	4326(2)	-1288(4)	108(1)
F(23B)	5929(2)	3335(2)	-2226(3)	93(1)
F(23C)	6427(2)	3660(2)	-115(3)	96(1)
C(24A)	2607(4)	-188(3)	238(6)	44(2)
F(24A)	2943(4)	-228(3)	-1018(6)	57(2)
F(24B)	1914(4)	-490(4)	-114(11)	51(2)
C(25A)	3065(4)	-706(3)	1331(7)	55(2)
F(25A)	3803(4)	-489(5)	1484(12)	120(4)
F(25B)	2820(6)	-622(5)	2691(7)	77(3)
C(26A)	3002(6)	-1516(4)	1046(11)	97(7)
F(26A)	3554(5)	-1812(5)	1894(10)	104(3)
F(26B)	2314(4)	-1733(4)	1425(9)	81(2)
F(26C)	3030(6)	-1706(5)	-283(8)	91(3)
C(24B)	2965(4)	-175(4)	1442(8)	45(3)
F(24C)	3737(4)	-153(4)	1720(10)	54(2)
F(24D)	2740(7)	-439(6)	2677(9)	63(4)
C(25B)	2774(4)	-752(3)	224(8)	47(3)
F(25C)	3144(6)	-557(5)	-938(8)	63(3)
F(25D)	2019(5)	-710(6)	-230(15)	54(3)
C(26B)	2995(7)	-1530(4)	586(13)	106(11)

F(26D)	3751(7)	-1539(8)	940(30)	329(18)
F(26E)	2649(15)	-1766(9)	1700(17)	310(20)
F(26F)	2834(9)	-1953(6)	-520(15)	94(4)
C(27)	-37(2)	1560(2)	4462(4)	45(1)
F(27A)	-132(1)	2003(1)	5619(2)	53(1)
F(27B)	49(1)	888(1)	5065(3)	57(1)
C(28)	-822(2)	1559(3)	3502(5)	49(1)
F(28A)	-922(2)	2196(2)	2822(3)	88(1)
F(28B)	-796(2)	1048(2)	2468(3)	97(1)
C(29)	-1541(3)	1420(3)	4236(6)	58(1)
F(29A)	-1655(2)	1925(3)	5189(4)	126(2)
F(29B)	-1501(2)	808(2)	4948(6)	146(2)
F(29C)	-2159(2)	1403(2)	3314(3)	79(1)

Table 3. Bond lengths [Å].

N(1)-C(4)	1.361(5)
N(1)-C(1)	1.374(5)
N(2)-C(9)	1.368(5)
N(2)-C(6)	1.373(5)
N(3)-C(11)	1.375(5)
N(3)-C(14)	1.382(5)
N(4)-C(19)	1.358(5)
N(4)-C(16)	1.375(5)
C(1)-C(20)	1.372(6)
C(1)-C(2)	1.437(6)
C(2)-C(3)	1.323(6)
C(3)-C(4)	1.458(6)
C(4)-C(5)	1.412(6)
C(5)-C(6)	1.403(6)
C(5)-C(21)	1.498(5)
C(6)-C(7)	1.441(6)
C(7)-C(8)	1.325(6)
C(8)-C(9)	1.440(6)
C(9)-C(10)	1.406(6)
C(10)-C(11)	1.428(6)
C(10)-C(24A)	1.551(7)
C(10)-C(24B)	1.586(8)
C(11)-C(12)	1.443(6)
C(12)-C(13)	1.318(6)
C(13)-C(14)	1.440(6)
C(14)-C(15)	1.406(5)
C(15)-C(16)	1.393(5)
C(15)-C(27)	1.514(6)
C(16)-C(17)	1.446(6)
C(17)-C(18)	1.341(6)
C(18)-C(19)	1.417(6)
C(19)-C(20)	1.393(6)
C(21)-F(21B)	1.357(4)
C(21)-F(21A)	1.367(4)
C(21)-C(22)	1.555(6)
C(22)-F(22B)	1.347(5)
C(22)-F(22A)	1.349(5)
C(22)-C(23)	1.519(6)
C(23)-F(23B)	1.299(5)
C(23)-F(23C)	1.320(6)
C(23)-F(23A)	1.325(6)
C(24A)-F(24A)	1.340(7)
C(24A)-F(24B)	1.340(7)
C(24A)-C(25A)	1.549(7)
C(25A)-F(25A)	1.339(7)
C(25A)-F(25B)	1.363(7)
C(25A)-C(26A)	1.521(7)
C(26A)-F(26C)	1.271(8)
C(26A)-F(26A)	1.298(9)
C(26A)-F(26B)	1.340(9)
C(24B)-F(24D)	1.323(8)
C(24B)-F(24C)	1.345(8)
C(24B)-C(25B)	1.555(7)
C(25B)-F(25C)	1.343(8)

C(25B)-F(25D)	1.343(8)
C(25B)-C(26B)	1.516(8)
C(26B)-F(26F)	1.288(9)
C(26B)-F(26E)	1.307(10)
C(26B)-F(26D)	1.327(10)
C(27)-F(27B)	1.360(5)
C(27)-F(27A)	1.361(5)
C(27)-C(28)	1.554(6)
C(28)-F(28A)	1.334(5)
C(28)-F(28B)	1.341(5)
C(28)-C(29)	1.498(6)
C(29)-F(29B)	1.303(6)
C(29)-F(29C)	1.303(5)
C(29)-F(29A)	1.305(6)

Table 4. Bond angles [deg].

C(4)-N(1)-C(1)	106.7(3)
C(9)-N(2)-C(6)	109.1(3)
C(11)-N(3)-C(14)	106.9(3)
C(19)-N(4)-C(16)	108.8(4)
C(20)-C(1)-N(1)	127.4(4)
C(20)-C(1)-C(2)	123.3(4)
N(1)-C(1)-C(2)	109.2(4)
C(3)-C(2)-C(1)	107.8(4)
C(2)-C(3)-C(4)	107.2(4)
N(1)-C(4)-C(5)	123.3(4)
N(1)-C(4)-C(3)	109.0(4)
C(5)-C(4)-C(3)	127.7(4)
C(6)-C(5)-C(4)	124.0(4)
C(6)-C(5)-C(21)	118.4(4)
C(4)-C(5)-C(21)	117.5(4)
N(2)-C(6)-C(5)	125.4(4)
N(2)-C(6)-C(7)	107.1(4)
C(5)-C(6)-C(7)	127.6(4)
C(8)-C(7)-C(6)	108.2(4)
C(7)-C(8)-C(9)	108.6(4)
N(2)-C(9)-C(10)	127.2(4)
N(2)-C(9)-C(8)	107.0(4)
C(10)-C(9)-C(8)	125.8(4)
C(9)-C(10)-C(11)	127.3(4)
C(9)-C(10)-C(24A)	114.6(4)
C(11)-C(10)-C(24A)	115.7(4)
C(9)-C(10)-C(24B)	115.3(5)
C(11)-C(10)-C(24B)	110.7(4)
C(24A)-C(10)-C(24B)	45.5(3)
N(3)-C(11)-C(10)	126.6(4)
N(3)-C(11)-C(12)	108.6(4)
C(10)-C(11)-C(12)	124.8(4)
C(13)-C(12)-C(11)	107.8(4)
C(12)-C(13)-C(14)	108.5(4)
N(3)-C(14)-C(15)	124.7(4)
N(3)-C(14)-C(13)	108.2(4)
C(15)-C(14)-C(13)	127.1(4)
C(16)-C(15)-C(14)	125.3(4)
C(16)-C(15)-C(27)	116.8(4)
C(14)-C(15)-C(27)	117.7(4)
N(4)-C(16)-C(15)	122.7(4)
N(4)-C(16)-C(17)	106.9(4)
C(15)-C(16)-C(17)	130.3(4)
C(18)-C(17)-C(16)	107.6(4)
C(17)-C(18)-C(19)	108.2(4)
N(4)-C(19)-C(20)	126.7(4)
N(4)-C(19)-C(18)	108.4(4)
C(20)-C(19)-C(18)	124.9(4)
C(1)-C(20)-C(19)	130.3(4)
F(21B)-C(21)-F(21A)	104.2(3)
F(21B)-C(21)-C(5)	113.1(3)
F(21A)-C(21)-C(5)	111.8(3)
F(21B)-C(21)-C(22)	105.8(3)
F(21A)-C(21)-C(22)	105.3(3)

C(5)-C(21)-C(22)	115.7(3)
F(22B)-C(22)-F(22A)	107.1(3)
F(22B)-C(22)-C(23)	107.0(4)
F(22A)-C(22)-C(23)	107.5(3)
F(22B)-C(22)-C(21)	107.9(3)
F(22A)-C(22)-C(21)	109.3(3)
C(23)-C(22)-C(21)	117.5(4)
F(23B)-C(23)-F(23C)	108.6(5)
F(23B)-C(23)-F(23A)	108.2(5)
F(23C)-C(23)-F(23A)	106.3(4)
F(23B)-C(23)-C(22)	112.5(4)
F(23C)-C(23)-C(22)	111.0(4)
F(23A)-C(23)-C(22)	110.0(5)
F(24A)-C(24A)-F(24B)	103.1(6)
F(24A)-C(24A)-C(25A)	106.3(5)
F(24B)-C(24A)-C(25A)	107.2(6)
F(24A)-C(24A)-C(10)	116.3(5)
F(24B)-C(24A)-C(10)	114.4(6)
C(25A)-C(24A)-C(10)	108.9(4)
F(25A)-C(25A)-F(25B)	104.5(7)
F(25A)-C(25A)-C(26A)	111.4(6)
F(25B)-C(25A)-C(26A)	104.2(6)
F(25A)-C(25A)-C(24A)	108.3(5)
F(25B)-C(25A)-C(24A)	109.4(6)
C(26A)-C(25A)-C(24A)	118.1(5)
F(26C)-C(26A)-F(26A)	111.3(8)
F(26C)-C(26A)-F(26B)	106.3(8)
F(26A)-C(26A)-F(26B)	110.4(7)
F(26C)-C(26A)-C(25A)	115.3(7)
F(26A)-C(26A)-C(25A)	105.9(7)
F(26B)-C(26A)-C(25A)	107.6(6)
F(24D)-C(24B)-F(24C)	102.7(7)
F(24D)-C(24B)-C(25B)	107.5(6)
F(24C)-C(24B)-C(25B)	107.3(6)
F(24D)-C(24B)-C(10)	114.4(7)
F(24C)-C(24B)-C(10)	114.8(6)
C(25B)-C(24B)-C(10)	109.6(5)
F(25C)-C(25B)-F(25D)	105.5(7)
F(25C)-C(25B)-C(26B)	107.3(7)
F(25D)-C(25B)-C(26B)	110.1(7)
F(25C)-C(25B)-C(24B)	107.4(6)
F(25D)-C(25B)-C(24B)	108.5(6)
C(26B)-C(25B)-C(24B)	117.4(6)
F(26F)-C(26B)-F(26E)	109.3(9)
F(26F)-C(26B)-F(26D)	108.8(9)
F(26E)-C(26B)-F(26D)	108.9(10)
F(26F)-C(26B)-C(25B)	111.8(8)
F(26E)-C(26B)-C(25B)	111.1(9)
F(26D)-C(26B)-C(25B)	106.8(8)
F(27B)-C(27)-F(27A)	104.4(3)
F(27B)-C(27)-C(15)	113.3(3)
F(27A)-C(27)-C(15)	111.4(3)
F(27B)-C(27)-C(28)	106.6(3)
F(27A)-C(27)-C(28)	106.0(3)
C(15)-C(27)-C(28)	114.4(3)
F(28A)-C(28)-F(28B)	107.6(4)

F(28A)-C(28)-C(29)	106.5(4)
F(28B)-C(28)-C(29)	106.3(4)
F(28A)-C(28)-C(27)	109.4(3)
F(28B)-C(28)-C(27)	108.3(4)
C(29)-C(28)-C(27)	118.3(4)
F(29B)-C(29)-F(29C)	107.7(4)
F(29B)-C(29)-F(29A)	106.8(5)
F(29C)-C(29)-F(29A)	106.4(4)
F(29B)-C(29)-C(28)	111.4(4)
F(29C)-C(29)-C(28)	112.8(4)
F(29A)-C(29)-C(28)	111.3(4)