Supplementary Material (ESI) for Chemical Communications

Electronic Supporting Information

meso-Alkylidene (*m*-benzi)pentaphyrin: A modified pentaphyrin bearing exocyclic double bonds at meso-positions

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Experimental Section

Proton NMR spectra (300 MHz, Bruker Avance™ and 400 MHz, Bruker DPX-400) were recorded using TMS as the internal standard. High resolution mass spectra were obtained on an Voyager-DE STR MALDI-TOF mass spectrometer. Column chromatography was performed over silica gel (Merck, 230-400 mesh). Pyrrole was distilled at atmospheric pressure from CaH_2. All other reagents were obtained from Aldrich and used as received unless noted otherwise.

6,26-Bis(diethoxycarbonylmethylidene)-11,16,21-tri(pentafluorophenyl)-27-(*m*-benzi)pentaphyrin(2)

Compound **1** (0.53 g, 0.96 mmol), pyrrole (0.08 g, 1.14 mmol) and pentafluorobenzaldehyde (0.27 mL, 2.19 mmol) were dissolved in CH_2Cl_2 (450 mL) and TFA (0.04 mL, 0.52 mmol) was added. The mixture was stirred for 7 day at room temperature. Then DDQ (0.85 g, 3.75 mmol) was added and stirred additional 1 hr. The reaction was stopped by adding TEA (0.50 mL, 3.59 mmol) and extracted with CH_2Cl_2. The organic layer was dried (Na_2SO_4) and solvent was removed in vacuo. The remaining solid was purified by column chromatography on silica ($CHCl_3$/EtOAc = 19/1) to obtain products **2**. Yield: 0.084 g (8%); UV-Vis. (CH_2Cl_2) λ_{max} (log ε) 460 (4.91), 754 (4.20); ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.19 (br s, 2H), 9.99 (br s, 1H), 7.60 (dd, 2H, J = 1.71, 7.71 Hz), 7.33 (t, 1H, J = 7.71 Hz), 6.83 (t, 1H, J = 1.71 Hz) 6.75 (d, 2H, J = 5.12 Hz), 6.58 (d, 2H, J = 3.93 Hz), 6.48 (d, 2H, J = 5.12 Hz), 5.92 (d, 2H, J = 3.93 Hz), 4.16 (q, 4H, J = 7.13 Hz), 3.97 (q, 4H, J = 7.10 Hz), 1.26 (t, 3H, J = 7.10 Hz), 1.02 (t, 3H, J = 7.13 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.31, 165.63, 159.55, 150.46, 144.03, 138.41, 137.45, 135.94, 133.15, 131.79, 129.49, 128.92, 125.84, 124.82, 119.33, 116.97, 107.41, 93.16, 61.98, 61.24, 13.88, 13.63; HRMS Calcd. for $C_{59}H_{35}F_{15}N_4O_8$ 1212.2215, Found 1212.2599.

Figure 1. ^{1}H NMR spectrum of 6,26-Bis(diethoxycarbonylmethylidene)-11,16,21-tri(pentafluorophenyl)-27-(*m*-benzi)penta-phyrin(**2**) in $CDCl_3$

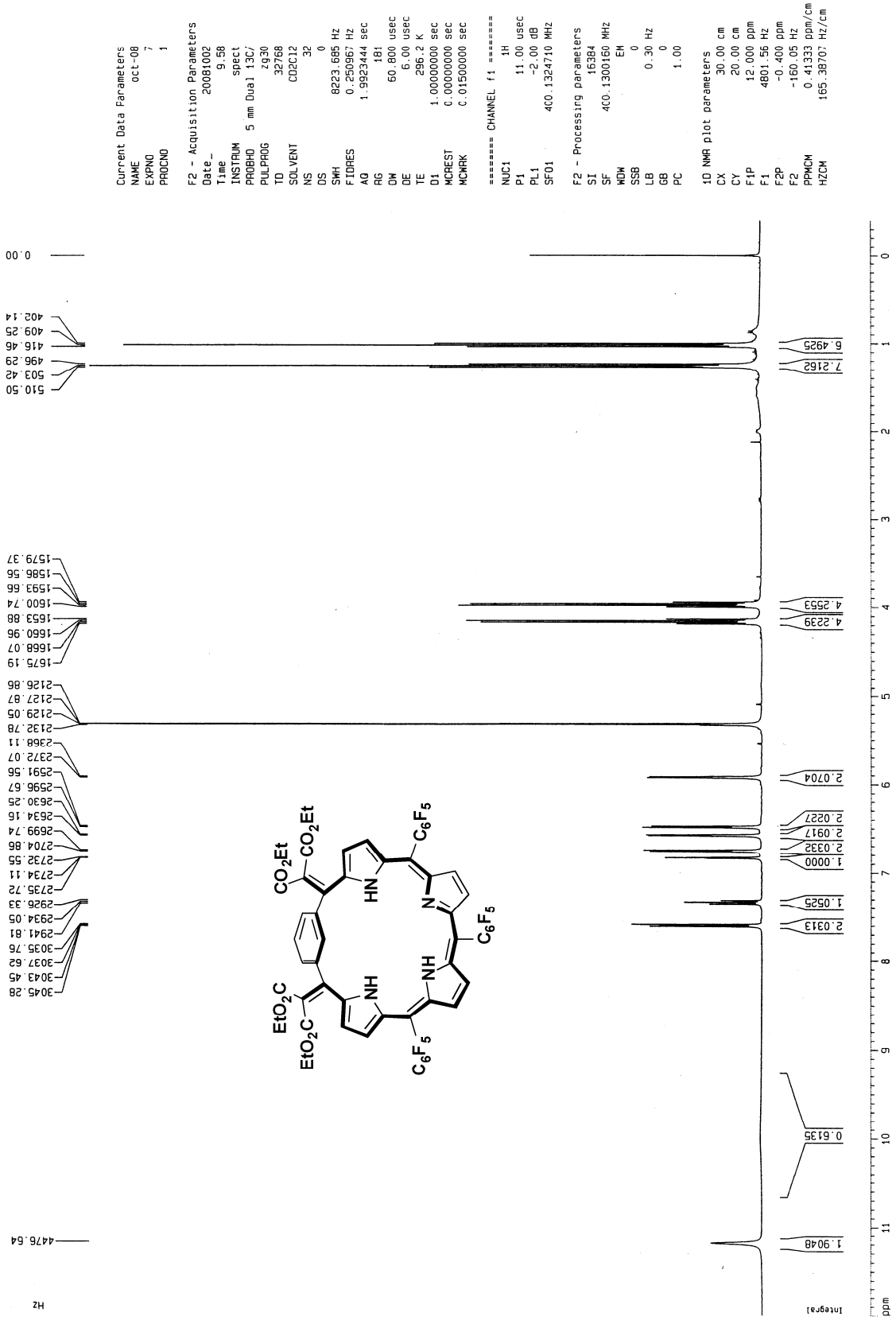


Figure 2. ^{13}C NMR spectrum of 6,26-Bis(diethoxycarbonylmethylidene)-11,16,21-tri(pentafluorophenyl)-27-(*m*-benzi)penta-phyrin(**2**) in $CDCl_3$

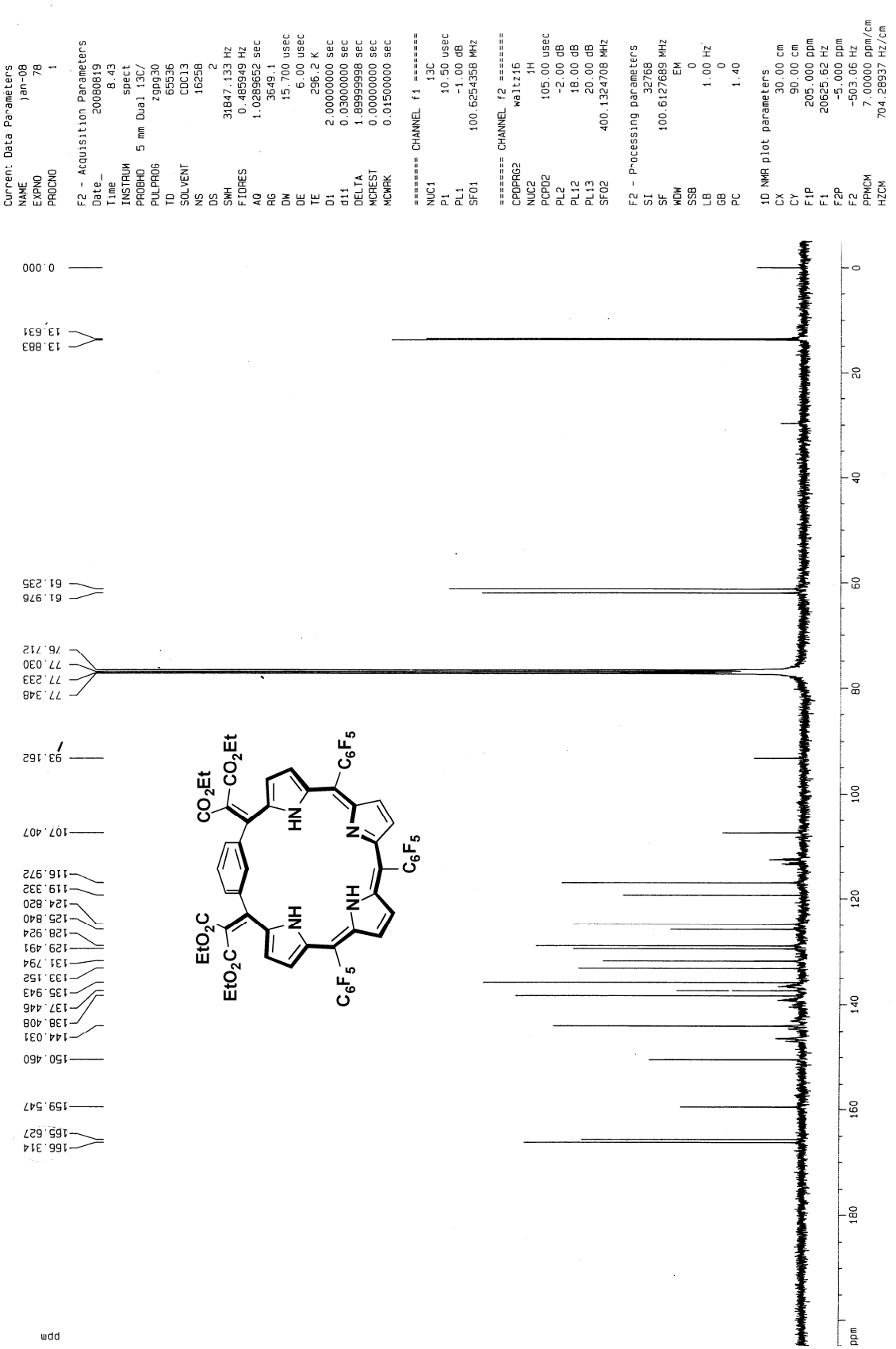


Figure 3. MALDI-TOF Mass spectrum of 6,26-Bis(diethoxycarbonylmethylidene)-11,16,21-tri(pentafluorophenyl)-27-(*m*-benzi)pentaphyrin(**2**) in CH_2Cl_2

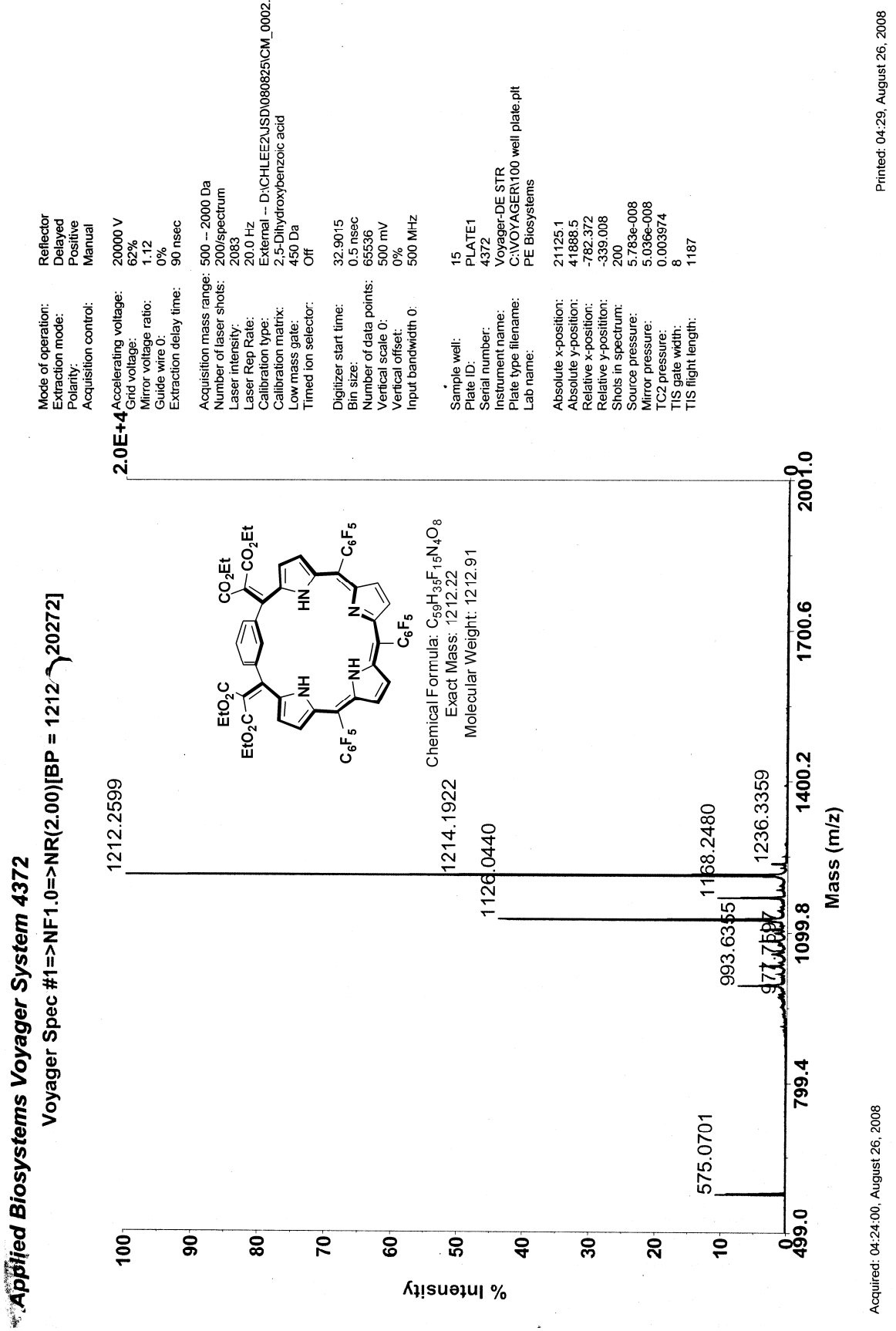
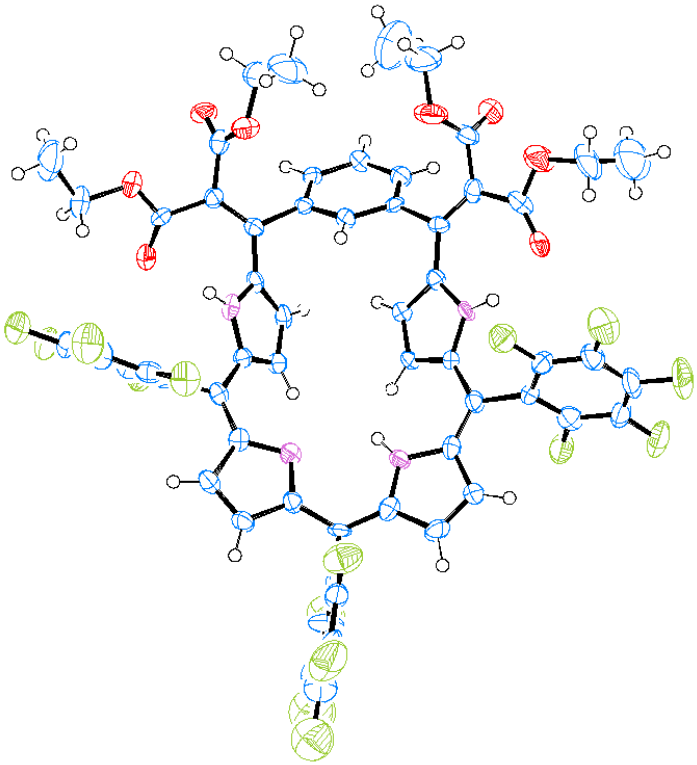


Figure 4. Solid state structure of (*m*-benzi)pentaphyrin (**2**) from X-ray diffraction analyses: A) top view and B) side view.

A)



B)

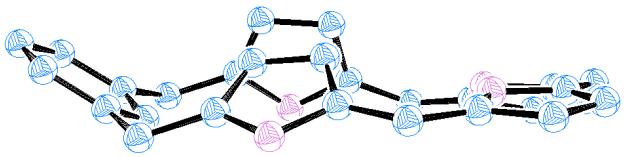


Figure 5. ^{1}H NMR spectral changes of (*m*-benzi)pentaphyrin in $CDCl_3$ upon the addition of trifluoroacetic acid (50.0 equiv.)

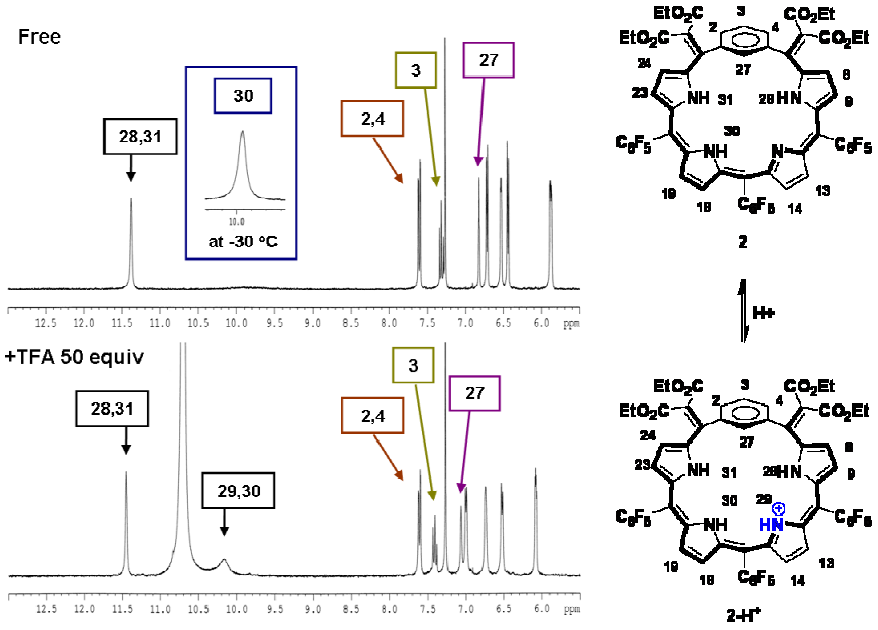


Figure 6. UV-vis absorption spectral changes of (*m*-benzi)pentaphyrin (2.6 x 10^{-5} M in CH_2Cl_2) upon the addition of trifluoroacetic acid 0-300 equiv.

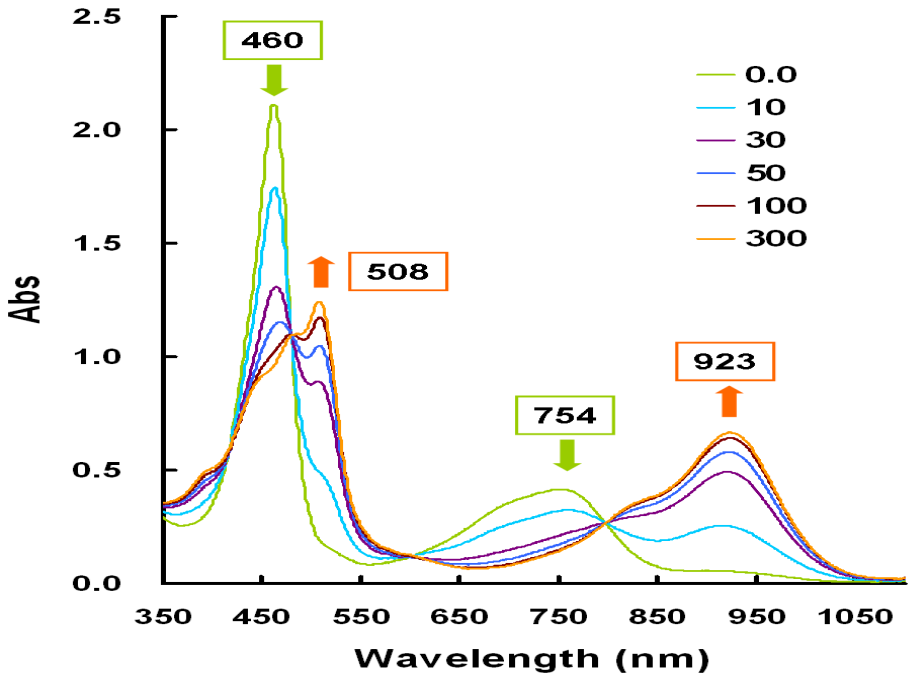


Figure 7. ^{1}H NMR spectral changes of (*m*-benzi)pentaphyrin in DMSO-d_6 upon the addition of TBAF A) 0.0 equiv. B) 3.0 equiv. C) 10.0 equiv.

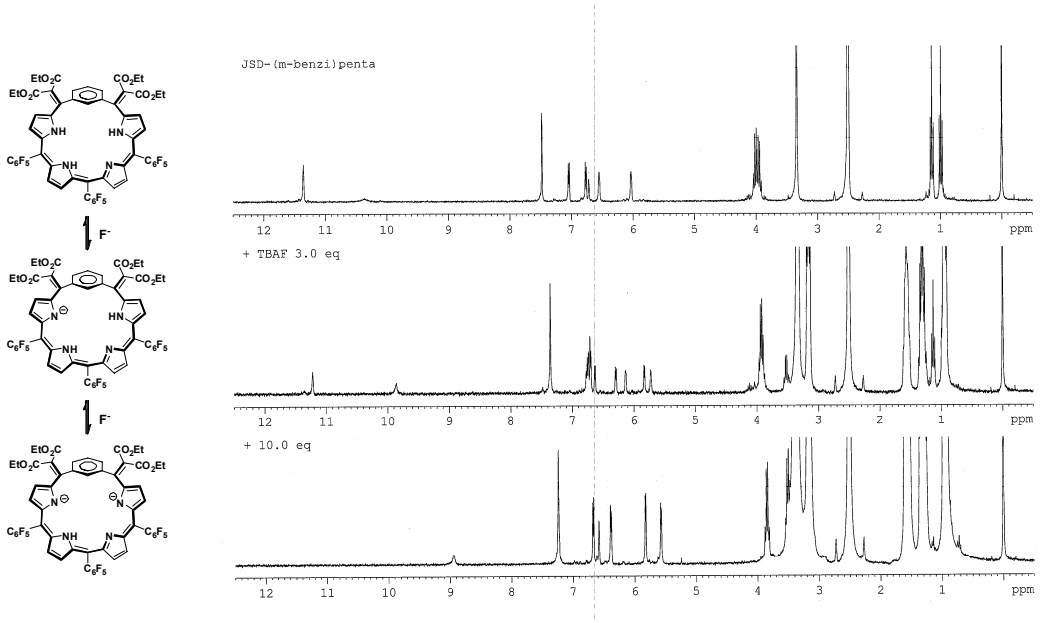


Figure 8. UV-vis absorption spectral changes of (*m*-benzi)pentaphyrin (2.6 x 10^{-5} M in CH_3CN) upon the addition of TBAF A) 0.0-5.0 equiv. B) 5.0-50.0 equiv.

A) B)

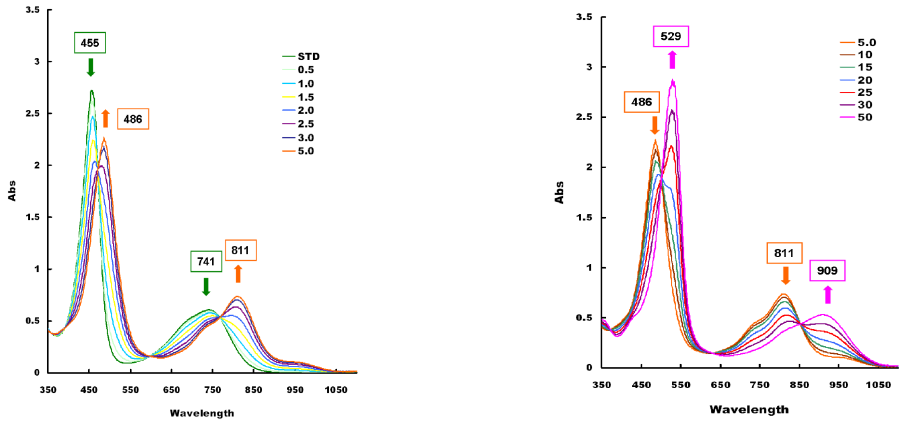


Figure 9. The color changes induced of (*m*-benzi)pentaphyrin (4.4 x 10^{-5} M in CH_3CN) upon the addition of TBAF. (From left to right, 0, 1, 3, 5, 10 equiv.)

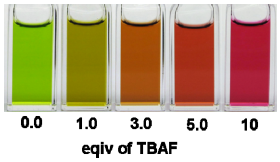


Figure 10. UV-vis absorption spectral changes of (*m*-benzi)pentaphyrin (2.6 x 10^{-5} M in CH_3CN) upon the addition of TBACN 0.0-5.0 equiv.

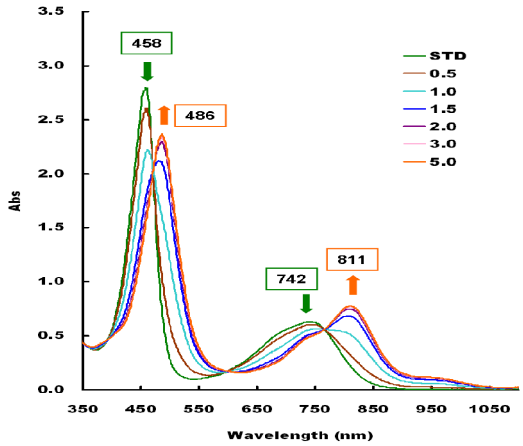


Figure 11. The color changes induced of (*m*-benzi)pentaphyrin (4.4 x 10^{-5} M in CH_3CN-1% H_2O) upon the addition of various anions. (5.0 equiv.)

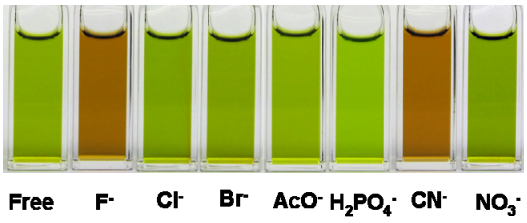


Table 1. Crystal data and structure refinement for ym157P-1.

Identification code	ym157p-1	
Empirical formula	C65 H53 F15 N4 O11 S3	
Formula weight	1447.29	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 14.0190(14) Å	α= 71.256(2)?
	b = 14.8954(15) Å	β= 74.778(2)?
	c = 17.1725(17) Å	γ = 85.907(2)?
Volume	3276.3(6) □3	
Z	2	
Density (calculated)	1.467 Mg/m^3	
Absorption coefficient	0.219 mm^{-1}	
F(000)	1484	
Crystal size	? x ? x ? mm^3	
Theta range for data collection	1.61 to 26.00□.	
Index ranges	-17<=h<=17, -13<=k<=18, -21<=l<=21	
Reflections collected	18343	
Independent reflections	12498 [R(int) = 0.0500]	
Completeness to theta = 26.00	97.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12498 / 12 / 866	
Goodness-of-fit on F^2	0.761	
Final R indices [I>2sigma(I)]	R1 = 0.0848, wR2 = 0.1911	
R indices (all data)	R1 = 0.2077, wR2 = 0.2226	
Largest diff. peak and hole	1.492 and -0.843 $e.^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}x 10^3) for ym157P-1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9390(4)	-331(4)	-1749(3)	23(1)
C(2)	8608(4)	-827(4)	-1095(3)	24(1)
C(3)	8618(4)	-1817(4)	-731(3)	23(1)
C(4)	9420(4)	-2305(4)	-1073(3)	26(1)
C(5)	10191(4)	-1818(4)	-1746(3)	30(2)
C(6)	10176(4)	-828(4)	-2060(4)	32(2)
C(7)	9376(4)	743(4)	-2044(3)	23(1)
C(8)	9202(4)	1111(4)	-1331(3)	25(1)
C(9)	9157(4)	617(4)	-489(3)	24(1)
C(10)	8913(4)	1213(4)	-14(3)	25(1)
C(11)	8802(4)	2126(4)	-558(3)	24(1)
C(12)	8551(4)	3006(4)	-378(3)	28(2)
C(13)	8053(4)	3074(4)	399(4)	29(2)
C(14)	7863(5)	3901(4)	656(4)	35(2)
C(15)	7352(5)	3650(4)	1469(4)	38(2)
C(16)	7136(4)	2662(4)	1764(4)	31(2)
C(17)	6523(4)	2119(4)	2532(3)	30(2)
C(18)	6183(4)	1178(4)	2700(3)	28(2)
C(19)	5350(4)	753(4)	3376(4)	33(2)
C(20)	5164(4)	-70(4)	3266(3)	34(2)
C(21)	5931(4)	-165(4)	2541(4)	29(2)
C(22)	6023(4)	-925(4)	2245(3)	26(2)
C(23)	6856(4)	-1140(4)	1667(3)	24(1)
C(24)	7879(4)	-1003(4)	1532(3)	30(2)
C(25)	8374(4)	-1453(4)	951(3)	31(2)
C(26)	7677(4)	-1840(4)	703(3)	25(1)
C(27)	7818(4)	-2282(4)	33(3)	26(2)
C(28)	9474(4)	1204(4)	-2889(4)	30(2)
C(29)	9587(5)	671(5)	-3506(4)	36(2)
C(30)	8839(7)	-258(7)	-4059(5)	95(3)
C(31)	9360(8)	-1291(7)	-3806(7)	121(4)
C(32)	9466(5)	2253(5)	-3303(4)	38(2)
C(33)	9382(7)	3419(6)	-4624(5)	77(3)

C(34)	10388(9)	3761(7)	-5036(6)	111(4)
C(35)	8853(4)	3912(4)	-1098(4)	26(1)
C(36)	8370(5)	4227(4)	-1732(4)	35(2)
C(37)	8593(5)	5070(5)	-2369(4)	43(2)
C(38)	9338(6)	5616(5)	-2391(4)	47(2)
C(39)	9859(5)	5335(5)	-1781(4)	41(2)
C(40)	9589(5)	4486(5)	-1151(4)	37(2)
C(41)	6038(4)	2617(3)	3155(3)	43(2)
C(42)	5220(4)	3184(3)	3050(3)	50(2)
C(43)	4751(3)	3605(3)	3661(3)	68(2)
C(44)	5100(4)	3460(4)	4379(3)	68(2)
C(45)	5918(4)	2894(4)	4484(3)	77(3)
C(46)	6387(3)	2473(3)	3872(3)	71(3)
C(47)	5182(4)	-1617(4)	2547(3)	26(1)
C(48)	4241(5)	-1388(5)	2411(4)	35(2)
C(49)	3511(4)	-2041(6)	2629(4)	44(2)
C(50)	3690(5)	-2977(5)	3012(4)	45(2)
C(51)	4579(5)	-3244(5)	3173(4)	34(2)
C(52)	5305(5)	-2581(5)	2950(4)	33(2)
C(53)	7293(4)	-3003(4)	62(4)	27(2)
C(54)	6552(5)	-3574(4)	839(4)	32(2)
C(55)	4999(5)	-4403(5)	1340(4)	59(2)
C(56)	4346(6)	-4839(6)	1033(5)	82(3)
C(57)	7378(4)	-3269(5)	-719(4)	35(2)
C(58)	7162(5)	-2674(5)	-2111(4)	52(2)
C(59)	6724(7)	-1785(5)	-2623(4)	83(3)
F(1)	7598(3)	3697(2)	-1696(2)	50(1)
F(2)	8073(3)	5355(3)	-2963(2)	64(1)
F(3)	9568(3)	6453(3)	-3013(2)	70(1)
F(4)	10579(3)	5878(3)	-1795(3)	65(1)
F(5)	10135(3)	4222(2)	-558(2)	52(1)
F(6)	4862(3)	3303(3)	2402(3)	68(1)
F(7)	3954(3)	4104(3)	3600(3)	107(2)
F(8)	4634(4)	3859(4)	4990(3)	107(2)
F(9)	6277(4)	2769(4)	5161(4)	137(2)
F(10)	7169(4)	1960(3)	3981(3)	92(2)
F(11)	4075(3)	-479(3)	1981(2)	52(1)
F(12)	2655(3)	-1787(3)	2412(3)	69(1)

F(13)	2969(3)	-3627(3)	3236(2)	68(1)
F(14)	4739(3)	-4154(3)	3562(2)	62(1)
F(15)	6177(3)	-2860(2)	3135(2)	42(1)
N(1)	9003(3)	2040(3)	-1344(3)	25(1)
N(2)	7618(3)	2324(3)	1112(3)	27(1)
N(3)	6556(3)	628(3)	2209(3)	28(1)
N(4)	6771(3)	-1651(3)	1146(3)	31(1)
O(1)	10351(3)	596(3)	-3988(3)	44(1)
O(2)	8753(4)	272(4)	-3465(3)	71(2)
O(3)	9503(3)	2870(3)	-3007(3)	48(1)
O(4)	9399(4)	2407(3)	-4093(3)	60(1)
O(5)	6570(3)	-3685(3)	1564(3)	46(1)
O(6)	5851(3)	-3942(3)	633(3)	50(1)
O(7)	7698(3)	-4003(3)	-835(2)	42(1)
O(8)	7057(3)	-2567(3)	-1294(3)	41(1)
O(1S)	5000(3)	1919(3)	-773(2)	43(1)
S(1S)	5177(1)	1348(2)	66(1)	57(1)
C(1S)	5470(6)	2183(6)	507(5)	77(3)
C(2S)	6390(5)	881(5)	-170(5)	64(2)
O(2S)	3757(5)	1754(4)	4693(5)	139(3)
S(2S)	2773(2)	1485(2)	5092(2)	107(1)
C(3S)	2340(7)	1827(8)	6005(6)	124(4)
C(4S)	2748(7)	292(6)	5631(7)	129(5)
O(3S)	9012(6)	4885(6)	3660(5)	191(5)
S(3S)	8216(3)	5603(3)	3586(2)	149(1)
C(5S)	8410(6)	6281(6)	2584(5)	90(3)
C(6S)	7491(8)	4982(5)	3414(6)	119(4)

Table 3. Bond lengths [? and angles [? for ym157P-1.

C(1)-C(6)	1.370(7)
C(1)-C(2)	1.394(7)
C(1)-C(7)	1.516(7)
C(2)-C(3)	1.405(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.396(7)
C(3)-C(27)	1.488(7)
C(4)-C(5)	1.396(7)
C(4)-H(4)	0.9500
C(5)-C(6)	1.399(8)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(28)	1.365(7)
C(7)-C(8)	1.455(7)
C(8)-C(9)	1.381(7)
C(8)-N(1)	1.387(7)
C(9)-C(10)	1.360(7)
C(9)-H(9)	0.9500
C(10)-C(11)	1.405(7)
C(10)-H(10)	0.9500
C(11)-N(1)	1.351(6)
C(11)-C(12)	1.439(8)
C(12)-C(13)	1.367(7)
C(12)-C(35)	1.505(7)
C(13)-N(2)	1.394(6)
C(13)-C(14)	1.423(8)
C(14)-C(15)	1.334(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.420(8)
C(15)-H(15)	0.9500
C(16)-N(2)	1.371(7)
C(16)-C(17)	1.396(7)
C(17)-C(18)	1.428(8)
C(17)-C(41)	1.489(6)
C(18)-N(3)	1.343(7)
C(18)-C(19)	1.427(7)

C(19)-C(20)	1.352(8)
C(19)-H(19)	0.9500
C(20)-C(21)	1.454(7)
C(20)-H(20)	0.9500
C(21)-C(22)	1.368(8)
C(21)-N(3)	1.393(7)
C(22)-C(23)	1.411(7)
C(22)-C(47)	1.493(8)
C(23)-N(4)	1.379(7)
C(23)-C(24)	1.410(8)
C(24)-C(25)	1.388(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.388(8)
C(25)-H(25)	0.9500
C(26)-N(4)	1.360(6)
C(26)-C(27)	1.464(8)
C(27)-C(53)	1.325(8)
C(28)-C(29)	1.487(8)
C(28)-C(32)	1.496(8)
C(29)-O(1)	1.192(7)
C(29)-O(2)	1.325(8)
C(30)-O(2)	1.455(8)
C(30)-C(31)	1.633(12)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-O(3)	1.193(7)
C(32)-O(4)	1.330(7)
C(33)-C(34)	1.448(11)
C(33)-O(4)	1.492(8)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(40)	1.352(8)

C(35)-C(36)	1.370(8)
C(36)-F(1)	1.362(7)
C(36)-C(37)	1.366(8)
C(37)-F(2)	1.348(7)
C(37)-C(38)	1.354(9)
C(38)-F(3)	1.349(7)
C(38)-C(39)	1.372(9)
C(39)-F(4)	1.330(7)
C(39)-C(40)	1.373(8)
C(40)-F(5)	1.373(7)
C(41)-C(42)	1.3900
C(41)-C(46)	1.3900
C(42)-F(6)	1.294(5)
C(42)-C(43)	1.3900
C(43)-F(7)	1.306(6)
C(43)-C(44)	1.3900
C(44)-F(8)	1.367(6)
C(44)-C(45)	1.3900
C(45)-F(9)	1.340(7)
C(45)-C(46)	1.3900
C(46)-F(10)	1.310(6)
C(47)-C(48)	1.400(8)
C(47)-C(52)	1.400(8)
C(48)-F(11)	1.355(7)
C(48)-C(49)	1.356(9)
C(49)-F(12)	1.342(7)
C(49)-C(50)	1.374(9)
C(50)-F(13)	1.342(7)
C(50)-C(51)	1.353(9)
C(51)-F(14)	1.337(7)
C(51)-C(52)	1.360(8)
C(52)-F(15)	1.348(7)
C(53)-C(57)	1.491(8)
C(53)-C(54)	1.501(8)
C(54)-O(5)	1.209(7)
C(54)-O(6)	1.333(7)
C(55)-C(56)	1.449(10)
C(55)-O(6)	1.480(7)

C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
C(57)-O(7)	1.208(7)
C(57)-O(8)	1.332(7)
C(58)-O(8)	1.429(7)
C(58)-C(59)	1.524(9)
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
N(1)-H(1)	0.8800
N(2)-H(2A)	0.8800
N(4)-H(4A)	0.8800
O(1S)-S(1S)	1.493(4)
S(1S)-C(1S)	1.770(8)
S(1S)-C(2S)	1.786(7)
C(1S)-H(1S1)	0.9800
C(1S)-H(1S2)	0.9800
C(1S)-H(1S3)	0.9800
C(2S)-H(2S1)	0.9800
C(2S)-H(2S2)	0.9800
C(2S)-H(2S3)	0.9800
O(2S)-S(2S)	1.392(6)
S(2S)-C(4S)	1.719(8)
S(2S)-C(3S)	1.748(8)
C(3S)-H(3S1)	0.9800
C(3S)-H(3S2)	0.9800
C(3S)-H(3S3)	0.9800
C(4S)-H(4S1)	0.9800
C(4S)-H(4S2)	0.9800
C(4S)-H(4S3)	0.9800
O(3S)-S(3S)	1.490(7)
S(3S)-C(6S)	1.563(8)
S(3S)-C(5S)	1.652(8)

C(5S)-H(5S1)	0.9800
C(5S)-H(5S2)	0.9800
C(5S)-H(5S3)	0.9800
C(6S)-H(6S1)	0.9800
C(6S)-H(6S2)	0.9800
C(6S)-H(6S3)	0.9800

C(6)-C(1)-C(2)	119.0(5)
C(6)-C(1)-C(7)	122.2(5)
C(2)-C(1)-C(7)	118.7(5)
C(1)-C(2)-C(3)	121.8(5)
C(1)-C(2)-H(2)	119.1
C(3)-C(2)-H(2)	119.1
C(4)-C(3)-C(2)	117.9(5)
C(4)-C(3)-C(27)	123.3(5)
C(2)-C(3)-C(27)	118.6(5)
C(3)-C(4)-C(5)	120.6(5)
C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	119.6(5)
C(4)-C(5)-H(5)	120.2
C(6)-C(5)-H(5)	120.2
C(1)-C(6)-C(5)	121.0(6)
C(1)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(28)-C(7)-C(8)	130.5(5)
C(28)-C(7)-C(1)	118.2(5)
C(8)-C(7)-C(1)	111.2(5)
C(9)-C(8)-N(1)	104.6(5)
C(9)-C(8)-C(7)	128.3(5)
N(1)-C(8)-C(7)	127.1(5)
C(10)-C(9)-C(8)	109.8(5)
C(10)-C(9)-H(9)	125.1
C(8)-C(9)-H(9)	125.1
C(9)-C(10)-C(11)	108.2(5)
C(9)-C(10)-H(10)	125.9
C(11)-C(10)-H(10)	125.9
N(1)-C(11)-C(10)	105.5(5)

N(1)-C(11)-C(12)	124.0(5)
C(10)-C(11)-C(12)	130.5(5)
C(13)-C(12)-C(11)	124.5(5)
C(13)-C(12)-C(35)	117.8(5)
C(11)-C(12)-C(35)	117.7(5)
C(12)-C(13)-N(2)	126.0(5)
C(12)-C(13)-C(14)	128.3(6)
N(2)-C(13)-C(14)	105.7(5)
C(15)-C(14)-C(13)	108.7(6)
C(15)-C(14)-H(14)	125.7
C(13)-C(14)-H(14)	125.7
C(14)-C(15)-C(16)	109.5(6)
C(14)-C(15)-H(15)	125.3
C(16)-C(15)-H(15)	125.3
N(2)-C(16)-C(17)	124.8(5)
N(2)-C(16)-C(15)	106.0(5)
C(17)-C(16)-C(15)	129.1(6)
C(16)-C(17)-C(18)	124.9(5)
C(16)-C(17)-C(41)	117.1(5)
C(18)-C(17)-C(41)	116.9(5)
N(3)-C(18)-C(19)	112.8(5)
N(3)-C(18)-C(17)	124.2(5)
C(19)-C(18)-C(17)	122.8(5)
C(20)-C(19)-C(18)	106.0(5)
C(20)-C(19)-H(19)	127.0
C(18)-C(19)-H(19)	127.0
C(19)-C(20)-C(21)	106.8(6)
C(19)-C(20)-H(20)	126.6
C(21)-C(20)-H(20)	126.6
C(22)-C(21)-N(3)	125.9(5)
C(22)-C(21)-C(20)	124.8(6)
N(3)-C(21)-C(20)	109.4(5)
C(21)-C(22)-C(23)	126.3(6)
C(21)-C(22)-C(47)	119.0(5)
C(23)-C(22)-C(47)	114.7(5)
N(4)-C(23)-C(24)	105.8(5)
N(4)-C(23)-C(22)	121.7(5)
C(24)-C(23)-C(22)	132.2(6)

C(25)-C(24)-C(23)	107.8(5)
C(25)-C(24)-H(24)	126.1
C(23)-C(24)-H(24)	126.1
C(24)-C(25)-C(26)	108.3(5)
C(24)-C(25)-H(25)	125.8
C(26)-C(25)-H(25)	125.8
N(4)-C(26)-C(25)	107.1(5)
N(4)-C(26)-C(27)	123.2(5)
C(25)-C(26)-C(27)	129.4(5)
C(53)-C(27)-C(26)	125.8(5)
C(53)-C(27)-C(3)	121.3(5)
C(26)-C(27)-C(3)	112.9(5)
C(7)-C(28)-C(29)	121.2(5)
C(7)-C(28)-C(32)	126.3(6)
C(29)-C(28)-C(32)	112.4(5)
O(1)-C(29)-O(2)	122.6(6)
O(1)-C(29)-C(28)	123.9(6)
O(2)-C(29)-C(28)	113.4(5)
O(2)-C(30)-C(31)	115.4(7)
O(2)-C(30)-H(30A)	108.4
C(31)-C(30)-H(30A)	108.4
O(2)-C(30)-H(30B)	108.4
C(31)-C(30)-H(30B)	108.4
H(30A)-C(30)-H(30B)	107.5
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
O(3)-C(32)-O(4)	123.8(6)
O(3)-C(32)-C(28)	128.6(6)
O(4)-C(32)-C(28)	107.6(6)
C(34)-C(33)-O(4)	109.0(7)
C(34)-C(33)-H(33A)	109.9
O(4)-C(33)-H(33A)	109.9
C(34)-C(33)-H(33B)	109.9
O(4)-C(33)-H(33B)	109.9

H(33A)-C(33)-H(33B)	108.3
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(40)-C(35)-C(36)	115.5(6)
C(40)-C(35)-C(12)	122.9(5)
C(36)-C(35)-C(12)	121.6(6)
F(1)-C(36)-C(37)	118.7(6)
F(1)-C(36)-C(35)	118.2(6)
C(37)-C(36)-C(35)	123.0(6)
F(2)-C(37)-C(38)	120.7(6)
F(2)-C(37)-C(36)	120.4(7)
C(38)-C(37)-C(36)	119.0(7)
F(3)-C(38)-C(37)	120.0(7)
F(3)-C(38)-C(39)	119.2(7)
C(37)-C(38)-C(39)	120.8(6)
F(4)-C(39)-C(38)	120.8(6)
F(4)-C(39)-C(40)	121.9(7)
C(38)-C(39)-C(40)	117.3(7)
C(35)-C(40)-C(39)	124.4(6)
C(35)-C(40)-F(5)	119.9(6)
C(39)-C(40)-F(5)	115.7(6)
C(42)-C(41)-C(46)	120.0
C(42)-C(41)-C(17)	121.0(4)
C(46)-C(41)-C(17)	118.9(4)
F(6)-C(42)-C(41)	121.1(4)
F(6)-C(42)-C(43)	118.9(4)
C(41)-C(42)-C(43)	120.0
F(7)-C(43)-C(44)	118.5(5)
F(7)-C(43)-C(42)	121.4(5)
C(44)-C(43)-C(42)	120.0
F(8)-C(44)-C(43)	120.5(5)
F(8)-C(44)-C(45)	119.5(5)
C(43)-C(44)-C(45)	120.0
F(9)-C(45)-C(46)	119.4(5)

F(9)-C(45)-C(44)	120.6(5)
C(46)-C(45)-C(44)	120.0
F(10)-C(46)-C(45)	118.6(4)
F(10)-C(46)-C(41)	121.4(4)
C(45)-C(46)-C(41)	120.0
C(48)-C(47)-C(52)	114.2(6)
C(48)-C(47)-C(22)	124.3(5)
C(52)-C(47)-C(22)	121.3(5)
F(11)-C(48)-C(49)	118.2(6)
F(11)-C(48)-C(47)	118.2(6)
C(49)-C(48)-C(47)	123.4(6)
F(12)-C(49)-C(48)	120.4(7)
F(12)-C(49)-C(50)	120.3(6)
C(48)-C(49)-C(50)	119.1(6)
F(13)-C(50)-C(51)	120.1(7)
F(13)-C(50)-C(49)	119.5(7)
C(51)-C(50)-C(49)	120.4(6)
F(14)-C(51)-C(50)	120.0(6)
F(14)-C(51)-C(52)	120.1(6)
C(50)-C(51)-C(52)	119.8(6)
F(15)-C(52)-C(51)	118.8(6)
F(15)-C(52)-C(47)	118.2(6)
C(51)-C(52)-C(47)	123.0(6)
C(27)-C(53)-C(57)	120.4(5)
C(27)-C(53)-C(54)	124.4(5)
C(57)-C(53)-C(54)	115.1(5)
O(5)-C(54)-O(6)	123.5(6)
O(5)-C(54)-C(53)	125.1(6)
O(6)-C(54)-C(53)	111.4(5)
C(56)-C(55)-O(6)	110.1(6)
C(56)-C(55)-H(55A)	109.6
O(6)-C(55)-H(55A)	109.6
C(56)-C(55)-H(55B)	109.6
O(6)-C(55)-H(55B)	109.6
H(55A)-C(55)-H(55B)	108.2
C(55)-C(56)-H(56A)	109.5
C(55)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5

C(55)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
O(7)-C(57)-O(8)	123.7(6)
O(7)-C(57)-C(53)	126.2(6)
O(8)-C(57)-C(53)	110.1(5)
O(8)-C(58)-C(59)	105.8(5)
O(8)-C(58)-H(58A)	110.6
C(59)-C(58)-H(58A)	110.6
O(8)-C(58)-H(58B)	110.6
C(59)-C(58)-H(58B)	110.6
H(58A)-C(58)-H(58B)	108.7
C(58)-C(59)-H(59A)	109.5
C(58)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(58)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(11)-N(1)-C(8)	111.8(4)
C(11)-N(1)-H(1)	124.1
C(8)-N(1)-H(1)	124.1
C(16)-N(2)-C(13)	110.0(5)
C(16)-N(2)-H(2A)	125.0
C(13)-N(2)-H(2A)	125.0
C(18)-N(3)-C(21)	104.8(5)
C(26)-N(4)-C(23)	110.9(5)
C(26)-N(4)-H(4A)	124.6
C(23)-N(4)-H(4A)	124.6
C(29)-O(2)-C(30)	114.8(5)
C(32)-O(4)-C(33)	116.4(6)
C(54)-O(6)-C(55)	116.4(5)
C(57)-O(8)-C(58)	117.4(5)
O(1S)-S(1S)-C(1S)	105.5(3)
O(1S)-S(1S)-C(2S)	105.7(3)
C(1S)-S(1S)-C(2S)	96.9(4)
S(1S)-C(1S)-H(1S1)	109.5
S(1S)-C(1S)-H(1S2)	109.5
H(1S1)-C(1S)-H(1S2)	109.5

S(1S)-C(1S)-H(1S3)	109.5
H(1S1)-C(1S)-H(1S3)	109.5
H(1S2)-C(1S)-H(1S3)	109.5
S(1S)-C(2S)-H(2S1)	109.5
S(1S)-C(2S)-H(2S2)	109.5
H(2S1)-C(2S)-H(2S2)	109.5
S(1S)-C(2S)-H(2S3)	109.5
H(2S1)-C(2S)-H(2S3)	109.5
H(2S2)-C(2S)-H(2S3)	109.5
O(2S)-S(2S)-C(4S)	107.4(4)
O(2S)-S(2S)-C(3S)	111.9(5)
C(4S)-S(2S)-C(3S)	95.0(5)
S(2S)-C(3S)-H(3S1)	109.5
S(2S)-C(3S)-H(3S2)	109.5
H(3S1)-C(3S)-H(3S2)	109.5
S(2S)-C(3S)-H(3S3)	109.5
H(3S1)-C(3S)-H(3S3)	109.5
H(3S2)-C(3S)-H(3S3)	109.5
S(2S)-C(4S)-H(4S1)	109.5
S(2S)-C(4S)-H(4S2)	109.5
H(4S1)-C(4S)-H(4S2)	109.5
S(2S)-C(4S)-H(4S3)	109.5
H(4S1)-C(4S)-H(4S3)	109.5
H(4S2)-C(4S)-H(4S3)	109.5
O(3S)-S(3S)-C(6S)	95.8(6)
O(3S)-S(3S)-C(5S)	108.9(4)
C(6S)-S(3S)-C(5S)	88.7(5)
S(3S)-C(5S)-H(5S1)	109.5
S(3S)-C(5S)-H(5S2)	109.5
H(5S1)-C(5S)-H(5S2)	109.5
S(3S)-C(5S)-H(5S3)	109.5
H(5S1)-C(5S)-H(5S3)	109.5
H(5S2)-C(5S)-H(5S3)	109.5
S(3S)-C(6S)-H(6S1)	109.5
S(3S)-C(6S)-H(6S2)	109.5
H(6S1)-C(6S)-H(6S2)	109.5
S(3S)-C(6S)-H(6S3)	109.5
H(6S1)-C(6S)-H(6S3)	109.5

H(6S2)-C(6S)-H(6S3) 109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (^{2}x 10^3) for ym157P-1. 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)	22(3)	26(4)	26(3)	-14(3)	-8(3)	-3(3)
C(2)	15(3)	28(4)	27(3)	-10(3)	-1(3)	2(3)
C(3)	19(3)	31(4)	23(3)	-13(3)	-4(3)	-3(3)
C(4)	26(4)	26(4)	26(3)	-11(3)	-4(3)	-1(3)
C(5)	31(4)	33(4)	25(3)	-7(3)	-6(3)	2(3)
C(6)	29(4)	38(4)	28(4)	-11(3)	-6(3)	-2(3)
C(7)	16(3)	34(4)	24(3)	-16(3)	-3(3)	1(3)
C(8)	26(4)	22(4)	24(3)	-4(3)	-6(3)	3(3)
C(9)	21(3)	25(4)	25(3)	-7(3)	-6(3)	3(3)
C(10)	32(4)	27(4)	14(3)	-2(3)	-6(3)	-4(3)
C(11)	26(4)	21(4)	21(3)	-5(3)	-3(3)	-5(3)
C(12)	31(4)	25(4)	23(3)	-2(3)	-7(3)	-2(3)
C(13)	31(4)	22(4)	30(4)	-1(3)	-9(3)	-3(3)
C(14)	49(4)	27(4)	25(4)	-7(3)	-4(3)	-5(3)
C(15)	42(4)	28(4)	47(4)	-22(4)	-5(3)	3(3)
C(16)	30(4)	28(4)	38(4)	-9(3)	-12(3)	-3(3)
C(17)	42(4)	31(4)	19(3)	-17(3)	-4(3)	3(3)
C(18)	30(4)	26(4)	24(3)	-4(3)	-4(3)	-1(3)
C(19)	35(4)	32(4)	27(4)	-12(3)	2(3)	2(3)
C(20)	34(4)	36(4)	24(3)	-6(3)	0(3)	0(3)
C(21)	26(4)	26(4)	32(4)	-7(3)	-7(3)	2(3)
C(22)	28(4)	23(4)	20(3)	2(3)	-9(3)	4(3)
C(23)	28(4)	20(3)	23(3)	-4(3)	-8(3)	1(3)
C(24)	37(4)	25(4)	26(3)	-6(3)	-7(3)	-2(3)
C(25)	25(4)	29(4)	30(4)	-3(3)	3(3)	-6(3)
C(26)	17(3)	26(4)	25(3)	-5(3)	2(3)	0(3)
C(27)	28(4)	28(4)	22(3)	-9(3)	-3(3)	0(3)
C(28)	21(4)	28(4)	36(4)	-8(3)	1(3)	-3(3)
C(29)	38(4)	50(5)	21(4)	-12(3)	-8(3)	-3(4)
C(30)	85(7)	154(10)	67(6)	-61(7)	-3(5)	-59(7)
C(31)	137(10)	66(7)	150(10)	-16(7)	-41(8)	-5(7)
C(32)	41(4)	46(5)	21(4)	-8(4)	-2(3)	4(4)
C(33)	120(8)	55(6)	32(4)	15(4)	-13(5)	-5(5)

C(34)	167(11)	70(7)	73(7)	0(6)	-22(7)	5(7)
C(35)	32(4)	20(4)	27(3)	-7(3)	-6(3)	-2(3)
C(36)	38(4)	29(4)	38(4)	-14(4)	-4(3)	-4(3)
C(37)	57(5)	32(4)	31(4)	-3(4)	-6(4)	4(4)
C(38)	60(5)	26(4)	35(4)	3(4)	6(4)	-2(4)
C(39)	44(5)	24(4)	49(5)	-10(4)	0(4)	-6(4)
C(40)	39(4)	35(4)	36(4)	-13(4)	-6(3)	10(4)
C(41)	67(5)	29(4)	22(4)	-6(3)	8(4)	-18(4)
C(42)	49(5)	34(4)	58(5)	-28(4)	24(4)	-9(4)
C(43)	55(6)	29(5)	109(7)	-26(5)	5(5)	-13(4)
C(44)	75(3)	66(3)	64(3)	-29(2)	-7(2)	-2(2)
C(45)	84(3)	77(3)	73(3)	-25(2)	-23(2)	1(2)
C(46)	92(7)	77(6)	52(5)	-49(5)	4(5)	-1(5)
C(47)	22(4)	35(4)	26(3)	-16(3)	-6(3)	-4(3)
C(48)	31(4)	44(5)	34(4)	-20(4)	-9(3)	9(4)
C(49)	12(4)	69(6)	52(5)	-21(4)	-2(3)	-10(4)
C(50)	47(5)	47(5)	38(4)	-8(4)	-3(4)	-28(4)
C(51)	38(4)	33(4)	26(4)	-8(3)	-1(3)	-12(4)
C(52)	42(4)	35(4)	21(3)	-10(3)	-3(3)	-5(4)
C(53)	32(4)	19(4)	29(4)	-8(3)	-3(3)	1(3)
C(54)	44(4)	25(4)	31(4)	-14(3)	-6(3)	-9(3)
C(55)	54(5)	55(5)	59(5)	-12(4)	4(4)	-32(4)
C(56)	55(6)	73(6)	104(7)	-23(6)	2(5)	-26(5)
C(57)	26(4)	36(4)	40(4)	-9(4)	-5(3)	-8(3)
C(58)	54(5)	60(5)	48(5)	-21(4)	-15(4)	-1(4)
C(59)	145(9)	64(6)	42(5)	-9(5)	-40(5)	15(6)
F(1)	58(3)	45(2)	45(2)	-8(2)	-19(2)	-1(2)
F(2)	75(3)	55(3)	53(3)	4(2)	-31(2)	12(2)
F(3)	75(3)	35(2)	64(3)	15(2)	5(2)	-3(2)
F(4)	65(3)	35(2)	84(3)	-10(2)	-6(2)	-19(2)
F(5)	58(3)	41(2)	54(2)	-5(2)	-19(2)	-12(2)
F(6)	58(3)	75(3)	88(3)	-46(3)	-26(2)	14(2)
F(7)	74(4)	77(4)	165(5)	-78(4)	32(3)	-6(3)
F(11)	43(2)	43(3)	65(3)	-9(2)	-16(2)	12(2)
F(12)	27(2)	83(3)	92(3)	-21(3)	-14(2)	-2(2)
F(13)	61(3)	77(3)	64(3)	-22(2)	-4(2)	-34(2)
F(14)	78(3)	34(3)	67(3)	-8(2)	-12(2)	-16(2)
F(15)	46(2)	32(2)	46(2)	-5(2)	-16(2)	1(2)

N(1)	34(3)	21(3)	13(3)	0(2)	0(2)	1(2)
N(2)	33(3)	26(3)	20(3)	-8(2)	-2(2)	2(2)
N(3)	33(3)	22(3)	27(3)	-5(3)	-7(2)	5(3)
N(4)	29(3)	22(3)	37(3)	-1(3)	-9(3)	-5(2)
O(1)	45(3)	46(3)	39(3)	-16(2)	-1(2)	-4(2)
O(2)	55(4)	124(5)	48(3)	-54(3)	4(3)	-34(3)
O(3)	79(4)	30(3)	25(2)	1(2)	-1(2)	-13(3)
O(4)	97(4)	46(3)	34(3)	-6(3)	-22(3)	8(3)
O(5)	59(3)	38(3)	35(3)	-3(2)	-5(2)	-21(2)
O(6)	52(3)	46(3)	46(3)	-14(2)	1(2)	-25(2)
O(7)	60(3)	30(3)	41(3)	-21(2)	-10(2)	6(2)
O(8)	51(3)	38(3)	39(3)	-17(2)	-18(2)	6(2)
O(1S)	40(3)	56(3)	37(3)	-17(2)	-18(2)	3(2)
S(1S)	44(1)	68(1)	51(1)	-3(1)	-19(1)	-9(1)
C(1S)	72(6)	114(7)	69(5)	-49(6)	-38(5)	27(5)
C(2S)	51(5)	61(5)	90(6)	-19(5)	-42(4)	17(4)
O(2S)	125(6)	79(5)	162(6)	-62(5)	90(5)	-43(4)
S(2S)	143(3)	64(2)	77(2)	-17(1)	24(2)	-2(2)
C(3S)	87(7)	213(12)	119(8)	-117(9)	-14(6)	-33(8)
C(4S)	70(7)	54(6)	218(12)	26(7)	-38(7)	-18(5)
O(3S)	139(7)	200(9)	147(7)	15(6)	-2(5)	112(7)
S(3S)	131(3)	152(3)	134(3)	-12(3)	-29(2)	19(3)
C(5S)	81(7)	76(6)	72(6)	1(5)	16(5)	21(5)
C(6S)	192(11)	30(5)	153(10)	18(6)	-118(9)	-49(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2}x 10 ^{3}) for ym157P-1.

	x	y	z	U(eq)
H(2)	8053	-485	-889	29
H(4)	9440	-2976	-845	31
H(5)	10723	-2156	-1989	37
H(6)	10719	-495	-2497	38
H(9)	9277	-42	-275	29
H(10)	8832	1043	583	30
H(14)	8066	4529	307	42
H(15)	7161	4067	1800	45
H(19)	4997	998	3816	39
H(20)	4634	-503	3597	40
H(24)	8176	-663	1792	36
H(25)	9071	-1490	757	37
H(30A)	9225	131	-4625	114
H(30B)	8169	-352	-4110	114
H(31A)	10080	-1210	-4007	181
H(31B)	9138	-1700	-4073	181
H(31C)	9174	-1583	-3187	181
H(33A)	9016	3474	-5057	93
H(33B)	9042	3806	-4262	93
H(34A)	10687	3879	-4621	166
H(34B)	10387	4352	-5501	166
H(34C)	10771	3284	-5264	166
H(55A)	5240	-4892	1790	71
H(55B)	4634	-3926	1589	71
H(56A)	4195	-4379	528	122
H(56B)	3732	-5045	1478	122
H(56C)	4669	-5389	885	122
H(58A)	6802	-3247	-2056	63
H(58B)	7868	-2729	-2389	63
H(59A)	6032	-1731	-2329	125
H(59B)	6760	-1827	-3188	125
H(59C)	7099	-1226	-2682	125

H(1)	9007	2517	-1809	30
H(2A)	7648	1723	1139	32
H(4A)	6206	-1832	1106	37
H(1S1)	6096	2506	156	116
H(1S2)	5534	1855	1085	116
H(1S3)	4943	2650	525	116
H(2S1)	6406	455	-505	96
H(2S2)	6566	529	362	96
H(2S3)	6866	1404	-495	96
H(3S1)	2795	1605	6372	187
H(3S2)	1683	1547	6312	187
H(3S3)	2300	2519	5843	187
H(4S1)	3369	9	5405	194
H(4S2)	2193	-11	5559	194
H(4S3)	2669	196	6237	194
H(5S1)	9055	6600	2402	135
H(5S2)	7890	6756	2530	135
H(5S3)	8398	5888	2225	135
H(6S1)	7840	4428	3294	179
H(6S2)	7245	5357	2925	179
H(6S3)	6934	4770	3917	179

Table 6. Torsion angles [? for ym157P-1.

C(6)-C(1)-C(2)-C(3)	1.9(8)
C(7)-C(1)-C(2)-C(3)	-173.5(5)
C(1)-C(2)-C(3)-C(4)	-3.1(8)
C(1)-C(2)-C(3)-C(27)	172.5(5)
C(2)-C(3)-C(4)-C(5)	1.0(8)
C(27)-C(3)-C(4)-C(5)	-174.4(5)
C(3)-C(4)-C(5)-C(6)	2.2(8)
C(2)-C(1)-C(6)-C(5)	1.5(8)
C(7)-C(1)-C(6)-C(5)	176.7(5)
C(4)-C(5)-C(6)-C(1)	-3.5(9)
C(6)-C(1)-C(7)-C(28)	58.7(7)
C(2)-C(1)-C(7)-C(28)	-126.1(6)
C(6)-C(1)-C(7)-C(8)	-124.3(6)
C(2)-C(1)-C(7)-C(8)	50.9(7)
C(28)-C(7)-C(8)-C(9)	-176.5(6)
C(1)-C(7)-C(8)-C(9)	7.0(8)
C(28)-C(7)-C(8)-N(1)	6.5(10)
C(1)-C(7)-C(8)-N(1)	-170.0(5)
N(1)-C(8)-C(9)-C(10)	1.7(6)
C(7)-C(8)-C(9)-C(10)	-175.9(5)
C(8)-C(9)-C(10)-C(11)	-0.4(6)
C(9)-C(10)-C(11)-N(1)	-1.1(6)
C(9)-C(10)-C(11)-C(12)	-180.0(6)
N(1)-C(11)-C(12)-C(13)	158.3(6)
C(10)-C(11)-C(12)-C(13)	-23.0(10)
N(1)-C(11)-C(12)-C(35)	-21.4(8)
C(10)-C(11)-C(12)-C(35)	157.3(6)
C(11)-C(12)-C(13)-N(2)	-7.4(9)
C(35)-C(12)-C(13)-N(2)	172.3(5)
C(11)-C(12)-C(13)-C(14)	172.9(6)
C(35)-C(12)-C(13)-C(14)	-7.4(9)
C(12)-C(13)-C(14)-C(15)	179.9(6)
N(2)-C(13)-C(14)-C(15)	0.2(7)
C(13)-C(14)-C(15)-C(16)	-3.4(7)
C(14)-C(15)-C(16)-N(2)	5.2(7)
C(14)-C(15)-C(16)-C(17)	-171.4(6)

N(2)-C(16)-C(17)-C(18)	-10.4(9)
C(15)-C(16)-C(17)-C(18)	165.7(6)
N(2)-C(16)-C(17)-C(41)	-178.2(5)
C(15)-C(16)-C(17)-C(41)	-2.1(9)
C(16)-C(17)-C(18)-N(3)	13.4(9)
C(41)-C(17)-C(18)-N(3)	-178.7(5)
C(16)-C(17)-C(18)-C(19)	-161.2(6)
C(41)-C(17)-C(18)-C(19)	6.7(8)
N(3)-C(18)-C(19)-C(20)	-3.8(7)
C(17)-C(18)-C(19)-C(20)	171.3(5)
C(18)-C(19)-C(20)-C(21)	3.2(6)
C(19)-C(20)-C(21)-C(22)	177.5(6)
C(19)-C(20)-C(21)-N(3)	-1.8(7)
N(3)-C(21)-C(22)-C(23)	13.3(9)
C(20)-C(21)-C(22)-C(23)	-165.9(5)
N(3)-C(21)-C(22)-C(47)	-167.1(5)
C(20)-C(21)-C(22)-C(47)	13.7(8)
C(21)-C(22)-C(23)-N(4)	-153.1(5)
C(47)-C(22)-C(23)-N(4)	27.4(7)
C(21)-C(22)-C(23)-C(24)	33.5(9)
C(47)-C(22)-C(23)-C(24)	-146.1(6)
N(4)-C(23)-C(24)-C(25)	-1.4(6)
C(22)-C(23)-C(24)-C(25)	172.8(6)
C(23)-C(24)-C(25)-C(26)	1.9(6)
C(24)-C(25)-C(26)-N(4)	-1.7(6)
C(24)-C(25)-C(26)-C(27)	171.9(5)
N(4)-C(26)-C(27)-C(53)	-42.1(9)
C(25)-C(26)-C(27)-C(53)	145.2(6)
N(4)-C(26)-C(27)-C(3)	136.2(5)
C(25)-C(26)-C(27)-C(3)	-36.5(8)
C(4)-C(3)-C(27)-C(53)	-56.8(8)
C(2)-C(3)-C(27)-C(53)	127.9(6)
C(4)-C(3)-C(27)-C(26)	124.9(6)
C(2)-C(3)-C(27)-C(26)	-50.5(7)
C(8)-C(7)-C(28)-C(29)	-176.0(6)
C(1)-C(7)-C(28)-C(29)	0.3(8)
C(8)-C(7)-C(28)-C(32)	2.8(10)
C(1)-C(7)-C(28)-C(32)	179.1(5)

C(7)-C(28)-C(29)-O(1)	-104.2(7)
C(32)-C(28)-C(29)-O(1)	76.8(8)
C(7)-C(28)-C(29)-O(2)	75.0(7)
C(32)-C(28)-C(29)-O(2)	-104.0(6)
C(7)-C(28)-C(32)-O(3)	10.7(11)
C(29)-C(28)-C(32)-O(3)	-170.4(7)
C(7)-C(28)-C(32)-O(4)	-168.8(6)
C(29)-C(28)-C(32)-O(4)	10.2(7)
C(13)-C(12)-C(35)-C(40)	72.1(8)
C(11)-C(12)-C(35)-C(40)	-108.1(7)
C(13)-C(12)-C(35)-C(36)	-105.5(7)
C(11)-C(12)-C(35)-C(36)	74.3(7)
C(40)-C(35)-C(36)-F(1)	-177.6(5)
C(12)-C(35)-C(36)-F(1)	0.2(8)
C(40)-C(35)-C(36)-C(37)	-1.3(9)
C(12)-C(35)-C(36)-C(37)	176.4(5)
F(1)-C(36)-C(37)-F(2)	-1.9(9)
C(35)-C(36)-C(37)-F(2)	-178.1(5)
F(1)-C(36)-C(37)-C(38)	177.7(6)
C(35)-C(36)-C(37)-C(38)	1.5(10)
F(2)-C(37)-C(38)-F(3)	-0.2(10)
C(36)-C(37)-C(38)-F(3)	-179.8(5)
F(2)-C(37)-C(38)-C(39)	179.0(6)
C(36)-C(37)-C(38)-C(39)	-0.6(10)
F(3)-C(38)-C(39)-F(4)	0.3(9)
C(37)-C(38)-C(39)-F(4)	-178.9(6)
F(3)-C(38)-C(39)-C(40)	178.9(5)
C(37)-C(38)-C(39)-C(40)	-0.3(10)
C(36)-C(35)-C(40)-C(39)	0.4(9)
C(12)-C(35)-C(40)-C(39)	-177.4(5)
C(36)-C(35)-C(40)-F(5)	-178.3(5)
C(12)-C(35)-C(40)-F(5)	3.9(9)
F(4)-C(39)-C(40)-C(35)	179.0(6)
C(38)-C(39)-C(40)-C(35)	0.4(10)
F(4)-C(39)-C(40)-F(5)	-2.3(9)
C(38)-C(39)-C(40)-F(5)	179.2(5)
C(16)-C(17)-C(41)-C(42)	77.2(6)
C(18)-C(17)-C(41)-C(42)	-91.6(5)

C(16)-C(17)-C(41)-C(46)	-105.9(5)
C(18)-C(17)-C(41)-C(46)	85.3(6)
C(46)-C(41)-C(42)-F(6)	-177.7(5)
C(17)-C(41)-C(42)-F(6)	-0.8(5)
C(46)-C(41)-C(42)-C(43)	0.0
C(17)-C(41)-C(42)-C(43)	176.9(5)
F(6)-C(42)-C(43)-F(7)	0.9(5)
C(41)-C(42)-C(43)-F(7)	-176.8(5)
F(6)-C(42)-C(43)-C(44)	177.7(5)
C(41)-C(42)-C(43)-C(44)	0.0
F(7)-C(43)-C(44)-F(8)	-2.1(6)
C(42)-C(43)-C(44)-F(8)	-178.9(5)
F(7)-C(43)-C(44)-C(45)	176.9(5)
C(42)-C(43)-C(44)-C(45)	0.0
F(8)-C(44)-C(45)-F(9)	-2.8(6)
C(43)-C(44)-C(45)-F(9)	178.2(6)
F(8)-C(44)-C(45)-C(46)	178.9(5)
C(43)-C(44)-C(45)-C(46)	0.0
F(9)-C(45)-C(46)-F(10)	0.3(6)
C(44)-C(45)-C(46)-F(10)	178.5(5)
F(9)-C(45)-C(46)-C(41)	-178.3(6)
C(44)-C(45)-C(46)-C(41)	0.0
C(42)-C(41)-C(46)-F(10)	-178.5(5)
C(17)-C(41)-C(46)-F(10)	4.6(6)
C(42)-C(41)-C(46)-C(45)	0.0
C(17)-C(41)-C(46)-C(45)	-177.0(4)
C(21)-C(22)-C(47)-C(48)	61.9(8)
C(23)-C(22)-C(47)-C(48)	-118.5(6)
C(21)-C(22)-C(47)-C(52)	-122.6(6)
C(23)-C(22)-C(47)-C(52)	57.0(7)
C(52)-C(47)-C(48)-F(11)	-176.3(5)
C(22)-C(47)-C(48)-F(11)	-0.5(8)
C(52)-C(47)-C(48)-C(49)	-1.4(9)
C(22)-C(47)-C(48)-C(49)	174.4(6)
F(11)-C(48)-C(49)-F(12)	0.9(9)
C(47)-C(48)-C(49)-F(12)	-174.0(5)
F(11)-C(48)-C(49)-C(50)	175.5(5)
C(47)-C(48)-C(49)-C(50)	0.6(10)

F(12)-C(49)-C(50)-F(13)	-5.8(10)
C(48)-C(49)-C(50)-F(13)	179.5(6)
F(12)-C(49)-C(50)-C(51)	175.0(6)
C(48)-C(49)-C(50)-C(51)	0.3(10)
F(13)-C(50)-C(51)-F(14)	-0.7(9)
C(49)-C(50)-C(51)-F(14)	178.6(6)
F(13)-C(50)-C(51)-C(52)	-179.6(5)
C(49)-C(50)-C(51)-C(52)	-0.3(10)
F(14)-C(51)-C(52)-F(15)	-0.5(8)
C(50)-C(51)-C(52)-F(15)	178.4(5)
F(14)-C(51)-C(52)-C(47)	-179.5(5)
C(50)-C(51)-C(52)-C(47)	-0.6(9)
C(48)-C(47)-C(52)-F(15)	-177.6(5)
C(22)-C(47)-C(52)-F(15)	6.5(8)
C(48)-C(47)-C(52)-C(51)	1.4(8)
C(22)-C(47)-C(52)-C(51)	-174.6(5)
C(26)-C(27)-C(53)-C(57)	168.2(5)
C(3)-C(27)-C(53)-C(57)	-9.9(9)
C(26)-C(27)-C(53)-C(54)	-8.8(9)
C(3)-C(27)-C(53)-C(54)	173.1(5)
C(27)-C(53)-C(54)-O(5)	-26.7(10)
C(57)-C(53)-C(54)-O(5)	156.2(6)
C(27)-C(53)-C(54)-O(6)	152.4(6)
C(57)-C(53)-C(54)-O(6)	-24.7(7)
C(27)-C(53)-C(57)-O(7)	115.2(7)
C(54)-C(53)-C(57)-O(7)	-67.5(8)
C(27)-C(53)-C(57)-O(8)	-64.1(7)
C(54)-C(53)-C(57)-O(8)	113.2(6)
C(10)-C(11)-N(1)-C(8)	2.2(6)
C(12)-C(11)-N(1)-C(8)	-178.8(5)
C(9)-C(8)-N(1)-C(11)	-2.5(6)
C(7)-C(8)-N(1)-C(11)	175.1(5)
C(17)-C(16)-N(2)-C(13)	171.8(5)
C(15)-C(16)-N(2)-C(13)	-5.1(6)
C(12)-C(13)-N(2)-C(16)	-176.6(6)
C(14)-C(13)-N(2)-C(16)	3.1(6)
C(19)-C(18)-N(3)-C(21)	2.6(6)
C(17)-C(18)-N(3)-C(21)	-172.5(5)

C(22)-C(21)-N(3)-C(18)	-179.8(5)
C(20)-C(21)-N(3)-C(18)	-0.5(6)
C(25)-C(26)-N(4)-C(23)	0.9(6)
C(27)-C(26)-N(4)-C(23)	-173.2(5)
C(24)-C(23)-N(4)-C(26)	0.3(6)
C(22)-C(23)-N(4)-C(26)	-174.7(5)
O(1)-C(29)-O(2)-C(30)	-0.5(10)
C(28)-C(29)-O(2)-C(30)	-179.8(6)
C(31)-C(30)-O(2)-C(29)	75.7(8)
O(3)-C(32)-O(4)-C(33)	0.6(10)
C(28)-C(32)-O(4)-C(33)	-179.9(6)
C(34)-C(33)-O(4)-C(32)	87.4(8)
O(5)-C(54)-O(6)-C(55)	7.7(9)
C(53)-C(54)-O(6)-C(55)	-171.4(5)
C(56)-C(55)-O(6)-C(54)	-175.0(6)
O(7)-C(57)-O(8)-C(58)	-4.3(9)
C(53)-C(57)-O(8)-C(58)	175.0(5)
C(59)-C(58)-O(8)-C(57)	179.1(6)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for ym157P-1 [?and ?.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)