March 1, 2023 **Subject: Iacono10**

Crystal Structure Report

For Dr. Scott Iacono

X-RAY CRYSTALLOGRAPHY

US AIR FORCE ACADEMY
DEPARTMENT OF CHEMISTRY AND
CHEMISTRY RESEARCH CENTER

Dr. Gary J. Balaich
Small Molecule Crystallography Lab
Gregory Hall 2N 224
US Air Force Academy
Colorado Springs, CO 80940
Tel: (719) 314-6007
gary.balaich@afacademy.af.edu

Experimental Summary

The single crystal X-ray diffraction studies were carried out on a Rigaku Synergy-i single crystal diffractometer equipped with a Mo K_α radiation source (λ = 0.71073) and a Bantam HyPIX-3000 direct photon counting detector. Crystals of the subject compound were obtained from ethanol. A 0.379 x 0.298 x 0.242 mm^3 translucent colorless prism crystal was mounted on a Cryoloop with Paratone-N oil.

Data were collected in a nitrogen gas stream at 100.00(15) K using ϖ scans. Crystal-to-detector distance was 40 mm using an exposure time of 10 seconds with a scan width of 0.50°. Data collection was 100.0 % complete to 25.242° in θ. A total of 81813 reflections were collected. 5176 reflections were found to be symmetry independent, with an R_{int} of 0.0340. Indexing and unit cell refinement indicated a **primitive orthorhombic** lattice. The space group was found to be **Pbca.** The data were integrated using the CrysAlisPro software program (Rigaku Oxford Diffraction, 2019, 1.171.40.53) and scaled using an empirical absorption correction implemented in the SCALE 3 ABSPACK software program as well as a numerical absorption correction based on Gaussian integration over a multifaceted crystal model. Solution by direct methods (SHELXT-2016) produced a complete phasing model consistent with the proposed structure.

All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2017). All carbon bonded hydrogen atoms were placed using a riding model with their positions constrained relative to their parent atom using the appropriate HFIX command in SHELXL.

Notes: Excellent data and stable refinement.

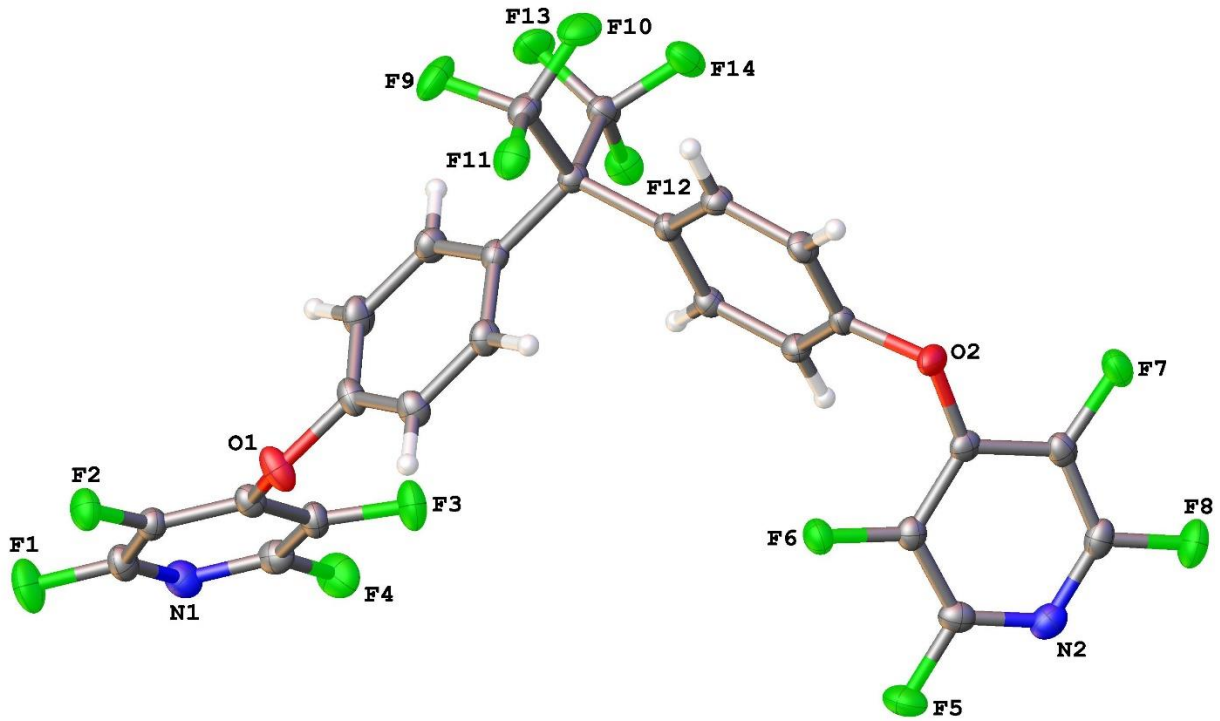

Figure 1. Thermal ellipsoid view of the PFP ether molecule $C_{25}H_8F_{14}N_2O_2$ (sample PFPEtherABS, Iacono10). Thermal ellipsoids are shown at the 50% probability level.

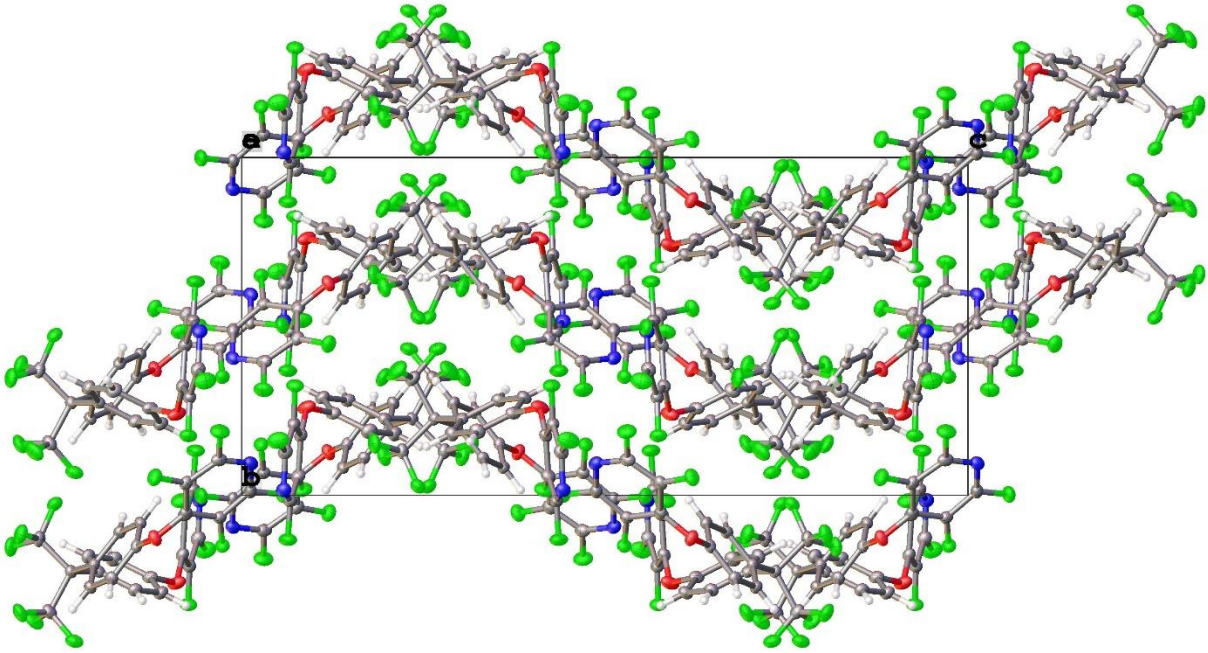

Figure 2. Packing diagram of the PFP ether molecule $C_{25}H_8F_{14}N_2O_2$ (sample PFPEtherABS, Iacono10), view along the a-axis direction. Thermal ellipsoids are shown at the 50% probability level.

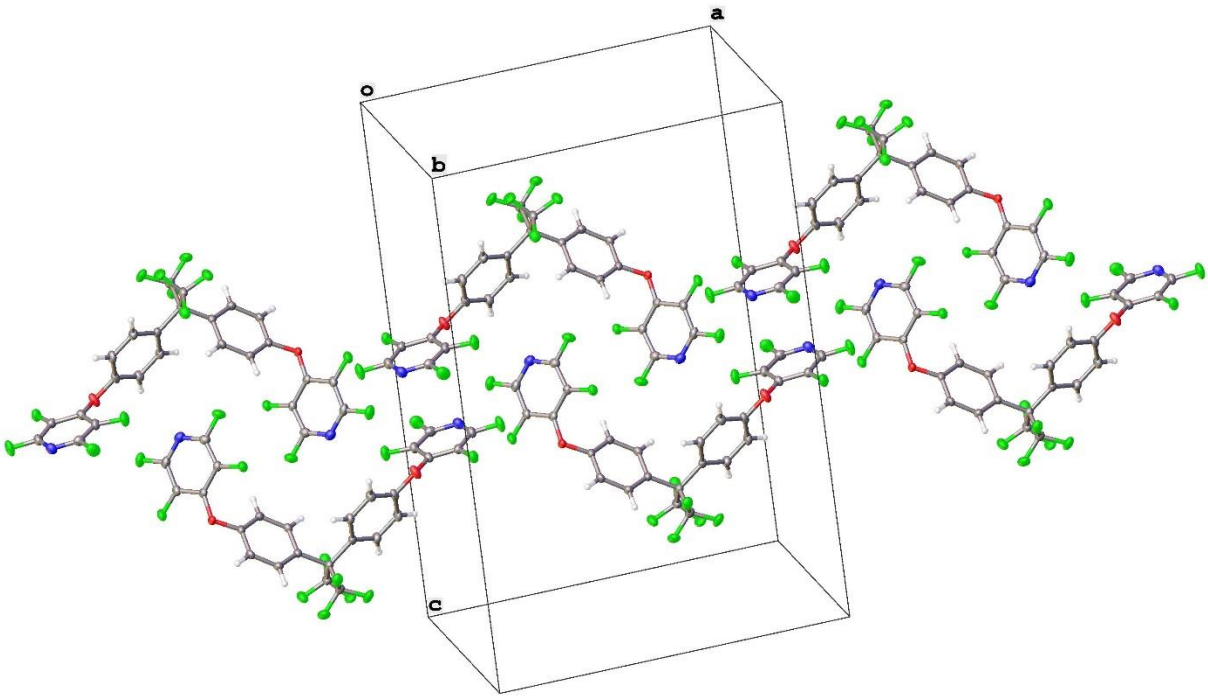

Figure 3. Packing diagram of the PFP ether molecule $C_{25}H_8F_{14}N_2O_2$ (sample PFPEtherABS, Iacono10), showing zig-zag motifs that run along the a-axis direction. Thermal ellipsoids are shown at the 50% probability level.

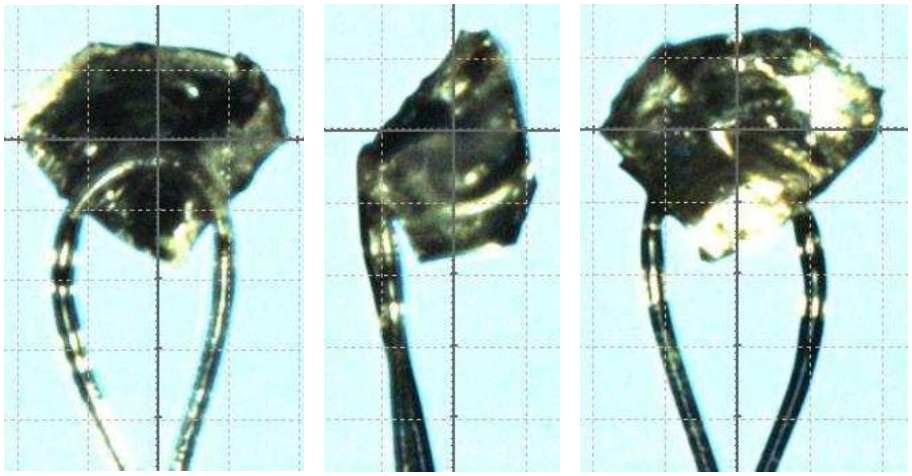

Figure 4. Images of the of the PFP ether crystal $C_{25}H_8F_{14}N_2O_2$ (sample PFPEtherABS, Iacono10), Crystal was obtained from ethanol (0.379 x 0.298 x 0.242 mm^3).

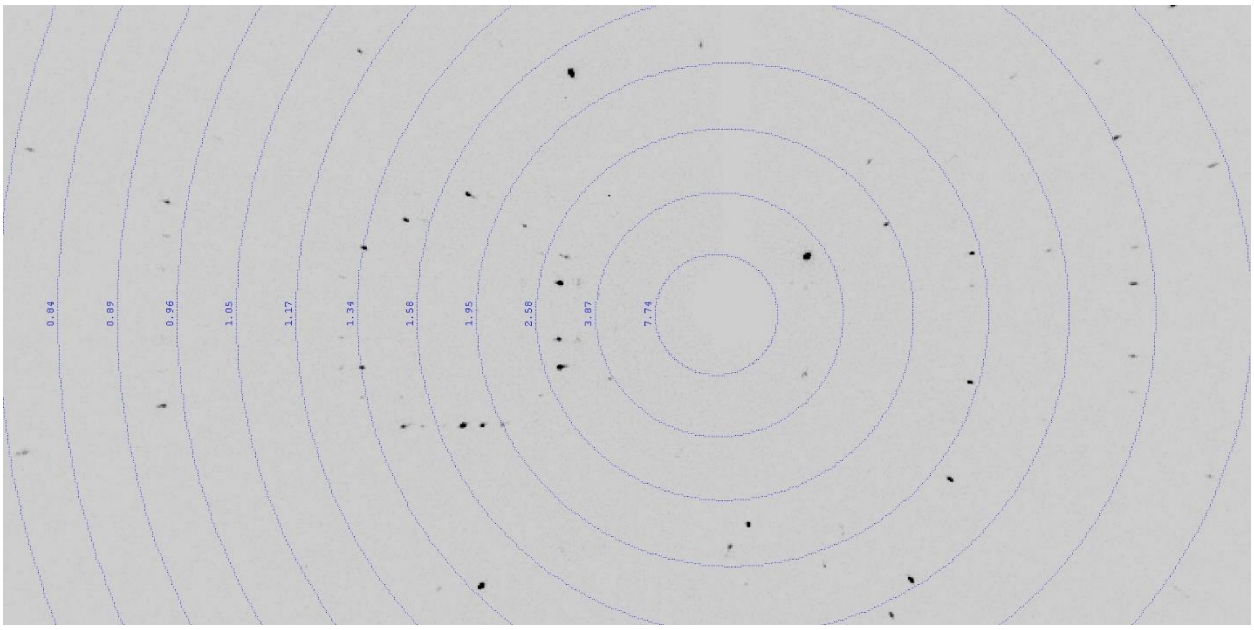

Figure 5. Example frame taken from the series of runs (run 3, frame 88), demonstrating excellent quality diffraction well beyond 0.84 Å for the selected crystal of sample PFPEtherABS (Iacono10).

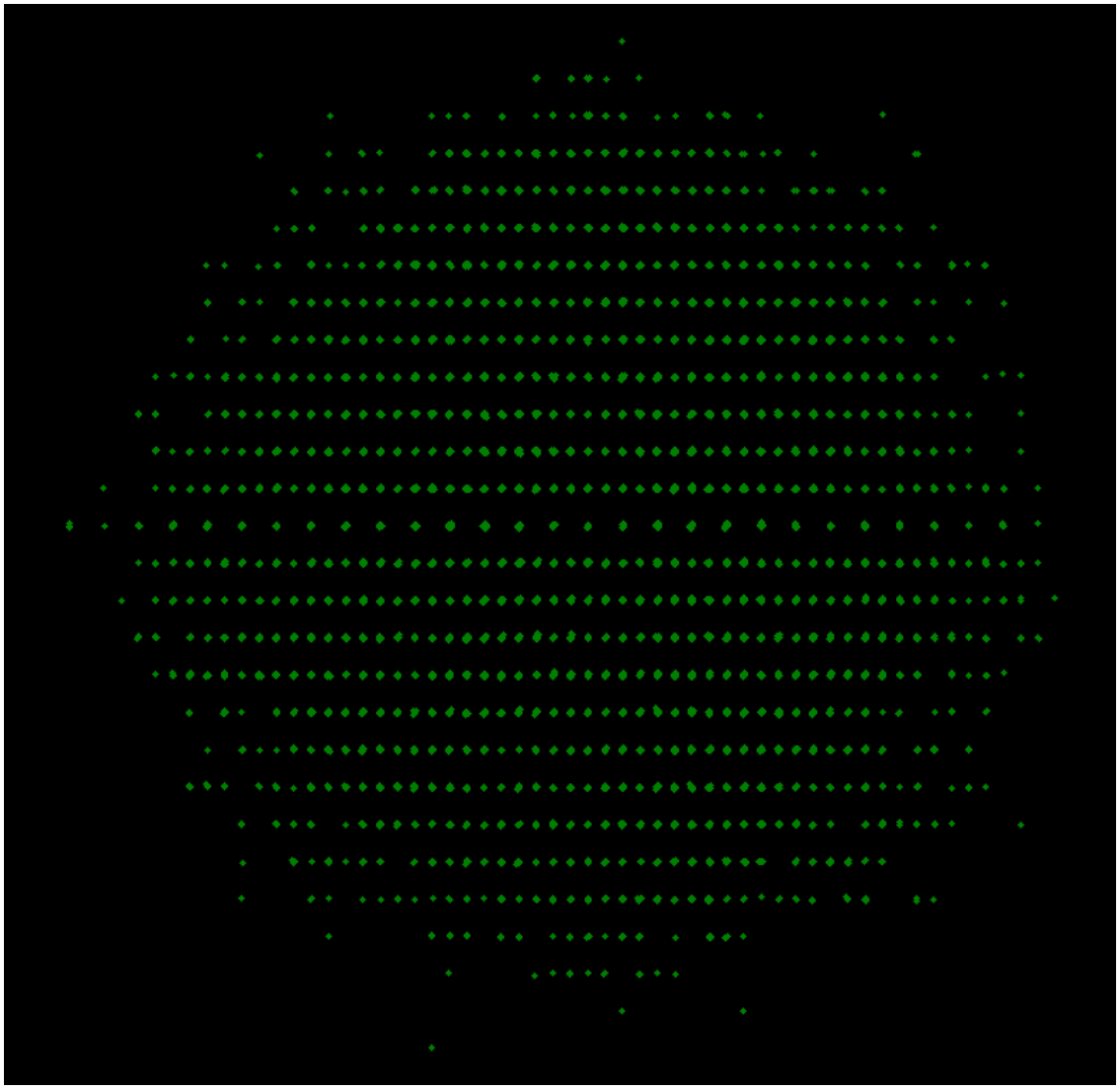

Figure 6. Reciprocal space plot for sample PFPEtherABS (Iacono10). View down the b* reciprocal lattice vector, showing good quality diffraction. Non-fitting reflections removed from this view.

Table 1. Crystal data and structure refinement for PFPEtherABS (Iacono10).

Identification code	pfpetherabs	
Empirical formula	C25 H8 F14 N2 O2	
Formula weight	634.33	
Temperature	100.00(15) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 16.4796(2) Å	α= 90°.
	b = 11.46540(10) Å	β= 90°.
	c = 24.7037(3) Å	γ = 90°.
Volume	4667.65(9) $Å^3$	
Z	8	
Density (calculated)	1.805 Mg/m^3	
Absorption coefficient	0.192 mm^{-1}	
F(000)	2512	
Crystal size	0.379 x 0.298 x 0.242 mm^3	
Theta range for data collection	1.649 to 27.467°.	
Index ranges	-19<=h<=21, -14<=k<=14, -30<=l<=31	
Reflections collected	81813	
Independent reflections	5176 [R(int) = 0.0340]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.276	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5176 / 0 / 389	
Goodness-of-fit on F^2	1.063	
Final R indices [I>2sigma(I)]	R1 = 0.0300, wR2 = 0.0765	
R indices (all data)	R1 = 0.0365, wR2 = 0.0800	
Extinction coefficient	0.00068(17)	
Largest diff. peak and hole	0.332 and -0.248 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for PFPEtherABS (Iacono10). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
F(1)	11573(1)	6621(1)	5502(1)	37(1)
F(2)	10440(1)	8240(1)	5735(1)	27(1)
F(3)	8532(1)	5161(1)	5834(1)	33(1)
F(4)	9766(1)	3682(1)	5635(1)	35(1)
F(5)	4081(1)	4977(1)	4440(1)	32(1)
F(6)	4294(1)	6500(1)	5266(1)	24(1)
F(7)	2217(1)	4472(1)	6197(1)	28(1)
F(8)	2049(1)	3118(1)	5300(1)	33(1)
F(9)	6929(1)	8711(1)	7855(1)	37(1)
F(10)	5666(1)	8489(1)	8051(1)	34(1)
F(11)	6020(1)	9324(1)	7304(1)	30(1)
F(12)	6448(1)	5263(1)	7573(1)	27(1)
F(13)	6797(1)	6528(1)	8174(1)	33(1)
F(14)	5537(1)	6147(1)	8040(1)	31(1)
O(1)	8885(1)	7601(1)	5894(1)	28(1)
O(2)	3283(1)	6271(1)	6193(1)	22(1)
N(1)	10668(1)	5153(1)	5577(1)	26(1)
N(2)	3066(1)	4058(1)	4876(1)	25(1)
C(1)	10812(1)	6280(1)	5600(1)	24(1)
C(2)	10240(1)	7110(1)	5718(1)	20(1)
C(3)	9445(1)	6764(1)	5814(1)	20(1)
C(4)	9287(1)	5572(1)	5779(1)	23(1)
C(5)	9921(1)	4828(1)	5670(1)	24(1)
C(6)	8244(1)	7427(1)	6262(1)	22(1)
C(7)	8354(1)	6893(1)	6757(1)	26(1)
C(8)	7699(1)	6811(1)	7111(1)	23(1)
C(9)	6944(1)	7261(1)	6969(1)	19(1)
C(10)	6859(1)	7805(1)	6466(1)	21(1)
C(11)	7506(1)	7891(1)	6111(1)	23(1)
C(12)	6202(1)	7261(1)	7348(1)	19(1)

C(13)	6251(1)	6297(1)	7788(1)	24(1)
C(14)	6204(1)	8453(1)	7644(1)	26(1)
C(15)	5411(1)	7052(1)	7031(1)	17(1)
C(16)	4712(1)	7726(1)	7085(1)	20(1)
C(17)	4018(1)	7467(1)	6790(1)	21(1)
C(18)	4018(1)	6511(1)	6450(1)	18(1)
C(19)	4699(1)	5816(1)	6393(1)	19(1)
C(20)	5394(1)	6101(1)	6681(1)	18(1)
C(21)	3263(1)	5530(1)	5764(1)	19(1)
C(22)	2690(1)	4638(1)	5764(1)	21(1)
C(23)	2613(1)	3955(1)	5310(1)	24(1)
C(24)	3614(1)	4884(1)	4880(1)	23(1)
C(25)	3734(1)	5657(1)	5301(1)	20(1)

Table 3. Bond lengths [Å] and angles [°] for PFPEtherABS (Iacono10).

F(1)-C(1)	1.3353(15)
F(2)-C(2)	1.3380(15)
F(3)-C(4)	1.3379(15)
F(4)-C(5)	1.3407(15)
F(5)-C(24)	1.3368(15)
F(6)-C(25)	1.3390(14)
F(7)-C(22)	1.3366(15)
F(8)-C(23)	1.3361(15)
F(9)-C(14)	1.3365(16)
F(10)-C(14)	1.3431(16)
F(11)-C(14)	1.3390(16)
F(12)-C(13)	1.3389(16)
F(13)-C(13)	1.3381(15)
F(14)-C(13)	1.3429(15)
O(1)-C(3)	1.3461(15)
O(1)-C(6)	1.4065(15)
O(2)-C(18)	1.3957(15)
O(2)-C(21)	1.3590(15)
N(1)-C(1)	1.3148(19)
N(1)-C(5)	1.3070(18)
N(2)-C(23)	1.3110(18)
N(2)-C(24)	1.3079(18)
C(1)-C(2)	1.3709(19)
C(2)-C(3)	1.3900(18)
C(3)-C(4)	1.3943(18)
C(4)-C(5)	1.3756(19)
C(6)-C(7)	1.3802(19)
C(6)-C(11)	1.3796(19)
C(7)-H(7)	0.9500
C(7)-C(8)	1.3920(19)
C(8)-H(8)	0.9500
C(8)-C(9)	1.3922(18)
C(9)-C(10)	1.3966(18)

C(9)-C(12)	1.5408(17)
C(10)-H(10)	0.9500
C(10)-C(11)	1.3833(18)
C(11)-H(11)	0.9500
C(12)-C(13)	1.5508(18)
C(12)-C(14)	1.5496(18)
C(12)-C(15)	1.5399(16)
C(15)-C(16)	1.3939(17)
C(15)-C(20)	1.3933(17)
C(16)-H(16)	0.9500
C(16)-C(17)	1.3874(18)
C(17)-H(17)	0.9500
C(17)-C(18)	1.3820(18)
C(18)-C(19)	1.3830(17)
C(19)-H(19)	0.9500
C(19)-C(20)	1.3863(17)
C(20)-H(20)	0.9500
C(21)-C(22)	1.3915(18)
C(21)-C(25)	1.3900(18)
C(22)-C(23)	1.3752(19)
C(24)-C(25)	1.3795(18)

C(3)-O(1)-C(6)	120.54(10)
C(21)-O(2)-C(18)	119.96(10)
C(5)-N(1)-C(1)	116.27(12)
C(24)-N(2)-C(23)	116.82(11)
F(1)-C(1)-C(2)	118.70(12)
N(1)-C(1)-F(1)	116.72(12)
N(1)-C(1)-C(2)	124.58(12)
F(2)-C(2)-C(1)	120.69(12)
F(2)-C(2)-C(3)	120.20(11)
C(1)-C(2)-C(3)	119.11(12)
O(1)-C(3)-C(2)	117.94(11)
O(1)-C(3)-C(4)	125.43(12)
C(2)-C(3)-C(4)	116.44(12)
F(3)-C(4)-C(3)	120.81(12)

F(3)-C(4)-C(5)	120.58(12)
C(5)-C(4)-C(3)	118.58(12)
F(4)-C(5)-C(4)	118.37(12)
N(1)-C(5)-F(4)	116.60(12)
N(1)-C(5)-C(4)	124.98(12)
C(7)-C(6)-O(1)	122.46(12)
C(11)-C(6)-O(1)	115.65(11)
C(11)-C(6)-C(7)	121.77(12)
C(6)-C(7)-H(7)	120.5
C(6)-C(7)-C(8)	118.99(12)
C(8)-C(7)-H(7)	120.5
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-C(7)	120.66(12)
C(9)-C(8)-H(8)	119.7
C(8)-C(9)-C(10)	118.61(12)
C(8)-C(9)-C(12)	123.74(11)
C(10)-C(9)-C(12)	117.55(11)
C(9)-C(10)-H(10)	119.4
C(11)-C(10)-C(9)	121.26(12)
C(11)-C(10)-H(10)	119.4
C(6)-C(11)-C(10)	118.71(12)
C(6)-C(11)-H(11)	120.6
C(10)-C(11)-H(11)	120.6
C(9)-C(12)-C(13)	112.66(10)
C(9)-C(12)-C(14)	106.56(10)
C(14)-C(12)-C(13)	107.40(11)
C(15)-C(12)-C(9)	111.23(10)
C(15)-C(12)-C(13)	106.81(10)
C(15)-C(12)-C(14)	112.20(10)
F(12)-C(13)-F(14)	106.41(11)
F(12)-C(13)-C(12)	111.46(10)
F(13)-C(13)-F(12)	107.14(10)
F(13)-C(13)-F(14)	106.53(10)
F(13)-C(13)-C(12)	113.19(11)
F(14)-C(13)-C(12)	111.70(10)
F(9)-C(14)-F(10)	106.91(11)

F(9)-C(14)-F(11)	106.38(11)
F(9)-C(14)-C(12)	112.32(11)
F(10)-C(14)-C(12)	112.24(11)
F(11)-C(14)-F(10)	107.39(11)
F(11)-C(14)-C(12)	111.26(11)
C(16)-C(15)-C(12)	124.46(11)
C(20)-C(15)-C(12)	117.09(11)
C(20)-C(15)-C(16)	118.42(11)
C(15)-C(16)-H(16)	119.6
C(17)-C(16)-C(15)	120.90(12)
C(17)-C(16)-H(16)	119.6
C(16)-C(17)-H(17)	120.4
C(18)-C(17)-C(16)	119.22(11)
C(18)-C(17)-H(17)	120.4
C(17)-C(18)-O(2)	115.66(11)
C(17)-C(18)-C(19)	121.28(11)
C(19)-C(18)-O(2)	122.99(11)
C(18)-C(19)-H(19)	120.6
C(18)-C(19)-C(20)	118.86(11)
C(20)-C(19)-H(19)	120.6
C(15)-C(20)-H(20)	119.3
C(19)-C(20)-C(15)	121.30(11)
C(19)-C(20)-H(20)	119.3
O(2)-C(21)-C(22)	118.35(11)
O(2)-C(21)-C(25)	124.24(11)
C(25)-C(21)-C(22)	117.20(11)
F(7)-C(22)-C(21)	120.07(12)
F(7)-C(22)-C(23)	121.22(12)
C(23)-C(22)-C(21)	118.69(12)
F(8)-C(23)-C(22)	119.20(12)
N(2)-C(23)-F(8)	116.51(12)
N(2)-C(23)-C(22)	124.29(12)
F(5)-C(24)-C(25)	118.57(12)
N(2)-C(24)-F(5)	116.61(11)
N(2)-C(24)-C(25)	124.81(12)
F(6)-C(25)-C(21)	120.94(11)

F(6)-C(25)-C(24)	120.94(11)
C(24)-C(25)-C(21)	118.11(12)

Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for PFPEtherABS (Iacono10). 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}
F(1)	16(1)	35(1)	59(1)	6(1)	7(1)	2(1)
F(2)	23(1)	20(1)	38(1)	-1(1)	3(1)	-4(1)
F(3)	22(1)	27(1)	50(1)	5(1)	3(1)	-7(1)
F(4)	44(1)	18(1)	42(1)	-1(1)	7(1)	-1(1)
F(5)	39(1)	34(1)	22(1)	-2(1)	9(1)	2(1)
F(6)	21(1)	24(1)	26(1)	1(1)	3(1)	-4(1)
F(7)	20(1)	37(1)	27(1)	5(1)	3(1)	-5(1)
F(8)	26(1)	26(1)	48(1)	-3(1)	-6(1)	-8(1)
F(9)	28(1)	40(1)	42(1)	-16(1)	-13(1)	-2(1)
F(10)	34(1)	41(1)	26(1)	-14(1)	1(1)	5(1)
F(11)	29(1)	21(1)	39(1)	-5(1)	-3(1)	0(1)
F(12)	27(1)	25(1)	29(1)	6(1)	0(1)	3(1)
F(13)	29(1)	48(1)	21(1)	4(1)	-9(1)	1(1)
F(14)	24(1)	46(1)	24(1)	8(1)	4(1)	2(1)
O(1)	22(1)	22(1)	41(1)	9(1)	11(1)	4(1)
O(2)	14(1)	31(1)	22(1)	-7(1)	-1(1)	1(1)
N(1)	25(1)	25(1)	29(1)	1(1)	3(1)	5(1)
N(2)	27(1)	23(1)	26(1)	-3(1)	-5(1)	3(1)
C(1)	17(1)	28(1)	27(1)	3(1)	1(1)	1(1)
C(2)	20(1)	20(1)	21(1)	1(1)	-1(1)	-2(1)
C(3)	18(1)	21(1)	22(1)	3(1)	1(1)	2(1)
C(4)	19(1)	24(1)	26(1)	3(1)	1(1)	-4(1)
C(5)	31(1)	18(1)	24(1)	1(1)	0(1)	-1(1)
C(6)	17(1)	19(1)	31(1)	1(1)	5(1)	-1(1)
C(7)	16(1)	28(1)	33(1)	4(1)	-2(1)	3(1)
C(8)	19(1)	27(1)	24(1)	3(1)	-3(1)	2(1)
C(9)	16(1)	19(1)	22(1)	-2(1)	-1(1)	-1(1)
C(10)	17(1)	21(1)	26(1)	2(1)	-2(1)	2(1)
C(11)	22(1)	21(1)	26(1)	5(1)	2(1)	1(1)
C(12)	16(1)	22(1)	18(1)	-2(1)	-2(1)	2(1)
C(13)	19(1)	32(1)	20(1)	2(1)	-1(1)	1(1)

C(14)	21(1)	29(1)	26(1)	-7(1)	-4(1)	1(1)
C(15)	15(1)	20(1)	16(1)	1(1)	0(1)	-1(1)
C(16)	19(1)	21(1)	19(1)	-3(1)	1(1)	2(1)
C(17)	16(1)	25(1)	22(1)	-1(1)	2(1)	4(1)
C(18)	14(1)	24(1)	17(1)	2(1)	0(1)	-2(1)
C(19)	19(1)	19(1)	18(1)	-2(1)	1(1)	-1(1)
C(20)	16(1)	20(1)	20(1)	1(1)	2(1)	3(1)
C(21)	15(1)	22(1)	20(1)	0(1)	-4(1)	4(1)
C(22)	15(1)	25(1)	23(1)	5(1)	-1(1)	2(1)
C(23)	19(1)	21(1)	32(1)	1(1)	-7(1)	-1(1)
C(24)	24(1)	25(1)	20(1)	1(1)	0(1)	5(1)
C(25)	17(1)	19(1)	23(1)	2(1)	-2(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for PFPEtherABS (Iacono10).

	x	y	z	U(eq)
H(7)	8869	6587	6855	31
H(8)	7768	6445	7452	28
H(10)	6348	8121	6366	26
H(11)	7442	8263	5770	28
H(16)	4711	8372	7326	24
H(17)	3548	7941	6823	25
H(19)	4690	5154	6162	22
H(20)	5868	5638	6637	22

Table 6. Torsion angles [°] for PFPEtherABS (Iacono10).

F(1)-C(1)-C(2)-F(2)	-0.11(19)
F(1)-C(1)-C(2)-C(3)	179.27(12)
F(2)-C(2)-C(3)-O(1)	3.64(18)
F(2)-C(2)-C(3)-C(4)	178.92(11)
F(3)-C(4)-C(5)-F(4)	-1.80(19)
F(3)-C(4)-C(5)-N(1)	175.60(13)
F(5)-C(24)-C(25)-F(6)	1.40(18)
F(5)-C(24)-C(25)-C(21)	-178.03(11)
F(7)-C(22)-C(23)-F(8)	0.73(19)
F(7)-C(22)-C(23)-N(2)	-178.73(12)
O(1)-C(3)-C(4)-F(3)	-1.2(2)
O(1)-C(3)-C(4)-C(5)	176.78(12)
O(1)-C(6)-C(7)-C(8)	176.50(12)
O(1)-C(6)-C(11)-C(10)	-176.74(11)
O(2)-C(18)-C(19)-C(20)	-177.65(11)
O(2)-C(21)-C(22)-F(7)	-5.02(17)
O(2)-C(21)-C(22)-C(23)	173.85(11)
O(2)-C(21)-C(25)-F(6)	4.80(19)
O(2)-C(21)-C(25)-C(24)	-175.76(11)
N(1)-C(1)-C(2)-F(2)	179.80(12)
N(1)-C(1)-C(2)-C(3)	-0.8(2)
N(2)-C(24)-C(25)-F(6)	-178.04(12)
N(2)-C(24)-C(25)-C(21)	2.5(2)
C(1)-N(1)-C(5)-F(4)	178.55(12)
C(1)-N(1)-C(5)-C(4)	1.1(2)
C(1)-C(2)-C(3)-O(1)	-175.74(12)
C(1)-C(2)-C(3)-C(4)	-0.46(19)
C(2)-C(3)-C(4)-F(3)	-176.07(11)
C(2)-C(3)-C(4)-C(5)	1.90(19)
C(3)-O(1)-C(6)-C(7)	40.87(19)
C(3)-O(1)-C(6)-C(11)	-143.10(13)
C(3)-C(4)-C(5)-F(4)	-179.77(12)
C(3)-C(4)-C(5)-N(1)	-2.4(2)
C(5)-N(1)-C(1)-F(1)	-179.55(12)

C(5)-N(1)-C(1)-C(2)	0.5(2)
C(6)-O(1)-C(3)-C(2)	-144.65(12)
C(6)-O(1)-C(3)-C(4)	40.53(19)
C(6)-C(7)-C(8)-C(9)	-0.1(2)
C(7)-C(6)-C(11)-C(10)	-0.7(2)
C(7)-C(8)-C(9)-C(10)	-0.5(2)
C(7)-C(8)-C(9)-C(12)	-176.75(12)
C(8)-C(9)-C(10)-C(11)	0.55(19)
C(8)-C(9)-C(12)-C(13)	-24.03(17)
C(8)-C(9)-C(12)-C(14)	93.50(14)
C(8)-C(9)-C(12)-C(15)	-143.93(12)
C(9)-C(10)-C(11)-C(6)	0.0(2)
C(9)-C(12)-C(13)-F(12)	-48.03(14)
C(9)-C(12)-C(13)-F(13)	72.83(14)
C(9)-C(12)-C(13)-F(14)	-166.93(10)
C(9)-C(12)-C(14)-F(9)	-49.18(14)
C(9)-C(12)-C(14)-F(10)	-169.68(10)
C(9)-C(12)-C(14)-F(11)	69.94(13)
C(9)-C(12)-C(15)-C(16)	-131.39(13)
C(9)-C(12)-C(15)-C(20)	50.56(15)
C(10)-C(9)-C(12)-C(13)	159.71(11)
C(10)-C(9)-C(12)-C(14)	-82.76(13)
C(10)-C(9)-C(12)-C(15)	39.81(15)
C(11)-C(6)-C(7)-C(8)	0.7(2)
C(12)-C(9)-C(10)-C(11)	177.01(12)
C(12)-C(15)-C(16)-C(17)	-178.85(12)
C(12)-C(15)-C(20)-C(19)	177.50(11)
C(13)-C(12)-C(14)-F(9)	71.78(14)
C(13)-C(12)-C(14)-F(10)	-48.72(13)
C(13)-C(12)-C(14)-F(11)	-169.10(10)
C(13)-C(12)-C(15)-C(16)	105.30(14)
C(13)-C(12)-C(15)-C(20)	-72.75(13)
C(14)-C(12)-C(13)-F(12)	-165.07(10)
C(14)-C(12)-C(13)-F(13)	-44.21(14)
C(14)-C(12)-C(13)-F(14)	76.04(13)
C(14)-C(12)-C(15)-C(16)	-12.13(17)

C(14)-C(12)-C(15)-C(20)	169.82(11)
C(15)-C(12)-C(13)-F(12)	74.38(12)
C(15)-C(12)-C(13)-F(13)	-164.76(10)
C(15)-C(12)-C(13)-F(14)	-44.51(14)
C(15)-C(12)-C(14)-F(9)	-171.14(11)
C(15)-C(12)-C(14)-F(10)	68.36(14)
C(15)-C(12)-C(14)-F(11)	-52.02(14)
C(15)-C(16)-C(17)-C(18)	1.44(19)
C(16)-C(15)-C(20)-C(19)	-0.67(18)
C(16)-C(17)-C(18)-O(2)	176.42(11)
C(16)-C(17)-C(18)-C(19)	-0.58(19)
C(17)-C(18)-C(19)-C(20)	-0.88(18)
C(18)-O(2)-C(21)-C(22)	130.65(12)
C(18)-O(2)-C(21)-C(25)	-54.82(17)
C(18)-C(19)-C(20)-C(15)	1.51(18)
C(20)-C(15)-C(16)-C(17)	-0.83(19)
C(21)-O(2)-C(18)-C(17)	165.09(11)
C(21)-O(2)-C(18)-C(19)	-17.97(17)
C(21)-C(22)-C(23)-F(8)	-178.13(11)
C(21)-C(22)-C(23)-N(2)	2.4(2)
C(22)-C(21)-C(25)-F(6)	179.39(11)
C(22)-C(21)-C(25)-C(24)	-1.18(18)
C(23)-N(2)-C(24)-F(5)	179.23(11)
C(23)-N(2)-C(24)-C(25)	-1.32(19)
C(24)-N(2)-C(23)-F(8)	179.30(11)
C(24)-N(2)-C(23)-C(22)	-1.2(2)
C(25)-C(21)-C(22)-F(7)	-179.93(11)
C(25)-C(21)-C(22)-C(23)	-1.06(18)