X-Ray crystallographic data of compound 2a

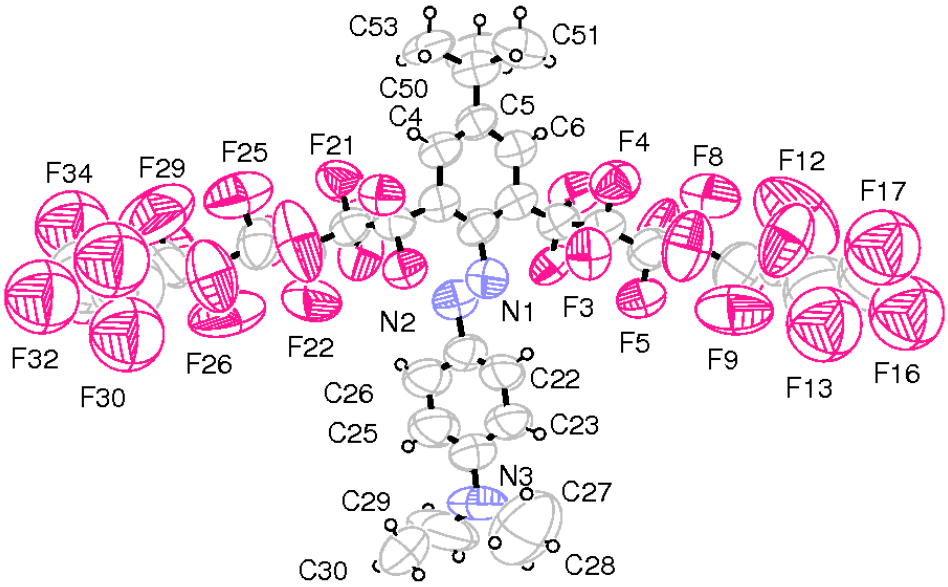
Crystallographic data were collected on a Enraf Nonius CAD4 diffractometer, using Mo-Kα radiation (λ=0.71073 Å) and a graphite crystal monochromator. Data were collected using ω-2ϑ scans. The space group was determined to be P-1 from the structure determination. The structure was solved by Direct Methods, using the program SHELXS-97 (Sheldrick, 2008). The positional parameters and the anisotropic thermal parameters of the non-H atoms were refined by full-matrix least-squares methods on F^2 using SHELXL-97 (Sheldrick, 2008) and converged to R = 0.196. All hydrogen atoms were considered as ideal and geometrically placed. Selected crystal and data collection parameters are reported in Table 1. Atomic scattering factors were taken from the *International Tables for Crystallography (Vol. C).* The terminal parts of the perfluorinated chains are rather delocalized and the corresponding atoms were refined only using isotropic thermal parameters and were restrained to reasonable geometries. A set of diffraction data measured at low temperature (173 K) gives rise to a similar behaviour indicating that the disorder is not dynamical and must be related to positional disorder probably due to the poorly interacting fluorine atoms with the neighbouring molecules. This explains the high value of the according R value, even the good behaviour of the refinement of the skeleton atoms.

Reference

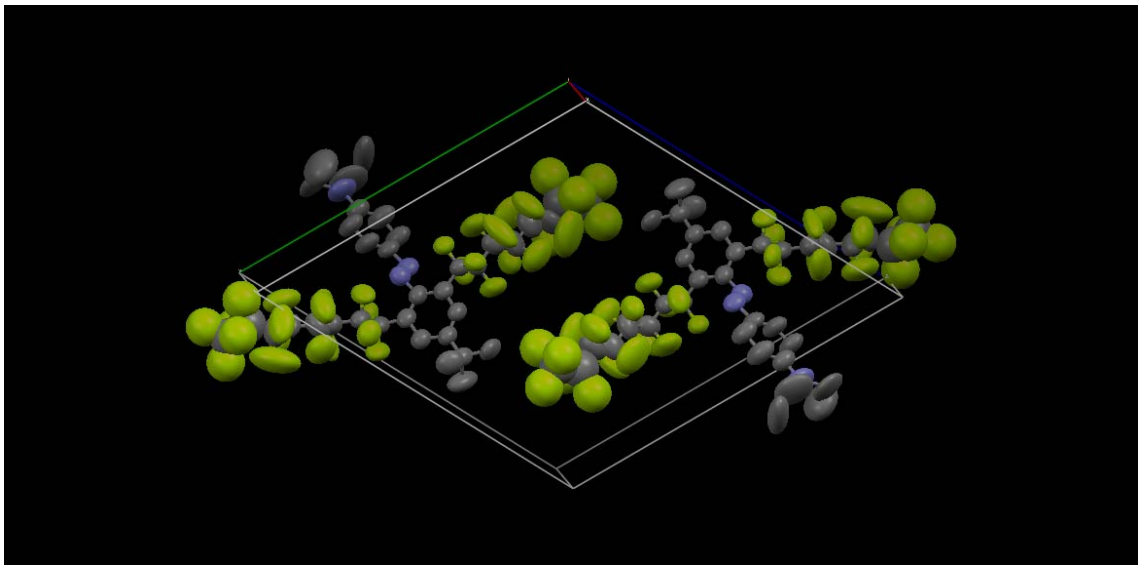
G.M.Sheldrick, *Acta Cryst*., **A64** (2008) 112-122

Table 1. Crystal data and structure refinement for **2a**.

Identification code	2a	
Empirical formula	C36 H25 F34 N3	
Formula weight	1145.59	
Temperature	294(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.4735(13) Å	α= 114.98(3)°.
	b = 19.729(6) Å	β= 96.59(2)°.
	c = 20.221(9) Å	γ = 97.04(2)°.
Volume	2283.1(13) $Å^3$	
Z	2	
Density (calculated)	1.666 Mg/m^3	
Absorption coefficient	0.196 mm^{-1}	
F(000)	1136	
Crystal size	0.34 x 0.28 x 0.17 mm^3	
Theta range for data collection	1.16 to 27.47°.	
Index ranges	-8<=h<=8, -25<=k<=23, 0<=l<=26	
Reflections collected	10474	
Independent reflections	10474	
Completeness to theta = 27.47°	100.0 %	
Max. and min. transmission	0.9674 and 0.9363	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10474 / 1014 / 575	
Goodness-of-fit on F^2	1.215	
Final R indices [I>2sigma(I)]	R1 = 0.1962, wR2 = 0.5129	
R indices (all data)	R1 = 0.3379, wR2 = 0.5806	
Largest diff. peak and hole	0.860 and -0.591 $e.Å^{-3}$	



Ortep view of **2a** showing atom labelling.



Perspective view of the unit cell of **2a**

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

	x	y	z	U(eq)
N(1)	2341(17)	7504(6)	2359(7)	123(3)
N(2)	653(18)	7223(7)	2389(6)	126(3)
N(3)	-5570(20)	6432(10)	-166(9)	215(7)
C(1)	4924(17)	8418(7)	3365(6)	106(2)
C(2)	3810(20)	7678(7)	3021(7)	115(3)
C(3)	4412(18)	7154(7)	3249(7)	110(3)
C(4)	6130(18)	7434(7)	3879(7)	112(3)
C(5)	7274(18)	8163(7)	4272(6)	110(3)
C(6)	6616(18)	8683(7)	4008(7)	115(3)
C(11)	4488(19)	9021(6)	3179(7)	114(3)
C(12)	5830(20)	9148(7)	2627(7)	120(3)
C(13)	5570(30)	9719(9)	2342(8)	154(4)
C(14)	7140(30)	9956(8)	2033(11)	183(5)
C(15)	6960(30)	10407(12)	1623(10)	183(5)
C(16)	8430(30)	10777(11)	1453(12)	206(7)
C(17)	7990(50)	11000(20)	858(14)	424(4)
C(18)	9740(40)	11577(14)	790(11)	424(4)
C(21)	-960(20)	7086(8)	1727(7)	127(4)
C(22)	-640(30)	7261(10)	1225(9)	170(7)
C(23)	-2130(30)	7103(11)	628(9)	174(7)
C(24)	-4010(20)	6634(9)	467(9)	141(5)
C(25)	-4270(30)	6472(12)	1046(11)	200(9)
C(26)	-2920(20)	6700(10)	1721(9)	167(6)
C(27)	-5160(40)	6685(15)	-813(12)	277(14)
C(28)	-3730(60)	6150(20)	-1220(16)	410(20)
C(29)	-7740(40)	6144(16)	-153(16)	367(18)
C(30)	-8130(50)	5262(16)	-564(19)	470(30)
C(31)	3492(17)	6328(7)	2953(6)	110(3)
C(32)	2040(20)	6052(7)	3291(7)	116(3)
C(33)	850(20)	5267(8)	3061(8)	143(3)
C(34)	-200(30)	4960(9)	3453(10)	163(4)

C(35)	-1580(30)	4260(11)	3268(10)	183(5)
C(36)	-2520(20)	3914(9)	3599(12)	189(5)
C(37)	-3670(50)	3231(18)	3342(15)	424(4)
C(38)	-4640(40)	2997(13)	3826(13)	424(4)
C(50)	8980(20)	8435(7)	4919(7)	127(4)
C(51)	11060(19)	8712(10)	4714(9)	181(6)
C(52)	8460(30)	9057(10)	5604(7)	206(8)
C(53)	9320(20)	7791(8)	5127(8)	161(5)
F(1)	2414(12)	8950(4)	2891(4)	138(2)
F(2)	4969(13)	9712(4)	3801(4)	158(3)
F(3)	5521(13)	8476(4)	2032(4)	155(3)
F(4)	7885(13)	9319(5)	2962(5)	172(3)
F(5)	3768(16)	9428(7)	1826(7)	244(5)
F(6)	5170(30)	10333(6)	2900(6)	270(7)
F(7)	7940(20)	9380(7)	1580(7)	249(6)
F(8)	8872(19)	10445(8)	2570(7)	259(6)
F(9)	6050(30)	9897(9)	916(8)	330(8)
F(10)	5620(20)	10872(7)	1879(7)	232(5)
F(11)	10020(20)	10395(9)	1211(9)	283(7)
F(12)	9450(40)	11422(12)	2103(15)	498(19)
F(13)	7830(40)	10473(14)	152(14)	424(4)
F(14)	6290(40)	11343(13)	885(13)	424(4)
F(15)	10000(30)	12248(10)	1380(11)	424(4)
F(16)	9120(30)	11697(13)	196(11)	424(4)
F(17)	11560(30)	11339(12)	735(12)	424(4)
F(18)	2627(10)	6047(4)	2203(4)	121(2)
F(19)	5146(10)	5916(4)	2914(4)	128(2)
F(20)	393(13)	6435(5)	3338(5)	170(3)
F(21)	2987(13)	6320(5)	4028(5)	174(3)
F(22)	-633(19)	5115(7)	2413(7)	262(6)
F(23)	2146(17)	4813(5)	2711(9)	269(7)
F(24)	-1113(14)	5519(5)	3925(6)	170(3)
F(25)	1340(20)	4876(9)	3988(8)	267(6)
F(26)	-3330(20)	4388(11)	2852(9)	334(8)
F(27)	-651(19)	3786(6)	2691(9)	258(6)
F(28)	-3400(20)	4473(7)	4139(9)	258(6)

F(29)	-760(30)	3868(17)	4055(14)	435(14)
F(30)	-4740(40)	2825(14)	2588(14)	424(4)
F(31)	-1960(40)	2802(15)	3276(15)	424(4)
F(32)	-5530(30)	2237(10)	3537(12)	424(4)
F(33)	-6230(30)	3347(12)	4154(13)	424(4)
F(34)	-3280(30)	3100(13)	4472(11)	424(4)

Table 3. Bond lengths [Å] and angles [°] for 2a.

N(1)-N(2)	1.183(12)
N(1)-C(2)	1.435(15)
N(2)-C(21)	1.504(16)
N(3)-C(24)	1.409(18)
N(3)-C(29)	1.46(3)
N(3)-C(27)	1.62(3)
C(1)-C(2)	1.379(15)
C(1)-C(11)	1.439(15)
C(1)-C(6)	1.457(15)
C(2)-C(3)	1.374(16)
C(3)-C(4)	1.447(15)
C(3)-C(31)	1.493(16)
C(4)-C(5)	1.374(14)
C(5)-C(6)	1.427(15)
C(5)-C(50)	1.468(15)
C(11)-F(1)	1.366(10)
C(11)-F(2)	1.377(10)
C(11)-C(12)	1.571(18)
C(12)-F(3)	1.333(10)
C(12)-F(4)	1.355(10)
C(12)-C(13)	1.484(19)
C(13)-F(6)	1.340(12)
C(13)-F(5)	1.353(12)
C(13)-C(14)	1.39(2)
C(14)-F(7)	1.330(13)
C(14)-F(8)	1.390(13)
C(14)-C(15)	1.46(3)
C(15)-C(16)	1.30(3)
C(15)-F(10)	1.328(13)
C(15)-F(9)	1.359(13)
C(16)-F(11)	1.364(14)
C(16)-F(12)	1.401(14)
C(16)-C(17)	1.45(3)
C(17)-F(13)	1.345(15)

C(17)-F(14)	1.359(15)
C(17)-C(18)	1.57(5)
C(18)-F(17)	1.319(15)
C(18)-F(15)	1.330(16)
C(18)-F(16)	1.343(16)
C(21)-C(22)	1.233(18)
C(21)-C(26)	1.393(18)
C(22)-C(23)	1.351(19)
C(23)-C(24)	1.352(19)
C(24)-C(25)	1.36(2)
C(25)-C(26)	1.39(2)
C(27)-C(28)	1.524(18)
C(29)-C(30)	1.550(18)
C(31)-F(18)	1.393(10)
C(31)-C(32)	1.408(16)
C(31)-F(19)	1.411(10)
C(32)-F(20)	1.372(10)
C(32)-F(21)	1.385(11)
C(32)-C(33)	1.491(18)
C(33)-F(23)	1.336(12)
C(33)-C(34)	1.37(2)
C(33)-F(22)	1.428(12)
C(34)-F(24)	1.369(13)
C(34)-C(35)	1.42(2)
C(34)-F(25)	1.461(13)
C(35)-C(36)	1.29(2)
C(35)-F(27)	1.404(13)
C(35)-F(26)	1.447(13)
C(36)-C(37)	1.31(4)
C(36)-F(28)	1.415(14)
C(36)-F(29)	1.421(14)
C(37)-C(38)	1.42(4)
C(37)-F(30)	1.427(16)
C(37)-F(31)	1.456(15)
C(38)-F(32)	1.376(16)
C(38)-F(33)	1.389(16)

C(38)-F(34)	1.407(16)
C(50)-C(52)	1.519(13)
C(50)-C(53)	1.529(13)
C(50)-C(51)	1.557(13)

N(2)-N(1)-C(2)	109.8(13)
N(1)-N(2)-C(21)	110.9(12)
C(24)-N(3)-C(29)	118.0(19)
C(24)-N(3)-C(27)	122.3(15)
C(29)-N(3)-C(27)	118.1(18)
C(2)-C(1)-C(11)	125.6(12)
C(2)-C(1)-C(6)	121.9(12)
C(11)-C(1)-C(6)	112.4(11)
C(3)-C(2)-C(1)	119.7(13)
C(3)-C(2)-N(1)	125.5(12)
C(1)-C(2)-N(1)	113.9(12)
C(2)-C(3)-C(4)	116.8(12)
C(2)-C(3)-C(31)	129.1(12)
C(4)-C(3)-C(31)	114.1(11)
C(5)-C(4)-C(3)	127.6(12)
C(4)-C(5)-C(6)	113.6(11)
C(4)-C(5)-C(50)	126.5(11)
C(6)-C(5)-C(50)	119.9(10)
C(5)-C(6)-C(1)	120.3(12)
F(1)-C(11)-F(2)	105.0(9)
F(1)-C(11)-C(1)	114.5(10)
F(2)-C(11)-C(1)	110.8(10)
F(1)-C(11)-C(12)	106.6(10)
F(2)-C(11)-C(12)	104.0(10)
C(1)-C(11)-C(12)	115.0(10)
F(3)-C(12)-F(4)	107.9(10)
F(3)-C(12)-C(13)	106.3(11)
F(4)-C(12)-C(13)	105.8(12)
F(3)-C(12)-C(11)	106.1(10)
F(4)-C(12)-C(11)	106.3(10)
C(13)-C(12)-C(11)	123.7(12)

F(6)-C(13)-F(5)	105.6(13)
F(6)-C(13)-C(14)	108.6(14)
F(5)-C(13)-C(14)	107.7(15)
F(6)-C(13)-C(12)	107.0(12)
F(5)-C(13)-C(12)	106.2(12)
C(14)-C(13)-C(12)	120.7(16)
F(7)-C(14)-C(13)	112.5(14)
F(7)-C(14)-F(8)	104.7(13)
C(13)-C(14)-F(8)	112.0(17)
F(7)-C(14)-C(15)	101.9(17)
C(13)-C(14)-C(15)	126.3(18)
F(8)-C(14)-C(15)	96.5(13)
C(16)-C(15)-F(10)	106(2)
C(16)-C(15)-F(9)	96.7(18)
F(10)-C(15)-F(9)	107.0(14)
C(16)-C(15)-C(14)	130(2)
F(10)-C(15)-C(14)	109.7(17)
F(9)-C(15)-C(14)	105.2(19)
C(15)-C(16)-F(11)	114.4(18)
C(15)-C(16)-F(12)	108(2)
F(11)-C(16)-F(12)	104.0(14)
C(15)-C(16)-C(17)	122(2)
F(11)-C(16)-C(17)	98(2)
F(12)-C(16)-C(17)	109(3)
F(13)-C(17)-F(14)	107.2(16)
F(13)-C(17)-C(16)	119(3)
F(14)-C(17)-C(16)	114(3)
F(13)-C(17)-C(18)	94(2)
F(14)-C(17)-C(18)	101(3)
C(16)-C(17)-C(18)	118(2)
F(17)-C(18)-F(15)	109.7(18)
F(17)-C(18)-F(16)	108.8(18)
F(15)-C(18)-F(16)	106.3(17)
F(17)-C(18)-C(17)	111.7(16)
F(15)-C(18)-C(17)	109.2(16)
F(16)-C(18)-C(17)	111.0(17)

C(22)-C(21)-C(26)	122.2(16)
C(22)-C(21)-N(2)	125.9(15)
C(26)-C(21)-N(2)	111.8(14)
C(21)-C(22)-C(23)	123.6(17)
C(24)-C(23)-C(22)	122.6(17)
C(23)-C(24)-C(25)	109.7(16)
C(23)-C(24)-N(3)	124.1(17)
C(25)-C(24)-N(3)	125.7(17)
C(24)-C(25)-C(26)	130.2(18)
C(25)-C(26)-C(21)	110.3(16)
C(28)-C(27)-N(3)	102.4(17)
N(3)-C(29)-C(30)	108(2)
F(18)-C(31)-C(32)	108.4(10)
F(18)-C(31)-F(19)	100.9(8)
C(32)-C(31)-F(19)	105.0(10)
F(18)-C(31)-C(3)	108.6(10)
C(32)-C(31)-C(3)	122.4(11)
F(19)-C(31)-C(3)	109.3(9)
F(20)-C(32)-F(21)	102.8(10)
F(20)-C(32)-C(31)	107.0(10)
F(21)-C(32)-C(31)	106.7(11)
F(20)-C(32)-C(33)	100.3(10)
F(21)-C(32)-C(33)	106.2(11)
C(31)-C(32)-C(33)	130.6(13)
F(23)-C(33)-C(34)	109.6(14)
F(23)-C(33)-F(22)	96.7(11)
C(34)-C(33)-F(22)	106.2(12)
F(23)-C(33)-C(32)	104.2(11)
C(34)-C(33)-C(32)	130.8(15)
F(22)-C(33)-C(32)	104.2(12)
F(24)-C(34)-C(33)	106.9(13)
F(24)-C(34)-C(35)	105.7(14)
C(33)-C(34)-C(35)	135.0(18)
F(24)-C(34)-F(25)	100.3(12)
C(33)-C(34)-F(25)	109.4(15)
C(35)-C(34)-F(25)	94.2(13)

C(36)-C(35)-F(27)	113.8(18)
C(36)-C(35)-C(34)	139(2)
F(27)-C(35)-C(34)	97.8(14)
C(36)-C(35)-F(26)	102.4(16)
F(27)-C(35)-F(26)	100.9(13)
C(34)-C(35)-F(26)	96.3(15)
C(35)-C(36)-C(37)	131(3)
C(35)-C(36)-F(28)	105.4(15)
C(37)-C(36)-F(28)	112.5(19)
C(35)-C(36)-F(29)	100.5(15)
C(37)-C(36)-F(29)	101(2)
F(28)-C(36)-F(29)	100.7(13)
C(36)-C(37)-C(38)	120(2)
C(36)-C(37)-F(30)	122(4)
C(38)-C(37)-F(30)	113(3)
C(36)-C(37)-F(31)	99(3)
C(38)-C(37)-F(31)	97(2)
F(30)-C(37)-F(31)	97.0(13)
F(32)-C(38)-F(33)	102.0(16)
F(32)-C(38)-F(34)	101.3(15)
F(33)-C(38)-F(34)	98.7(15)
F(32)-C(38)-C(37)	116.3(16)
F(33)-C(38)-C(37)	119.8(16)
F(34)-C(38)-C(37)	115.7(15)
C(5)-C(50)-C(52)	112.2(9)
C(5)-C(50)-C(53)	110.6(10)
C(52)-C(50)-C(53)	105.6(13)
C(5)-C(50)-C(51)	108.3(10)
C(52)-C(50)-C(51)	111.6(14)
C(53)-C(50)-C(51)	108.6(12)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2a. 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}
N(1)	122(6)	115(6)	124(8)	43(6)	24(5)	37(5)
N(2)	135(6)	144(8)	94(6)	37(6)	38(5)	50(6)
N(3)	179(10)	246(16)	158(12)	61(12)	-63(9)	14(11)
C(1)	109(6)	127(5)	90(7)	43(5)	34(4)	57(5)
C(2)	137(8)	120(6)	94(8)	45(6)	23(5)	48(6)
C(3)	116(7)	118(5)	91(7)	37(5)	28(5)	35(5)
C(4)	127(7)	119(6)	91(7)	41(5)	18(5)	52(5)
C(5)	123(6)	121(7)	87(6)	42(5)	19(5)	42(5)
C(6)	114(6)	132(7)	100(8)	48(6)	26(5)	39(6)
C(11)	142(7)	100(5)	89(7)	27(4)	17(6)	43(6)
C(12)	142(7)	114(6)	94(7)	30(5)	17(6)	50(7)
C(13)	199(10)	136(8)	121(12)	57(7)	12(7)	24(8)
C(14)	192(11)	122(9)	241(14)	86(9)	47(8)	21(7)
C(15)	234(15)	201(13)	137(11)	79(9)	71(9)	72(9)
C(16)	279(18)	176(14)	220(20)	120(13)	76(14)	79(10)
C(21)	148(8)	140(10)	73(7)	31(7)	17(6)	24(8)
C(22)	177(12)	202(15)	92(10)	58(10)	-14(8)	-38(11)
C(23)	168(12)	232(18)	100(11)	76(12)	-11(8)	-16(11)
C(24)	137(8)	173(13)	104(9)	53(10)	12(7)	37(8)
C(25)	171(12)	280(20)	119(13)	83(14)	5(9)	-22(13)
C(26)	151(10)	230(18)	102(10)	68(12)	15(8)	8(11)
C(27)	260(20)	360(30)	157(18)	112(19)	-113(15)	0(20)
C(28)	550(60)	470(50)	250(30)	180(40)	130(30)	140(40)
C(29)	211(15)	460(40)	290(30)	130(30)	-116(19)	-110(30)
C(30)	540(50)	430(30)	450(40)	360(30)	-260(40)	-190(30)
C(31)	108(5)	110(5)	96(6)	31(5)	7(5)	31(4)
C(32)	132(7)	115(6)	103(7)	45(6)	19(6)	43(5)
C(33)	107(7)	137(7)	161(10)	46(7)	17(6)	24(5)
C(34)	164(11)	146(8)	218(14)	105(9)	56(8)	56(8)
C(35)	149(10)	165(9)	258(17)	103(10)	55(8)	58(8)
C(36)	133(10)	139(10)	260(18)	76(10)	8(9)	-20(8)

C(50)	133(7)	136(9)	98(8)	32(6)	13(6)	61(6)
C(51)	124(7)	212(16)	173(15)	62(12)	4(8)	19(10)
C(52)	224(16)	223(16)	110(10)	3(10)	8(10)	119(14)
C(53)	183(12)	176(11)	110(10)	61(9)	-30(9)	50(10)
F(1)	152(5)	157(6)	138(6)	90(5)	22(4)	62(4)
F(2)	206(7)	129(5)	110(5)	15(4)	24(5)	78(5)
F(3)	209(7)	124(5)	119(6)	28(4)	76(5)	41(5)
F(4)	137(5)	215(9)	180(8)	98(7)	30(5)	54(5)
F(5)	173(7)	297(12)	300(12)	211(9)	-71(8)	-8(8)
F(6)	550(20)	155(7)	208(10)	118(6)	180(11)	169(10)
F(7)	350(16)	210(9)	263(13)	135(8)	152(11)	114(9)
F(8)	190(9)	309(14)	242(12)	121(9)	-36(9)	-6(9)
F(9)	343(17)	312(17)	192(11)	13(9)	-57(12)	30(12)
F(10)	272(12)	266(12)	243(12)	163(9)	77(10)	138(10)
F(11)	331(16)	373(17)	305(15)	234(13)	200(14)	184(14)
F(12)	480(30)	280(20)	450(30)	-53(17)	60(20)	-66(16)
F(18)	135(5)	122(4)	97(4)	35(4)	24(4)	39(4)
F(19)	129(4)	111(4)	119(5)	27(4)	17(4)	38(3)
F(20)	176(6)	182(7)	210(9)	110(7)	100(6)	96(6)
F(21)	172(7)	191(8)	107(5)	38(5)	6(5)	-24(6)
F(22)	265(11)	269(13)	166(10)	68(9)	-62(8)	-53(8)
F(23)	230(9)	133(6)	470(20)	113(9)	214(11)	70(7)
F(24)	187(7)	161(6)	180(9)	86(6)	63(6)	22(5)
F(25)	215(10)	387(18)	223(13)	152(12)	8(8)	108(10)
F(26)	212(10)	510(20)	312(17)	210(16)	-29(10)	131(11)
F(27)	284(12)	132(6)	338(16)	67(8)	132(12)	46(7)
F(28)	295(12)	196(10)	292(15)	107(10)	133(12)	8(9)
F(29)	311(19)	660(40)	500(30)	420(30)	19(18)	170(20)