SUPPORTING INFORMATION FOR

Synthesis, Structure, and Evaluation of the Effect of Multiple Stacking on the Electron-Donor Properties of -Stacked Polyfluorenes

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The spectral data for **F1**-**F4**, ^{13}C NMR spectra (Figure S1), photoelectron spectra (Figure S2) and the X-ray crystal structure data for **F2** and **F4** together with the ORTEP diagrams (Figure S3 and S4) are included.

Various polyfluorenes (**F2**-**F4**) were fully characterized by ^{1}H and ^{13}C NMR spectroscopy including mass spectroscopy and elemental analyses. Spectral data for the purified -stacked polyfluorenes **F1**-**F4** prepared according the Scheme 1, are given below:

F1. m.p. 92-94 ^{o}C (CH_2Cl_2-CH_3OH) (lit.[S1] mp 96 ^{o}C); ^{1}H NMR ($CDCl_3$) 1.25 (s, 6H, $2CH_3$) and 7.31-7.80 (m, 8H, Ar-H); ^{13}C NMR ($CDCl_3$) 27.8, 47.3, 119.77, 122.35, 126.65, 126.94, 138.79, 153.05. GC-MS: m/z = 194 (M^+) calcd for $C_{15}H_{14}$.

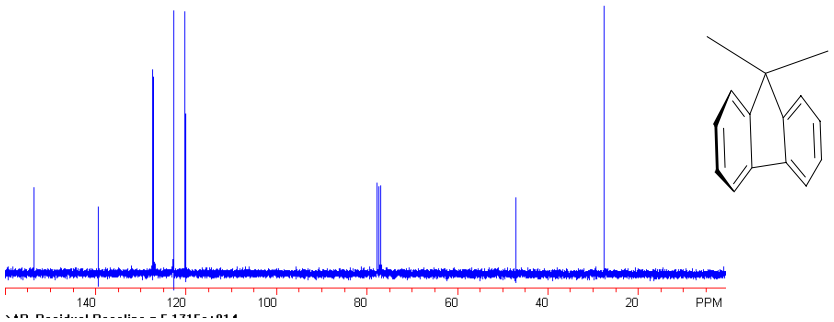
F2. mp 175-177 ^{o}C (CH_2Cl_2-CH_3OH); ^{1}H NMR ($CDCl_3$) 1.32 (s, 6H, $2CH_3$), 3.13 (s, 2H, CH_2) and 6.81-7.12 (m, 8H, Ar-H); ^{13}C NMR ($CDCl_3$) 30.28, 4956, 49.92, 118.81, 123.02, 125.55, 139.27, 149.6. GC-MS: m/z = 372 (M^+) calcd for $C_{29}H_{24}$.

F3. mp 227-229 ^{o}C (CH_2Cl_2-CH_3OH); ^{1}H NMR($CDCl_3$) 1.14 (s, 6H, $2CH_3$), 2.92 (s, 4H, $2CH_2$) and 6.27-7.12 (m,16H, Ar-H); ^{13}C NMR ($CDCl_3$) 30.57, 49.66, 51.08, 53.16, 118.10, 118.62, 122.86, 124.22, 124.82, 125.31, 125.39, 139.01, 140.27, 145.77, 149.69. GC-MS: m/z = 550 (M^+) calcd for $C_{43}H_{34}$.

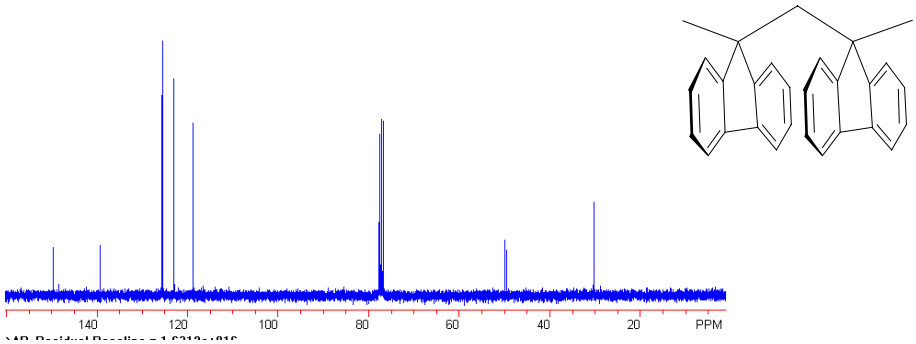
F4. m.p. 215-217 ^{o}C (CH_2Cl_2-CH_3OH); ^{1}H NMR ($CDCl_3$) 1.04 (6H, s, $2CH_3$), 2.71 (2H, s, CH_2), 2.714 (4H, s, $2CH_2$), 6.09-6.99 (16H, m, Ar-H); ^{13}C NMR ($CDCl_3$) 30.61, 49.58, 51.61, 53.14, 117.93, 118.58, 122.79, 124.14, 124.59, 125.24, 125.34, 138.95, 140.04, 145.96,149.68. FAB: m/z = 728 (M^+) calcd for $C_{57}H_{44}$.

The ^{13}C spectra of **F1**-**F4** recorded in $CDCl_3$ at 22 ^{o}C are also shown in Figure S1.

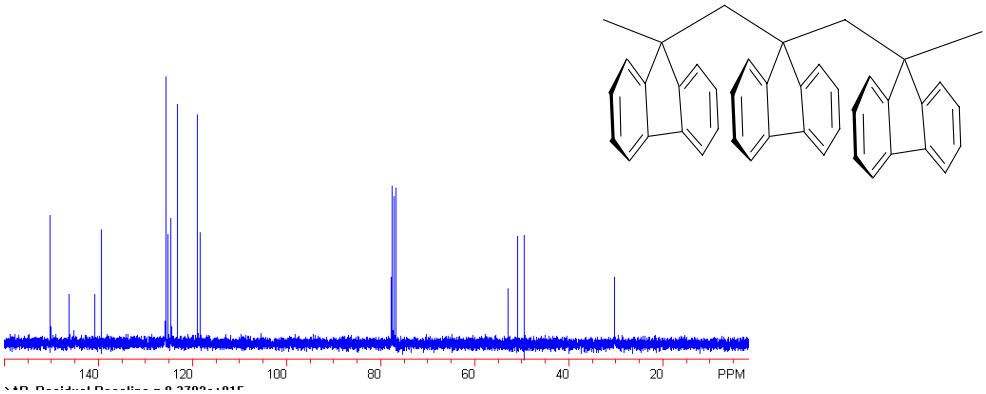
F1



F2



F3



F4

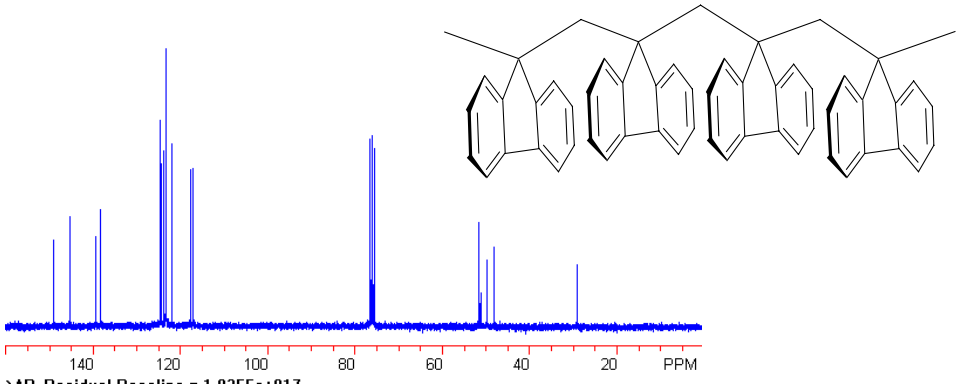


Figure S1. ^{13}C-NMR spectra of **F1-F4** recorded in $CDCl_3$ at 22^{o}C.

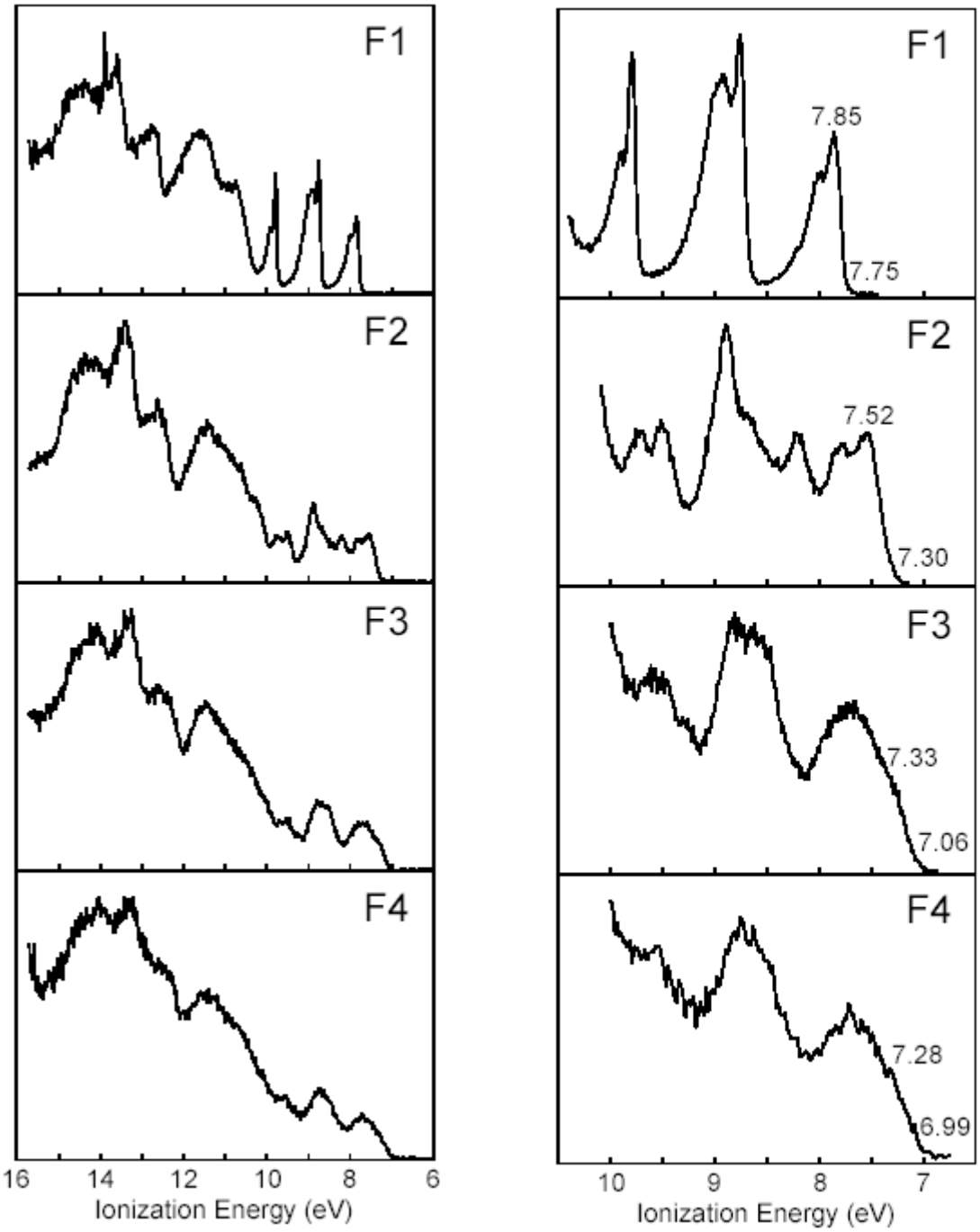


Figure S2. Photoelectron spectra of **F1-F4** showing the full valence region (left), and the closeup of low-energy region (right).

X-ray Crystallography. The intensity data were collected on a Bruker CCD-1000 diffractometer with Mo K_α (λ = 0.71073 Å) radiation at 173(2) K. The structures were solved by direct methods[S2] and refined by full matrix least-squares procedure. [The details of the X-ray structures of the polyfluorene donors **F2** [CCDC Deposition No. 207410] and **F3** [CCDC Deposition No. 207411] are on deposit and can be obtained from Cambridge Crystallographic Data Center, U.K.] *Crystal Data for **F2** [$C_{29}H_{24}$].* A suitable crystal with approximate dimensions (0.44 x 0.42 x 0.36 mm^3) was obtained from a mixture of methanol-dichloromethane solution of **F2**. Note that there are two symmetry independent molecules with essentially identical geometries in the asymmetric unit. MW = 372.48 x 2, triclinic, space group $P2_1/n$, a = 15.5455(15), b = 16.0998(16), and c = 17.0201(17) Å, = 90°, = 107.628(2)°, = 90°, Dc = 1.219 Mg m^3, V = 4059.8(7) $Å^3$, Z = 4. The final least-squares refinement of 527 parameters against 8271 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0463 and 0.1132, respectively. Crystal Data for **F3** [$C_{43}H_{34}$]. An X-ray quality crystal (0.4 x 0.3 x 0.3 mm^3) of **F3** was obtained by crystallization from ethanol-dichloromethane at 22 °C. MW = 550.70, monoclinic, space group $P2_1/c$, a = 10.9630(17), b = 21.074(4), and c = 13.470(3) Å, = 90°, = 103.575(4)°, = 90°, Dc = 1.209 Mg m^3, V = 3025.1(9) $Å^3$, Z = 4. The final least-squares refinement of 387 parameters against 5869 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0588 and 0.1338, respectively.

Tables of X-ray structure data, coordinates, bond lengths and bond angles for **F2** and **F3** are given below:

Table 1. Crystal data and structure refinement for **F2**.

Identification code	raj05
Empirical formula	$(C_{29}H_{24})$ x 2 = $C_{58}H48$
Formula weight	372.48 x 2 = 744.96
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 15.5455(15) Å = 90°. b = 16.0998(16) Å = 107.628(2)°. c = 17.0201(17) Å = 90°.
Volume	4059.8(7) $Å^3$
Z	4
Density (calculated)	1.219 Mg/m^3
Absorption coefficient	0.069 mm^{-1}
F(000)	1584
Crystal size	0.44 x 0.42 x 0.36 mm^3
Theta range for data collection	2.12 to 26.38°.
Index ranges	-19<=h<=19, -20<=k<=20, -21<=l<=21
Reflections collected	33086
Independent reflections	8271 [R(int) = 0.0390]
Completeness to theta = 26.38°	99.5 %
Absorption correction	Multiscan with SADABS
Max. and min. transmission	0.9757 and 0.9704
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8271 / 0 / 527
Goodness-of-fit on F^2	0.973
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.1132
R indices (all data)	R1 = 0.0620, wR2 = 0.1238
Largest diff. peak and hole	0.343 and -0.193 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **F2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5767(1)	3486(1)	8912(1)	24(1)
C(2)	5053(1)	2992(1)	9184(1)	19(1)
C(3)	4157(1)	3485(1)	8884(1)	19(1)
C(4)	3325(1)	3244(1)	9159(1)	19(1)
C(5)	2520(1)	3746(1)	8611(1)	25(1)
C(6)	5004(1)	2115(1)	8844(1)	20(1)
C(7)	4754(1)	1864(1)	8029(1)	23(1)
C(8)	4778(1)	1023(1)	7847(1)	28(1)
C(9)	5074(1)	446(1)	8476(1)	30(1)
C(10)	5340(1)	694(1)	9297(1)	28(1)
C(11)	5300(1)	1531(1)	9481(1)	22(1)
C(12)	5526(1)	1980(1)	10267(1)	23(1)
C(13)	5824(1)	1692(1)	11078(1)	32(1)
C(14)	5972(1)	2264(1)	11715(1)	37(1)
C(15)	5856(1)	3108(1)	11557(1)	32(1)
C(16)	5570(1)	3399(1)	10750(1)	26(1)
C(17)	5388(1)	2831(1)	10108(1)	21(1)
C(18)	3118(1)	2316(1)	9123(1)	20(1)
C(19)	2897(1)	1787(1)	8450(1)	23(1)
C(20)	2739(1)	952(1)	8566(1)	26(1)
C(21)	2789(1)	651(1)	9343(1)	28(1)
C(22)	2993(1)	1177(1)	10020(1)	26(1)
C(23)	3154(1)	2012(1)	9906(1)	21(1)
C(24)	3344(1)	2708(1)	10491(1)	20(1)
C(25)	3405(1)	2745(1)	11325(1)	24(1)
C(26)	3522(1)	3514(1)	11714(1)	25(1)
C(27)	3593(1)	4230(1)	11287(1)	25(1)
C(28)	3557(1)	4193(1)	10459(1)	22(1)
C(29)	3433(1)	3431(1)	10065(1)	19(1)
C(30)	3893(1)	8110(1)	3535(1)	24(1)
C(31)	4687(1)	7704(1)	4198(1)	19(1)
C(32)	4376(1)	7558(1)	4973(1)	20(1)
C(33)	5067(1)	7344(1)	5822(1)	19(1)
C(34)	4516(1)	6989(1)	6365(1)	24(1)
C(35)	4964(1)	6904(1)	3861(1)	19(1)
C(36)	4449(1)	6202(1)	3571(1)	22(1)
C(37)	4839(1)	5539(1)	3279(1)	26(1)
C(38)	5730(1)	5578(1)	3272(1)	27(1)

C(39)	6247(1)	6286(1)	3549(1)	23(1)
C(40)	5856(1)	6949(1)	3840(1)	19(1)
C(41)	6212(1)	7775(1)	4133(1)	18(1)
C(42)	7038(1)	8141(1)	4179(1)	24(1)
C(43)	7178(1)	8960(1)	4433(1)	27(1)
C(44)	6513(1)	9411(1)	4639(1)	27(1)
C(45)	5688(1)	9046(1)	4592(1)	23(1)
C(46)	5540(1)	8226(1)	4340(1)	18(1)
C(47)	5814(1)	6736(1)	5803(1)	17(1)
C(48)	5740(1)	5924(1)	5523(1)	20(1)
C(49)	6521(1)	5471(1)	5582(1)	21(1)
C(50)	7366(1)	5827(1)	5932(1)	22(1)
C(51)	7451(1)	6633(1)	6232(1)	21(1)
C(52)	6669(1)	7087(1)	6168(1)	18(1)
C(53)	6548(1)	7928(1)	6448(1)	19(1)
C(54)	7182(1)	8517(1)	6860(1)	23(1)
C(55)	6876(1)	9272(1)	7070(1)	28(1)
C(56)	5957(1)	9432(1)	6873(1)	29(1)
C(57)	5324(1)	8844(1)	6466(1)	25(1)
C(58)	5621(1)	8090(1)	6248(1)	20(1)

Table 3. Bond lengths [Å] and angles [°] for **F2**.

C(1)-C(2)	1.547(2)	C(30)-C(31)	1.544(2)
C(2)-C(6)	1.520(2)	C(31)-C(35)	1.524(2)
C(2)-C(17)	1.522(2)	C(31)-C(46)	1.526(2)
C(2)-C(3)	1.549(2)	C(31)-C(32)	1.554(2)
C(3)-C(4)	1.552(2)	C(32)-C(33)	1.556(2)
C(4)-C(18)	1.526(2)	C(33)-C(58)	1.526(2)
C(4)-C(29)	1.529(2)	C(33)-C(47)	1.527(2)
C(4)-C(5)	1.544(2)	C(33)-C(34)	1.548(2)
C(6)-C(7)	1.381(2)	C(35)-C(36)	1.387(2)
C(6)-C(11)	1.403(2)	C(35)-C(40)	1.400(2)
C(7)-C(8)	1.392(2)	C(36)-C(37)	1.392(2)
C(8)-C(9)	1.386(2)	C(37)-C(38)	1.390(2)
C(9)-C(10)	1.390(2)	C(38)-C(39)	1.392(2)
C(10)-C(11)	1.390(2)	C(39)-C(40)	1.392(2)
C(11)-C(12)	1.468(2)	C(40)-C(41)	1.467(2)
C(12)-C(13)	1.395(2)	C(41)-C(42)	1.393(2)
C(12)-C(17)	1.401(2)	C(41)-C(46)	1.403(2)
C(13)-C(14)	1.386(3)	C(42)-C(43)	1.383(2)
C(14)-C(15)	1.386(3)	C(43)-C(44)	1.392(2)
C(15)-C(16)	1.390(2)	C(44)-C(45)	1.391(2)
C(16)-C(17)	1.385(2)	C(45)-C(46)	1.386(2)
C(18)-C(19)	1.385(2)	C(47)-C(48)	1.384(2)
C(18)-C(23)	1.405(2)	C(47)-C(52)	1.405(2)
C(19)-C(20)	1.391(2)	C(48)-C(49)	1.393(2)
C(20)-C(21)	1.389(2)	C(49)-C(50)	1.391(2)
C(21)-C(22)	1.388(2)	C(50)-C(51)	1.387(2)
C(22)-C(23)	1.392(2)	C(51)-C(52)	1.393(2)
C(23)-C(24)	1.469(2)	C(52)-C(53)	1.466(2)
C(24)-C(25)	1.395(2)	C(53)-C(54)	1.394(2)
C(24)-C(29)	1.401(2)	C(53)-C(58)	1.401(2)
C(25)-C(26)	1.391(2)	C(54)-C(55)	1.390(2)
C(26)-C(27)	1.385(2)	C(55)-C(56)	1.389(2)
C(27)-C(28)	1.394(2)	C(56)-C(57)	1.390(2)
C(28)-C(29)	1.383(2)	C(57)-C(58)	1.389(2)
C(6)-C(2)-C(17)	101.42(12)	C(5)-C(4)-C(3)	106.46(12)
C(6)-C(2)-C(1)	108.74(12)	C(7)-C(6)-C(11)	120.45(14)
C(17)-C(2)-C(1)	110.16(12)	C(7)-C(6)-C(2)	128.34(14)
C(6)-C(2)-C(3)	114.45(12)	C(11)-C(6)-C(2)	111.14(13)
C(17)-C(2)-C(3)	114.85(12)	C(6)-C(7)-C(8)	119.27(15)
C(1)-C(2)-C(3)	107.07(12)	C(9)-C(8)-C(7)	120.31(16)
C(2)-C(3)-C(4)	121.37(12)	C(8)-C(9)-C(10)	120.83(15)
C(18)-C(4)-C(29)	101.03(12)	C(11)-C(10)-C(9)	118.94(15)
C(18)-C(4)-C(5)	111.47(12)	C(10)-C(11)-C(6)	120.18(15)
C(29)-C(4)-C(5)	109.09(12)	C(10)-C(11)-C(12)	131.92(15)
C(18)-C(4)-C(3)	114.69(12)	C(6)-C(11)-C(12)	107.90(14)
C(29)-C(4)-C(3)	114.08(12)	C(13)-C(12)-C(17)	120.11(16)

C(13)-C(12)-C(11)	130.92(16)	C(34)-C(33)-C(32)	106.59(12)
C(17)-C(12)-C(11)	108.96(13)	C(36)-C(35)-C(40)	120.28(14)
C(14)-C(13)-C(12)	118.65(17)	C(36)-C(35)-C(31)	128.59(14)
C(13)-C(14)-C(15)	121.17(16)	C(40)-C(35)-C(31)	111.09(13)
C(14)-C(15)-C(16)	120.38(16)	C(35)-C(36)-C(37)	118.93(15)
C(17)-C(16)-C(15)	118.99(16)	C(38)-C(37)-C(36)	120.80(15)
C(16)-C(17)-C(12)	120.64(14)	C(37)-C(38)-C(39)	120.60(15)
C(16)-C(17)-C(2)	128.81(15)	C(38)-C(39)-C(40)	118.63(15)
C(12)-C(17)-C(2)	110.54(13)	C(39)-C(40)-C(35)	120.73(14)
C(19)-C(18)-C(23)	119.93(14)	C(39)-C(40)-C(41)	130.95(14)
C(19)-C(18)-C(4)	129.22(14)	C(35)-C(40)-C(41)	108.29(13)
C(23)-C(18)-C(4)	110.84(13)	C(42)-C(41)-C(46)	120.71(14)
C(18)-C(19)-C(20)	119.19(15)	C(42)-C(41)-C(40)	130.47(14)
C(21)-C(20)-C(19)	120.71(15)	C(46)-C(41)-C(40)	108.72(13)
C(22)-C(21)-C(20)	120.72(15)	C(43)-C(42)-C(41)	118.40(15)
C(21)-C(22)-C(23)	118.62(15)	C(42)-C(43)-C(44)	121.21(15)
C(22)-C(23)-C(18)	120.81(14)	C(45)-C(44)-C(43)	120.43(15)
C(22)-C(23)-C(24)	130.53(15)	C(46)-C(45)-C(44)	118.96(15)
C(18)-C(23)-C(24)	108.62(13)	C(45)-C(46)-C(41)	120.29(14)
C(25)-C(24)-C(29)	120.32(14)	C(45)-C(46)-C(31)	128.98(13)
C(25)-C(24)-C(23)	131.32(14)	C(41)-C(46)-C(31)	110.64(13)
C(29)-C(24)-C(23)	108.30(13)	C(48)-C(47)-C(52)	120.10(13)
C(26)-C(25)-C(24)	118.77(14)	C(48)-C(47)-C(33)	128.96(13)
C(27)-C(26)-C(25)	120.73(14)	C(52)-C(47)-C(33)	110.86(13)
C(26)-C(27)-C(28)	120.67(15)	C(47)-C(48)-C(49)	119.31(14)
C(29)-C(28)-C(27)	119.03(14)	C(50)-C(49)-C(48)	120.37(14)
C(28)-C(29)-C(24)	120.44(14)	C(51)-C(50)-C(49)	120.95(14)
C(28)-C(29)-C(4)	128.37(13)	C(50)-C(51)-C(52)	118.63(14)
C(24)-C(29)-C(4)	111.11(13)	C(51)-C(52)-C(47)	120.61(14)
C(35)-C(31)-C(46)	101.23(12)	C(51)-C(52)-C(53)	130.82(14)
C(35)-C(31)-C(30)	109.75(12)	C(47)-C(52)-C(53)	108.54(13)
C(46)-C(31)-C(30)	110.30(12)	C(54)-C(53)-C(58)	120.92(14)
C(35)-C(31)-C(32)	112.79(12)	C(54)-C(53)-C(52)	130.63(14)
C(46)-C(31)-C(32)	115.31(12)	C(58)-C(53)-C(52)	108.44(13)
C(30)-C(31)-C(32)	107.35(12)	C(55)-C(54)-C(53)	118.67(15)
C(31)-C(32)-C(33)	121.13(12)	C(56)-C(55)-C(54)	120.44(15)
C(58)-C(33)-C(47)	101.01(12)	C(55)-C(56)-C(57)	120.99(15)
C(58)-C(33)-C(34)	109.98(12)	C(58)-C(57)-C(56)	119.09(15)
C(47)-C(33)-C(34)	109.71(12)	C(57)-C(58)-C(53)	119.88(14)
C(58)-C(33)-C(32)	113.54(12)	C(57)-C(58)-C(33)	128.95(14)
C(47)-C(33)-C(32)	115.94(12)	C(53)-C(58)-C(33)	111.14(13)

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **F2**. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(1)	27(1)	22(1)	-1(1)	10(1)	-6(1)
C(2)	20(1)	22(1)	16(1)	1(1)	5(1)	-2(1)
C(3)	23(1)	18(1)	17(1)	3(1)	5(1)	-1(1)
C(4)	18(1)	19(1)	19(1)	-1(1)	4(1)	1(1)
C(5)	23(1)	24(1)	25(1)	1(1)	2(1)	3(1)
C(6)	15(1)	23(1)	23(1)	3(1)	8(1)	-1(1)
C(7)	21(1)	25(1)	23(1)	2(1)	8(1)	1(1)
C(8)	26(1)	30(1)	31(1)	-5(1)	15(1)	-1(1)
C(9)	30(1)	22(1)	44(1)	-1(1)	22(1)	1(1)
C(10)	25(1)	26(1)	38(1)	12(1)	17(1)	6(1)
C(11)	16(1)	28(1)	25(1)	8(1)	10(1)	3(1)
C(12)	14(1)	34(1)	23(1)	7(1)	8(1)	2(1)
C(13)	24(1)	46(1)	27(1)	15(1)	11(1)	10(1)
C(14)	24(1)	66(1)	19(1)	12(1)	5(1)	11(1)
C(15)	20(1)	56(1)	20(1)	-4(1)	5(1)	3(1)
C(16)	15(1)	39(1)	22(1)	-1(1)	5(1)	-1(1)
C(17)	13(1)	32(1)	19(1)	3(1)	6(1)	-1(1)
C(18)	13(1)	21(1)	26(1)	1(1)	5(1)	2(1)
C(19)	16(1)	27(1)	25(1)	-2(1)	5(1)	0(1)
C(20)	20(1)	25(1)	33(1)	-8(1)	7(1)	-3(1)
C(21)	23(1)	20(1)	42(1)	2(1)	9(1)	-3(1)
C(22)	22(1)	25(1)	31(1)	5(1)	9(1)	-2(1)
C(23)	13(1)	24(1)	26(1)	0(1)	6(1)	1(1)
C(24)	12(1)	23(1)	25(1)	2(1)	6(1)	2(1)
C(25)	19(1)	29(1)	25(1)	7(1)	9(1)	1(1)
C(26)	21(1)	36(1)	19(1)	0(1)	7(1)	2(1)
C(27)	23(1)	27(1)	24(1)	-4(1)	5(1)	2(1)
C(28)	23(1)	20(1)	23(1)	1(1)	6(1)	2(1)
C(29)	12(1)	25(1)	20(1)	3(1)	3(1)	3(1)
C(30)	19(1)	28(1)	25(1)	5(1)	6(1)	1(1)
C(31)	17(1)	20(1)	20(1)	2(1)	6(1)	0(1)
C(32)	16(1)	23(1)	22(1)	1(1)	7(1)	0(1)
C(33)	18(1)	21(1)	19(1)	1(1)	8(1)	1(1)
C(34)	21(1)	29(1)	23(1)	3(1)	9(1)	1(1)
C(35)	22(1)	20(1)	14(1)	5(1)	5(1)	0(1)
C(36)	24(1)	24(1)	16(1)	4(1)	4(1)	-5(1)
C(37)	39(1)	21(1)	17(1)	1(1)	4(1)	-7(1)
C(38)	43(1)	20(1)	19(1)	2(1)	11(1)	6(1)

C(39)	26(1)	24(1)	20(1)	5(1)	8(1)	4(1)
C(40)	22(1)	20(1)	14(1)	5(1)	5(1)	1(1)
C(41)	18(1)	20(1)	15(1)	5(1)	3(1)	2(1)
C(42)	18(1)	28(1)	25(1)	4(1)	5(1)	1(1)
C(43)	20(1)	30(1)	30(1)	5(1)	4(1)	-7(1)
C(44)	31(1)	20(1)	27(1)	0(1)	4(1)	-5(1)
C(45)	26(1)	21(1)	21(1)	2(1)	7(1)	3(1)
C(46)	17(1)	21(1)	16(1)	5(1)	4(1)	0(1)
C(47)	18(1)	22(1)	14(1)	5(1)	7(1)	2(1)
C(48)	20(1)	21(1)	18(1)	3(1)	7(1)	-2(1)
C(49)	28(1)	15(1)	23(1)	1(1)	11(1)	0(1)
C(50)	22(1)	22(1)	26(1)	4(1)	10(1)	5(1)
C(51)	18(1)	24(1)	21(1)	2(1)	5(1)	0(1)
C(52)	20(1)	19(1)	14(1)	2(1)	7(1)	-1(1)
C(53)	22(1)	22(1)	15(1)	2(1)	8(1)	1(1)
C(54)	23(1)	26(1)	20(1)	-2(1)	8(1)	-2(1)
C(55)	33(1)	25(1)	26(1)	-8(1)	10(1)	-7(1)
C(56)	38(1)	23(1)	30(1)	-6(1)	17(1)	3(1)
C(57)	24(1)	27(1)	26(1)	-1(1)	12(1)	4(1)
C(58)	23(1)	23(1)	15(1)	1(1)	9(1)	1(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **F2**.

	x	y	z	U(eq)
H(1A)	6347	3194	9095	36
H(1B)	5834	4042	9159	36
H(1C)	5573	3536	8310	36
H(3A)	3962	3470	8274	23
H(3B)	4300	4071	9047	23
H(5A)	2417	3594	8032	38
H(5B)	2654	4341	8683	38
H(5C)	1978	3622	8770	38
H(7)	4567	2261	7598	27
H(8)	4591	843	7289	33
H(9)	5095	-125	8345	36
H(10)	5547	297	9726	34
H(13)	5923	1117	11192	38
H(14)	6158	2074	12269	44
H(15)	5972	3490	12002	38
H(16)	5500	3977	10640	31
H(19)	2855	1991	7916	27
H(20)	2594	584	8108	31
H(21)	2683	78	9412	34
H(22)	3021	972	10551	31
H(25)	3368	2253	11622	29
H(26)	3553	3549	12279	30
H(27)	3668	4751	11561	30
H(28)	3616	4684	10170	27
H(30A)	3752	8648	3736	36
H(30B)	3362	7748	3419	36
H(30C)	4059	8192	3029	36
H(32A)	3927	7102	4837	24
H(32B)	4051	8064	5051	24
H(34A)	4916	6905	6928	35
H(34B)	4248	6457	6138	35
H(34C)	4037	7381	6375	35
H(36)	3839	6173	3573	26
H(37)	4493	5054	3081	32
H(38)	5988	5118	3076	33
H(39)	6855	6315	3541	28
H(42)	7495	7836	4040	28
H(43)	7737	9218	4467	33
H(44)	6624	9972	4814	32

H(45)	5233	9354	4730	27
H(48)	5163	5679	5292	23
H(49)	6475	4917	5383	25
H(50)	7893	5512	5965	27
H(51)	8029	6871	6475	25
H(54)	7810	8405	6995	27
H(55)	7299	9681	7350	33
H(56)	5758	9952	7018	35
H(57)	4697	8956	6338	30

Table 6. Torsion angles [°] for **F2**.

C(6)-C(2)-C(3)-C(4)	68.65(17)	C(1)-C(2)-C(17)-C(12)	-114.09(14)
C(17)-C(2)-C(3)-C(4)	-48.11(18)	C(3)-C(2)-C(17)-C(12)	124.93(13)
C(1)-C(2)-C(3)-C(4)	-170.76(13)	C(29)-C(4)-C(18)-C(19)	175.67(14)
C(2)-C(3)-C(4)-C(18)	-45.07(18)	C(5)-C(4)-C(18)-C(19)	59.9(2)
C(2)-C(3)-C(4)-C(29)	70.79(17)	C(3)-C(4)-C(18)-C(19)	-61.2(2)
C(2)-C(3)-C(4)-C(5)	-168.83(13)	C(29)-C(4)-C(18)-C(23)	-2.98(15)
C(17)-C(2)-C(6)-C(7)	-178.86(14)	C(5)-C(4)-C(18)-C(23)	-118.75(14)
C(1)-C(2)-C(6)-C(7)	-62.76(19)	C(3)-C(4)-C(18)-C(23)	120.20(13)
C(3)-C(2)-C(6)-C(7)	56.9(2)	C(23)-C(18)-C(19)-C(20)	-1.8(2)
C(17)-C(2)-C(6)-C(11)	-1.82(15)	C(4)-C(18)-C(19)-C(20)	179.69(14)
C(1)-C(2)-C(6)-C(11)	114.28(13)	C(18)-C(19)-C(20)-C(21)	0.8(2)
C(3)-C(2)-C(6)-C(11)	-126.06(13)	C(19)-C(20)-C(21)-C(22)	0.5(2)
C(11)-C(6)-C(7)-C(8)	1.5(2)	C(20)-C(21)-C(22)-C(23)	-0.7(2)
C(2)-C(6)-C(7)-C(8)	178.27(14)	C(21)-C(22)-C(23)-C(18)	-0.4(2)
C(6)-C(7)-C(8)-C(9)	-1.8(2)	C(21)-C(22)-C(23)-C(24)	177.10(15)
C(7)-C(8)-C(9)-C(10)	0.8(2)	C(19)-C(18)-C(23)-C(22)	1.6(2)
C(8)-C(9)-C(10)-C(11)	0.5(2)	C(4)-C(18)-C(23)-C(22)	-179.62(13)
C(9)-C(10)-C(11)-C(6)	-0.8(2)	C(19)-C(18)-C(23)-C(24)	-176.38(13)
C(9)-C(10)-C(11)-C(12)	179.83(15)	C(4)-C(18)-C(23)-C(24)	2.41(16)
C(7)-C(6)-C(11)-C(10)	-0.2(2)	C(22)-C(23)-C(24)-C(25)	-1.0(3)
C(2)-C(6)-C(11)-C(10)	-177.51(13)	C(18)-C(23)-C(24)-C(25)	176.66(15)
C(7)-C(6)-C(11)-C(12)	179.32(13)	C(22)-C(23)-C(24)-C(29)	-178.40(15)
C(2)-C(6)-C(11)-C(12)	2.01(16)	C(18)-C(23)-C(24)-C(29)	-0.69(16)
C(10)-C(11)-C(12)-C(13)	-2.6(3)	C(29)-C(24)-C(25)-C(26)	2.4(2)
C(6)-C(11)-C(12)-C(13)	178.00(15)	C(23)-C(24)-C(25)-C(26)	-174.70(14)
C(10)-C(11)-C(12)-C(17)	178.09(16)	C(24)-C(25)-C(26)-C(27)	-1.2(2)
C(6)-C(11)-C(12)-C(17)	-1.35(16)	C(25)-C(26)-C(27)-C(28)	-0.5(2)
C(17)-C(12)-C(13)-C(14)	0.5(2)	C(26)-C(27)-C(28)-C(29)	1.0(2)
C(11)-C(12)-C(13)-C(14)	-178.82(15)	C(27)-C(28)-C(29)-C(24)	0.1(2)
C(12)-C(13)-C(14)-C(15)	-1.9(2)	C(27)-C(28)-C(29)-C(4)	176.72(14)
C(13)-C(14)-C(15)-C(16)	1.2(3)	C(25)-C(24)-C(29)-C(28)	-1.8(2)
C(14)-C(15)-C(16)-C(17)	1.1(2)	C(23)-C(24)-C(29)-C(28)	175.85(13)
C(15)-C(16)-C(17)-C(12)	-2.6(2)	C(25)-C(24)-C(29)-C(4)	-178.99(13)
C(15)-C(16)-C(17)-C(2)	178.70(14)	C(23)-C(24)-C(29)-C(4)	-1.29(16)
C(13)-C(12)-C(17)-C(16)	1.8(2)	C(18)-C(4)-C(29)-C(28)	-174.31(14)
C(11)-C(12)-C(17)-C(16)	-178.76(13)	C(5)-C(4)-C(29)-C(28)	-56.79(19)
C(13)-C(12)-C(17)-C(2)	-179.26(13)	C(3)-C(4)-C(29)-C(28)	62.10(19)
C(11)-C(12)-C(17)-C(2)	0.17(17)	C(18)-C(4)-C(29)-C(24)	2.55(15)
C(6)-C(2)-C(17)-C(16)	179.78(14)	C(5)-C(4)-C(29)-C(24)	120.07(13)
C(1)-C(2)-C(17)-C(16)	64.73(19)	C(3)-C(4)-C(29)-C(24)	-121.05(13)
C(3)-C(2)-C(17)-C(16)	-56.2(2)	C(35)-C(31)-C(32)-C(33)	72.96(17)
C(6)-C(2)-C(17)-C(12)	0.95(15)	C(46)-C(31)-C(32)-C(33)	-42.66(18)

C(30)-C(31)-C(32)-C(33)	-166.02(13)
C(31)-C(32)-C(33)-C(58)	75.34(17)
C(31)-C(32)-C(33)-C(47)	-40.99(19)
C(31)-C(32)-C(33)-C(34)	-163.42(13)
C(46)-C(31)-C(35)-C(36)	-176.05(14)
C(30)-C(31)-C(35)-C(36)	-59.49(19)
C(32)-C(31)-C(35)-C(36)	60.16(19)
C(46)-C(31)-C(35)-C(40)	1.80(15)
C(30)-C(31)-C(35)-C(40)	118.36(13)
C(32)-C(31)-C(35)-C(40)	-121.99(13)
C(40)-C(35)-C(36)-C(37)	1.5(2)
C(31)-C(35)-C(36)-C(37)	179.14(14)
C(35)-C(36)-C(37)-C(38)	-0.3(2)
C(36)-C(37)-C(38)-C(39)	-0.7(2)
C(37)-C(38)-C(39)-C(40)	0.5(2)
C(38)-C(39)-C(40)-C(35)	0.7(2)
C(38)-C(39)-C(40)-C(41)	-176.97(14)
C(36)-C(35)-C(40)-C(39)	-1.7(2)
C(31)-C(35)-C(40)-C(39)	-179.74(13)
C(36)-C(35)-C(40)-C(41)	176.45(13)
C(31)-C(35)-C(40)-C(41)	-1.61(16)
C(39)-C(40)-C(41)-C(42)	2.3(3)
C(35)-C(40)-C(41)-C(42)	-175.54(15)
C(39)-C(40)-C(41)-C(46)	178.55(15)
C(35)-C(40)-C(41)-C(46)	0.68(16)
C(46)-C(41)-C(42)-C(43)	-0.1(2)
C(40)-C(41)-C(42)-C(43)	175.71(14)
C(41)-C(42)-C(43)-C(44)	0.1(2)
C(42)-C(43)-C(44)-C(45)	-0.2(2)
C(43)-C(44)-C(45)-C(46)	0.3(2)
C(44)-C(45)-C(46)-C(41)	-0.4(2)
C(44)-C(45)-C(46)-C(31)	-176.64(14)
C(42)-C(41)-C(46)-C(45)	0.3(2)
C(40)-C(41)-C(46)-C(45)	-176.39(13)
C(42)-C(41)-C(46)-C(31)	177.16(13)
C(40)-C(41)-C(46)-C(31)	0.51(16)
C(35)-C(31)-C(46)-C(45)	175.19(14)
C(30)-C(31)-C(46)-C(45)	59.0(2)
C(32)-C(31)-C(46)-C(45)	-62.7(2)
C(35)-C(31)-C(46)-C(41)	-1.37(15)
C(30)-C(31)-C(46)-C(41)	-117.52(14)
C(32)-C(31)-C(46)-C(41)	120.69(14)
C(58)-C(33)-C(47)-C(48)	176.78(14)
C(34)-C(33)-C(47)-C(48)	60.70(19)
C(32)-C(33)-C(47)-C(48)	-60.1(2)
C(58)-C(33)-C(47)-C(52)	0.05(15)
C(34)-C(33)-C(47)-C(52)	-116.02(13)
C(32)-C(33)-C(47)-C(52)	123.22(13)
C(52)-C(47)-C(48)-C(49)	-2.0(2)
C(33)-C(47)-C(48)-C(49)	-178.48(14)
C(47)-C(48)-C(49)-C(50)	1.0(2)
C(48)-C(49)-C(50)-C(51)	0.4(2)
C(49)-C(50)-C(51)-C(52)	-0.8(2)
C(50)-C(51)-C(52)-C(47)	-0.3(2)
C(50)-C(51)-C(52)-C(53)	177.77(14)
C(48)-C(47)-C(52)-C(51)	1.7(2)
C(33)-C(47)-C(52)-C(51)	178.75(13)
C(48)-C(47)-C(52)-C(53)	-176.76(12)
C(33)-C(47)-C(52)-C(53)	0.30(16)
C(51)-C(52)-C(53)-C(54)	0.1(3)
C(47)-C(52)-C(53)-C(54)	178.36(15)
C(51)-C(52)-C(53)-C(58)	-178.80(15)
C(47)-C(52)-C(53)-C(58)	-0.56(16)
C(58)-C(53)-C(54)-C(55)	0.0(2)
C(52)-C(53)-C(54)-C(55)	-178.78(15)
C(53)-C(54)-C(55)-C(56)	0.1(2)
C(54)-C(55)-C(56)-C(57)	0.2(2)
C(55)-C(56)-C(57)-C(58)	-0.6(2)
C(56)-C(57)-C(58)-C(53)	0.8(2)
C(56)-C(57)-C(58)-C(33)	178.32(14)
C(54)-C(53)-C(58)-C(57)	-0.5(2)
C(52)-C(53)-C(58)-C(57)	178.57(13)
C(54)-C(53)-C(58)-C(33)	-178.44(13)
C(52)-C(53)-C(58)-C(33)	0.61(16)
C(47)-C(33)-C(58)-C(57)	-178.14(15)
C(34)-C(33)-C(58)-C(57)	-62.3(2)
C(32)-C(33)-C(58)-C(57)	57.1(2)
C(47)-C(33)-C(58)-C(53)	-0.41(15)
C(34)-C(33)-C(58)-C(53)	115.46(14)
C(32)-C(33)-C(58)-C(53)	-125.22(13)

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Symmetry transformations used to generate equivalent atoms.

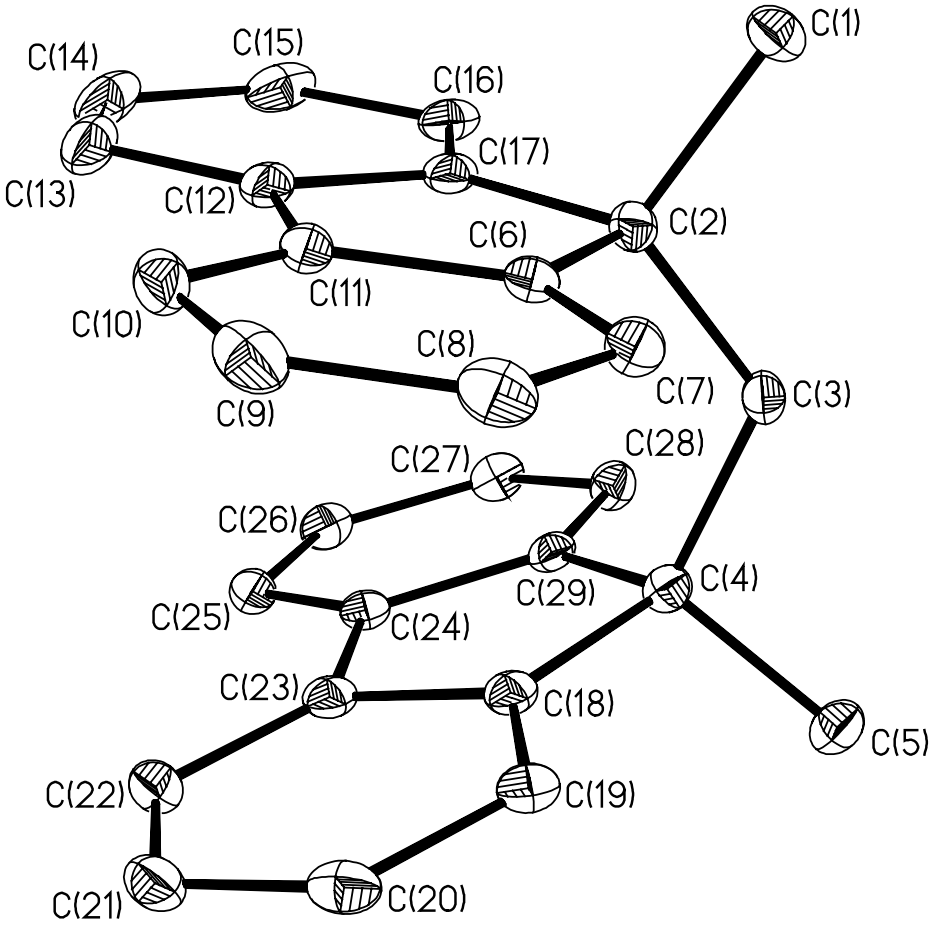

Figure S3. ORTEP Diagram of **F2**, thermal ellipsoid shown in 30% probability.

Table 1. Crystal data and structure refinement for **F3**.

Identification code	raj04
Empirical formula	$C_{43} H_{34}$
Formula weight	550.70
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 10.9630(17) Å = 90°. b = 21.074(4) Å = 103.575(4)°. c = 13.470(3) Å = 90°.
Volume	3025.1(9) $Å^3$
Z	4
Density (calculated)	1.209 Mg/m^3
Absorption coefficient	0.068 mm^{-1}
F(000)	1168
Crystal size	0.40 x 0.30 x 0.30 mm^3
Theta range for data collection	1.83 to 26.00°.
Index ranges	-7<=h<=13, -25<=k<=22, -16<=l<=16
Reflections collected	14273
Independent reflections	5869 [R(int) = 0.0422]
Completeness to theta = 26.00°	98.7 %
Absorption correction	Empirical with SADABS
Max. and min. transmission	0.9798 and 0.9732
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5869 / 0 / 387
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0588, wR2 = 0.1338
R indices (all data)	R1 = 0.1189, wR2 = 0.1498
Largest diff. peak and hole	0.164 and -0.145 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **F3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2292(2)	943(1)	4159(2)	71(1)
C(2)	3174(2)	1150(1)	3473(2)	50(1)
C(3)	2846(2)	796(1)	2462(2)	58(1)
C(4)	2859(2)	152(1)	2287(2)	88(1)
C(5)	2490(3)	-65(2)	1284(4)	128(2)
C(6)	2127(4)	355(3)	502(3)	138(2)
C(7)	2055(3)	999(2)	658(2)	110(1)
C(8)	2436(2)	1229(1)	1659(2)	68(1)
C(9)	2424(2)	1861(1)	2066(2)	66(1)
C(10)	2048(2)	2443(2)	1581(2)	96(1)
C(11)	2109(2)	2970(1)	2176(3)	115(1)
C(12)	2524(2)	2951(1)	3222(3)	101(1)
C(13)	2886(2)	2376(1)	3696(2)	77(1)
C(14)	2857(2)	1830(1)	3125(2)	55(1)
C(15)	4531(2)	1071(1)	4113(2)	52(1)
C(16)	5699(2)	1102(1)	3651(1)	44(1)
C(17)	5770(2)	519(1)	2993(2)	48(1)
C(18)	5819(2)	-113(1)	3269(2)	64(1)
C(19)	5898(2)	-573(1)	2542(3)	86(1)
C(20)	5919(2)	-397(1)	1561(2)	88(1)
C(21)	5864(2)	230(1)	1282(2)	73(1)
C(22)	5781(2)	693(1)	1998(2)	51(1)
C(23)	5709(2)	1383(1)	1924(2)	51(1)
C(24)	5682(2)	1781(1)	1099(2)	73(1)
C(25)	5627(2)	2422(2)	1244(2)	86(1)
C(26)	5598(2)	2680(1)	2180(2)	80(1)
C(27)	5610(2)	2282(1)	3004(2)	61(1)
C(28)	5666(2)	1633(1)	2873(1)	45(1)
C(29)	6851(2)	1126(1)	4585(1)	50(1)
C(30)	8199(2)	1275(1)	4471(1)	52(1)
C(31)	8602(2)	944(1)	3589(2)	52(1)
C(32)	8742(2)	306(1)	3427(2)	63(1)
C(33)	9171(2)	110(1)	2582(2)	74(1)
C(34)	9482(2)	557(1)	1934(2)	77(1)
C(35)	9375(2)	1195(1)	2100(2)	68(1)
C(36)	8946(2)	1392(1)	2944(2)	55(1)
C(37)	8824(2)	2027(1)	3338(2)	58(1)
C(38)	9109(2)	2620(1)	3009(2)	77(1)
C(39)	8948(3)	3154(1)	3555(2)	91(1)
C(40)	8535(3)	3097(1)	4439(2)	83(1)

C(41)	8261(2)	2507(1)	4785(2)	70(1)
C(42)	8397(2)	1972(1)	4234(2)	54(1)
C(43)	9105(2)	1093(1)	5491(2)	71(1)

Table 3. Bond lengths [Å] and angles [°] for **F3**.

C(1)-C(2)	1.549(3)	C(21)-C(22)	1.390(3)
C(2)-C(3)	1.520(3)	C(22)-C(23)	1.458(3)
C(2)-C(14)	1.522(3)	C(23)-C(24)	1.387(3)
C(2)-C(15)	1.544(3)	C(23)-C(28)	1.393(3)
C(3)-C(4)	1.380(3)	C(24)-C(25)	1.369(3)
C(3)-C(8)	1.404(3)	C(25)-C(26)	1.379(4)
C(4)-C(5)	1.393(4)	C(26)-C(27)	1.389(3)
C(5)-C(6)	1.364(5)	C(27)-C(28)	1.382(3)
C(6)-C(7)	1.377(5)	C(29)-C(30)	1.553(3)
C(7)-C(8)	1.401(3)	C(30)-C(31)	1.529(3)
C(8)-C(9)	1.442(3)	C(30)-C(42)	1.529(3)
C(9)-C(14)	1.396(3)	C(30)-C(43)	1.543(3)
C(9)-C(10)	1.405(3)	C(31)-C(32)	1.376(3)
C(10)-C(11)	1.362(4)	C(31)-C(36)	1.394(3)
C(11)-C(12)	1.375(4)	C(32)-C(33)	1.393(3)
C(12)-C(13)	1.384(3)	C(33)-C(34)	1.381(3)
C(13)-C(14)	1.380(3)	C(34)-C(35)	1.373(3)
C(15)-C(16)	1.551(3)	C(35)-C(36)	1.392(3)
C(16)-C(17)	1.527(3)	C(36)-C(37)	1.459(3)
C(16)-C(28)	1.528(2)	C(37)-C(38)	1.386(3)
C(16)-C(29)	1.560(3)	C(37)-C(42)	1.398(3)
C(17)-C(18)	1.382(3)	C(38)-C(39)	1.379(3)
C(17)-C(22)	1.392(3)	C(39)-C(40)	1.375(4)
C(18)-C(19)	1.396(3)	C(40)-C(41)	1.385(3)
C(19)-C(20)	1.378(4)	C(41)-C(42)	1.377(3)
C(20)-C(21)	1.372(4)		
C(3)-C(2)-C(14)	101.36(17)	C(14)-C(9)-C(10)	120.5(2)
C(3)-C(2)-C(15)	116.20(17)	C(14)-C(9)-C(8)	108.27(19)
C(14)-C(2)-C(15)	113.17(16)	C(10)-C(9)-C(8)	131.2(2)
C(3)-C(2)-C(1)	110.31(17)	C(11)-C(10)-C(9)	118.0(3)
C(14)-C(2)-C(1)	108.67(16)	C(10)-C(11)-C(12)	122.49(18)
C(15)-C(2)-C(1)	106.94(16)	C(11)-C(12)-C(13)	119.29(18)
C(4)-C(3)-C(8)	121.4(2)	C(14)-C(13)-C(12)	120.4(3)
C(4)-C(3)-C(2)	128.8(2)	C(13)-C(14)-C(9)	119.2(2)
C(8)-C(3)-C(2)	109.73(19)	C(13)-C(14)-C(2)	129.7(2)
C(3)-C(4)-C(5)	118.4(3)	C(9)-C(14)-C(2)	110.93(18)
C(6)-C(5)-C(4)	120.1(4)	C(2)-C(15)-C(16)	123.38(16)
C(5)-C(6)-C(7)	122.6(4)	C(17)-C(16)-C(28)	100.79(15)
C(6)-C(7)-C(8)	118.2(3)	C(17)-C(16)-C(15)	111.04(15)
C(7)-C(8)-C(3)	119.1(3)	C(28)-C(16)-C(15)	114.63(15)
C(7)-C(8)-C(9)	131.1(3)	C(17)-C(16)-C(29)	110.61(15)
C(3)-C(8)-C(9)	109.68(19)	C(28)-C(16)-C(29)	114.44(15)

C(15)-C(16)-C(29)	105.44(14)	C(42)-C(30)-C(43)	109.34(16)
C(18)-C(17)-C(22)	120.32(19)	C(31)-C(30)-C(29)	116.08(16)
C(18)-C(17)-C(16)	128.56(19)	C(42)-C(30)-C(29)	113.55(16)
C(22)-C(17)-C(16)	111.12(16)	C(43)-C(30)-C(29)	106.89(16)
C(17)-C(18)-C(19)	119.1(2)	C(32)-C(31)-C(36)	120.4(2)
C(20)-C(19)-C(18)	120.2(2)	C(32)-C(31)-C(30)	129.2(2)
C(21)-C(20)-C(19)	120.9(2)	C(36)-C(31)-C(30)	110.21(18)
C(20)-C(21)-C(22)	119.5(2)	C(31)-C(32)-C(33)	119.4(2)
C(21)-C(22)-C(17)	120.0(2)	C(34)-C(33)-C(32)	119.7(2)
C(21)-C(22)-C(23)	131.6(2)	C(35)-C(34)-C(33)	121.5(2)
C(17)-C(22)-C(23)	108.38(17)	C(34)-C(35)-C(36)	118.9(2)
C(24)-C(23)-C(28)	120.5(2)	C(35)-C(36)-C(31)	120.1(2)
C(24)-C(23)-C(22)	130.4(2)	C(35)-C(36)-C(37)	130.4(2)
C(28)-C(23)-C(22)	109.14(17)	C(31)-C(36)-C(37)	109.48(19)
C(25)-C(24)-C(23)	118.4(2)	C(38)-C(37)-C(42)	119.9(2)
C(24)-C(25)-C(26)	122.0(2)	C(38)-C(37)-C(36)	131.6(2)
C(25)-C(26)-C(27)	119.7(2)	C(42)-C(37)-C(36)	108.38(19)
C(28)-C(27)-C(26)	119.2(2)	C(39)-C(38)-C(37)	119.9(2)
C(27)-C(28)-C(23)	120.25(18)	C(40)-C(39)-C(38)	120.0(2)
C(27)-C(28)-C(16)	129.19(18)	C(39)-C(40)-C(41)	120.8(2)
C(23)-C(28)-C(16)	110.56(16)	C(42)-C(41)-C(40)	119.6(2)
C(30)-C(29)-C(16)	122.41(15)	C(41)-C(42)-C(37)	119.8(2)
C(31)-C(30)-C(42)	101.24(16)	C(41)-C(42)-C(30)	129.5(2)
C(31)-C(30)-C(43)	109.60(16)	C(37)-C(42)-C(30)	110.69(18)

Symmetry transformations used to generate equivalent atoms.

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **F3**. The anisotropic displacement factor exponent takes the form: $-2\ ^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	50(1)	101(2)	63(2)	14(1)	18(1)	0(1)
C(2)	45(1)	61(1)	45(1)	1(1)	12(1)	-2(1)
C(3)	42(1)	74(2)	60(2)	-15(1)	14(1)	-10(1)
C(4)	58(2)	90(2)	117(2)	-39(2)	22(2)	-17(1)
C(5)	76(2)	147(4)	168(4)	-92(3)	42(3)	-35(2)
C(6)	85(3)	235(6)	102(3)	-100(3)	39(2)	-50(3)
C(7)	75(2)	202(4)	54(2)	-23(2)	16(2)	-27(2)
C(8)	45(1)	117(2)	40(1)	-6(1)	9(1)	-16(1)
C(9)	46(1)	89(2)	59(2)	17(1)	7(1)	-8(1)
C(10)	62(2)	121(2)	102(2)	48(2)	12(2)	-3(2)
C(11)	62(2)	96(2)	185(4)	45(3)	26(2)	8(2)
C(12)	71(2)	68(2)	166(3)	-12(2)	33(2)	3(1)
C(13)	58(2)	77(2)	98(2)	-15(2)	22(1)	2(1)
C(14)	39(1)	66(1)	61(2)	-2(1)	12(1)	0(1)
C(15)	47(1)	69(1)	39(1)	4(1)	10(1)	-1(1)
C(16)	43(1)	51(1)	37(1)	3(1)	9(1)	2(1)
C(17)	42(1)	53(1)	47(1)	1(1)	8(1)	0(1)
C(18)	61(2)	55(1)	76(2)	8(1)	18(1)	2(1)
C(19)	70(2)	54(2)	134(3)	-9(2)	26(2)	1(1)
C(20)	79(2)	85(2)	99(2)	-36(2)	19(2)	2(2)
C(21)	64(2)	97(2)	58(2)	-22(1)	12(1)	2(1)
C(22)	43(1)	67(1)	41(1)	-4(1)	7(1)	0(1)
C(23)	41(1)	70(2)	40(1)	9(1)	9(1)	2(1)
C(24)	67(2)	99(2)	51(1)	25(1)	13(1)	2(1)
C(25)	69(2)	102(2)	86(2)	50(2)	17(2)	8(2)
C(26)	58(2)	58(2)	122(2)	28(2)	17(2)	6(1)
C(27)	45(1)	59(1)	76(2)	7(1)	9(1)	2(1)
C(28)	34(1)	53(1)	46(1)	8(1)	5(1)	0(1)
C(29)	49(1)	63(1)	37(1)	1(1)	7(1)	4(1)
C(30)	43(1)	69(1)	40(1)	2(1)	2(1)	3(1)
C(31)	34(1)	67(1)	51(1)	1(1)	2(1)	6(1)
C(32)	47(1)	75(2)	63(2)	3(1)	8(1)	10(1)
C(33)	56(2)	86(2)	79(2)	-18(2)	12(1)	10(1)
C(34)	49(1)	122(2)	58(2)	-23(2)	10(1)	2(1)
C(35)	49(1)	104(2)	52(1)	-1(1)	12(1)	-4(1)
C(36)	35(1)	80(2)	48(1)	5(1)	3(1)	-1(1)
C(37)	41(1)	72(2)	55(1)	6(1)	3(1)	-4(1)
C(38)	67(2)	90(2)	74(2)	11(2)	14(1)	-15(1)
C(39)	95(2)	74(2)	96(2)	5(2)	9(2)	-22(2)

C(40)	91(2)	66(2)	82(2)	-9(1)	3(2)	-9(1)
C(41)	66(2)	76(2)	62(2)	-8(1)	7(1)	-2(1)
C(42)	40(1)	68(2)	49(1)	-2(1)	-1(1)	-1(1)
C(43)	56(1)	95(2)	51(1)	5(1)	-8(1)	8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **F3**.

	x	y	z	U(eq)
H(1A)	1437	1023	3811	106
H(1B)	2491	1179	4786	106
H(1C)	2402	498	4307	106
H(4)	3108	-132	2826	105
H(5)	2490	-498	1148	154
H(6)	1921	202	-164	166
H(7)	1761	1273	114	132
H(10)	1766	2468	875	116
H(11)	1862	3358	1863	138
H(12)	2560	3320	3606	121
H(13)	3151	2357	4404	92
H(15A)	4565	664	4454	62
H(15B)	4652	1392	4644	62
H(18)	5801	-231	3931	76
H(19)	5937	-1001	2720	103
H(20)	5971	-707	1081	106
H(21)	5882	345	619	88
H(24)	5700	1616	463	87
H(25)	5610	2692	695	103
H(26)	5570	3118	2258	96
H(27)	5580	2450	3636	73
H(29A)	6656	1437	5055	60
H(29B)	6889	717	4923	60
H(32)	8551	8	3878	75
H(33)	9247	-320	2454	89
H(34)	9771	423	1372	92
H(35)	9586	1491	1656	82
H(38)	9409	2658	2420	93
H(39)	9119	3554	3326	109
H(40)	8439	3458	4809	99
H(41)	7987	2472	5385	83
H(43A)	9943	1216	5476	106
H(43B)	9077	642	5589	106
H(43C)	8859	1306	6042	106

Table 6. Torsion angles [°] for **F3**.

C(14)-C(2)-C(3)-C(4)	-175.4(2)	C(2)-C(15)-C(16)-C(28)	43.0(2)
C(15)-C(2)-C(3)-C(4)	61.5(3)	C(2)-C(15)-C(16)-C(29)	169.75(17)
C(1)-C(2)-C(3)-C(4)	-60.4(3)	C(28)-C(16)-C(17)-C(18)	-179.71(19)
C(14)-C(2)-C(3)-C(8)	1.5(2)	C(15)-C(16)-C(17)-C(18)	-57.9(3)
C(15)-C(2)-C(3)-C(8)	-121.60(19)	C(29)-C(16)-C(17)-C(18)	58.9(3)
C(1)-C(2)-C(3)-C(8)	116.50(19)	C(28)-C(16)-C(17)-C(22)	0.2(2)
C(8)-C(3)-C(4)-C(5)	1.9(3)	C(15)-C(16)-C(17)-C(22)	122.06(18)
C(2)-C(3)-C(4)-C(5)	178.5(2)	C(29)-C(16)-C(17)-C(22)	-121.23(18)
C(3)-C(4)-C(5)-C(6)	0.0(5)	C(22)-C(17)-C(18)-C(19)	0.9(3)
C(4)-C(5)-C(6)-C(7)	-2.9(6)	C(16)-C(17)-C(18)-C(19)	-179.2(2)
C(5)-C(6)-C(7)-C(8)	3.6(5)	C(17)-C(18)-C(19)-C(20)	-0.4(4)
C(6)-C(7)-C(8)-C(3)	-1.5(4)	C(18)-C(19)-C(20)-C(21)	0.0(4)
C(6)-C(7)-C(8)-C(9)	-177.2(3)	C(19)-C(20)-C(21)-C(22)	-0.3(4)
C(4)-C(3)-C(8)-C(7)	-1.2(3)	C(20)-C(21)-C(22)-C(17)	0.8(3)
C(2)-C(3)-C(8)-C(7)	-178.4(2)	C(20)-C(21)-C(22)-C(23)	-180.0(2)
C(4)-C(3)-C(8)-C(9)	175.33(19)	C(18)-C(17)-C(22)-C(21)	-1.1(3)
C(2)-C(3)-C(8)-C(9)	-1.9(2)	C(16)-C(17)-C(22)-C(21)	178.93(18)
C(7)-C(8)-C(9)-C(14)	177.4(2)	C(18)-C(17)-C(22)-C(23)	179.47(17)
C(3)-C(8)-C(9)-C(14)	1.4(2)	C(16)-C(17)-C(22)-C(23)	-0.5(2)
C(7)-C(8)-C(9)-C(10)	-1.4(4)	C(21)-C(22)-C(23)-C(24)	1.2(4)
C(3)-C(8)-C(9)-C(10)	-177.3(2)	C(17)-C(22)-C(23)-C(24)	-179.5(2)
C(14)-C(9)-C(10)-C(11)	-0.6(3)	C(21)-C(22)-C(23)-C(28)	-178.8(2)
C(8)-C(9)-C(10)-C(11)	178.1(2)	C(17)-C(22)-C(23)-C(28)	0.5(2)
C(9)-C(10)-C(11)-C(12)	0.1(3)	C(28)-C(23)-C(24)-C(25)	0.8(3)
C(10)-C(11)-C(12)-C(13)	-0.48(17)	C(22)-C(23)-C(24)-C(25)	-179.2(2)
C(11)-C(12)-C(13)-C(14)	1.3(3)	C(23)-C(24)-C(25)-C(26)	-0.1(4)
C(12)-C(13)-C(14)-C(9)	-1.7(3)	C(24)-C(25)-C(26)-C(27)	-0.7(4)
C(12)-C(13)-C(14)-C(2)	-178.22(19)	C(25)-C(26)-C(27)-C(28)	0.8(3)
C(10)-C(9)-C(14)-C(13)	1.4(3)	C(26)-C(27)-C(28)-C(23)	-0.1(3)
C(8)-C(9)-C(14)-C(13)	-177.52(19)	C(26)-C(27)-C(28)-C(16)	179.54(19)
C(10)-C(9)-C(14)-C(2)	178.48(19)	C(24)-C(23)-C(28)-C(27)	-0.7(3)
C(8)-C(9)-C(14)-C(2)	-0.4(2)	C(22)-C(23)-C(28)-C(27)	179.27(16)
C(3)-C(2)-C(14)-C(13)	176.1(2)	C(24)-C(23)-C(28)-C(16)	179.60(18)
C(15)-C(2)-C(14)-C(13)	-58.8(3)	C(22)-C(23)-C(28)-C(16)	-0.4(2)
C(1)-C(2)-C(14)-C(13)	59.9(3)	C(17)-C(16)-C(28)-C(27)	-179.50(18)
C(3)-C(2)-C(14)-C(9)	-0.6(2)	C(15)-C(16)-C(28)-C(27)	61.2(2)
C(15)-C(2)-C(14)-C(9)	124.53(19)	C(29)-C(16)-C(28)-C(27)	-60.8(2)
C(1)-C(2)-C(14)-C(9)	-116.84(19)	C(17)-C(16)-C(28)-C(23)	0.13(19)
C(3)-C(2)-C(15)-C(16)	44.1(3)	C(15)-C(16)-C(28)-C(23)	-119.16(18)
C(14)-C(2)-C(15)-C(16)	-72.7(2)	C(29)-C(16)-C(28)-C(23)	118.83(17)
C(1)-C(2)-C(15)-C(16)	167.72(18)	C(17)-C(16)-C(29)-C(30)	70.6(2)
C(2)-C(15)-C(16)-C(17)	-70.4(2)	C(28)-C(16)-C(29)-C(30)	-42.4(2)

C(15)-C(16)-C(29)-C(30)	-169.32(17)
C(16)-C(29)-C(30)-C(31)	-43.5(2)
C(16)-C(29)-C(30)-C(42)	73.2(2)
C(16)-C(29)-C(30)-C(43)	-166.13(17)
C(42)-C(30)-C(31)-C(32)	173.53(19)
C(43)-C(30)-C(31)-C(32)	58.1(3)
C(29)-C(30)-C(31)-C(32)	-63.1(3)
C(42)-C(30)-C(31)-C(36)	-1.2(2)
C(43)-C(30)-C(31)-C(36)	-116.63(18)
C(29)-C(30)-C(31)-C(36)	122.20(18)
C(36)-C(31)-C(32)-C(33)	-3.2(3)
C(30)-C(31)-C(32)-C(33)	-177.5(2)
C(31)-C(32)-C(33)-C(34)	1.8(3)
C(32)-C(33)-C(34)-C(35)	-0.3(4)
C(33)-C(34)-C(35)-C(36)	0.2(3)
C(34)-C(35)-C(36)-C(31)	-1.6(3)
C(34)-C(35)-C(36)-C(37)	175.3(2)
C(32)-C(31)-C(36)-C(35)	3.2(3)
C(30)-C(31)-C(36)-C(35)	178.44(18)
C(32)-C(31)-C(36)-C(37)	-174.36(17)
C(30)-C(31)-C(36)-C(37)	0.9(2)
C(35)-C(36)-C(37)-C(38)	-1.0(4)
C(31)-C(36)-C(37)-C(38)	176.2(2)
C(35)-C(36)-C(37)-C(42)	-177.4(2)
C(31)-C(36)-C(37)-C(42)	-0.2(2)
C(42)-C(37)-C(38)-C(39)	-1.3(3)
C(36)-C(37)-C(38)-C(39)	-177.3(2)
C(37)-C(38)-C(39)-C(40)	1.6(4)
C(38)-C(39)-C(40)-C(41)	-0.8(4)
C(39)-C(40)-C(41)-C(42)	-0.4(4)
C(40)-C(41)-C(42)-C(37)	0.7(3)
C(40)-C(41)-C(42)-C(30)	177.8(2)
C(38)-C(37)-C(42)-C(41)	0.1(3)
C(36)-C(37)-C(42)-C(41)	176.92(17)
C(38)-C(37)-C(42)-C(30)	-177.48(18)
C(36)-C(37)-C(42)-C(30)	-0.6(2)
C(31)-C(30)-C(42)-C(41)	-176.1(2)
C(43)-C(30)-C(42)-C(41)	-60.5(3)
C(29)-C(30)-C(42)-C(41)	58.7(3)
C(31)-C(30)-C(42)-C(37)	1.1(2)
C(43)-C(30)-C(42)-C(37)	116.7(2)
C(29)-C(30)-C(42)-C(37)	-124.02(18)

Symmetry transformations used to generate equivalent atoms.

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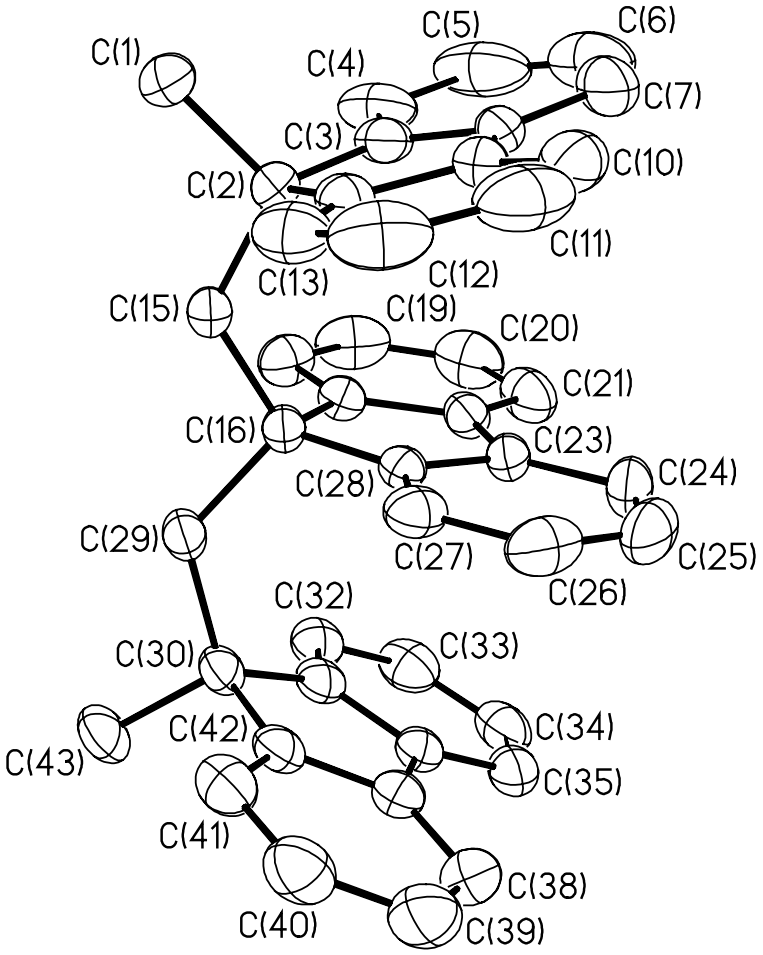

Figure S4. ORTEP Diagram of **F3**, thermal ellipsoid shown in 30% probability.

References

S1. Greenbow, E.J.; McNeil, D. *J. Chem. Soc.* **1956**, 3204.

S2. All software and sources of the scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-Ray Systems, Madison, WI).