Supporting Information

Highly Efficient Deep-Blue Organic Electroluminescent Devices Doped with Hexaphenylanthracene Fluorophores

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A. X-ray data for compound (3bb)

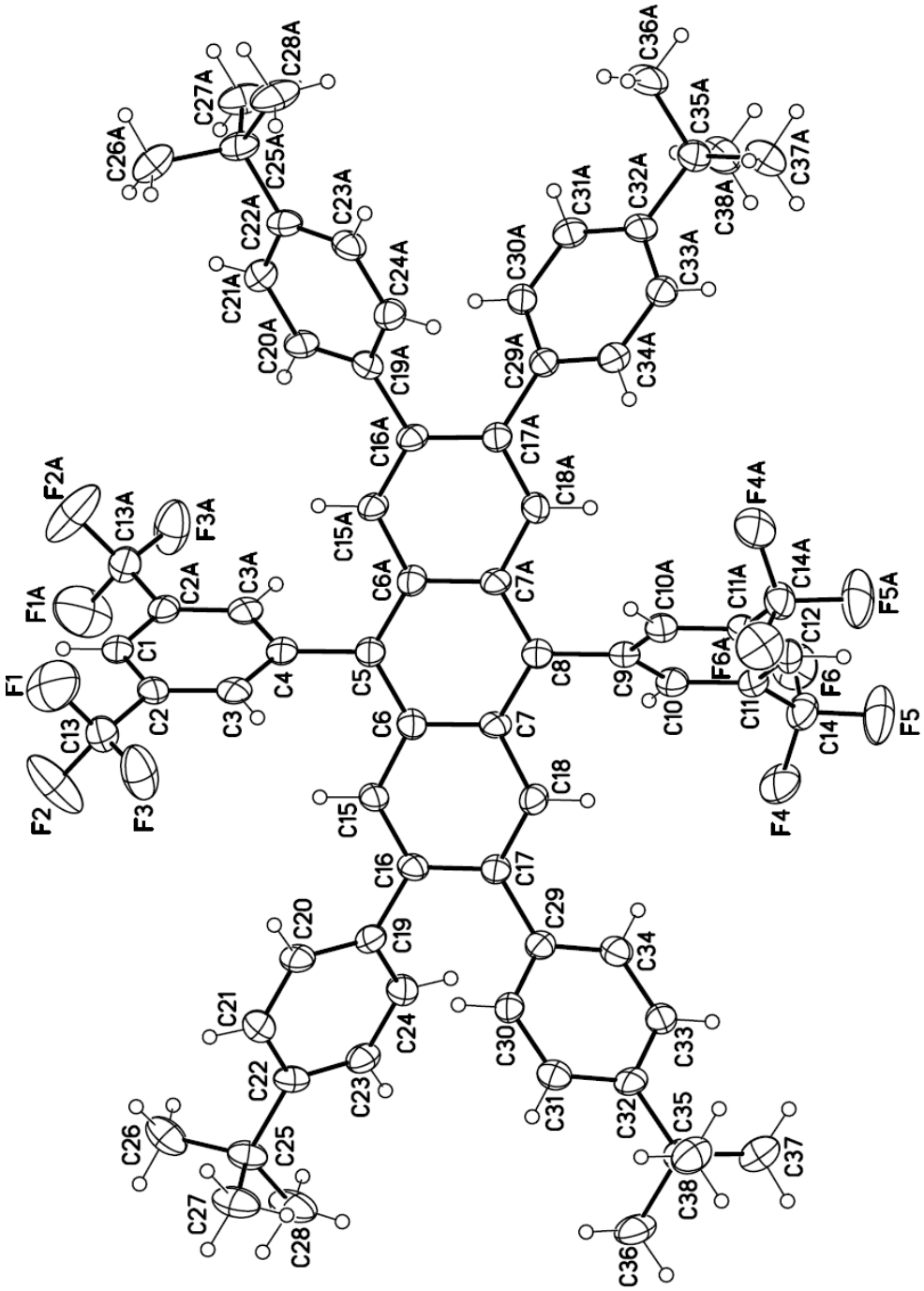


Table 1. Crystal data and structure refinement for **3bb**.

Identification code	090802lt_0m	
Empirical formula	C35 H31 F6	
Formula weight	565.60	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 19.118(3) Å	α= 90°.
	b = 27.955(5) Å	β= 123.128(6)°.
	c = 13.258(2) Å	γ = 90°.
Volume	5934.1(18) $Å^3$	
Z	8	
Density (calculated)	1.266 Mg/m^3	
Absorption coefficient	0.099 mm^{-1}	
F(000)	2360	
Crystal size	0.12 x 0.02 x 0.02 mm^3	
Theta range for data collection	1.46 to 26.43°.	
Index ranges	-22≤h≤23, -34≤k≤34, -16≤l≤14	
Reflections collected	44436	
Independent reflections	6082 [R(int) = 0.2174]	
Completeness to theta = 26.43°	99.4 %	
Absorption correction	Empirical	
Max. and min. transmission	0.7454 and 0.5824	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6082 / 0 / 376	
Goodness-of-fit on F^2	0.963	
Final R indices [I>2sigma(I)]	R1 = 0.0768, wR2 = 0.1674	
R indices (all data)	R1 = 0.2254, wR2 = 0.2436	
Extinction coefficient	0.0048(5)	
Largest diff. peak and hole	0.635 and -0.495 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	5000	-1899(2)	7500	27(1)
C(2)	5200(3)	-1649(2)	6792(4)	29(1)
C(3)	5208(3)	-1153(2)	6802(4)	29(1)
C(4)	5000	-896(2)	7500	27(1)
C(5)	5000	-357(2)	7500	26(2)
C(6)	4461(3)	-103(2)	6418(4)	27(1)
C(7)	4473(3)	408(2)	6418(4)	25(1)
C(8)	5000	662(2)	7500	25(2)
C(9)	5000	1195(2)	7500	29(2)
C(10)	4285(3)	1453(2)	7187(4)	32(1)
C(11)	4280(3)	1948(2)	7192(4)	31(1)
C(12)	5000	2199(2)	7500	35(2)
C(13)	5406(3)	-1924(2)	6028(5)	40(1)
C(14)	3510(3)	2212(2)	6866(5)	41(1)
C(15)	3857(3)	-338(2)	5319(4)	27(1)
C(16)	3331(3)	-98(2)	4274(4)	26(1)
C(17)	3409(3)	413(2)	4237(4)	26(1)
C(18)	3962(3)	647(2)	5292(4)	29(1)
C(19)	2668(3)	-364(2)	3207(4)	29(1)
C(20)	2843(3)	-789(2)	2842(4)	32(1)
C(21)	2230(3)	-1031(2)	1830(4)	34(1)
C(22)	1416(3)	-858(2)	1116(4)	30(1)
C(23)	1238(3)	-445(2)	1506(4)	32(1)
C(24)	1850(3)	-199(2)	2521(4)	32(1)
C(25)	775(3)	-1132(2)	-26(4)	37(1)
C(26)	668(4)	-1642(2)	297(5)	51(2)
C(27)	1095(3)	-1156(2)	-859(4)	49(2)
C(28)	-80(3)	-884(2)	-697(5)	52(2)
C(29)	2944(3)	693(2)	3083(4)	27(1)
C(30)	2894(3)	531(2)	2055(4)	27(1)
C(31)	2525(3)	814(2)	1023(4)	30(1)

C(32)	2214(3)	1264(2)	988(4)	30(1)
C(33)	2257(3)	1420(2)	2018(4)	30(1)
C(34)	2619(3)	1137(2)	3052(4)	31(1)
C(35)	1864(3)	1577(2)	-145(4)	33(1)
C(36)	1192(3)	1297(2)	-1260(4)	43(1)
C(37)	1493(3)	2037(2)	-50(5)	46(2)
C(38)	2593(3)	1695(2)	-291(5)	46(2)
F(1)	6083(3)	-2203(1)	6685(3)	90(1)
F(2)	4816(2)	-2226(1)	5303(3)	82(1)
F(3)	5583(2)	-1667(1)	5371(3)	63(1)
F(4)	2851(2)	2068(1)	5798(3)	55(1)
F(5)	3571(2)	2683(1)	6808(3)	67(1)
F(6)	3288(2)	2126(1)	7655(3)	58(1)

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

C(1)-C(2)	1.380(6)
C(1)-C(2)#1	1.380(6)
C(1)-H(1)	0.9300
C(2)-C(3)	1.388(6)
C(2)-C(13)	1.487(7)
C(3)-C(4)	1.390(6)
C(3)-H(3)	0.9300
C(4)-C(3)#1	1.390(6)
C(4)-C(5)	1.507(8)
C(5)-C(6)	1.417(5)
C(5)-C(6)#1	1.417(5)
C(6)-C(7)	1.428(6)
C(6)-C(15)	1.430(6)
C(7)-C(8)	1.414(5)
C(7)-C(18)	1.427(6)
C(8)-C(7)#1	1.414(5)
C(8)-C(9)	1.489(9)
C(9)-C(10)#1	1.393(6)
C(9)-C(10)	1.393(6)
C(10)-C(11)	1.384(6)
C(10)-H(10)	0.9300
C(11)-C(12)	1.393(6)
C(11)-C(14)	1.484(7)
C(12)-C(11)#1	1.393(6)
C(12)-H(12)	0.9300
C(13)-F(3)	1.309(6)
C(13)-F(2)	1.313(6)
C(13)-F(1)	1.343(6)
C(14)-F(5)	1.329(5)
C(14)-F(4)	1.343(5)
C(14)-F(6)	1.347(6)
C(15)-C(16)	1.363(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.441(6)

C(16)-C(19)	1.483(6)
C(17)-C(18)	1.372(6)
C(17)-C(29)	1.502(6)
C(18)-H(18)	0.9300
C(19)-C(24)	1.390(6)
C(19)-C(20)	1.390(6)
C(20)-C(21)	1.383(6)
C(20)-H(20)	0.9300
C(21)-C(22)	1.392(6)
C(21)-H(21)	0.9300
C(22)-C(23)	1.383(6)
C(22)-C(25)	1.533(6)
C(23)-C(24)	1.389(6)
C(23)-H(23)	0.9300
C(24)-H(24)	0.9300
C(25)-C(27)	1.528(7)
C(25)-C(28)	1.533(7)
C(25)-C(26)	1.534(7)
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-C(34)	1.381(6)
C(29)-C(30)	1.389(6)
C(30)-C(31)	1.394(6)
C(30)-H(30)	0.9300
C(31)-C(32)	1.380(6)
C(31)-H(31)	0.9300
C(32)-C(33)	1.394(6)
C(32)-C(35)	1.540(6)
C(33)-C(34)	1.396(6)

C(33)-H(33)	0.9300
C(34)-H(34)	0.9300
C(35)-C(37)	1.507(7)
C(35)-C(36)	1.540(7)
C(35)-C(38)	1.545(7)
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
C(37)-H(37A)	0.9600
C(37)-H(37B)	0.9600
C(37)-H(37C)	0.9600
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600

C(2)-C(1)-C(2)#1	119.3(6)
C(2)-C(1)-H(1)	120.3
C(2)#1-C(1)-H(1)	120.3
C(1)-C(2)-C(3)	120.3(5)
C(1)-C(2)-C(13)	118.5(4)
C(3)-C(2)-C(13)	121.2(4)
C(2)-C(3)-C(4)	121.2(5)
C(2)-C(3)-H(3)	119.4
C(4)-C(3)-H(3)	119.4
C(3)#1-C(4)-C(3)	117.7(6)
C(3)#1-C(4)-C(5)	121.1(3)
C(3)-C(4)-C(5)	121.1(3)
C(6)-C(5)-C(6)#1	119.9(6)
C(6)-C(5)-C(4)	120.0(3)
C(6)#1-C(5)-C(4)	120.0(3)
C(5)-C(6)-C(7)	119.8(4)
C(5)-C(6)-C(15)	122.5(4)
C(7)-C(6)-C(15)	117.5(4)
C(8)-C(7)-C(18)	121.8(4)
C(8)-C(7)-C(6)	120.4(4)
C(18)-C(7)-C(6)	117.8(4)

C(7)#1-C(8)-C(7)	119.5(6)
C(7)#1-C(8)-C(9)	120.2(3)
C(7)-C(8)-C(9)	120.2(3)
C(10)#1-C(9)-C(10)	117.7(6)
C(10)#1-C(9)-C(8)	121.2(3)
C(10)-C(9)-C(8)	121.2(3)
C(11)-C(10)-C(9)	121.6(5)
C(11)-C(10)-H(10)	119.2
C(9)-C(10)-H(10)	119.2
C(10)-C(11)-C(12)	119.9(5)
C(10)-C(11)-C(14)	120.2(4)
C(12)-C(11)-C(14)	119.9(4)
C(11)#1-C(12)-C(11)	119.4(6)
C(11)#1-C(12)-H(12)	120.3
C(11)-C(12)-H(12)	120.3
F(3)-C(13)-F(2)	107.4(4)
F(3)-C(13)-F(1)	104.1(5)
F(2)-C(13)-F(1)	103.9(5)
F(3)-C(13)-C(2)	115.5(4)
F(2)-C(13)-C(2)	112.9(5)
F(1)-C(13)-C(2)	112.1(4)
F(5)-C(14)-F(4)	107.3(4)
F(5)-C(14)-F(6)	107.2(4)
F(4)-C(14)-F(6)	104.7(4)
F(5)-C(14)-C(11)	113.9(4)
F(4)-C(14)-C(11)	111.6(4)
F(6)-C(14)-C(11)	111.6(4)
C(16)-C(15)-C(6)	123.2(4)
C(16)-C(15)-H(15)	118.4
C(6)-C(15)-H(15)	118.4
C(15)-C(16)-C(17)	119.3(4)
C(15)-C(16)-C(19)	119.7(4)
C(17)-C(16)-C(19)	121.0(4)
C(18)-C(17)-C(16)	118.3(4)
C(18)-C(17)-C(29)	119.3(4)
C(16)-C(17)-C(29)	122.4(4)

C(17)-C(18)-C(7)	123.3(4)
C(17)-C(18)-H(18)	118.3
C(7)-C(18)-H(18)	118.3
C(24)-C(19)-C(20)	117.0(4)
C(24)-C(19)-C(16)	121.8(4)
C(20)-C(19)-C(16)	121.2(4)
C(21)-C(20)-C(19)	121.2(5)
C(21)-C(20)-H(20)	119.4
C(19)-C(20)-H(20)	119.4
C(20)-C(21)-C(22)	122.0(5)
C(20)-C(21)-H(21)	119.0
C(22)-C(21)-H(21)	119.0
C(23)-C(22)-C(21)	116.5(4)
C(23)-C(22)-C(25)	123.9(4)
C(21)-C(22)-C(25)	119.5(4)
C(22)-C(23)-C(24)	121.8(5)
C(22)-C(23)-H(23)	119.1
C(24)-C(23)-H(23)	119.1
C(23)-C(24)-C(19)	121.4(5)
C(23)-C(24)-H(24)	119.3
C(19)-C(24)-H(24)	119.3
C(27)-C(25)-C(22)	108.4(4)
C(27)-C(25)-C(28)	108.7(4)
C(22)-C(25)-C(28)	111.8(4)
C(27)-C(25)-C(26)	109.1(4)
C(22)-C(25)-C(26)	110.1(4)
C(28)-C(25)-C(26)	108.6(5)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5

C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(34)-C(29)-C(30)	118.4(4)
C(34)-C(29)-C(17)	120.3(4)
C(30)-C(29)-C(17)	121.1(4)
C(29)-C(30)-C(31)	120.3(4)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(32)-C(31)-C(30)	121.9(4)
C(32)-C(31)-H(31)	119.0
C(30)-C(31)-H(31)	119.0
C(31)-C(32)-C(33)	117.4(4)
C(31)-C(32)-C(35)	120.0(4)
C(33)-C(32)-C(35)	122.6(4)
C(32)-C(33)-C(34)	121.1(5)
C(32)-C(33)-H(33)	119.5
C(34)-C(33)-H(33)	119.5
C(29)-C(34)-C(33)	120.9(5)
C(29)-C(34)-H(34)	119.6
C(33)-C(34)-H(34)	119.6
C(37)-C(35)-C(36)	109.3(4)
C(37)-C(35)-C(32)	112.2(4)
C(36)-C(35)-C(32)	109.8(4)
C(37)-C(35)-C(38)	109.0(4)
C(36)-C(35)-C(38)	108.9(4)
C(32)-C(35)-C(38)	107.6(4)
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5

C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(35)-C(37)-H(37A)	109.5
C(35)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(35)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(35)-C(38)-H(38A)	109.5
C(35)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(35)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3bb**. 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)	12(2)	29(3)	26(3)	0	2(2)	0
C(2)	20(3)	30(3)	24(3)	-3(2)	5(2)	1(2)
C(3)	12(2)	37(3)	24(3)	0(2)	1(2)	-2(2)
C(4)	12(2)	29(3)	26(3)	0	2(2)	0
C(5)	21(4)	26(4)	27(4)	0	10(3)	0
C(6)	19(3)	25(3)	30(3)	-2(2)	10(2)	-1(2)
C(7)	16(2)	30(3)	22(3)	0(2)	5(2)	-5(2)
C(8)	19(4)	28(4)	27(4)	0	12(3)	0
C(9)	30(4)	28(4)	20(3)	0	8(3)	0
C(10)	26(3)	32(3)	27(3)	1(2)	8(2)	-2(2)
C(11)	29(3)	27(3)	26(3)	2(2)	7(2)	2(2)
C(12)	37(5)	20(4)	37(4)	0	14(4)	0
C(13)	40(3)	31(3)	40(3)	-2(3)	17(3)	-1(3)
C(14)	30(3)	29(3)	45(4)	4(3)	8(3)	0(2)
C(15)	20(3)	27(3)	25(3)	-3(2)	6(2)	2(2)
C(16)	19(3)	30(3)	23(3)	-3(2)	7(2)	0(2)
C(17)	18(3)	26(3)	27(3)	0(2)	8(2)	-1(2)
C(18)	25(3)	24(3)	30(3)	3(2)	10(2)	-2(2)
C(19)	27(3)	29(3)	25(3)	4(2)	9(2)	3(2)
C(20)	21(3)	37(3)	25(3)	0(2)	3(2)	-3(2)
C(21)	33(3)	32(3)	32(3)	-4(2)	14(3)	-4(2)
C(22)	23(3)	39(3)	21(3)	-1(2)	8(2)	-3(2)
C(23)	24(3)	35(3)	28(3)	6(2)	9(2)	3(2)
C(24)	27(3)	30(3)	31(3)	-2(2)	11(2)	0(2)
C(25)	23(3)	47(3)	27(3)	-5(2)	5(2)	-6(2)
C(26)	44(4)	50(4)	46(3)	-19(3)	17(3)	-18(3)
C(27)	30(3)	71(4)	31(3)	-10(3)	7(3)	-4(3)
C(28)	26(3)	72(4)	36(3)	-16(3)	4(3)	-5(3)
C(29)	20(3)	27(3)	26(3)	1(2)	8(2)	-5(2)
C(30)	20(3)	25(3)	29(3)	1(2)	9(2)	1(2)
C(31)	21(3)	36(3)	28(3)	-3(2)	11(2)	-3(2)

C(32)	16(3)	33(3)	26(3)	3(2)	3(2)	-1(2)
C(33)	25(3)	29(3)	29(3)	-1(2)	11(2)	2(2)
C(34)	31(3)	32(3)	27(3)	-3(2)	13(2)	-4(2)
C(35)	28(3)	32(3)	31(3)	3(2)	11(2)	2(2)
C(36)	31(3)	52(4)	30(3)	9(3)	6(3)	4(3)
C(37)	41(3)	49(4)	39(3)	13(3)	17(3)	11(3)
C(38)	44(4)	47(3)	42(3)	11(3)	21(3)	1(3)
F(1)	102(3)	94(3)	76(3)	10(2)	50(2)	56(3)
F(2)	92(3)	91(3)	97(3)	-65(2)	73(3)	-60(2)
F(3)	101(3)	41(2)	84(3)	-12(2)	74(2)	-17(2)
F(4)	31(2)	50(2)	55(2)	9(2)	4(2)	10(2)
F(5)	47(2)	29(2)	112(3)	3(2)	35(2)	8(2)
F(6)	46(2)	65(2)	68(2)	-2(2)	36(2)	8(2)

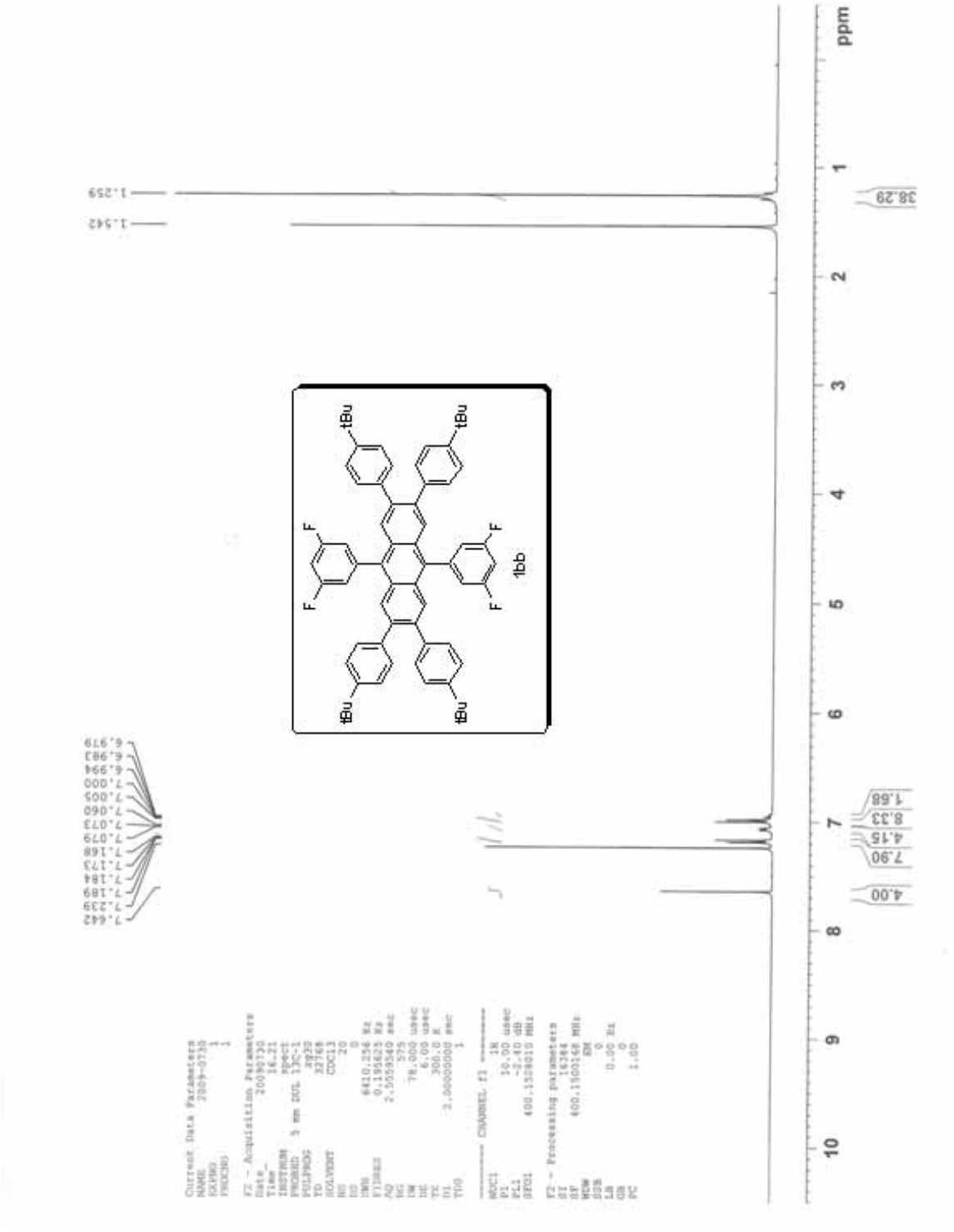
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3bb**.

	x	y	z	U(eq)
H(1)	5000	-2231	7500	32
H(3)	5355	-989	6334	34
H(10)	3799	1288	6970	38
H(12)	5000	2532	7500	41
H(15)	3821	-669	5319	33
H(18)	4006	977	5272	35
H(20)	3382	-912	3286	39
H(21)	2365	-1317	1621	41
H(23)	694	-328	1076	38
H(24)	1709	81	2747	38
H(26A)	1193	-1807	677	76
H(26B)	262	-1809	-422	76
H(26C)	483	-1629	839	76
H(27A)	1153	-837	-1076	74
H(27B)	705	-1331	-1573	74
H(27C)	1627	-1313	-451	74
H(28A)	-275	-853	-169	77
H(28B)	-470	-1071	-1387	77
H(28C)	-29	-572	-955	77
H(30)	3108	232	2055	32
H(31)	2487	697	338	36
H(33)	2040	1719	2016	35
H(34)	2641	1250	3730	37
H(36A)	751	1207	-1157	65
H(36B)	1437	1015	-1356	65
H(36C)	971	1495	-1962	65
H(37A)	1055	1966	77	68
H(37B)	1268	2217	-782	68
H(37C)	1919	2222	615	68
H(38A)	2391	1888	-998	68

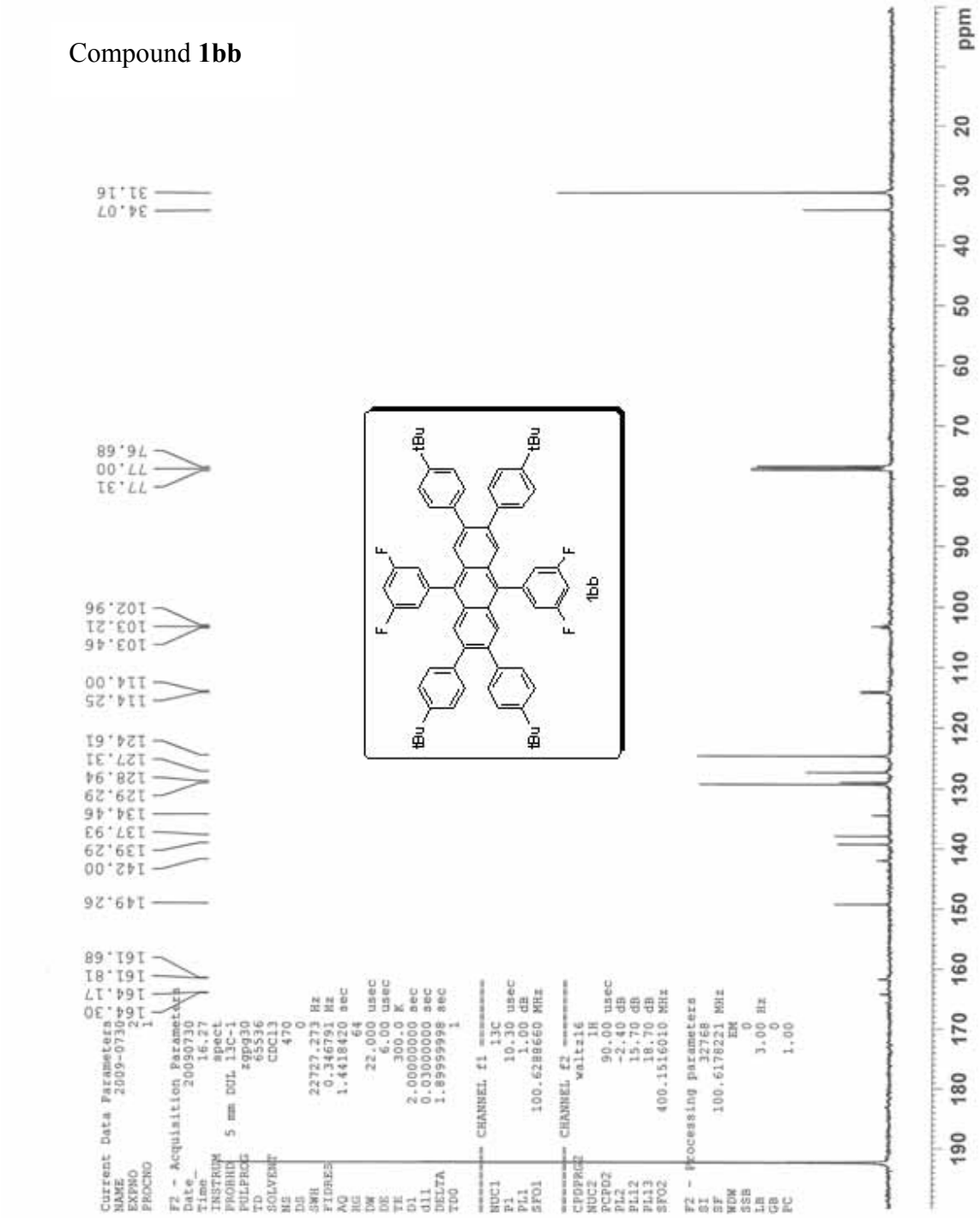
H(38B)	2825	1404	-370	68
H(38C)	3017	1868	403	68

B. NMR spectral- data for key compounds:

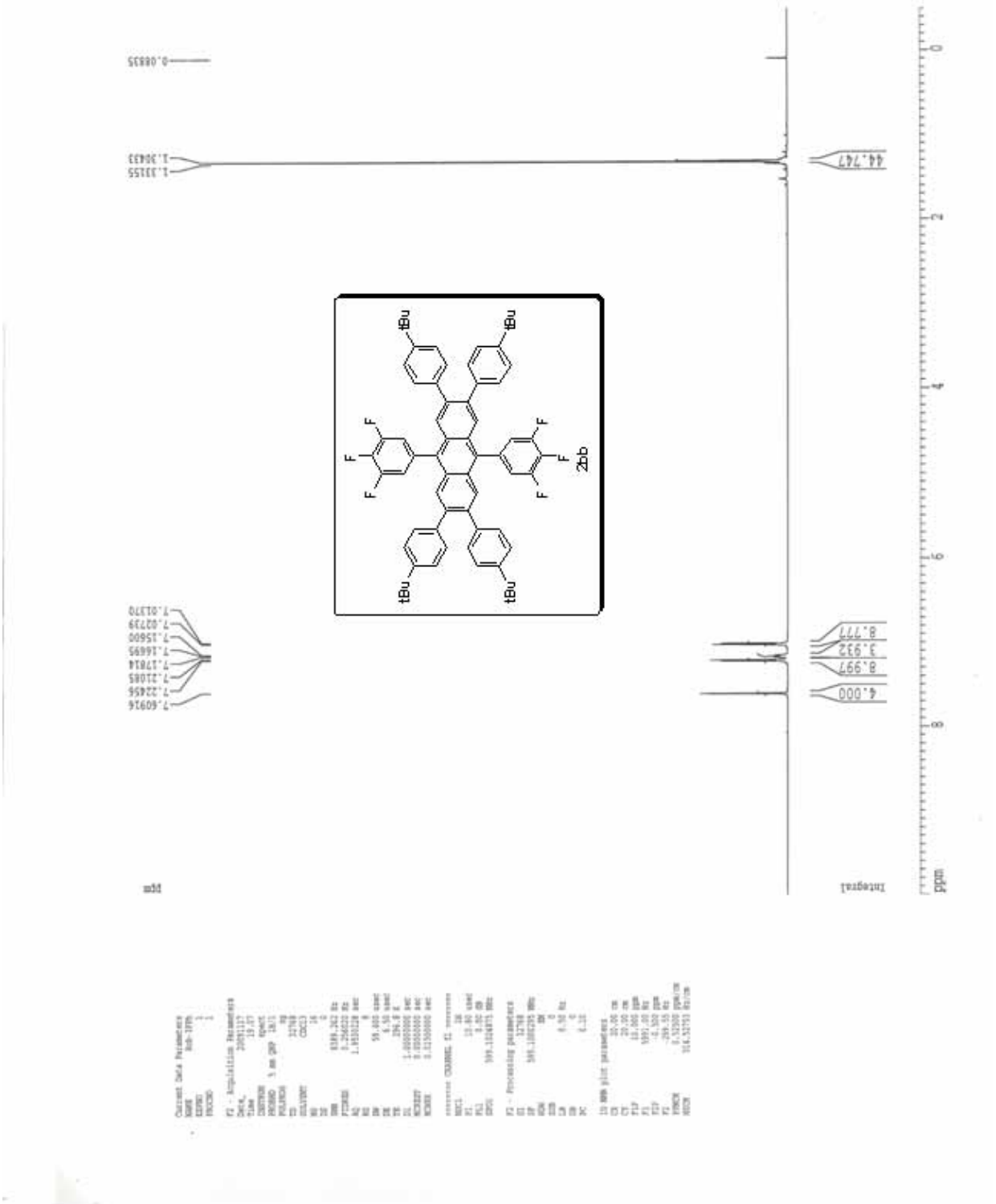
Compound **1bb**



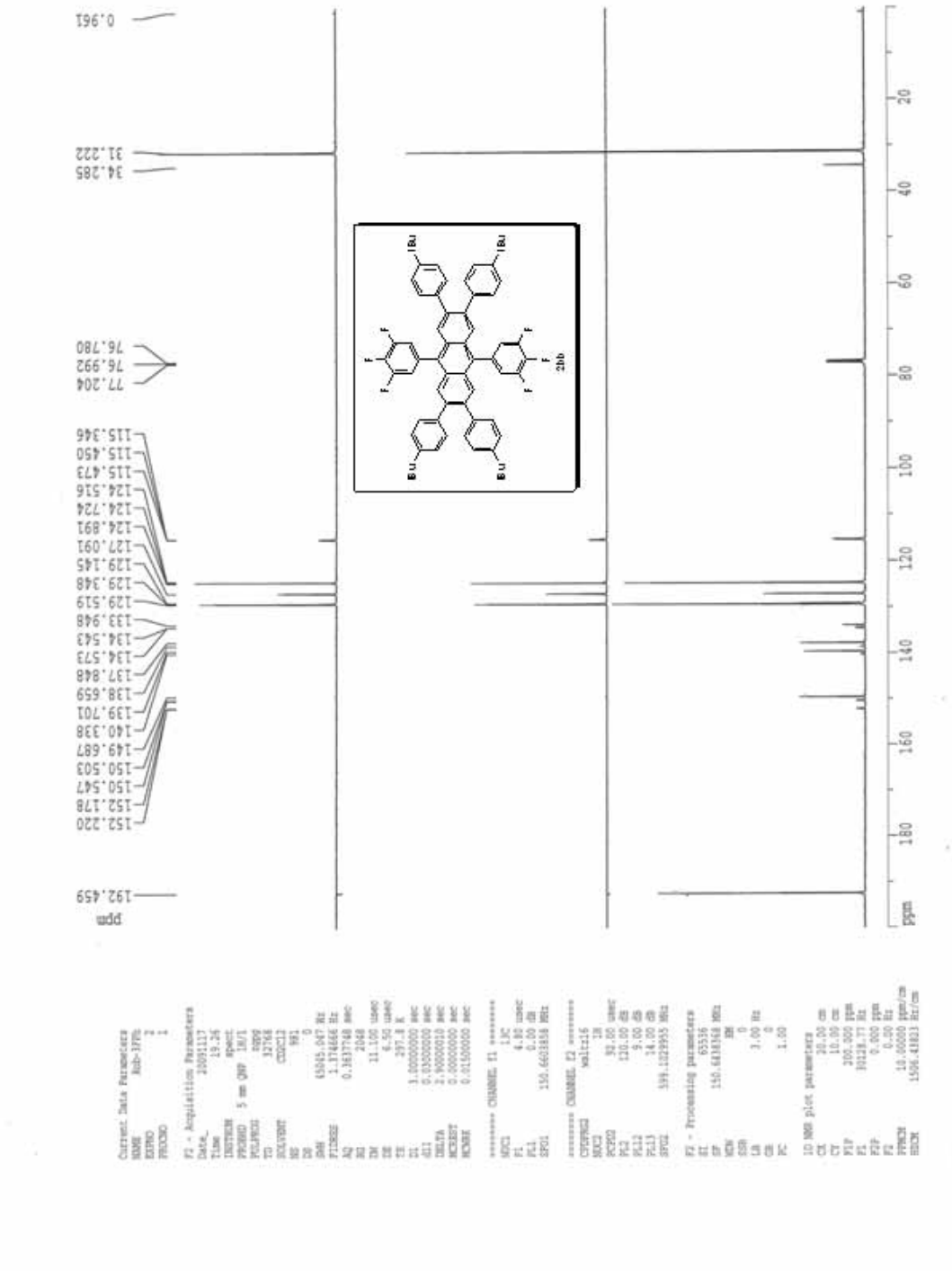
Compound **1bb**



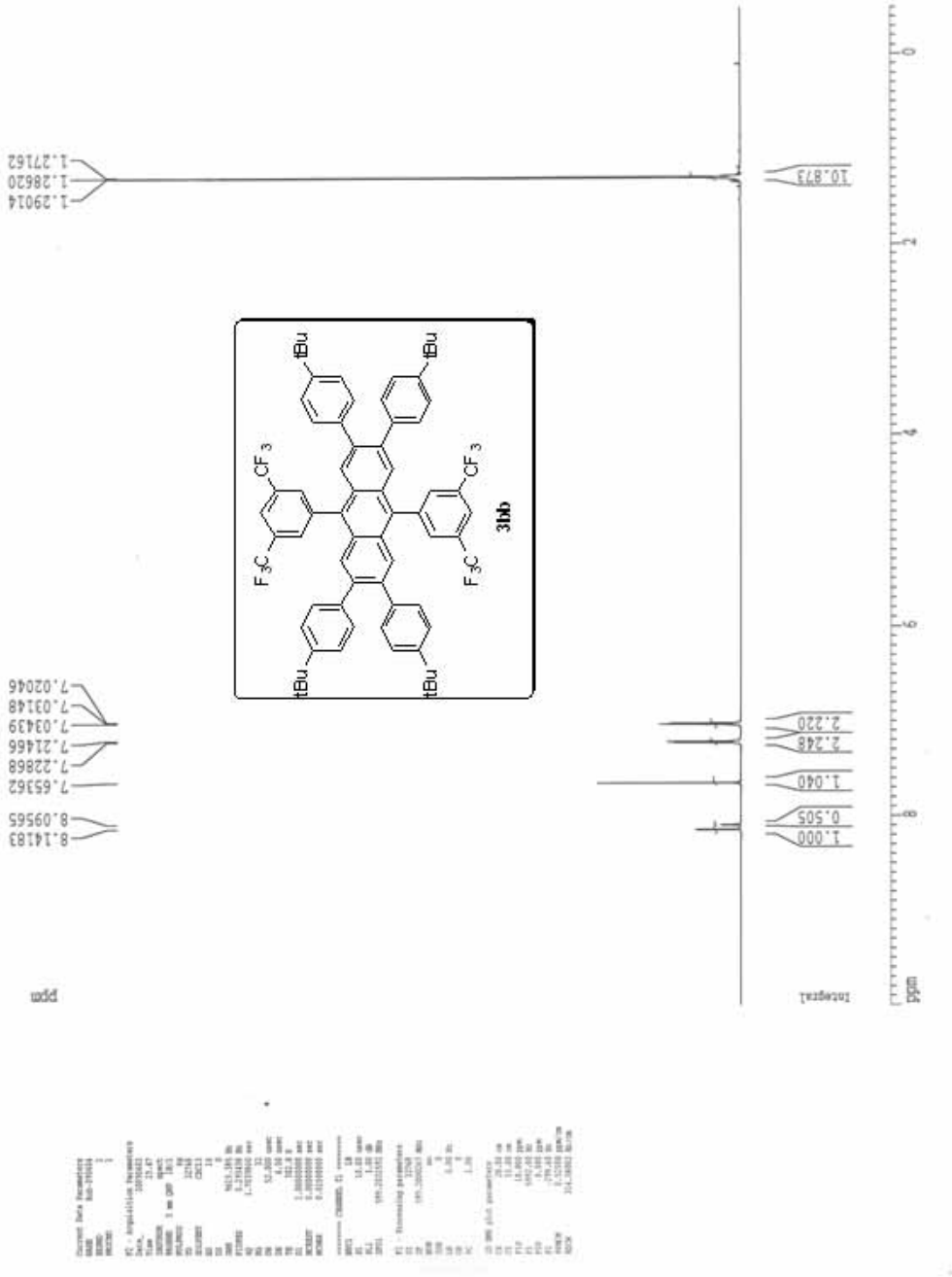
Compound **2bb**



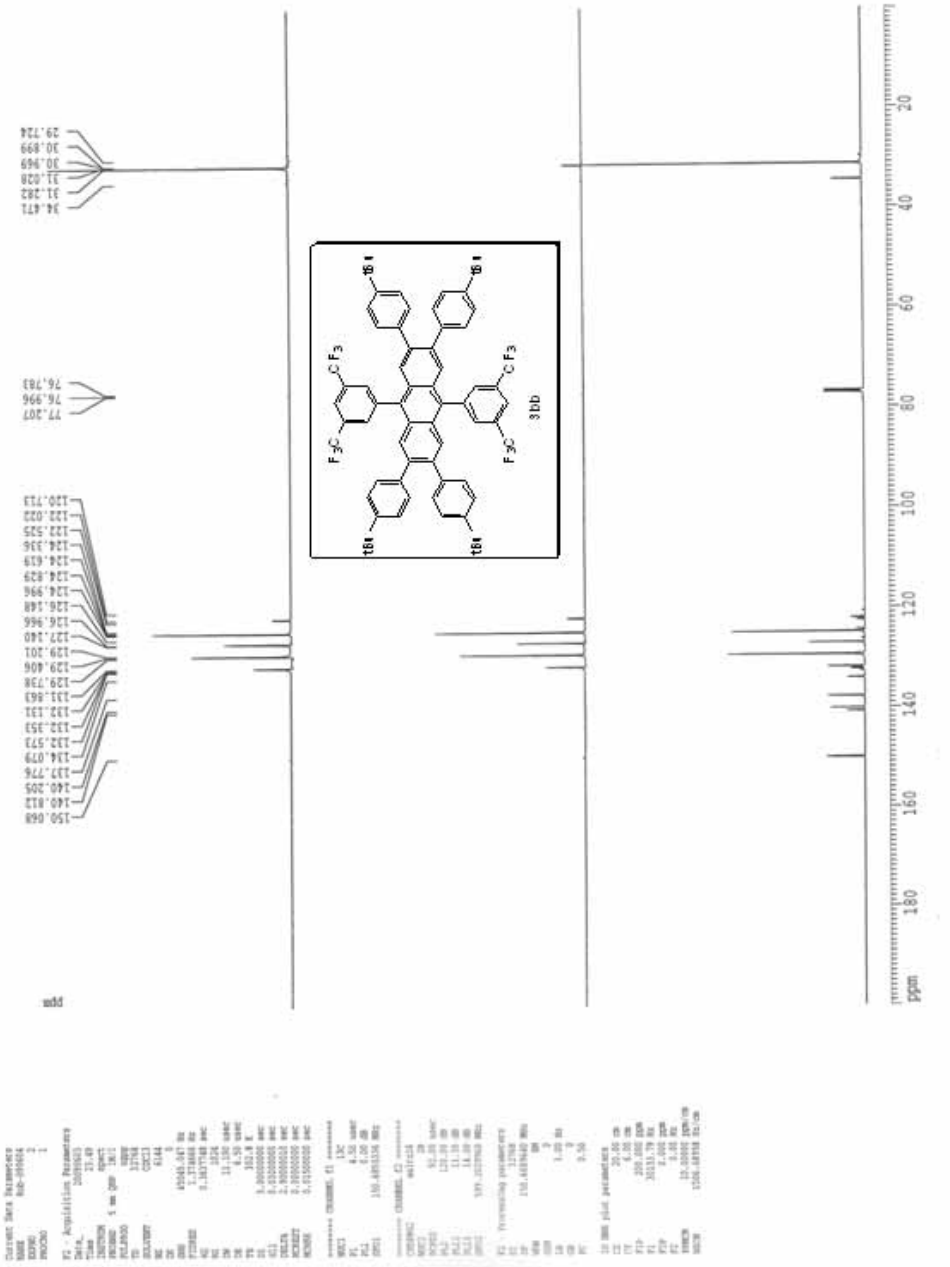
Compound **2bb**



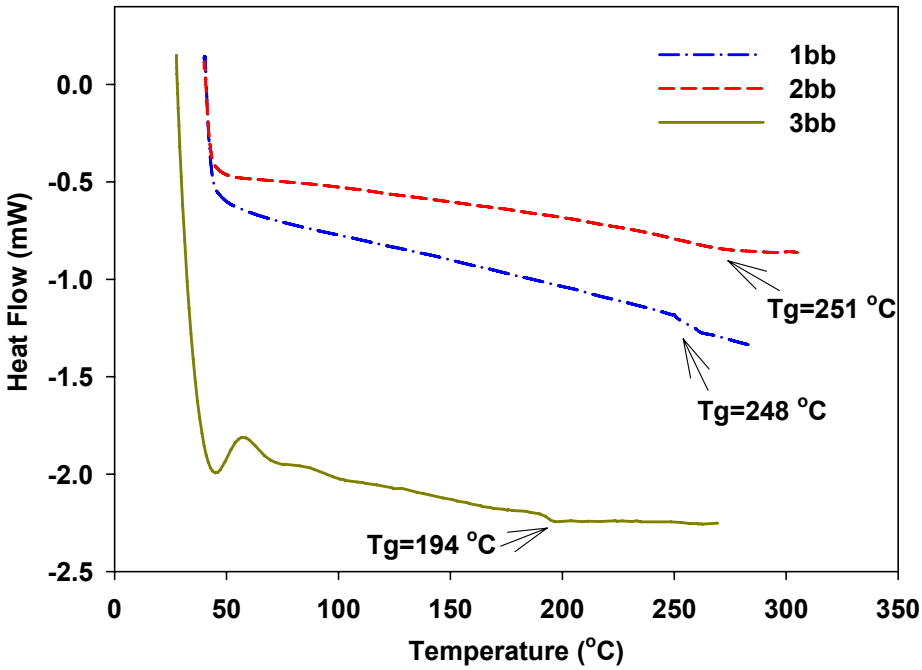
Compound **3bb**



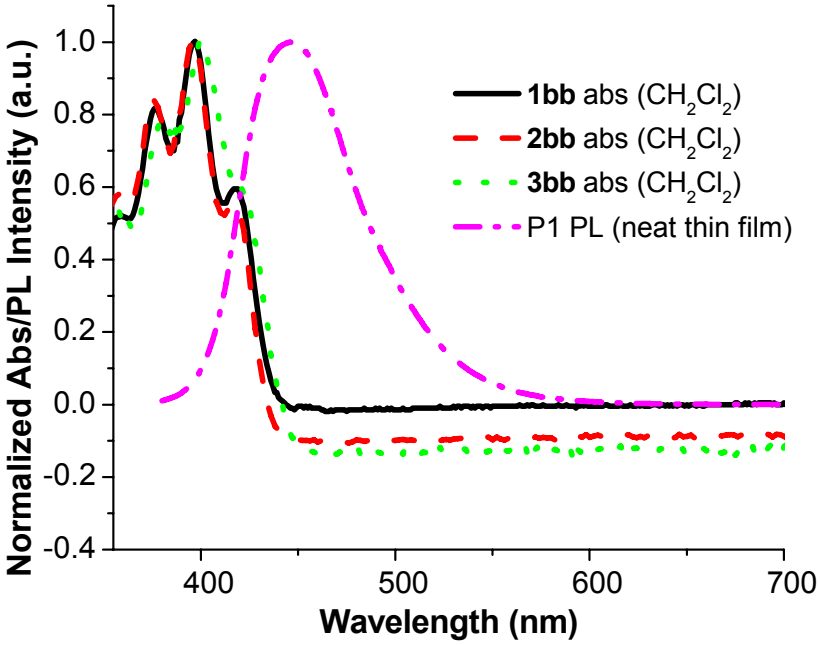
Compound **3bb**



C) DSC curve of **1bb**, **2bb** and **3bb.**



D) Figure S1. Absorption spectra of the **HPhAn** dopants in solution and the PL spectrum of DMPPP



i) As shown in this figure, the structured low energy absorption band and emission band of the **HPhAn** dopants at 350—440 nm and ca. 450 nm overlap well with the emission band of the DMPPP host efficient energy transfer from the DMPPP host to **HPhAn** dopants is expected.

ii) the EL spectra of the **HPhAn**-doped devices shown in Figs. 4 and 8 display a little vibrational structure similar to that observed in the **HPhAn** solution PL spectra (Fig. 2). Such vibrational structure can not be found in the DMPPP PL spectrum.

Based on i) and ii), it is clear that the EL peak of the doped device is originated from the **HPhAn** dopant.