Supporting Information

Stable, Solution-processed High-mobility Substituted Pentacene Semiconductors

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Single crystal X-ray diffraction data for 6,13-bis(4-pentylphenylethynyl)pentacene (3)

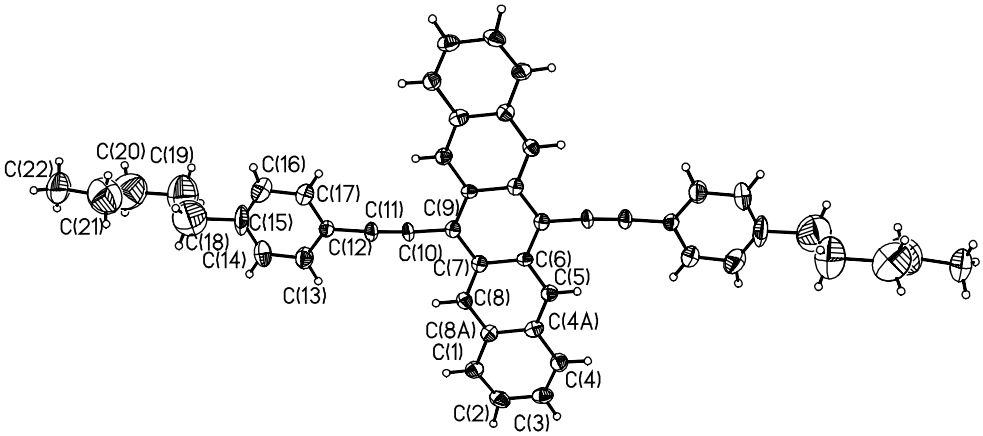

Table 1. Crystal data and structure refinement for *6,13-Bis(4-pentylphenylethynyl)pentacene (**3**)*.

Identification code	**3**	
Empirical formula	C48 H42	
Formula weight	618.82	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 16.867(14) Å	α= 90°.

	b = 5.225(4) Å	β= 98.257(19)°.
	c = 20.485(15) Å	γ = 90°.
Volume	1787(2) $Å^3$	
Z	2	
Density (calculated)	1.150 Mg/m^3	
Absorption coefficient	0.486 mm^{-1}	
F(000)	660	
Crystal size	0.50 x 0.04 x 0.01 mm^3	
θ range for data collection	2.65 to 68.20°.	
Index ranges	$-20 \leq h \leq 13$, $-5 \leq k \leq 5$, $-18 \leq l \leq 17$	
Reflections collected	5023	
Independent reflections	2373 [R(int) = 0.0534]	
Completeness to θ = 68.20°	72.5 %	
Absorption correction	Sadabs	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2373 / 144 / 233	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2σ(I)]	R1 = 0.1455, wR2 = 0.3440	
R indices (all data)	R1 = 0.2421, wR2 = 0.3894	
Largest diff. peak and hole	0.273 and -0.207 $e.Å^{-3}$	
Ratio of min. to max. apparent transmission	0.71	

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

	x	y	z	U(eq)
C(1)	15566(5)	11343(16)	3206(4)	59(2)
C(2)	16103(6)	13194(19)	3187(5)	65(3)
C(3)	16676(6)	13721(19)	3746(5)	61(3)
C(4A)	16134(4)	10378(15)	4356(4)	47(2)
C(4)	16693(4)	12372(15)	4301(4)	58(2)
C(5)	16119(5)	8950(15)	4914(5)	45(2)
C(6)	15573(4)	6997(14)	4975(4)	38(2)
C(7)	14981(4)	6463(14)	4397(4)	41(2)
C(8A)	15543(4)	9862(14)	3780(4)	45(2)
C(8)	15000(4)	7933(15)	3832(4)	47(2)
C(9)	14420(4)	4460(14)	4446(4)	39(2)
C(10)	13820(4)	3884(13)	3896(3)	41(2)
C(11)	13315(4)	3259(14)	3464(4)	46(2)
C(12)	12677(4)	2432(15)	2970(4)	45(2)
C(13)	12460(5)	3698(17)	2384(5)	73(3)
C(14)	11828(6)	2940(20)	1930(5)	100(4)
C(15)	11387(6)	930(30)	2052(7)	113(4)
C(16)	11596(7)	-460(30)	2620(8)	113(4)
C(17)	12239(5)	334(19)	3080(4)	84(3)
C(18)	10716(11)	-280(40)	1460(9)	220(8)
C(19)	10068(12)	260(40)	1580(9)	232(9)
C(20)	9194(12)	-470(40)	954(11)	239(10)
C(21)	9319(13)	-2310(40)	678(9)	227(9)
C(22)	8400(7)	-2640(30)	174(6)	163(5)

Table 3. Bond lengths [Å] and angles [°].

C(1)-C(2)	1.330(10)	C(4)-C(4A)-C(8A)	117.1(8)
C(1)-C(8A)	1.412(10)	C(3)-C(4)-C(4A)	121.5(8)
C(2)-C(3)	1.415(11)	C(4A)-C(5)-C(6)	124.6(8)
C(3)-C(4)	1.335(11)	C(5)-C(6)-C(9)#1	123.2(7)
C(4A)-C(5)	1.367(10)	C(5)-C(6)-C(7)	116.7(8)
C(4A)-C(4)	1.420(10)	C(9)#1-C(6)-C(7)	120.1(7)
C(4A)-C(8A)	1.458(10)	C(8)-C(7)-C(9)	123.9(7)
C(5)-C(6)	1.392(9)	C(8)-C(7)-C(6)	118.3(7)
C(6)-C(9)#1	1.407(9)	C(9)-C(7)-C(6)	117.8(7)
C(6)-C(7)	1.462(9)	C(8)-C(8A)-C(1)	124.3(7)
C(7)-C(8)	1.393(9)	C(8)-C(8A)-C(4A)	117.2(7)
C(7)-C(9)	1.424(9)	C(1)-C(8A)-C(4A)	118.4(7)
C(8A)-C(8)	1.377(9)	C(8A)-C(8)-C(7)	124.3(7)
C(9)-C(6)#1	1.407(9)	C(6)#1-C(9)-C(7)	122.1(7)
C(9)-C(10)	1.435(9)	C(6)#1-C(9)-C(10)	117.9(7)
C(10)-C(11)	1.182(8)	C(7)-C(9)-C(10)	120.0(7)
C(11)-C(12)	1.434(10)	C(11)-C(10)-C(9)	175.4(8)
C(12)-C(17)	1.359(10)	C(10)-C(11)-C(12)	176.6(8)
C(12)-C(13)	1.374(10)	C(17)-C(12)-C(13)	116.7(7)
C(13)-C(14)	1.369(11)	C(17)-C(12)-C(11)	119.9(8)
C(14)-C(15)	1.328(14)	C(13)-C(12)-C(11)	123.4(8)
C(15)-C(16)	1.376(17)	C(14)-C(13)-C(12)	122.6(9)
C(15)-C(18)	1.661(19)	C(15)-C(14)-C(13)	120.2(10)
C(16)-C(17)	1.394(14)	C(14)-C(15)-C(16)	119.7(11)
C(18)-C(19)	1.188(18)	C(14)-C(15)-C(18)	120.3(14)
C(19)-C(20)	1.85(2)	C(16)-C(15)-C(18)	118.7(14)
C(20)-C(21)	1.15(2)	C(15)-C(16)-C(17)	119.5(12)
C(21)-C(22)	1.74(2)	C(12)-C(17)-C(16)	121.2(11)
		C(19)-C(18)-C(15)	108.0(18)
C(2)-C(1)-C(8A)	121.5(8)	C(18)-C(19)-C(20)	118(2)
C(1)-C(2)-C(3)	120.5(9)	C(21)-C(20)-C(19)	109(2)
C(4)-C(3)-C(2)	121.0(10)	C(20)-C(21)-C(22)	99(2)
C(5)-C(4A)-C(4)	124.1(8)		
C(5)-C(4A)-C(8A)	118.9(8)		

Symmetry transformations used to generate

equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3). 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)	75(6)	44(6)	58(6)	8(5)	11(5)	-15(5)
C(2)	90(7)	56(6)	50(7)	15(5)	17(6)	0(5)
C(3)	72(6)	46(6)	69(8)	5(5)	26(6)	-7(5)
C(4A)	50(4)	31(5)	62(6)	1(5)	17(5)	3(4)
C(4)	67(5)	50(6)	54(6)	3(5)	3(4)	-8(5)
C(5)	49(5)	39(5)	48(6)	2(5)	6(5)	-2(4)
C(6)	42(4)	35(5)	39(5)	4(4)	11(4)	-2(4)
C(7)	42(4)	36(5)	45(5)	-5(4)	6(4)	5(4)
C(8A)	46(4)	35(5)	52(6)	4(4)	5(4)	4(4)
C(8)	52(5)	47(5)	41(5)	2(4)	3(4)	2(4)
C(9)	42(4)	34(5)	43(5)	-6(4)	6(4)	3(4)
C(10)	40(4)	46(5)	34(5)	-12(4)	-7(4)	2(4)
C(11)	43(4)	48(5)	45(5)	-18(4)	-1(4)	0(4)
C(12)	43(4)	49(5)	43(6)	-6(4)	5(4)	-5(4)
C(13)	65(5)	80(7)	69(7)	-1(6)	-8(5)	-5(5)
C(14)	89(7)	130(9)	71(7)	-8(7)	-25(6)	-13(7)
C(15)	81(7)	148(11)	97(9)	-50(8)	-31(7)	-22(7)
C(16)	101(8)	122(11)	114(10)	-21(9)	10(8)	-49(8)
C(17)	77(6)	99(7)	72(6)	-6(6)	0(5)	-33(6)
C(18)	152(12)	299(17)	214(15)	-34(13)	43(12)	18(13)
C(19)	189(14)	265(16)	223(15)	-18(13)	-34(13)	3(14)
C(20)	206(15)	240(17)	273(18)	-6(15)	41(14)	-7(14)
C(21)	252(17)	227(16)	203(15)	-20(13)	35(13)	7(14)
C(22)	119(8)	215(12)	141(9)	-2(10)	-35(8)	-43(9)

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

	x	y	z	U(eq)
H(1A)	15196	11017	2833	71
H(4A)	17079	12746	4659	69
H(8A)	14620	7590	3467	56
H(13A)	12753	5127	2292	87
H(14A)	11707	3826	1535	120
H(17A)	12370	-588	3469	100
H(18A)	10794	421	1036	264
H(18B)	10773	-2124	1444	264
H(19A)	10063	2088	1668	278
H(19B)	9992	-603	1985	278
H(20A)	8721	-700	1167	287
H(20B)	9096	938	645	287
H(21A)	9432	-3756	975	273
H(21B)	9756	-2094	422	273
H(22A)	8407	-4146	-92	245
H(22B)	8306	-1163	-106	245
H(22C)	7981	-2780	444	245
H(2A)	16150(30)	14370(110)	2840(30)	25(18)
H(3A)	16990(40)	15100(140)	3690(30)	50(20)
H(5A)	16490(40)	9300(120)	5260(30)	50(20)
H(16A)	11470(60)	-2000(200)	2780(50)	140(50)

Table 6. Torsion angles [°].

C(8A)-C(1)-C(2)-C(3)	0.4(12)
C(1)-C(2)-C(3)-C(4)	0.4(13)
C(2)-C(3)-C(4)-C(4A)	-0.7(12)
C(5)-C(4A)-C(4)-C(3)	-179.4(7)
C(8A)-C(4A)-C(4)-C(3)	0.2(10)
C(4)-C(4A)-C(5)-C(6)	179.8(6)
C(8A)-C(4A)-C(5)-C(6)	0.1(11)
C(4A)-C(5)-C(6)-C(9)#1	179.1(7)
C(4A)-C(5)-C(6)-C(7)	0.2(10)
C(5)-C(6)-C(7)-C(8)	-0.4(9)
C(9)#1-C(6)-C(7)-C(8)	-179.4(6)
C(5)-C(6)-C(7)-C(9)	179.5(6)
C(9)#1-C(6)-C(7)-C(9)	0.5(10)
C(2)-C(1)-C(8A)-C(8)	179.6(7)
C(2)-C(1)-C(8A)-C(4A)	-0.8(11)
C(5)-C(4A)-C(8A)-C(8)	-0.2(9)
C(4)-C(4A)-C(8A)-C(8)	-179.9(6)
C(5)-C(4A)-C(8A)-C(1)	-179.8(6)
C(4)-C(4A)-C(8A)-C(1)	0.5(9)
C(1)-C(8A)-C(8)-C(7)	179.6(7)
C(4A)-C(8A)-C(8)-C(7)	0.0(10)
C(9)-C(7)-C(8)-C(8A)	-179.6(6)
C(6)-C(7)-C(8)-C(8A)	0.3(10)
C(8)-C(7)-C(9)-C(6)#1	179.3(6)
C(6)-C(7)-C(9)-C(6)#1	-0.5(10)
C(8)-C(7)-C(9)-C(10)	-1.1(10)
C(6)-C(7)-C(9)-C(10)	179.1(6)
C(6)#1-C(9)-C(10)-C(11)	-12(9)
C(7)-C(9)-C(10)-C(11)	168(9)
C(9)-C(10)-C(11)-C(12)	33(19)
C(10)-C(11)-C(12)-C(17)	-27(12)
C(10)-C(11)-C(12)-C(13)	151(12)

C(17)-C(12)-C(13)-C(14)	0.9(12)
C(11)-C(12)-C(13)-C(14)	-177.3(7)
C(12)-C(13)-C(14)-C(15)	1.3(14)
C(13)-C(14)-C(15)-C(16)	-3.7(17)
C(13)-C(14)-C(15)-C(18)	-170.3(10)
C(14)-C(15)-C(16)-C(17)	3.8(19)
C(18)-C(15)-C(16)-C(17)	170.7(11)
C(13)-C(12)-C(17)-C(16)	-0.7(13)
C(11)-C(12)-C(17)-C(16)	177.6(9)
C(15)-C(16)-C(17)-C(12)	-1.6(17)
C(14)-C(15)-C(18)-C(19)	-108(2)
C(16)-C(15)-C(18)-C(19)	85(2)
C(15)-C(18)-C(19)-C(20)	172.4(14)
C(18)-C(19)-C(20)-C(21)	33(3)
C(19)-C(20)-C(21)-C(22)	176.5(12)

Symmetry transformations used to generate equivalent atoms:

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