Supplementary Material (ESI) for Journal of Materials Chemistry

High Mobility Organic Single Crystal Transistors Based on Soluble Triisopropylsilylethynyl Anthracene Derivatives

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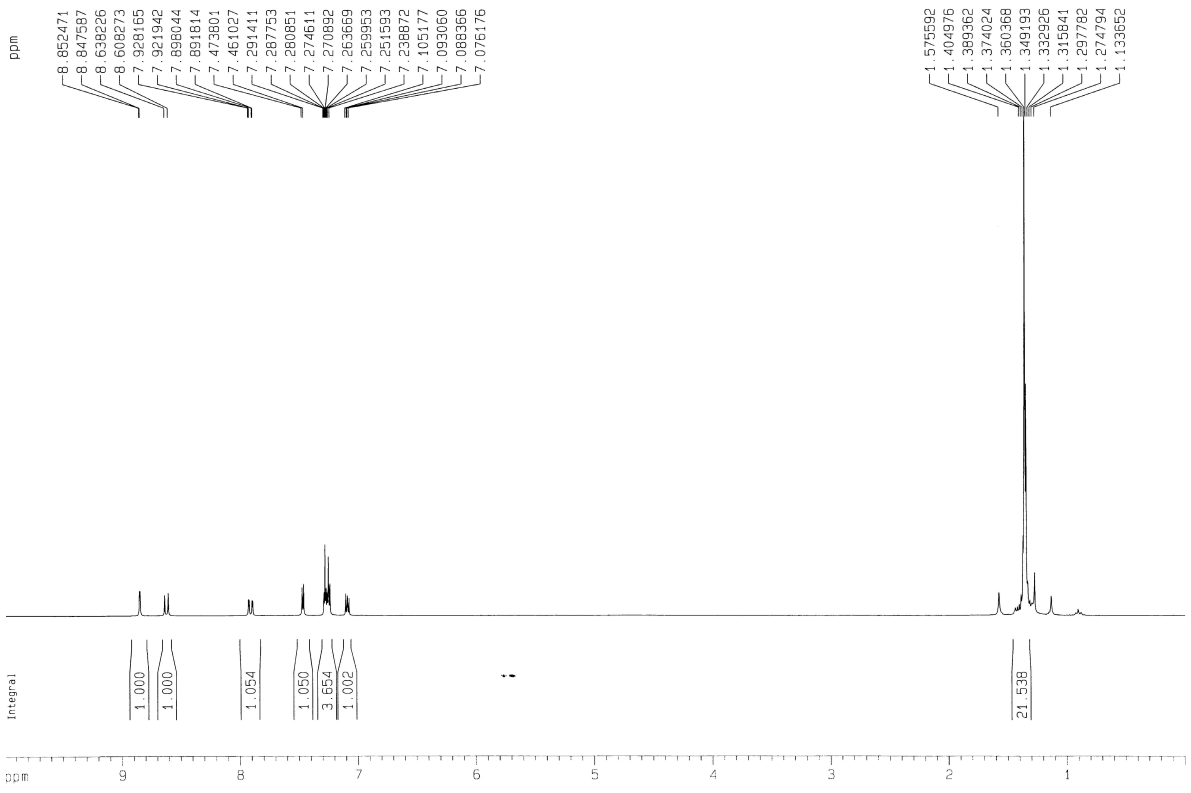
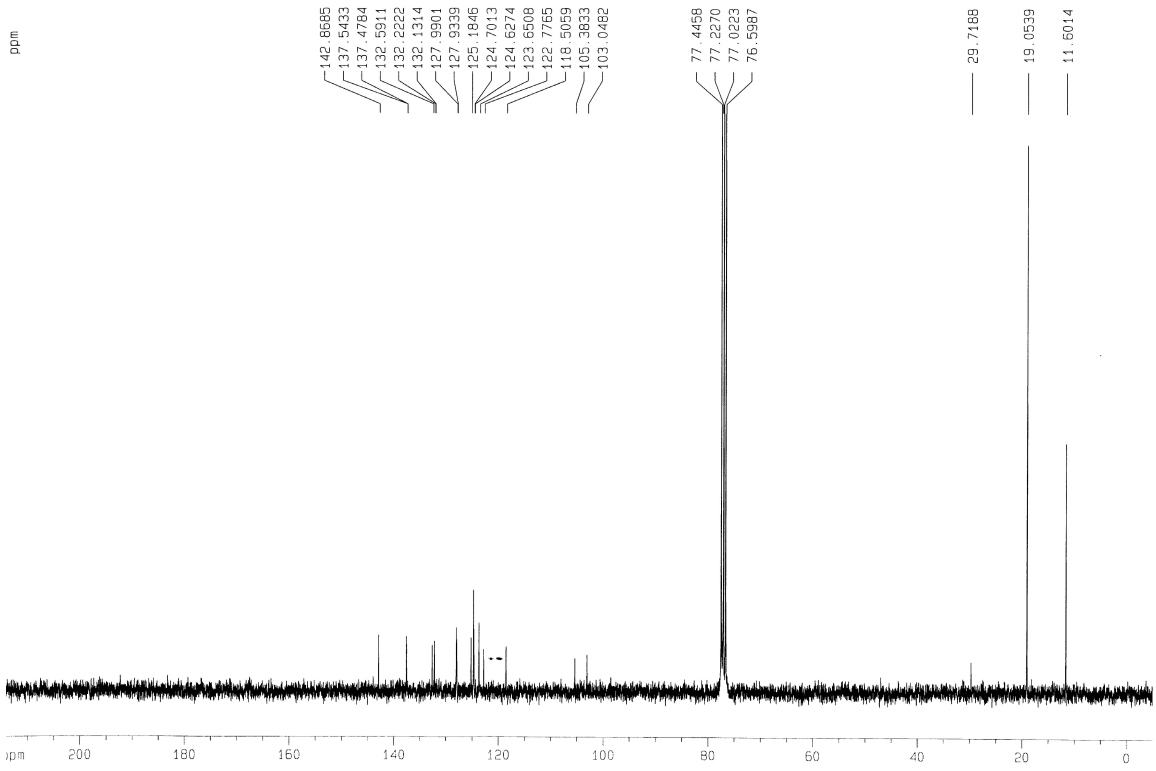
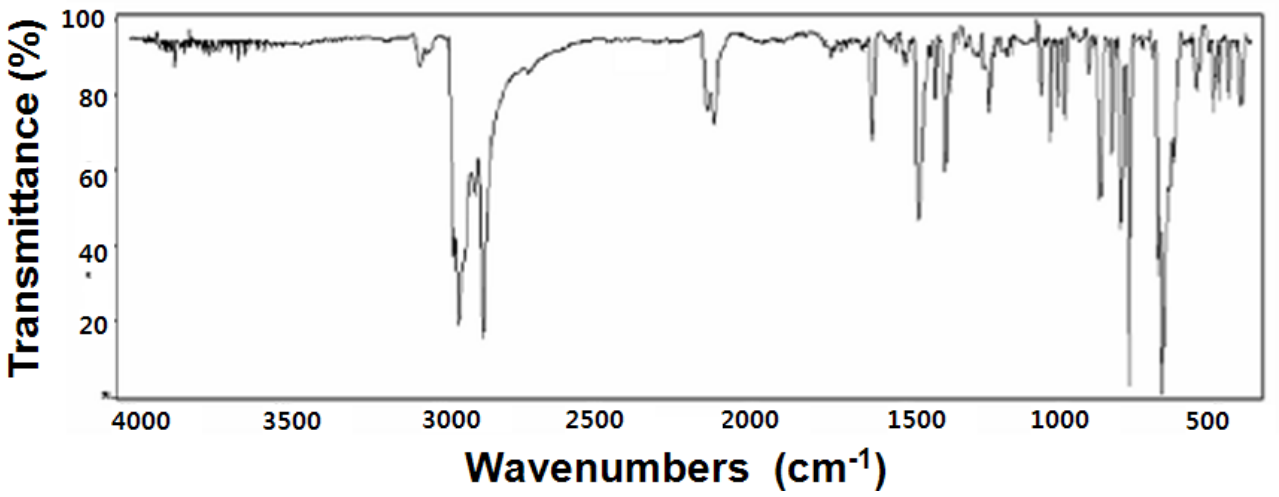


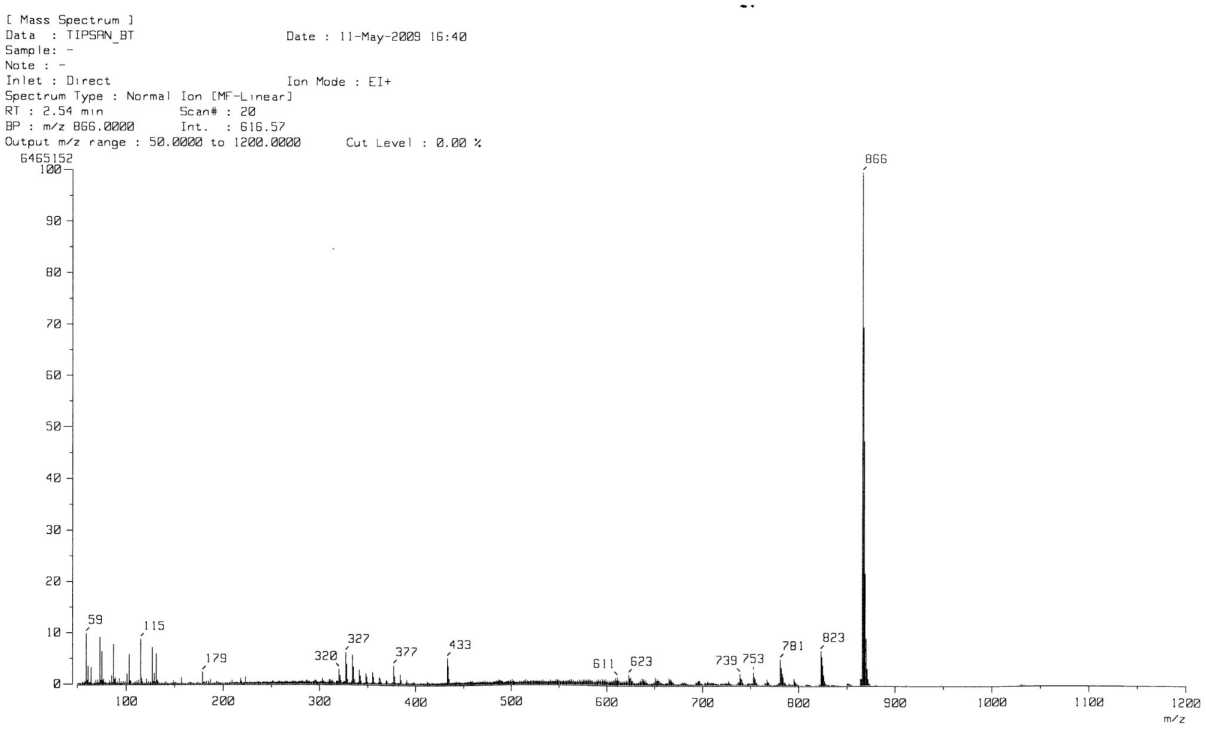
S 1. ^{1}H-NMR spectra of TIPSAntBT



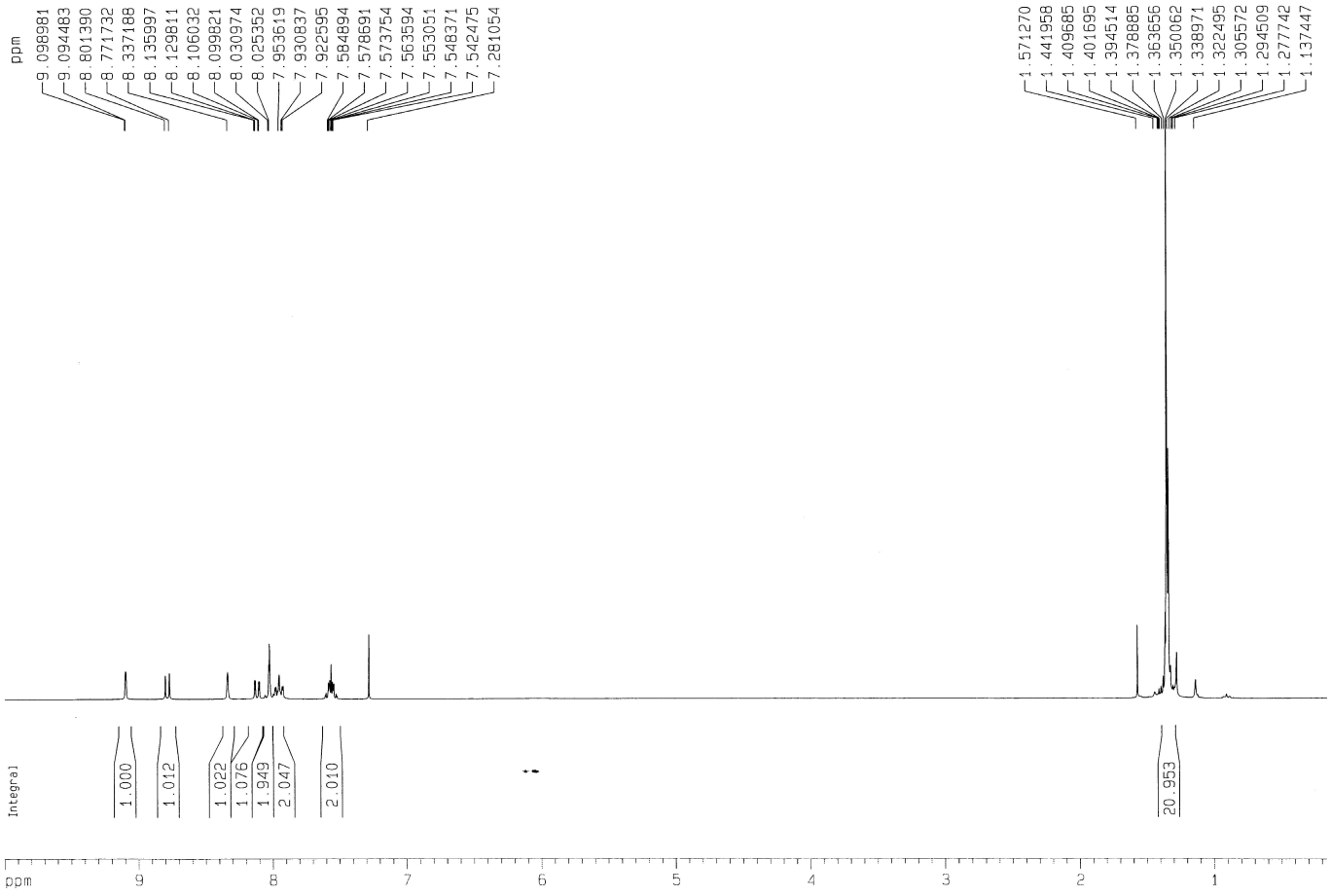
S 2. C-NMR spectra of TIPSAntBT



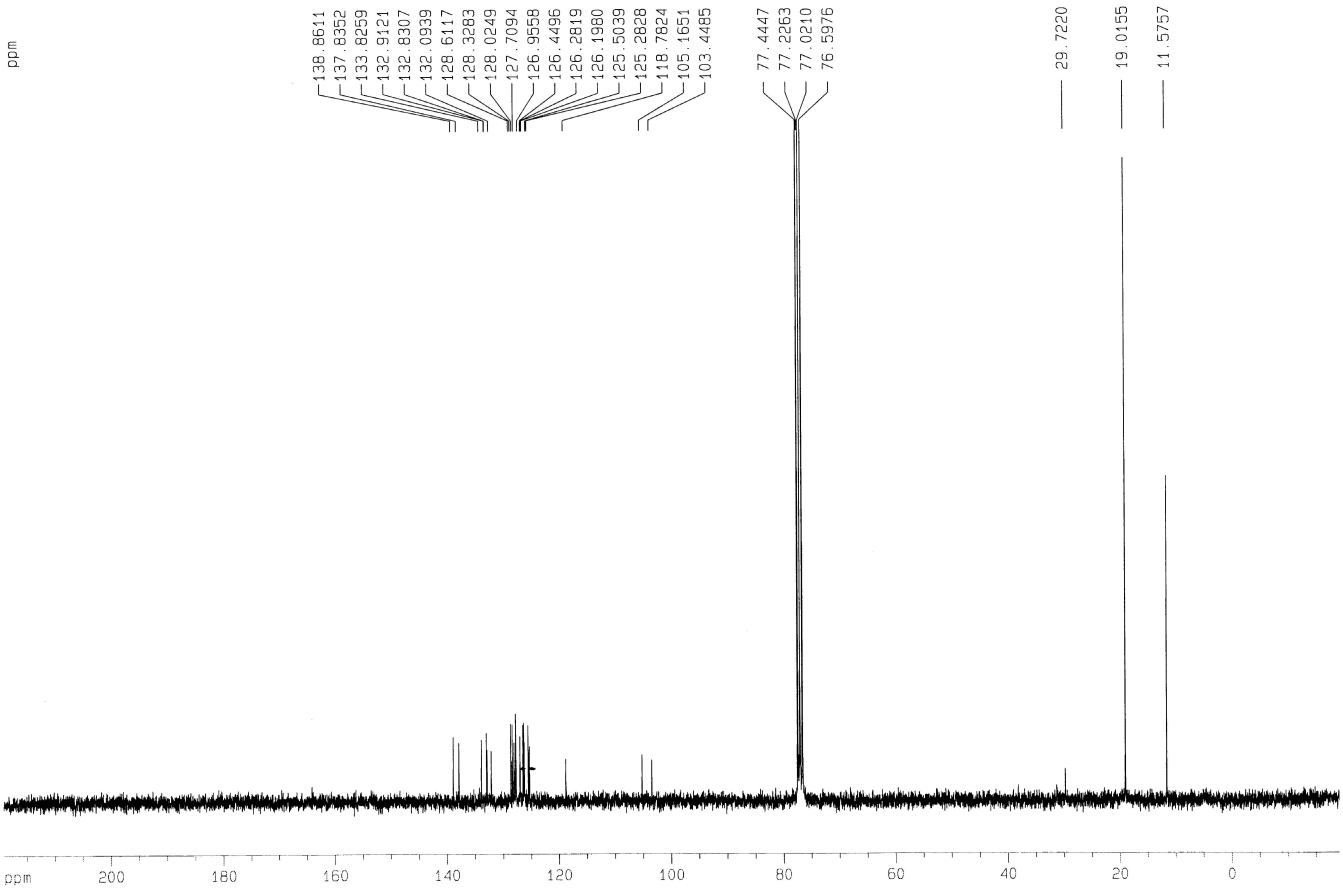
S 3. IR spectra of TIPSAntBT



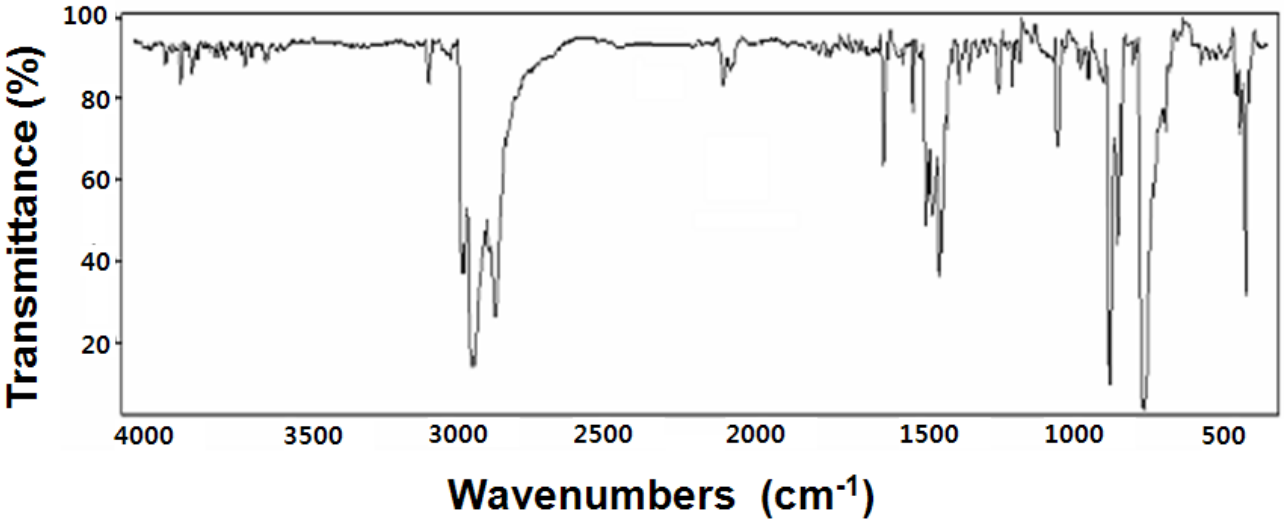
S 4. Mass spectra of TIPSAntBT



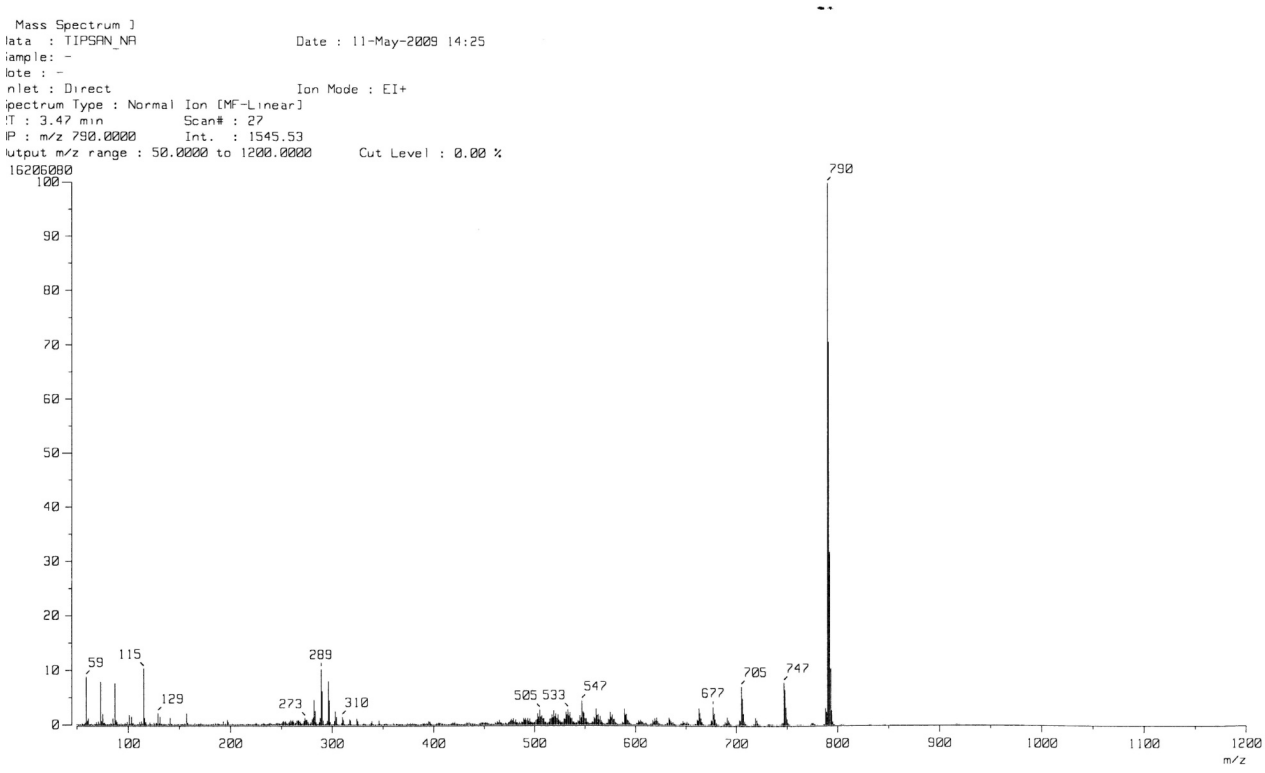
S 5. ^{1}H-NMR spectra of TIPSAntNa



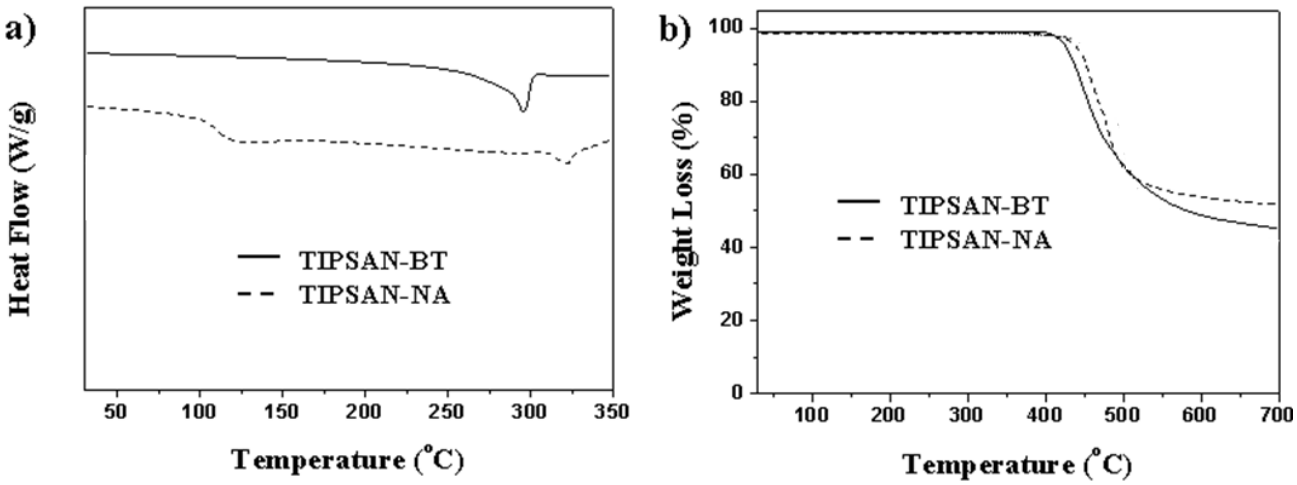
S 6. C-NMR spectra of TIPSAntNa



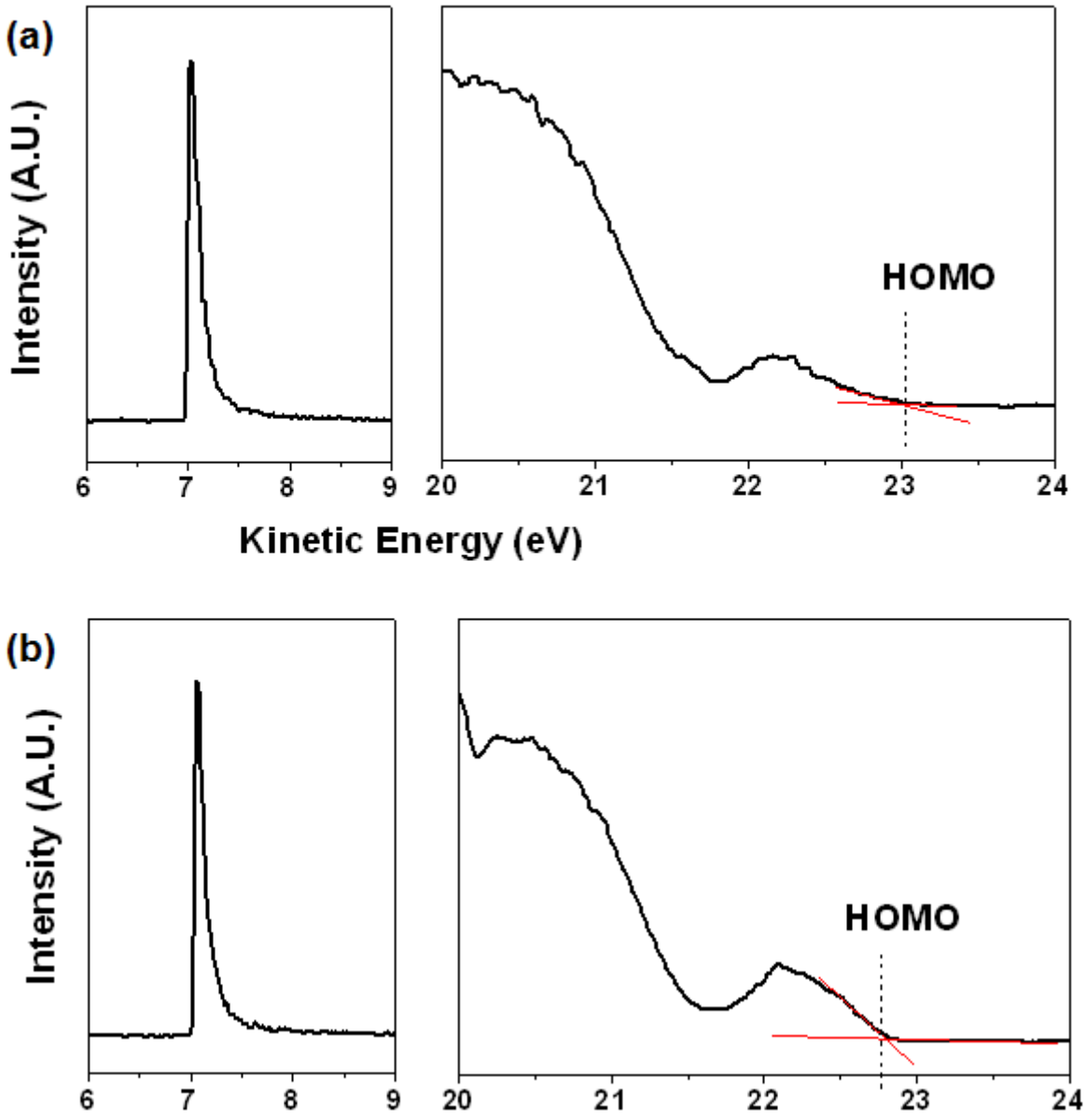
S 7. IR spectra of TIPSAntNa



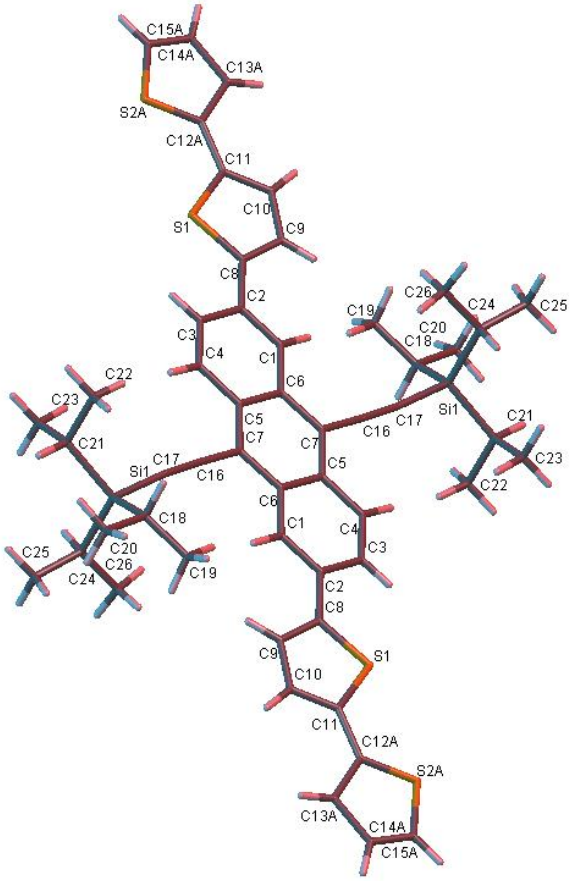
S 8. Mass spectra of TIPSAntNa



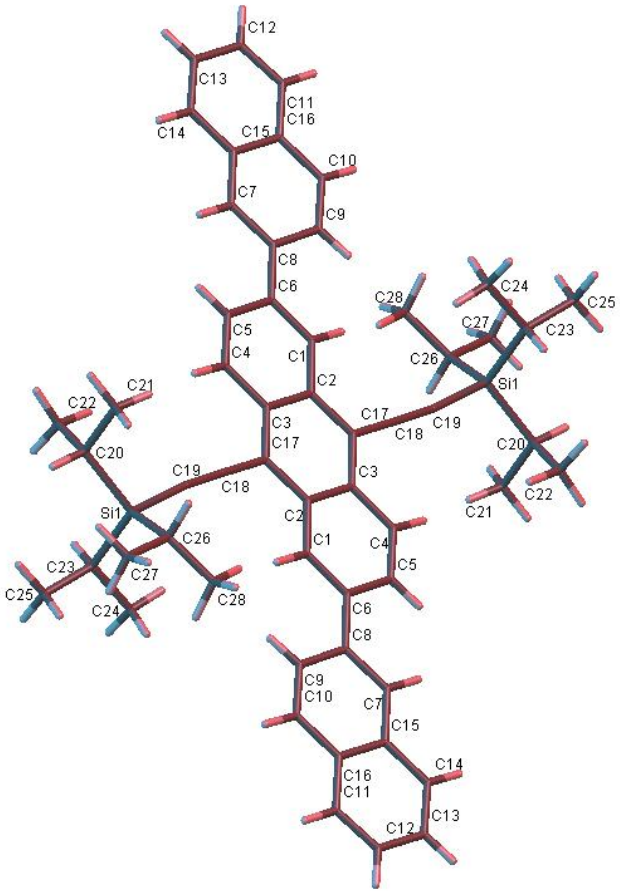
S 9. Thermal properties of the TIPSAntBT and TIPSAntNa: a) DSC curves. b) TGA thermograms.



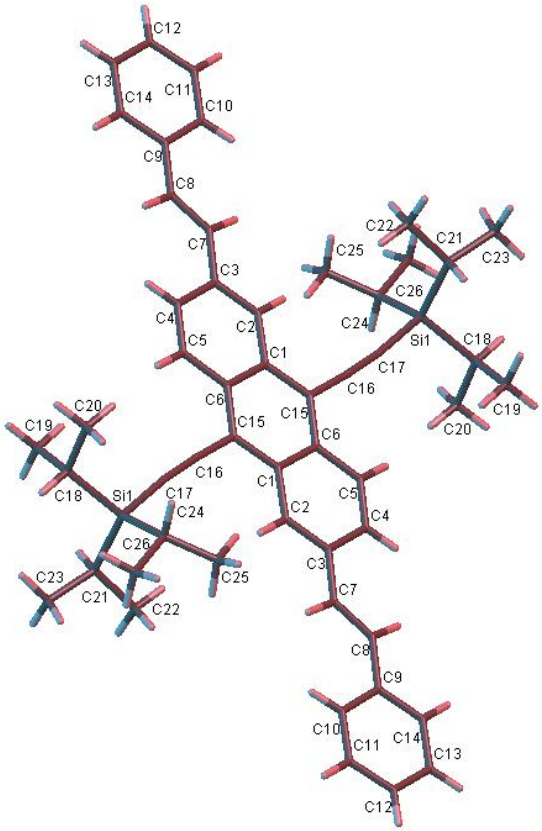
S 10. UPS energy distribution curves of TIPSAntBT (a) and TIPSAntNa (b).



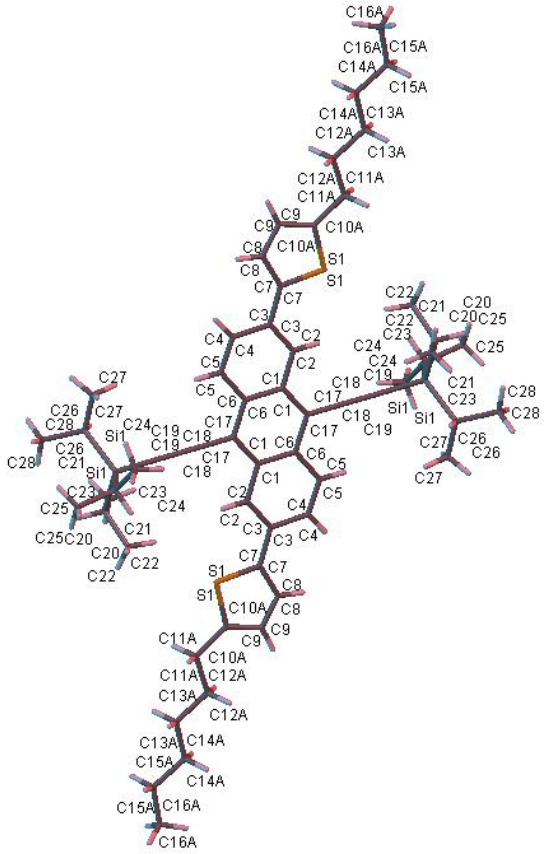
S 11. Labelled plots of TIPSAntBT (View along the crystallographic b axis)



S 12. Labelled plots of TIPSAntNa (View along the crystallographic b axis)



S 13. Labelled plots of TIPSAntPV (View along the crystallographic b axis)



S 14. Labelled plots of TIPSAntHT (View along the crystallographic b axis)

Identification code	TIPSAntBT	
Empirical formula	$Si_2C_{52}H_{58}S_4$	
Formula weight	867.40	
Temperature	100(2) K	
Wavelength	0.75000 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 8.2340(16) Å	α= 81.48(3)°.
	b = 11.958(2) Å	β= 85.50(3)°.
	c = 12.198(2) Å	γ = 87.63(3)°.
Volume	1183.6(4) $Å^3$	
Z	1	
Density (calculated)	1.217 Mg/m^3	
Absorption coefficient	0.286 mm^{-1}	
F(000)	462	
Crystal size	0.22 x 0.03 x 0.03 mm^3	
Theta range for data collection	2.73 to 26.00°.	
Index ranges	-9<=h<=9, -13<=k<=13, -14<=l<=14	
Reflections collected	7087	
Independent reflections	3595 [R(int) = 0.0347]	
Completeness to theta = 26.00°	90.8 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9915 and 0.9398	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3595 / 0 / 269	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0517, wR2 = 0.1513	
R indices (all data)	R1 = 0.0538, wR2 = 0.1540	
Largest diff. peak and hole	0.341 and -0.248 $e.Å^{-3}$	

S 15. Table of Crystallographic data for TIPSAntBT

Identification code	TIPSAntNa	
Empirical formula	$Si_2C_{56}H_{62}$	
Formula weight	791.24	
Temperature	100(2) K	
Wavelength	0.75000 Å	
Crystal system	Triclinic	
Space group	P $\bar{1}$	
Unit cell dimensions	a = 8.1903(16) Å	α= 78.37(3)°.
	b = 11.438(2) Å	β= 88.17(3)°.
	c = 12.144(2) Å	γ = 85.10(3)°.
Volume	1110.1(4) $Å^3$	
Z	1	
Density (calculated)	1.184 Mg/m^3	
Absorption coefficient	0.117 mm^{-1}	
F(000)	426	
Crystal size	0.22 x 0.05 x 0.05 mm^3	
Theta range for data collection	3.14 to 26.00.	
Index ranges	-9<=h<=9, -13<=k<=13, -14<=l<=14	
Reflections collected	5557	
Independent reflections	3408 [R(int) = 0.0377]	
Completeness to theta = 26.00°	91.3 %	
Absorption correction	Empirical	
Max. and min. transmission	0.9942 and 0.9746	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3408 / 0 / 268	
Goodness-of-fit on F^2	1.096	
Final R indices [I>2sigma(I)]	R1 = 0.0429, wR2 = 0.1104	
R indices (all data)	R1 = 0.0532, wR2 = 0.1359	
Largest diff. peak and hole	0.256 and -0.390 $e.Å^{-3}$	

S 16. Table of Crystallographic data for TIPSAntNa