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 TIPSAnNa
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 TIPSAnBT (a) and TIPSAnNa (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$_2$C$_{52}$H$_{58}$S$_4$
Formula weight  867.40
Temperature  100(2) K
Wavelength  0.75000 Å
Crystal system  Triclinic
Space group  P$ar{1}$
Unit cell dimensions  
  a = 8.2340(16) Å  \( \alpha = 81.48(3)^\circ \)
  b = 11.958(2) Å  \( \beta = 85.50(3)^\circ \)
  c = 12.198(2) Å  \( \gamma = 87.63(3)^\circ \)
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\( \leq h \leq 9 \), -13\( \leq k \leq 13 \), -14\( \leq l \leq 14 \)
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
Table of Crystallographic data for TIPSAntNa

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Identification code TIPSAntNa
Empirical formula Si$_2$C$_{56}$H$_{62}$
Formula weight 791.24
Temperature 100(2) K
Wavelength 0.75000 Å
Crystal system Triclinic
Space group $P \overline{1}$

Unit cell dimensions
\[a = 8.1903(16) \text{ Å} \quad \alpha = 78.37(3)^\circ,\]
\[b = 11.438(2) \text{ Å} \quad \beta = 88.17(3)^\circ,\]
\[c = 12.144(2) \text{ Å} \quad \gamma = 85.10(3)^\circ.\]

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$^{-3}$