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Supplementary materials for

Synthesis and characterization of amino-capped oligothiophene-based hole-transport materials

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Table 1. Crystal data and collection parameters for **DBAT1** and **-2**:

Compound	DBAT1	DBAT2
Formula	(C ₃₆ H ₅₀ N ₂ S)	(C ₄₀ H ₅₂ N ₂ S ₂)
Formula weight	542.84	624.96
Space group	P2 ₁ /n (#14)	P-1 (#2)
Temp	-116 °C	-116 °C
a (Å)	12.301(5)	12.0888(6)
b (Å)	16.426(6)	12.1517(7)
c (Å)	16.316(7)	12.8142
Volume (Å ³)	3256(2)	1792.92(16)
α (deg)	90	84.4140(10)
β (deg)	99.026(9)	73.1610(10)
γ (deg)	90	87.552(2)
Z	4	2
Dcalc (g/cm ³)	1.107	1.158
Diffractionmeter	Siemens SMART	Siemens SMART
Radiation	Mo-Kα	Mo-Kα
Monochromator	Graphite	Graphite
Detector	CCD area detector	CCD area detector
Scan type, deg	ω scans, 0.3	ω scans, 0.3
frame collection type (s)	30	30
reflections measured	hemisphere	hemisphere
2θ range (°)	3.5-55.0	3.5-55.0
μ (cm ⁻¹)	0.125	0.178
Tmin, Tmax	0.943, 0.956	0.924, 0.982
Crystal Dimensions (mm ⁻¹)	0.48 X 0.43 X 0.36	0.45 X 0.42 X 0.10
no. of reflections measured	18719	14383
no. of observations	7394	8224
no. of restraints	4	0
no. of parameters	347	391
R Int	0.0974	0.0659
R	0.0877 for 4536 data F ₀ > 4σ(F ₀); 0.1388 for all data	0.1022 for 3229 data F ₀ > 4σ(F ₀); 0.2211 for all data
wR2	0.2232 for 4536 data F ₀ > 4σ(F ₀); 0.2592 for all data	0.2708 for 3229 data F ₀ > 4σ(F ₀); 0.3438 for all data

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GOF	1.036	1.010
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Table 2. Selected Bond Distances and Angles for **DBAT1**

C9-C10	1.37	C27-C28	1.36	N1-C11	1.46
C8-C9	1.45	C26-C27	1.45	N1-C15	1.45
C7-C8	1.34	C25-C26	1.34	N2-C29	1.45
C4-C7	1.46	C22-C25	1.46	N2-C33	1.45
N1-C1	1.38	N2-C19	1.38	S1-C9	1.74
S1-C27	1.74	C25-C26-C27	125.70	C7-C8-C9	126.61
C4-C7-C8	125.69	C22-C25-C26	127.64	C9-S1-C27	92.23
C11-N1-C15	117.42	C29-N2-C33	117.26	C1-N1-C11	121.21

Table 3. Selected Bond Distances and Angles for **DBAT2**

N1-C1	1.37	N2-C21	1.37	S1-C12	1.73
S1-C9	1.74	S2-C29	1.74	S2-C32	1.71
C7-C8	1.36	C27-C28	1.35	C8-C9	1.43
C28-C29	1.43	C4-C7	1.44	C24-C27	1.45
S1-C9-C8	122.7	S2-C29-C28	121.5	C27-C28-C29	125.3
C7-C8-C9	126.7	C3-C4-C7	124.0	C23-C24-C27	123.9
C1-N1-C17	121.5	C1-N1-C13	120.4	C21-N2-C33	123.2
C21-N2-C37	120.2	C4-C7-C8	128.8	C24-C27-C28	128.3