Supporting Information for:

Easily-Soluble Heteroacene Bis(benzothieno)silole Derivatives for Nitro Explosives Sensing

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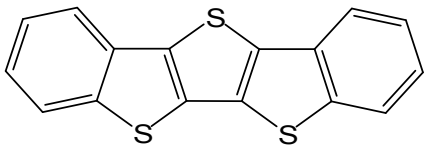

DBTDT

Scheme S1. Chemical structure of DBTDT.

Table S1, S2 and S3 gives the crystallographic data for the derivatives **4** and **6**.

Table S1. Crystal data and structure refinement parameters for **4** and **6**.

	BBTS-DM (4)	**BBTS-M (6)**
Molecular formula	C18 H14 S2 Si	C17H11S2Si
CCDC number	930047	930048
Molecular weight	322.5	307.46
a(Å)	22.468(2)	15.5429(17)
b(Å)	22.468(2)	13.1602(15)
c(Å)	13.1835(15)	7.4458(9)

α º)	90	90
β(º)	90	90
γ(º)	90	90
V(Å ^{3})	655.4(13)	1523.0(3)
Z	16	8
Dc(g.cm^{-3})	1.287	1.341
Crystal system	Tetragonal	Orthorhombic
space g oup	I4(1)/a	Cmc2(1)
Temperature (K)	296	296
Wavelength Mo-Kα(Å)	0.71073	0.71073
Crystal size(mm)	0.32*0.2 *0.20	0.31*0.27*0.23
μ(mm^{-1})	0.382	0.414
(000)	2688	636
Θlimit(º)	1.81~24.99	2.62~27.52
Index ranges hkl	-26<=h<=23	-10<=h<=20
	-23<=k<=25	-17<=k<=17
	-14<=l<=15	-5<=l<=9
Reflections collected	12466	2829
Independent reflections	2909	1222
Data/re traints/parameters	2909 / 0 / 192	1222 / 1 95
Goodness-of-fit on F^2	1.053	1.109
FinalRindices[I>2σ (I)]	R1 = 0.0468	R1 = 0.0342
	wR2 = 0.12 1	wR2 = 0.0969
R indices (all data)	R1 = 0.0647	R1 = 0.0375
	wR2 = 0.1369	wR2 = 0.1008
Largest diff peak and hole(e Å $^{-3}$)	0.431 and -0.409	0.450 and 0.224

Table S2: Selected bond lengths [Å] for compounds **BBTS-DM (4)**

Si1-C18	1.850(4)
Si1-C17	1.855(3)
Si1-C10	1.877(3)
Si1-C1	1.879(3)
S2-C8	1.727(3)

S2-C7	1.738(3)
S2-C12	1.693(5)
S2-C9	1.730(3)
C8-C1	1.362(4)
C8-C9	1.450(4)）
C1-C2	1.431(4)
C10-C9	1.367(4)
C10-C11	1.424(4)
C11-C16	1.393(5)
C11-C12	1.437(5)
C7-C6	1.388(5)
C7-C2	1.416(4)
C2-C3	1.399(4)
C3-C4	1.373(5)
C4-C5	1.371(6)
C12-C13	1.394(6)
C16-C15	1.391(6)
C13-C14	1.368(8)
C6-C5	1.370(6)

Table S3: Selected bond lengths [Å] for compounds **BBTS-DM (6)**

Si1-C10	1.836(5)
Si1-C3	1.864(3)
S1-C1	1.725(2)
S1-C4	1.741(3)
C1-C3	1.369(3)
C1-C1A	1.465(5)
C2-C6	1.388(4)
C2-C7	1.402(4)
C3-C7	1.434(4)
C4-C5	1.395(3)
C4-C7	1.418(3)
C5-C8	1.377(5)
C6-C8	1.394(4)