



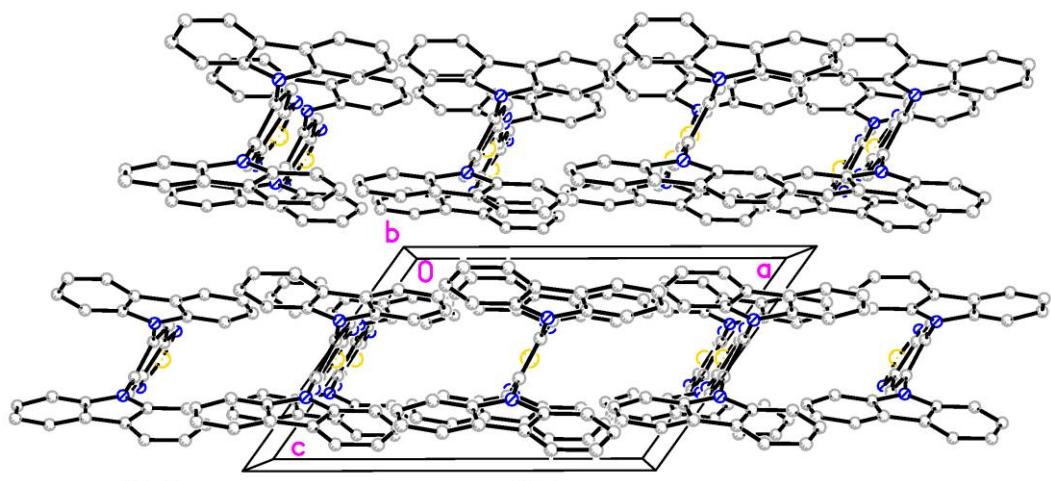
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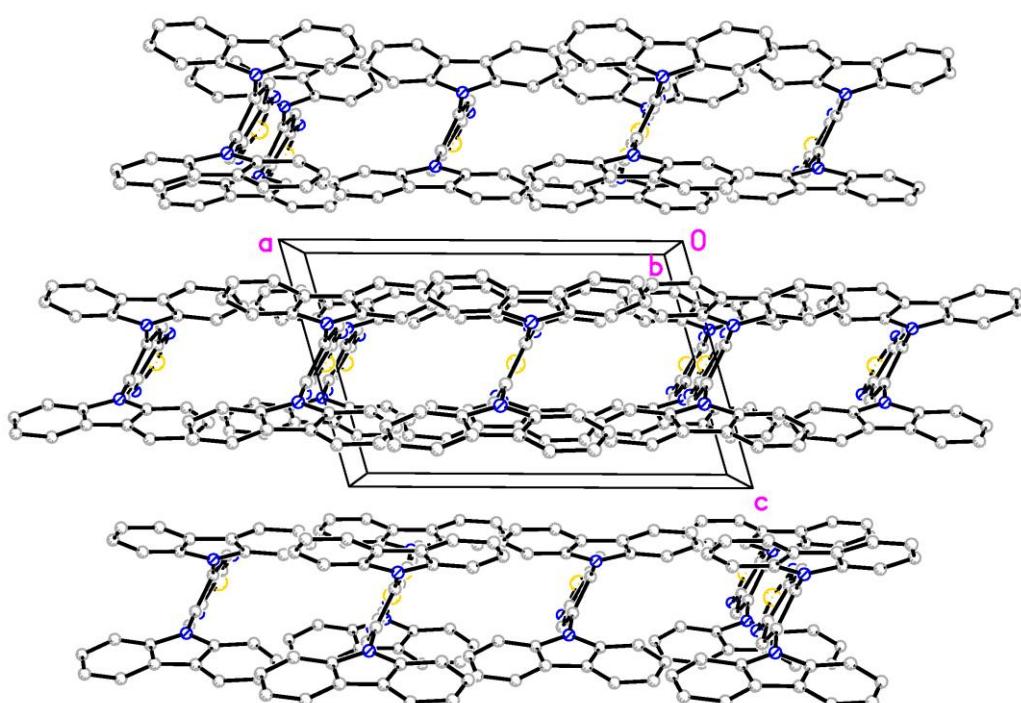
**Supporting information for article:**

**Crystal structure of 5,6-bis(9*H*-carbazol-9-yl)benzo[*c*][1,2,5]thiadiazole:  
distortion from a hypothetical higher-symmetry structure**

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**Structure 1**



**Structure 2**

**Fig. S1. Molecular packing of DCBT in two hypothetical crystal structures with the *C*2 space group.**

Table S1. Geometrical parameters ( $\text{\AA}$ ) for benzothiadiazole fragments. Topologically equivalent bonds are placed in the same cells.

Bond	(I)	(Ia), molecule A	(Ia), molecule B	B3LYP	M06	CSD (23 hits)	benzothiadiazole
S1-N1	1.616(2)	1.616(1)	1.607(2)	1.641	1.628	1.615	1.619, 1.614
S1-N2	1.614(2)	1.616(1)	1.616(2)				
N1-C1	1.347(2)	1.348(2)	1.351(2)	1.336	1.331	1.351	1.351, 1.347
N2-C2	1.350(2)	1.349(2)	1.351(2)				
C1-C2	1.433(2)	1.428(2)	1.422(2)	1.444	1.438	1.434	1.442
C1-C6	1.421(2)	1.411(2)	1.413(2)	1.418	1.416	1.415	1.417, 1.416
C2-C3	1.417(2)	1.416(2)	1.418(2)				
C3-C4	1.366(2)	1.371(2)	1.368(2)	1.373	1.365	1.365	1.371, 1.366
C5-C6	1.363(2)	1.363(2)	1.369(2)				
C4-C5	1.452(2)	1.450(2)	1.445(2)	1.457	1.453	1.444	1.427
N3-C5	1.415(2)	1.418(2)	1.414(2)	1.416	1.409		
N4-C4	1.415(2)	1.411(2)	1.417(2)				

Table S2. Geometrical parameters ( $\text{\AA}$ ) for carbazole fragments. Topologically equivalent bonds are placed in the same cells.

Bond	(I)	(Ia), molecule A	(Ia), molecule A	B3LYP	M06	CSD (304 hits)	Carbazole
N(3)-C(7)	1.397(2)	1.393(2)	1.400(2)	1.404	1.396	1.395	1.384
N(3)-C(18)	1.396(2)	1.402(2)	1.404(2)	1.404	1.398		
N(4)-C(19)	1.396(2)	1.404(2)	1.399(2)	1.404	1.396		
N(4)-C(30)	1.396(2)	1.406(2)	1.398(2)	1.404	1.398		
C(7)-C(8)	1.389(2)	1.382(2)	1.390(2)	1.393	1.387	1.387	1.395
C(17)-C(18)	1.390(2)	1.391(2)	1.393(2)	1.395	1.388		
C(19)-C(20)	1.389(2)	1.389(2)	1.392(2)	1.395	1.388		
C(29)-C(30)	1.392(2)	1.388(2)	1.391(2)	1.393	1.387		
C(8)-C(9)	1.390(3)	1.395(2)	1.388(2)	1.391	1.385	1.381	1.385
C(16)-C(17)	1.394(3)	1.388(2)	1.387(2)	1.392	1.386		
C(20)-C(21)	1.386(3)	1.389(2)	1.389(2)	1.392	1.386		
C(28)-C(29)	1.390(2)	1.388(2)	1.384(2)	1.391	1.385		
C(9)-C(10)	1.394(3)	1.402(4)	1.397(2)	1.402	1.397	1.390	1.401
C(15)-C(16)	1.397(3)	1.388(3)	1.392(3)	1.402	1.397		
C(21)-C(22)	1.401(3)	1.396(2)	1.394(2)	1.402	1.397		
C(27)-C(28)	1.404(3)	1.398(2)	1.395(3)	1.402	1.397		
C(10)-C(11)	1.386(3)	1.362(4)	1.378(3)	1.389	1.384	1.374	1.383
C(14)-C(15)	1.381(3)	1.377(3)	1.378(3)	1.390	1.384		
C(22)-C(23)	1.389(3)	1.376(2)	1.381(2)	1.390	1.384		
C(26)-C(27)	1.384(3)	1.382(2)	1.382(2)	1.389	1.384		
C(11)-C(12)	1.400(2)	1.399(2)	1.395(2)	1.397	1.392	1.394	1.397
C(13)-C(14)	1.400(2)	1.410(2)	1.406(2)	1.414	1.391		
C(23)-C(24)	1.400(2)	1.393(2)	1.394(2)	1.397	1.391		
C(25)-C(26)	1.402(2)	1.393(2)	1.395(2)	1.397	1.392		
C(7)-C(12)	1.412(2)	1.414(2)	1.409(2)	1.415	1.406	1.406	1.415
C(18)-C(13)	1.411(2)	1.408(2)	1.404(2)	1.397	1.407		
C(19)-C(24)	1.412(2)	1.408(2)	1.411(2)	1.414	1.407		
C(30)-C(25)	1.408(2)	1.403(2)	1.405(2)	1.415	1.406		
C(12)-C(13)	1.446(2)	1.440(3)	1.445(2)	1.447	1.442	1.441	1.453
C(24)-C(25)	1.443(2)	1.439(2)	1.440(2)	1.447	1.442		