

Electronic Supplementary Information for:

**A conjugated polymer based on 5,5'-bibenzo[c][1,2,5]thiadiazole for  
high-performance solar cells<sup>†</sup>**

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BBT dibromide could have four possible isomers: 4,7-dibromo (**4**), 7,7'-dibromo (**4a**), 4,4'-dibromo (**4b**), 4,7'-dibromo (**4c**) isomer (Fig. S1). The <sup>1</sup>H NMR spectrum of the isolated compound clearly demonstrates that its chemical structure is **4** other than **4a-c**. The <sup>1</sup>H NMR spectrum of **4** shows one singlet peak (H<sub>6</sub>) and one doublet-doublet peak (H<sub>6</sub>') (Fig. S3). **4** should have two more doublet-doublet peaks (H<sub>4</sub>' and H<sub>7</sub>'), which are not resolved due to overlap of H<sub>4</sub>'/H<sub>7</sub>' peaks. If the chemical structure were **4a**, there should be two doublet peaks (H<sub>4</sub>/H<sub>6</sub> and H<sub>4</sub>'/H<sub>6</sub>', *J* (H<sub>4</sub>-H<sub>6</sub>) ~ 1.7 Hz). If the chemical structure were **4b**, there should be two doublet peaks (H<sub>6</sub>/H<sub>7</sub> and H<sub>6</sub>'/H<sub>7</sub>', *J* (H<sub>6</sub>-H<sub>7</sub>) ~ 8.9 Hz). If the chemical structure were **4c**, there should be two doublet peaks (H<sub>4</sub>' and H<sub>6</sub>', *J* (H<sub>4</sub>'-H<sub>6</sub>') ~ 1.7 Hz) and two doublet peaks (H<sub>6</sub> and H<sub>7</sub>, *J* (H<sub>6</sub>-H<sub>7</sub>) ~ 8.9 Hz).

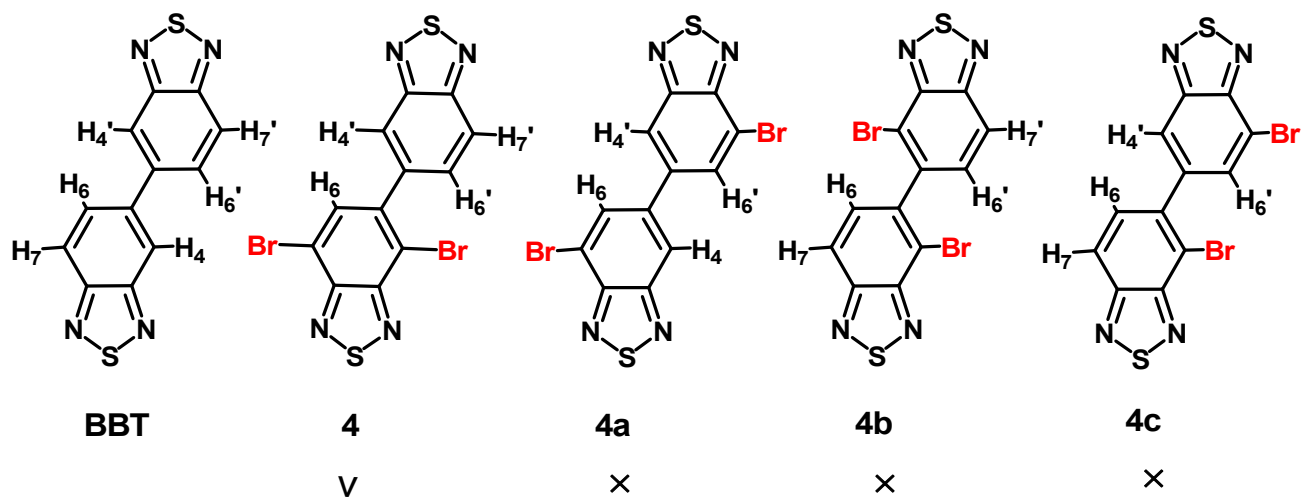


Fig. S1 Possible 4 isomers of BBT dibromide.

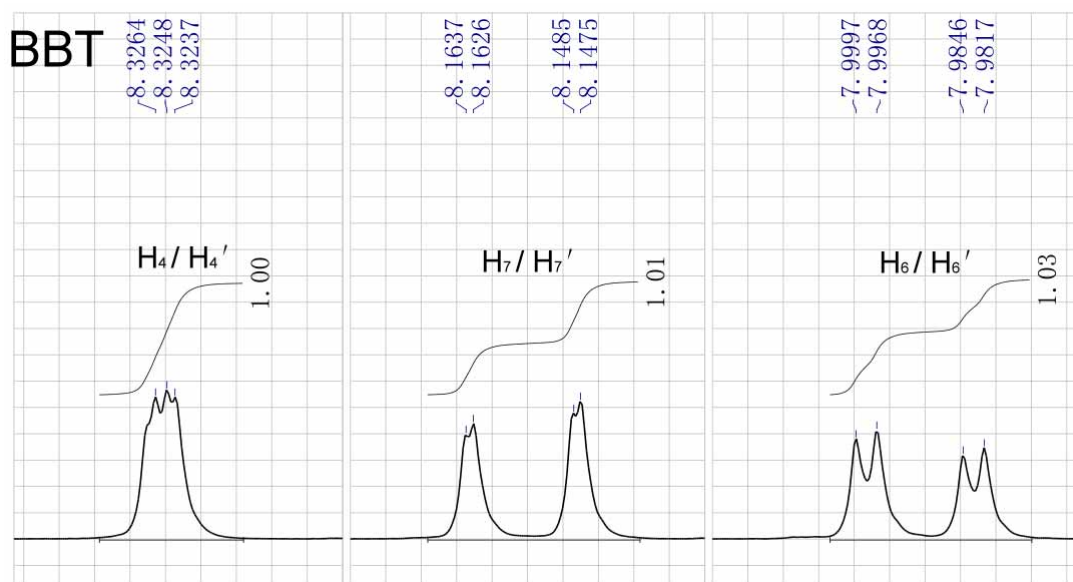
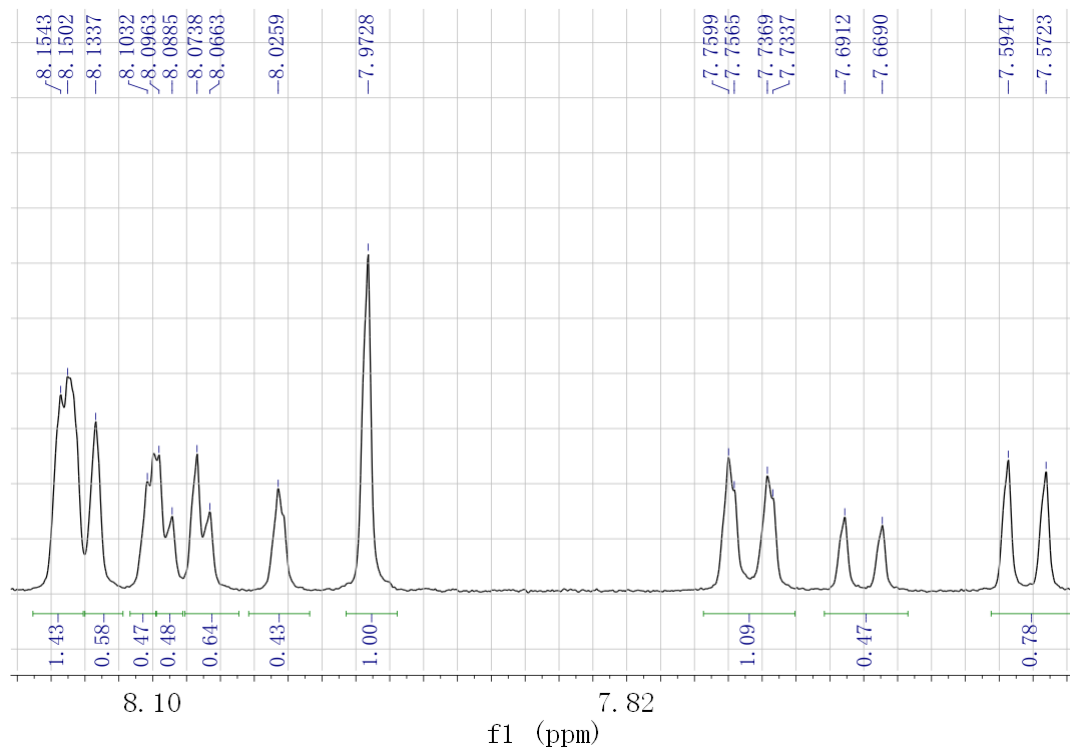
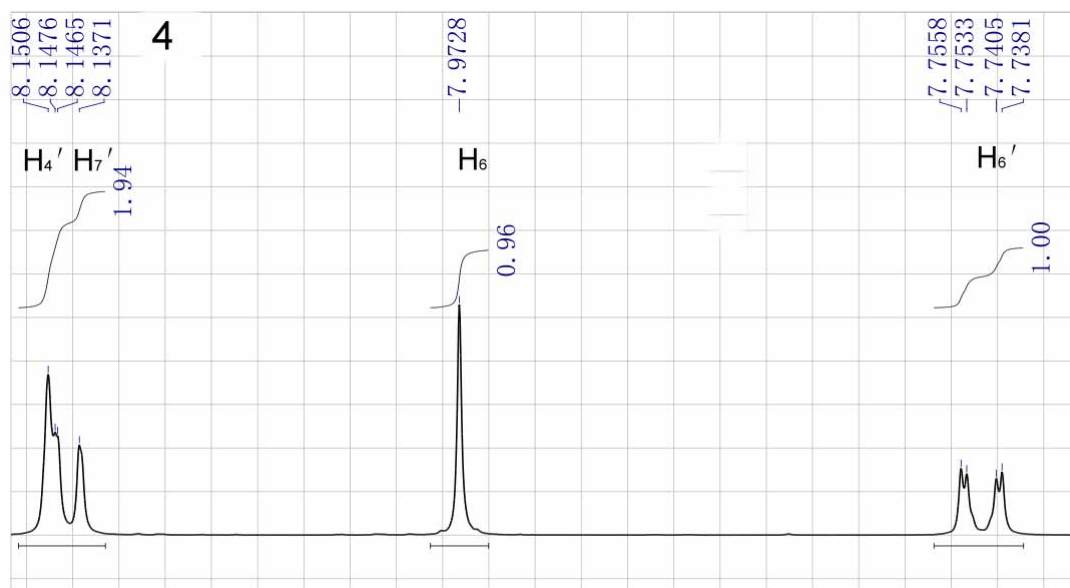


Fig. S2  $^1\text{H}$  NMR of **BBT**.  $J(H_6-H_7) = 9.1$  Hz,  $J(H_4-H_6) = 1.7$  Hz,  $J(H_4-H_7) = 0.7$  Hz.



**Fig. S3**  $^1\text{H}$  NMR of **BBT** dibromide isomers mixture.



**Fig. S4**  $^1\text{H}$  NMR of **4**.  $J(\text{H}_6'-\text{H}_7') = 9.1$  Hz,  $J(\text{H}_4'-\text{H}_6') = 1.5$  Hz, can not calculate  $J(\text{H}_4'-\text{H}_7')$  due to overlap of  $\text{H}_4'/\text{H}_7'$  peaks.