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### Preparation and Determination of 4,8-Diethylbenzo-[1,2-*d*]:4,5-*d*]bis[1,2,3]trithiole Dication [DEBBT(2)]

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## Preparation and Determination of 4,8-Diethylbenzo-[1,2-*d*:4,5-*d'*]bis[1,2,3]trithiole Dication [DEBBT(2+)]

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*Preparation and detection of DEBBT(2+)-S and DEBBT(2+)-T are reported.*

**Keywords** Dication; trithiole

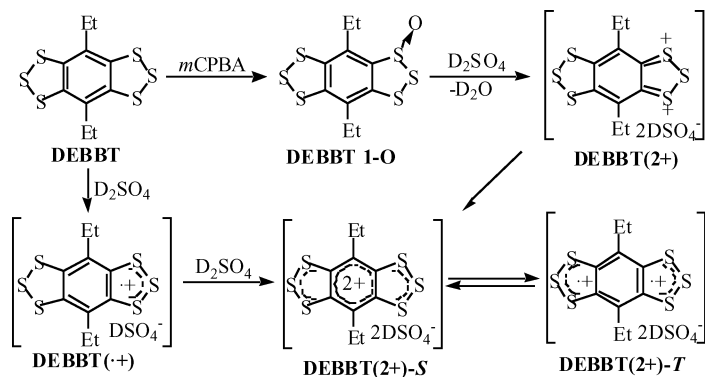
## RESULTS AND DISCUSSION

DEBBT was oxidized with  $D_2SO_4$ , leading to the generation of radical cation DEBBT( $\cdot+$ ) which was further oxidized to produce a singlet-state dication DEBBT(2+)-S. DEBBT(2+)-S was also prepared by treating DEBBT 1-O with  $D_2SO_4$  via DEBBT(2+) and was verified by  $^1H$  and  $^{13}C$ -NMR. These results reveal that the positive charges, initially generated on one trithiole ring, delocalize to the whole molecule by  $\pi$ -conjugation.

The ESR signal of the dication generated from DEBBT 1-O was observed in the  $D_2SO_4$  solution, which implies that DEBBT(2+)-S partially isomerizes to the triplet-state dication DEBBT(2+)-T, and that two molecules of DEBBT(2+)-T further form a spin pair at one trithiole ring with sufficient distance between two radical centers. The oxidation of DEBBT with two equivalents of  $NOPF_6$  produced the dication, which was isolated into a stable form. However, the dication is silent for NMR in  $CD_3CN$ , while ESR is active, suggesting that the dication produced by this procedure is DEBBT(2+)-T. MO calculation shows that

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DEBBT(2+)-S is more stable than DEBBT(2+)-T. It appears that their electronic states are strongly affected by the solvent.

## REFERENCE

- [1] T. Kimura, T. Sasaki, H. Yamaki, E. Suzuki, and S. Niizuma, *Eur J. Org. Chem.*, 4902 (2003).