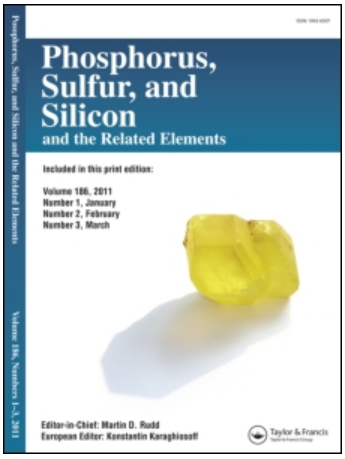

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Preparation and Determination of 4,8-Diethylbenzo-[1,2-d :4,5-d ']bis[1,2,3]trithiole Dication [DEBBT(2)]

Takeshi Kimura[a]; Takashi Sasaki[a]; Hiroaki Yamaki[a]; Eiichi Suzuki[a]
[a] Center for Instrumental Analysis and Department of Chemical Engineering, Iwate University, Morioka, Iwate, Japan

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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+)]

Takeshi Kimura
Takashi Sasaki
Hiroaki Yamaki
Eiichi Suzuki
Center for Instrumental Analysis and Department of Chemical Engineering, Iwate University, Morioka, Iwate, Japan

*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(·+) 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 ^{1}H and ^{13}C-NMR. These results reveal that the positive charges, initially generated on one trithiole ring, delocalize to the whole molecule by π-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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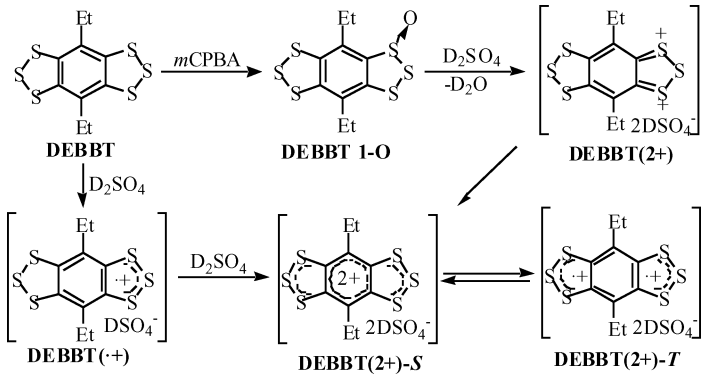
Address correspondence to Takeshi Kimura, Center for Instrumental Analysis and Department of Chemical Engineering, Iwate University, Morioka, Iwate 020-8551, Japan. E-mail: kimura@iwate-u.ac.jp



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

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