Electronic Supplementary Material (ESI) for New Journal of Chemistry.

EPR spectroscopy study of di-o-quinone bridged with π-extended TTF: redox behavior and binding modes as a ligand.

Nikolay O. Chalkov, Vladimir K. Cherkasov, Gleb A. Abakumov, Andrey G. Starikov and Viacheslav A. Kuropatov

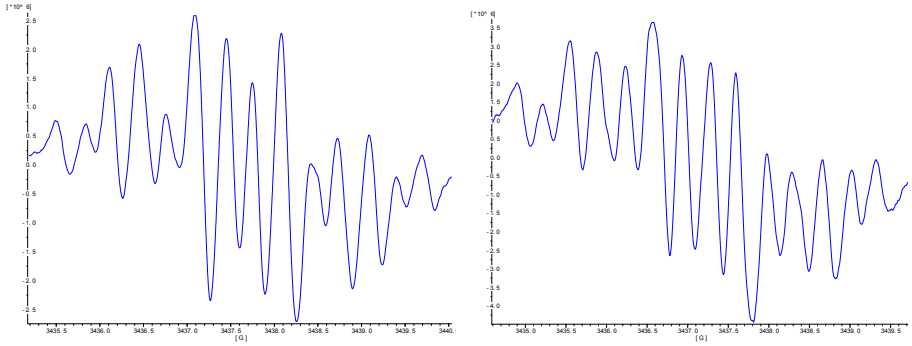

Figure S1. EPR spectrum of **1a** (left) and **1c** (M=Na) (right) in THF, 298 K

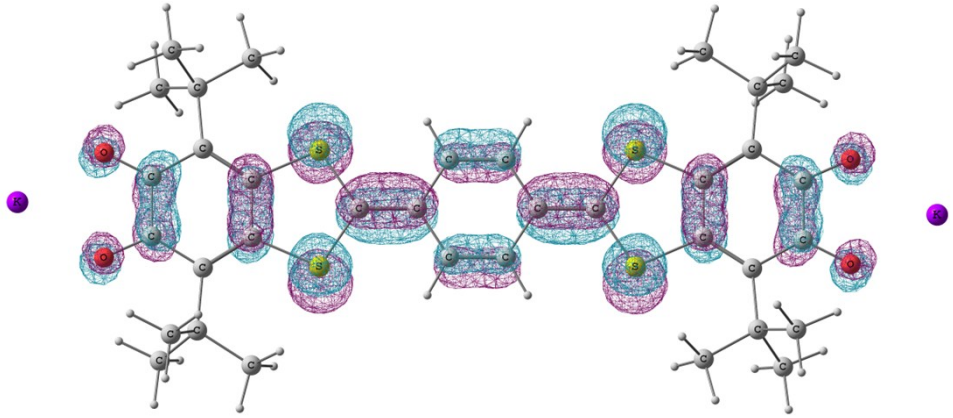

Figure S2. TD DFT B3LYP/6-311++G(d,p) calculated α-SOMO orbital of $\mathbf{1^{2-}K_2}$ for singlet biradical state.

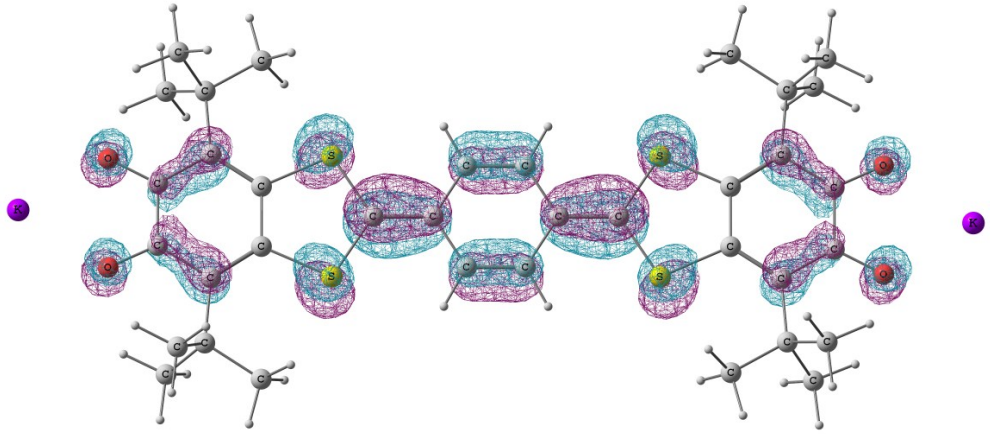

Figure S3. TD DFT B3LYP/6-311++G(d,p) calculated β-SOMO orbital of $\mathbf{1^{2-}K_2}$ for singlet biradical state.

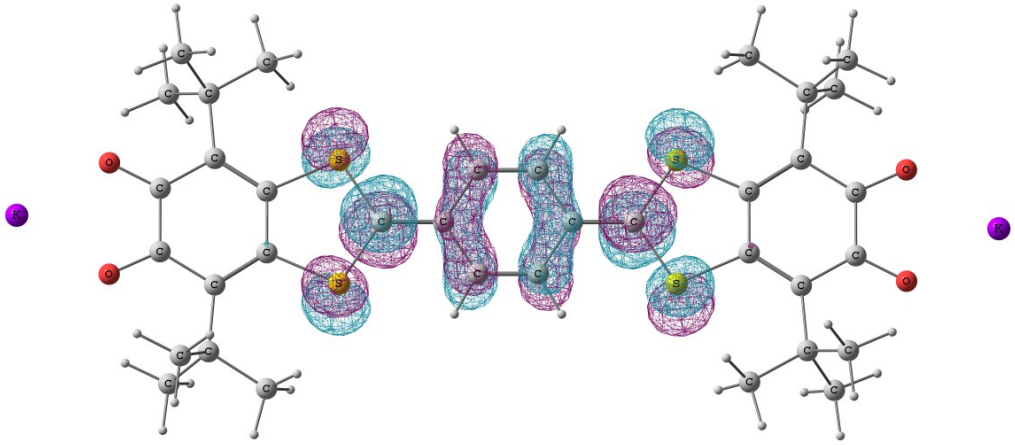

Figure S4. TD DFT B3LYP/6-311++G(d,p) calculated α-LUMO orbital of $\mathbf{1^{2-}K_2}$ for singlet biradical state.

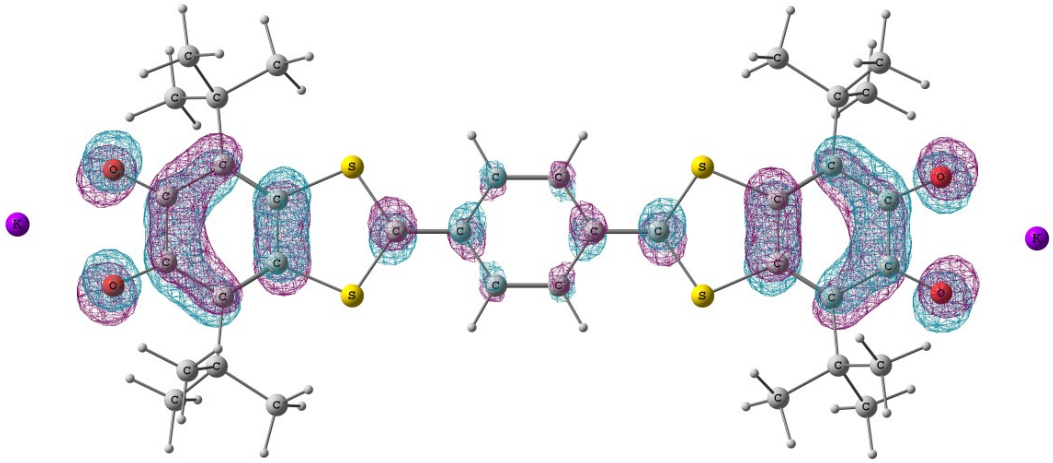

Figure S5. TD DFT B3LYP/6-311++G(d,p) calculated β-LUMO orbital of $\mathbf{1^{2-}K_2}$ for singlet biradical state.

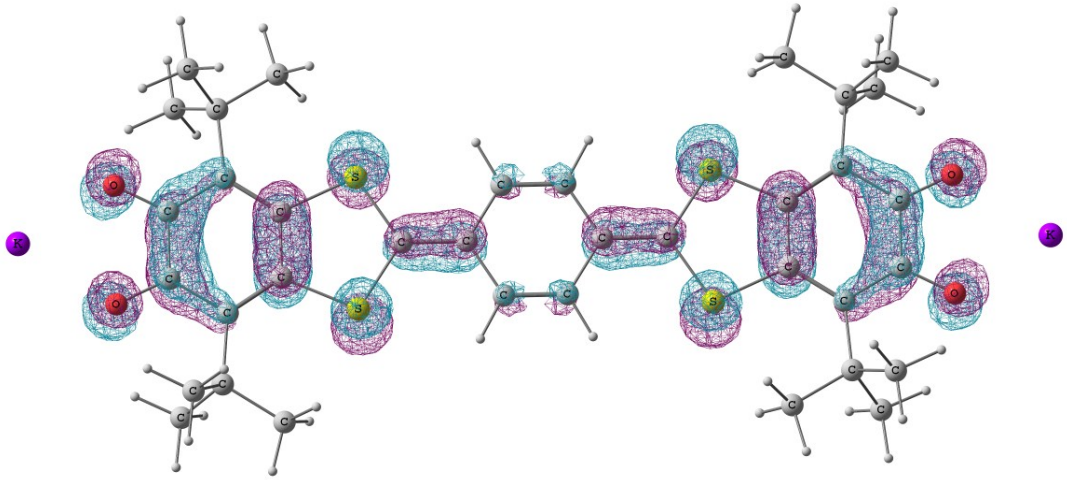

Figure S6. TD DFT B3LYP/6-311++G(d,p) calculated β-LUMO+1 orbital of $\mathbf{1^{2-}K_2}$ for singlet biradical state.

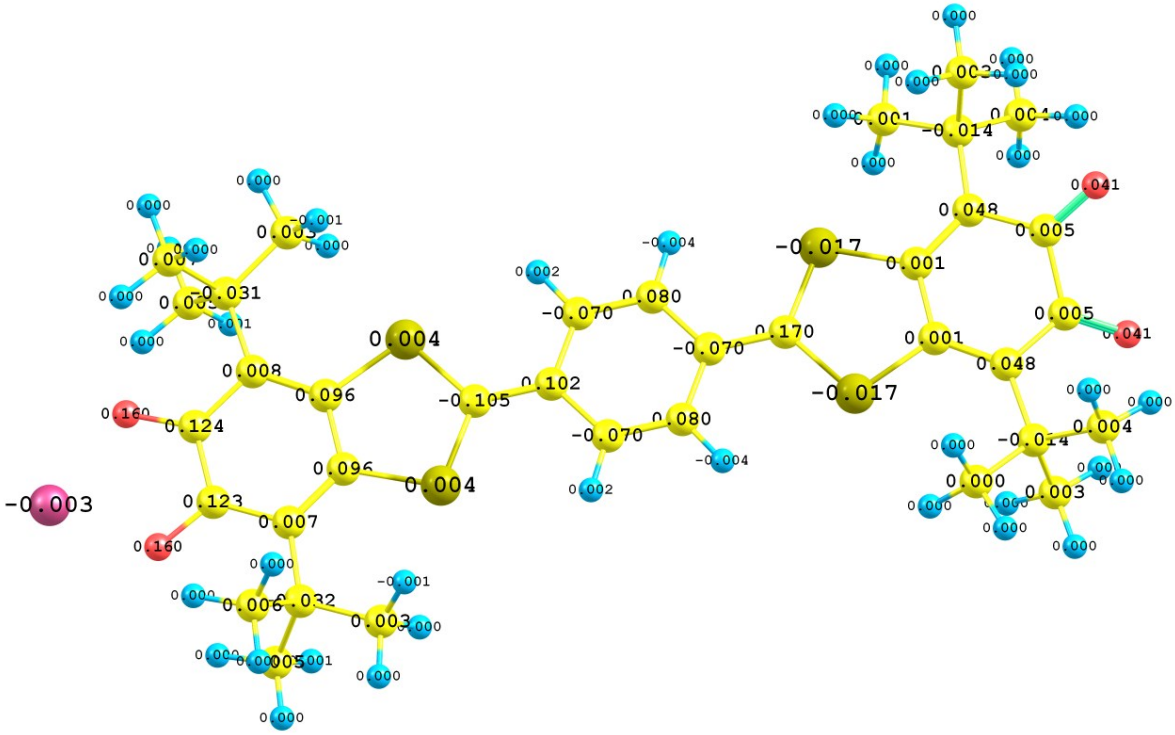

Figure S7. Spin density distribution for the broken-symmetry state of **1**$^{\cdot-}$**K**, calculated by UB3LYP/6-311++G(d,p) level of theory.

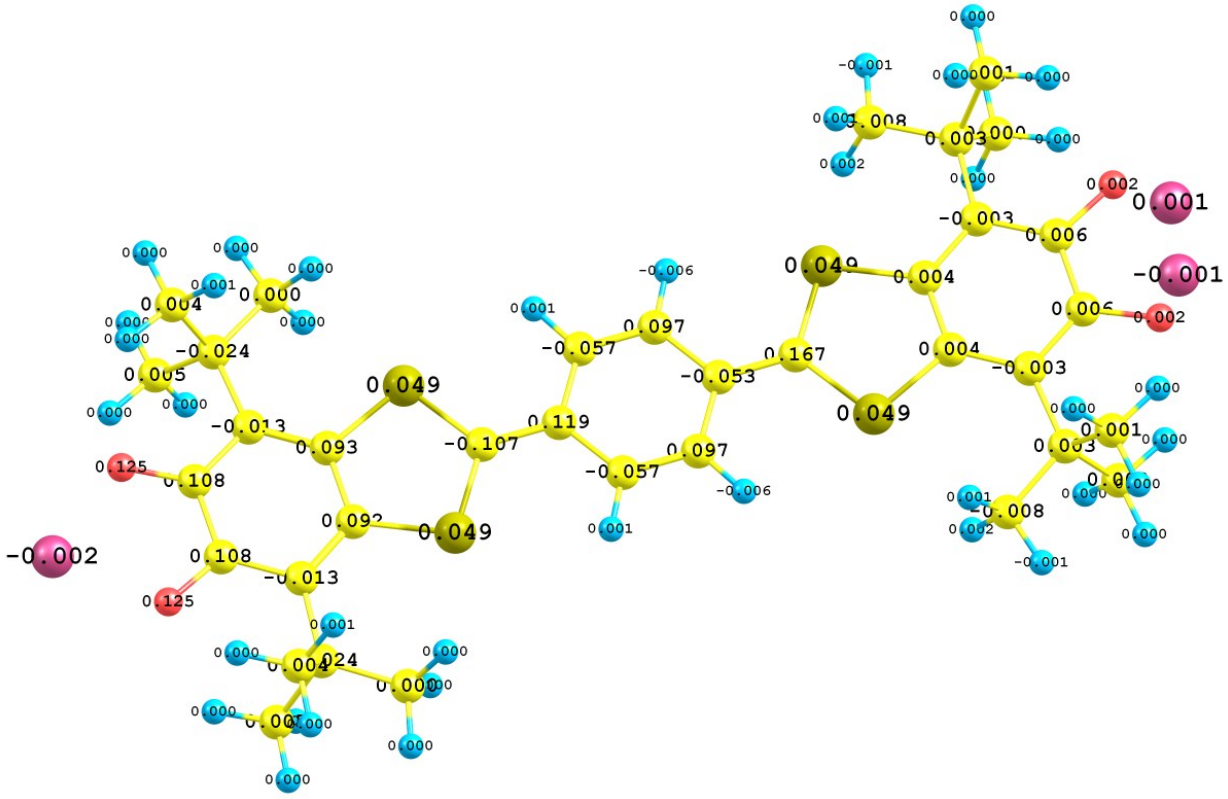

Figure S8. Spin density distribution for the broken-symmetry state of **1**$^{3-\cdot}$**K**$_3$, calculated by UB3LYP/6-311++G(d,p) level of theory.

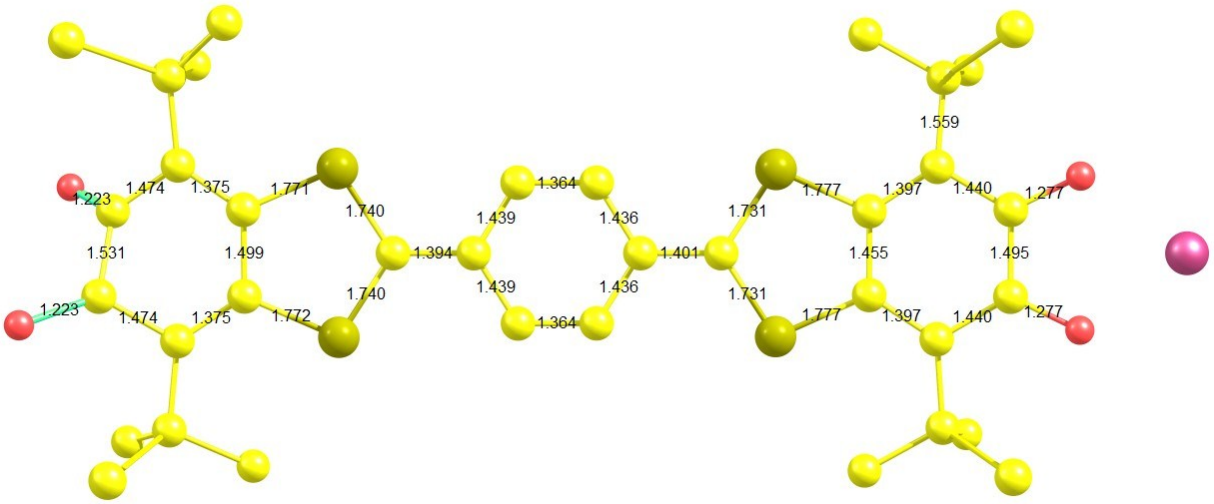

Figure S9. Bond lengths in the TD DFT B3LYP/6-311++G(d,p) calculated structure for of **1**$^{-}$·**K**.

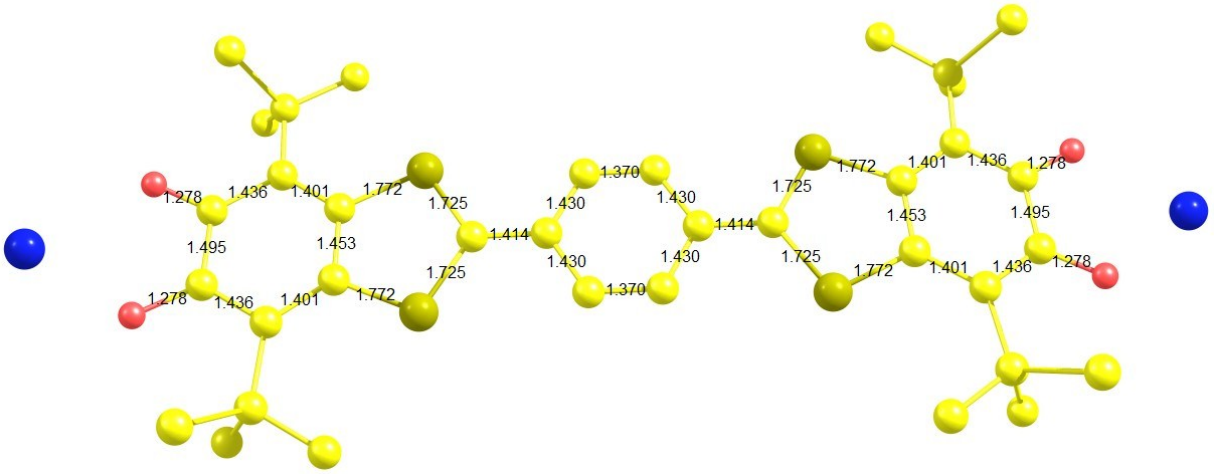

Figure S10. Bond lengths in the TD DFT B3LYP/6-311++G(d,p) calculated structure for of **1**$^{2-}$**K**$_2$.

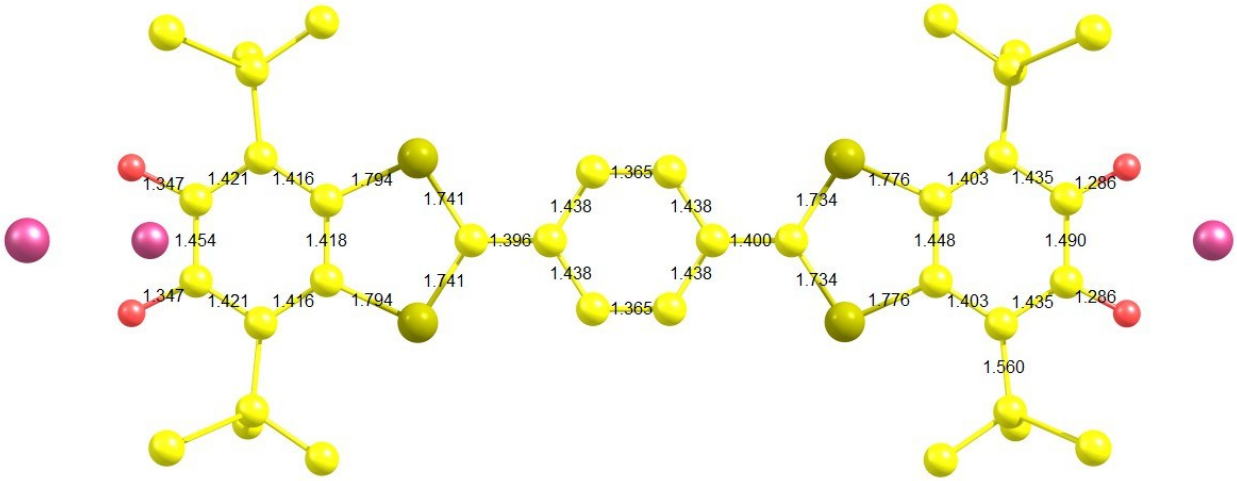

Figure S11. Bond lengths in the TD DFT B3LYP/6-311++G(d,p) calculated structure for of **1**$^{3-}$·**K**$_3$.

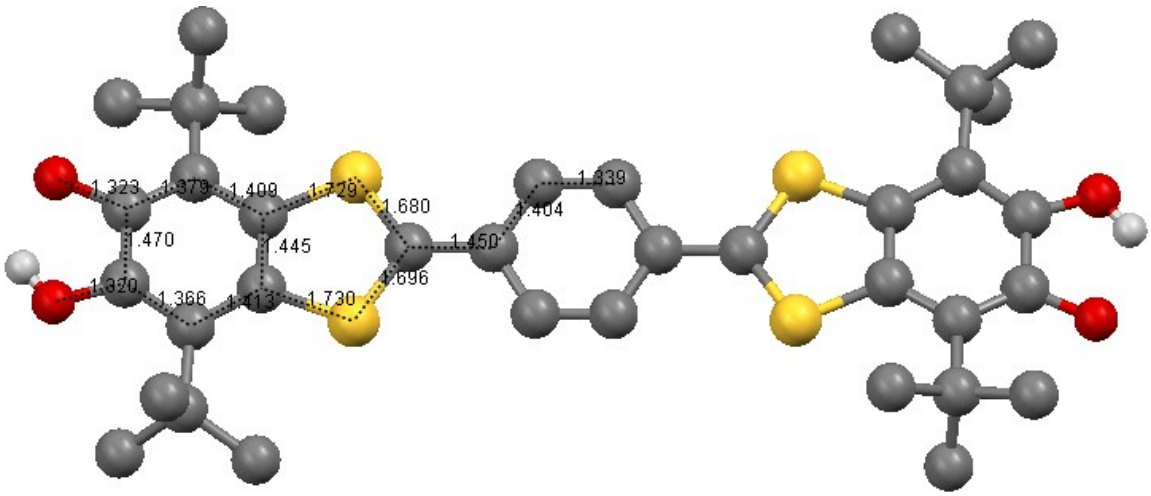

Figure S12. Bond lengths from the structural data for of $\mathbf{1^{2-}H_2}$.

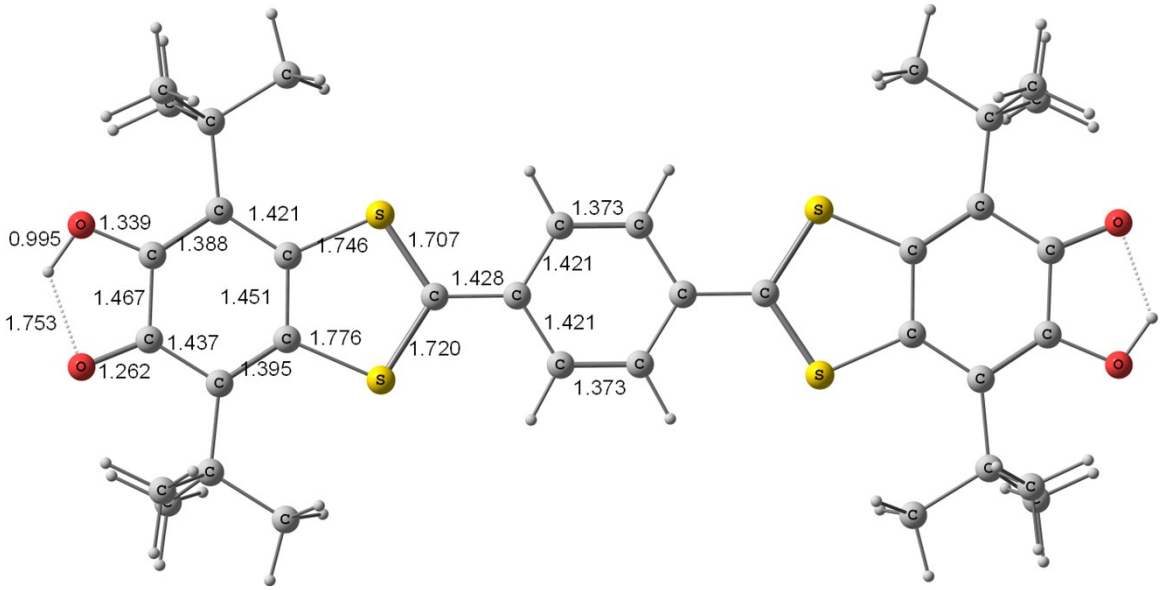

Figure S13. Bond lengths in the TD DFT B3LYP/6-311++G(d,p) calculated structure for of $\mathbf{1^{2-}H_2}$.

Figure S14. Ampoule for EPR experiment.