Supporting Information

for

Protonated paramagnetic redox forms of di-*o*-quinone bridged with *p*-phenylene-extended TTF: A EPR spectroscopy study

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Additional material

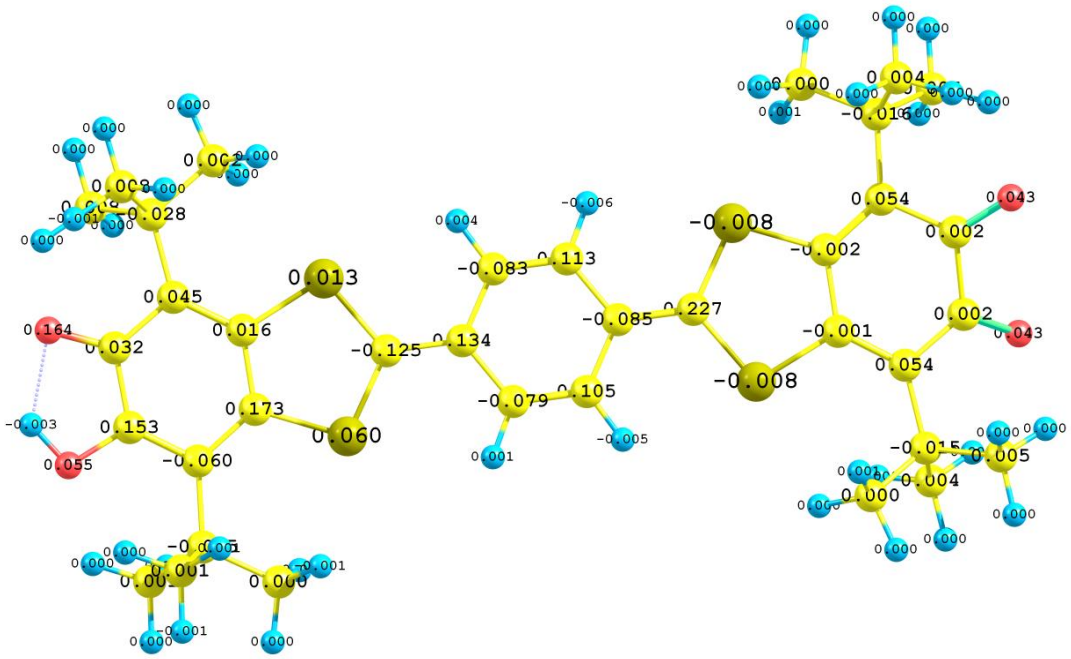

Figure S1: Spin-density distribution for the broken-symmetry state of (**1**˙)**H**, calculated by UB3LYP/6-311++G(d,p) level of theory.

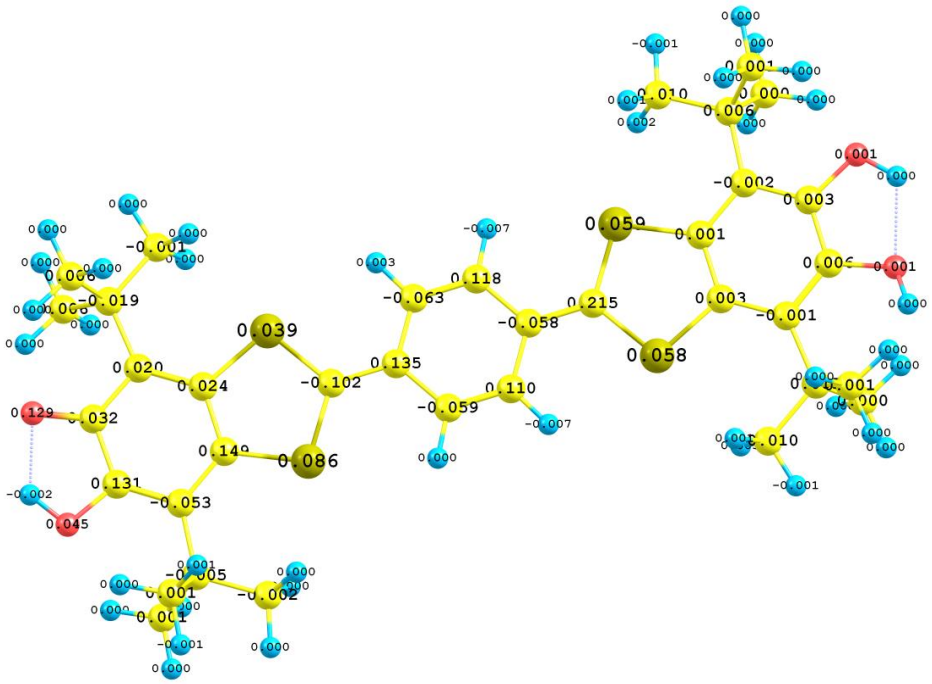

Figure S2: Spin-density distribution for the broken-symmetry state of (**1**˙)$\mathbf{H_3}$, calculated by UB3LYP/6-311++G(d,p) level of theory.

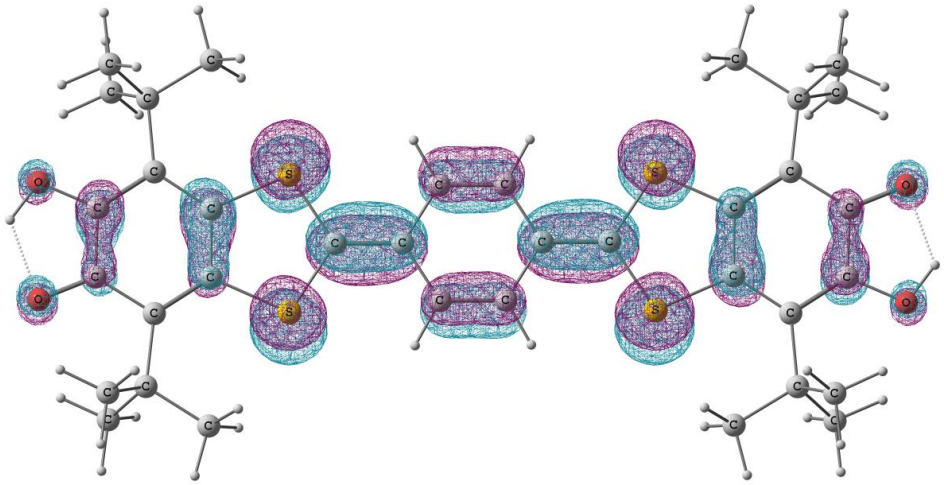

Figure S3: TD DFT B3LYP/6-311++G(d,p) calculated α-SOMO orbital of **(1)H_2** for singlet biradical state.

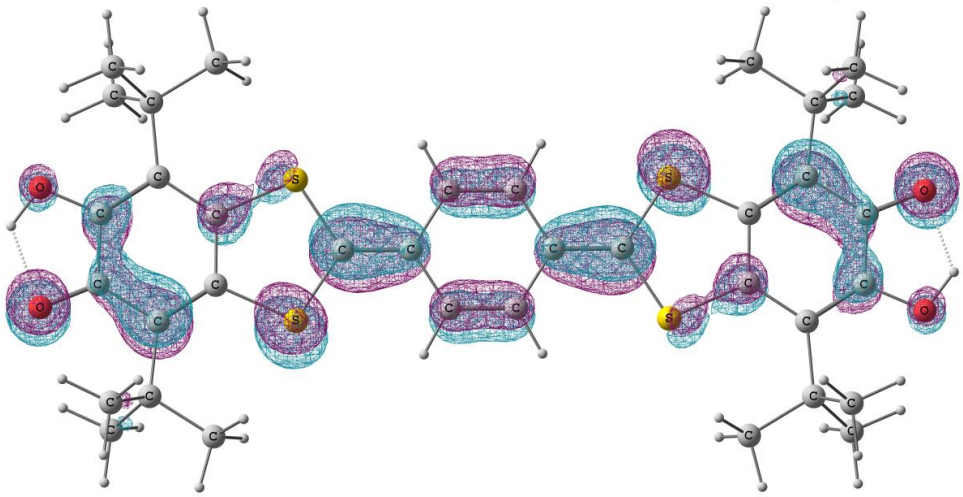

Figure S4: TD DFT B3LYP/6-311++G(d,p) calculated β-SOMO orbital of **(1)H_2** for singlet biradical state.

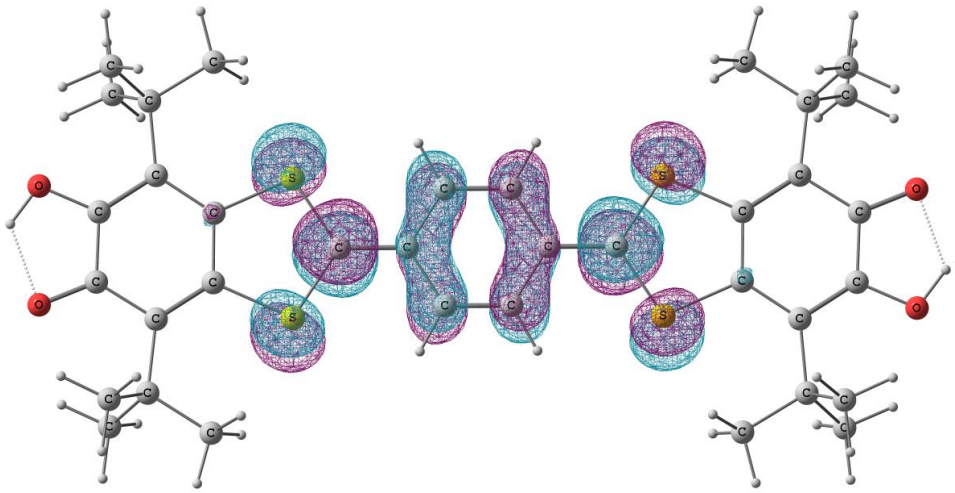

Figure S5: TD DFT B3LYP/6-311++G(d,p) calculated α-LUMO orbital of **(1)H_2** for singlet biradical state.

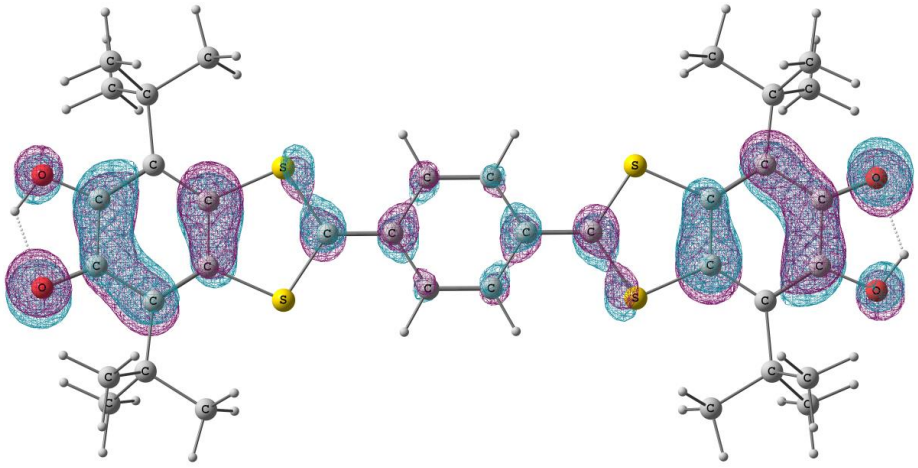

Figure S6: TD DFT B3LYP/6-311++G(d,p) calculated β-LUMO orbital of **(1)H_2** for singlet biradical state.