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Supporting Information

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# Oxidation of End-Capped Pentathienoacenes and Characterization of Their Radical Cations

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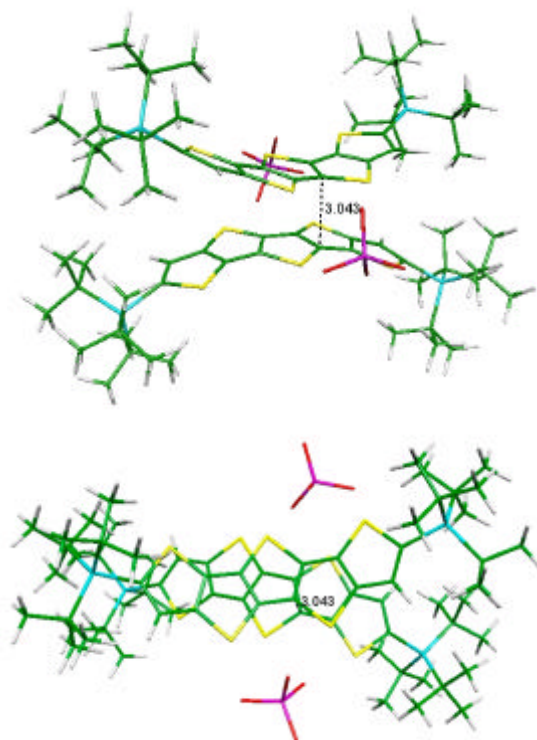
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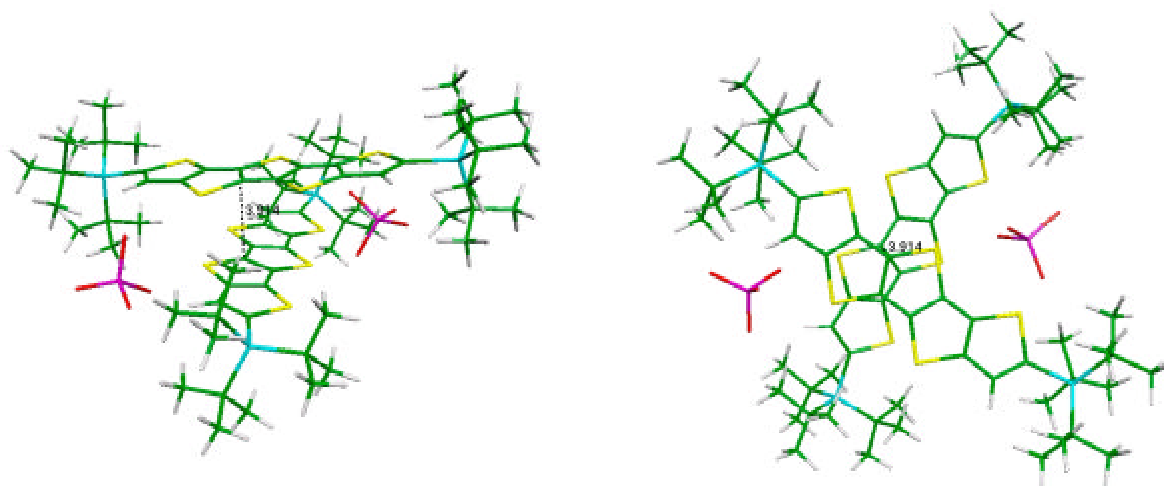
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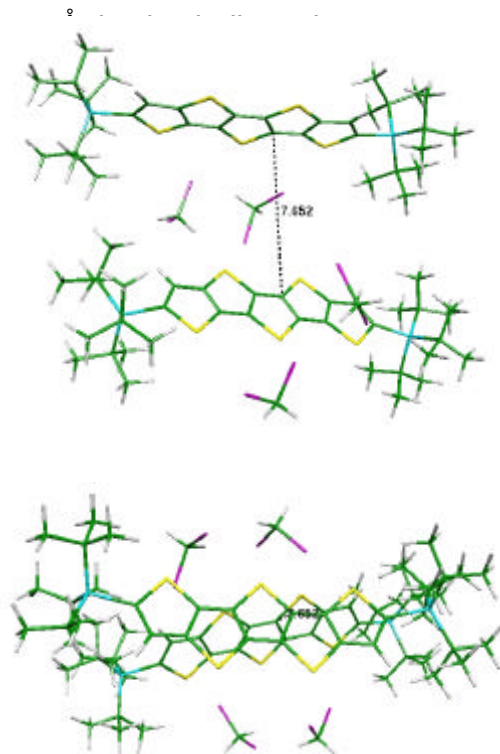
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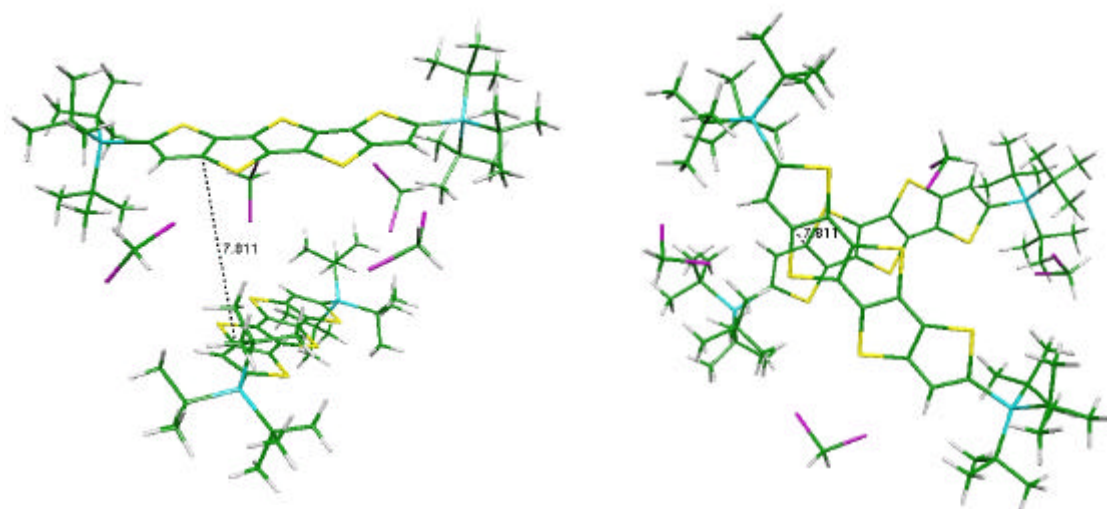
**Figure S1.** Lateral and top views of the optimum geometry of the antiparallel  $([\text{TIPS-T5-TIPS}]^+)_2(\text{ClO}_4^-)_2$  aggregate computed at the B3LYP/3-21G level. The shortest inter-radical C...C distance, 3.043 Å, is also indicated.



**Figure S2.** Lateral and top views of the optimum geometry of the crossed ( $[\text{TIPS-T5-TIPS}]^+$ )<sub>2</sub>(ClO<sub>4</sub><sup>-</sup>)<sub>2</sub> aggregate computed at the B3LYP/3-21G level. The shortest inter-radical C••C distance, 3.



**Figure S3.** Lateral and top views of the optimum geometry of the antiparallel ( $[\text{TIPS-T5-TIPS}]^+$ )<sub>2</sub>(CH<sub>2</sub>Cl<sub>2</sub>)<sub>4</sub> aggregate computed at the B3LYP/3-21G level. The shortest inter-radical C••C distance, 7.652 Å, is also indicated.



**Figure S4.** Lateral and top views of the optimum geometry of the crossed  $([\text{TIPS-T5-TIPS}]^+)_2(\text{CH}_2\text{Cl}_2)_4$  aggregate computed at the B3LYP/3-21G level. The shortest inter-radical  $\text{C}\bullet\bullet\text{C}$  distance, 7.811 Å, is also indicated.