Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Role of Sulfur Oxidation in Controlling Electronic Properties of the Sulfur-Containing Host Molecules for Phosphorescent Organic Light-Emitting Diodes

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Supporting Information
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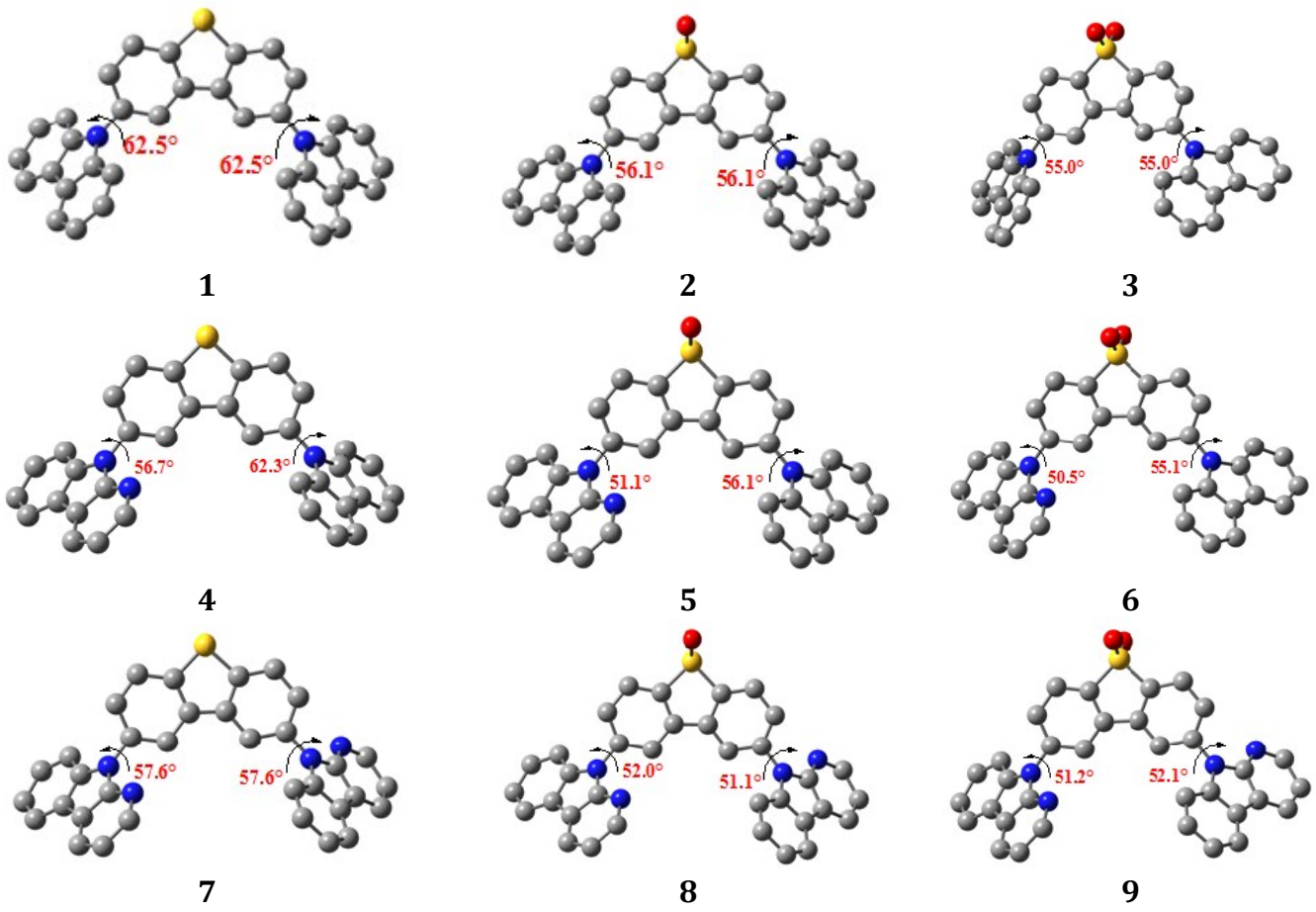
Figure S1: Optimized geometries of host molecules along with some selected dihedral angles.

Figure S2: Optimized geometries of 3, 7-substituted host along with some selected dihedral angles

Figure S3: Calculated and experimental triplet energy (E_T) of hosts **1**, **4**, and **7** in B3LYP/6-31+G* method.



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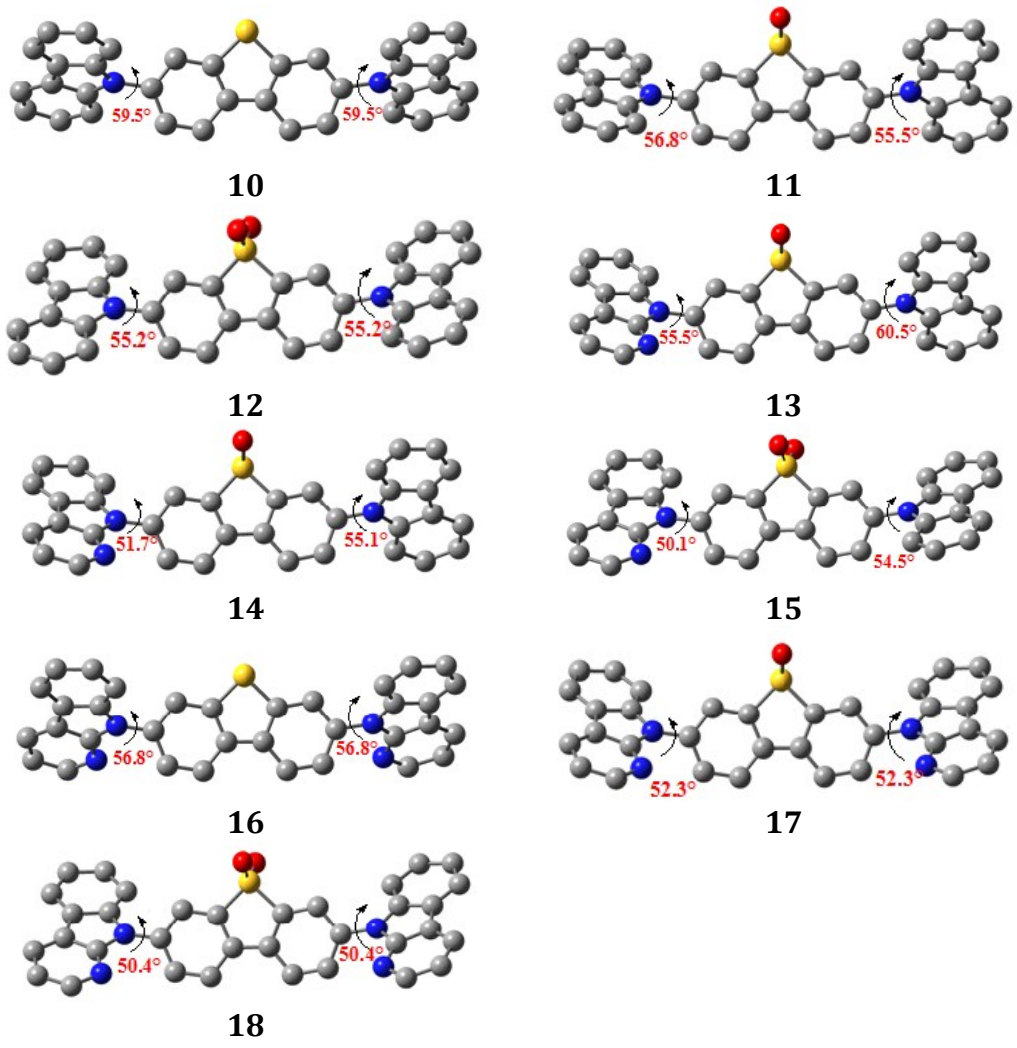

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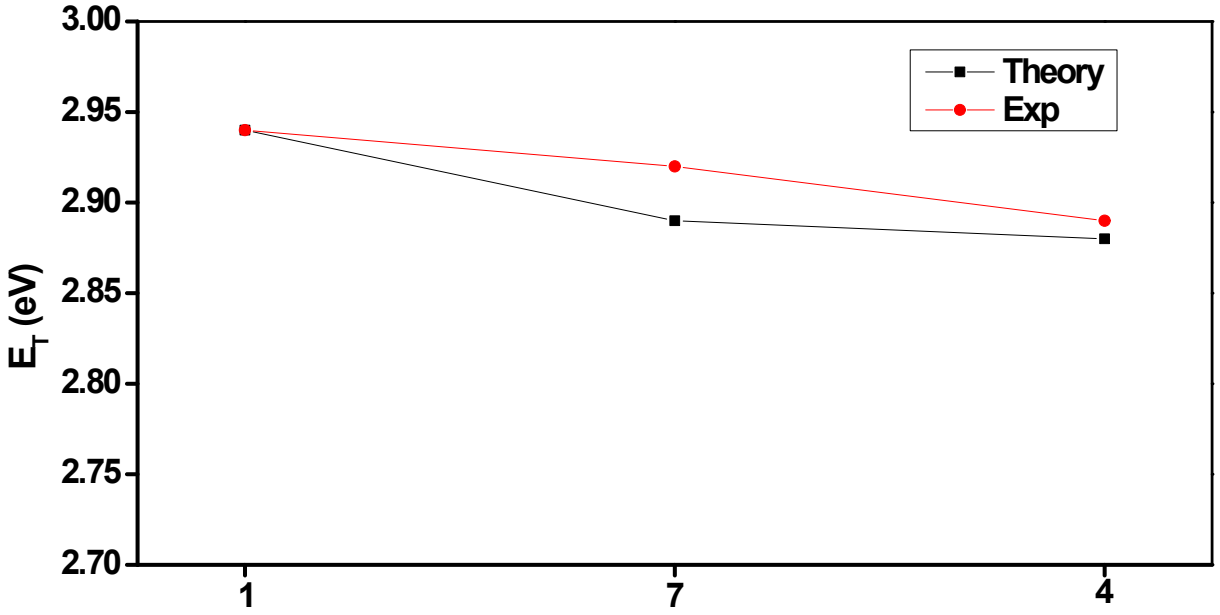

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