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

E. Varathan\textsuperscript{1,2} and V. Subramanian\textsuperscript{1,2,*}

CSIR-Network of Institutes for Solar Energy
\textsuperscript{1}Chemical laboratory, CSIR-Central Leather Research Institute, Adyar, Chennai-600 020
\textsuperscript{2}Academy of Scientific and Innovative Research (AcSIR), New Delhi 110025, India
E-mail: subuchem@hotmail.com, subbu@clri.res.in.
Tel.: +91 44 24411630. Fax: +91 44 24911589.

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