

Supplementary Materials

N-Methyl- and N-Phenylpiperazine Functionalized Styryl Dyes inside Cucurbiturils: Theoretical Assessment of the Factors Governing the Host-Guest Recognition

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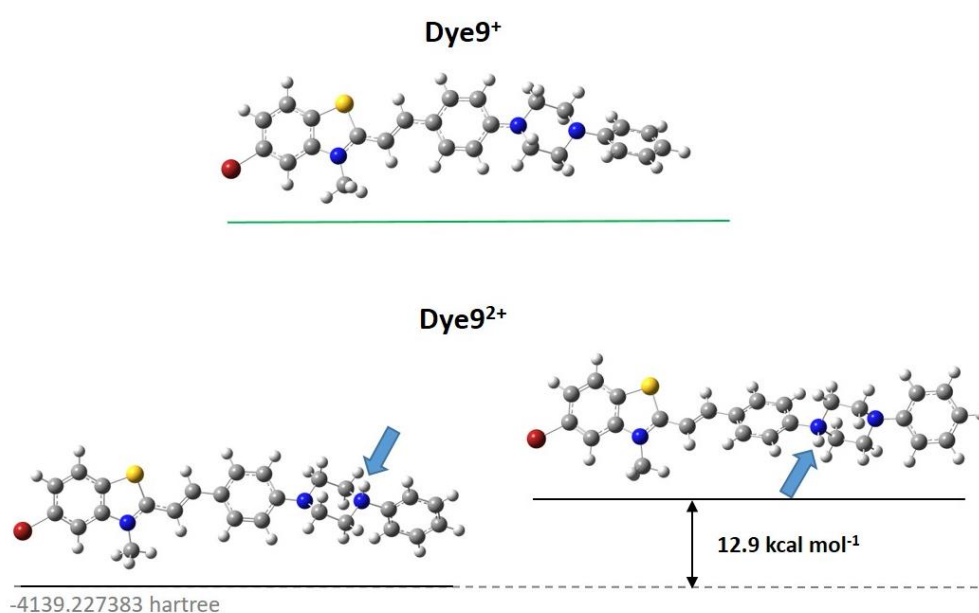


Figure S1. Optimized structures of dye9 in its mono- (Dye9⁺) and dicationic (Dye9²⁺) forms. The energetically preferred form of Dye9²⁺ is the N1-protonated (left).