**ESI of TMPH-2019-0286.R1**

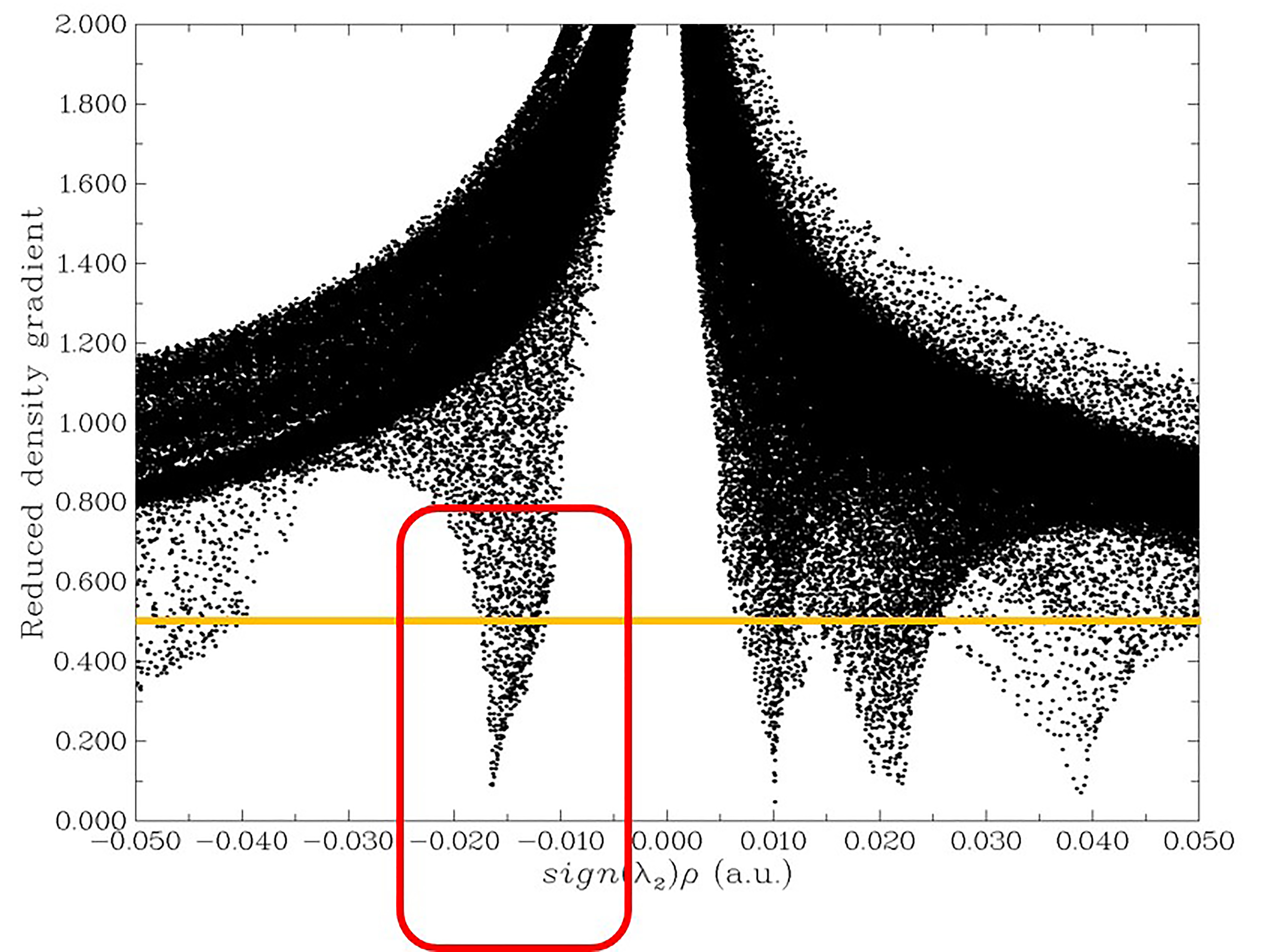
**Theoretical insights into elaborating and regulating excited state dynamics for the novel 6-cyano-2-(2’-hydroxyphenyl)imidazo[1,2a]pyridine system in polar and nonpolar solvents**

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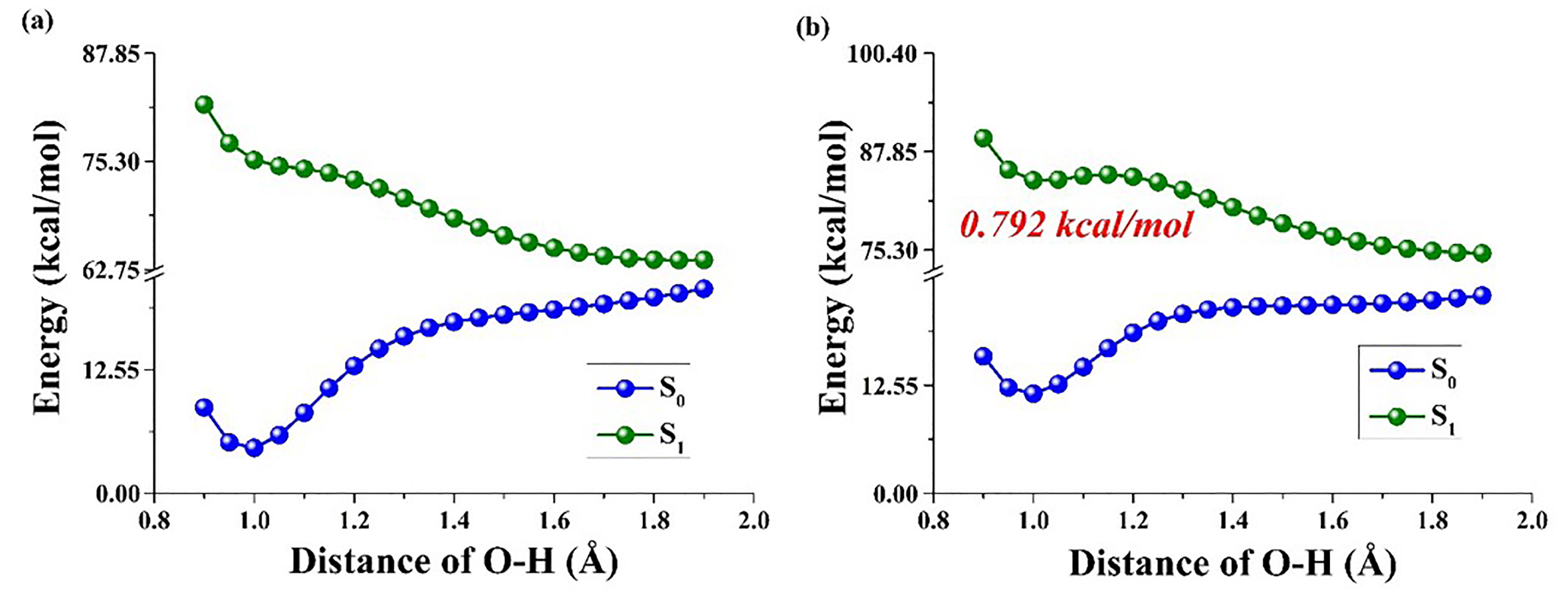
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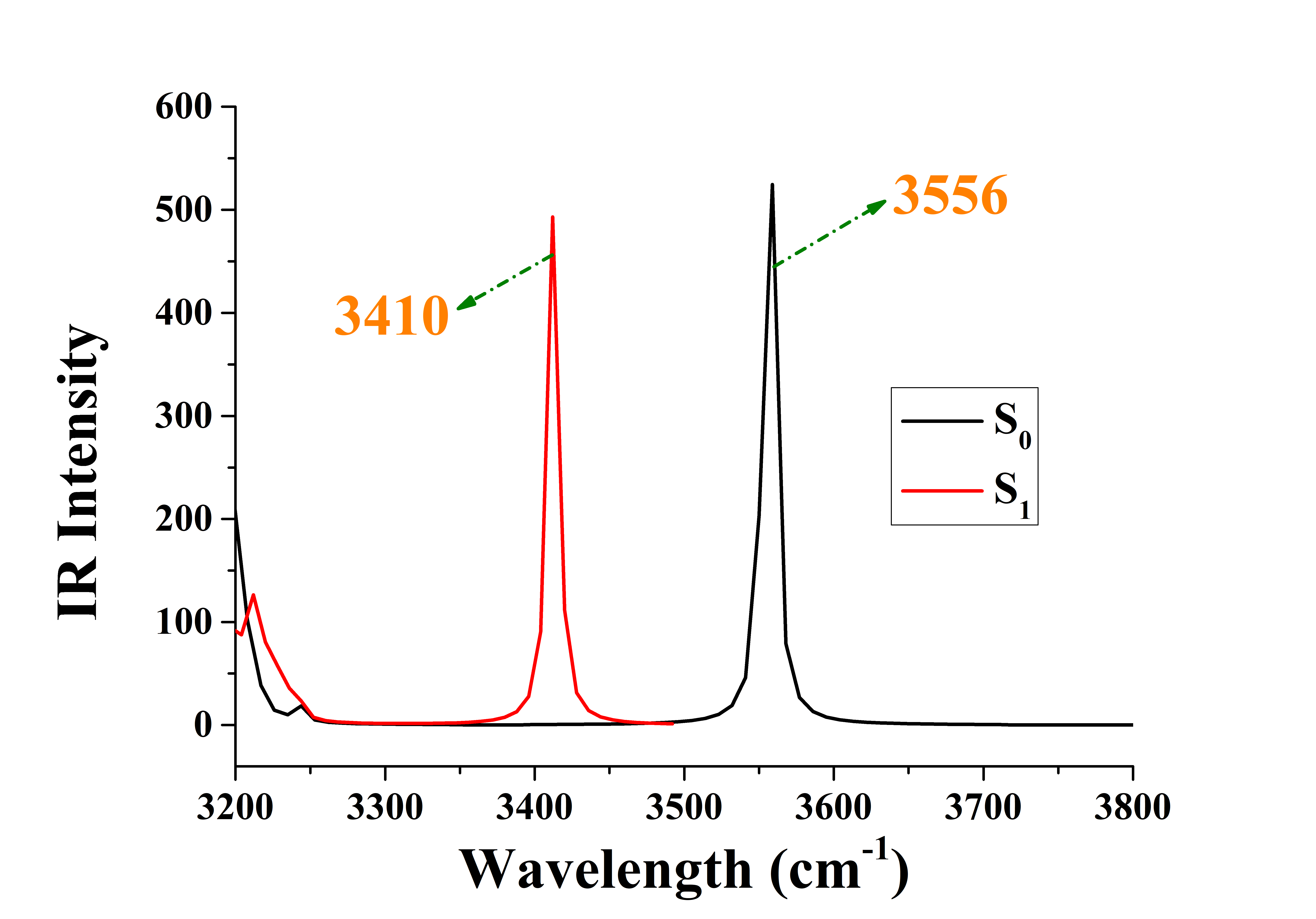
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**Figure S1.** The RDG (Y-axis) versus sign(λ2)ρ (X-axis) for 6-CN-HPIP system in the ground state. Herein, the weak interactions could be revealed according to RDG principle (i.e., negative values of sign(λ2)ρ refer to hydrogen bonding interactions; positive values of sign(λ2)ρ stand for steric effects; values of sign(λ2)ρ near zero exhibit van der Waal (VDW) interactions).



**Figure S2.** The constructed potential energy curves along with the ESIPT path in CCl4 (a) and DMSO (b) solvents using the Cam-B3LYP functional for 6-CN-HPIP system in both S0 and S1 states.



**Figure S3.** The theoretical IR vibrational spectra at the spectral region of O-H stretching vibration mode for 6-CN-HPIP forms in DMSO solvent.