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

SUPPLEMENTARY INFORMATION

HYDROGEN BOND VS π-STACKING INTERACTIONS IN THE *p*-AMINOPHENOL…*p*-CRESOL DIMER: AN EXPERIMENTAL AND THEORETICAL STUDY

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Table S1: Optimized structures of the isomers of *p*-AmPhOH...*p*-CreOH dimer in the S_0 and S_1 states, relative energies, vertical and adiabatic energies and oscillator strengths for the $S_1 \leftarrow S_0$ transition, calculated at the RI-CC2/cc-pVDZ level of theory.

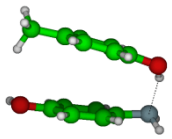
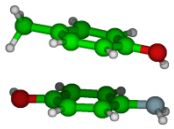
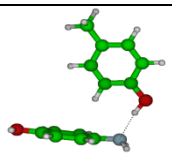
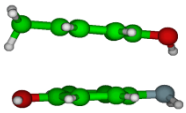
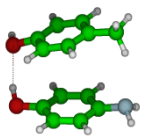
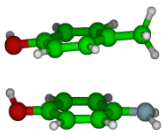
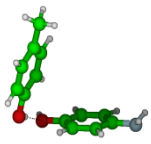
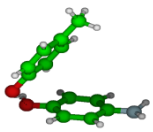
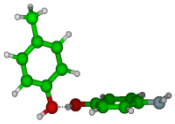
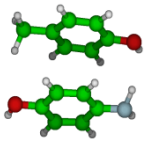
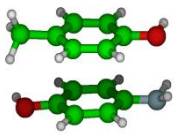
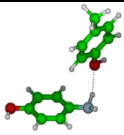
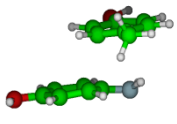
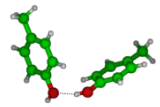
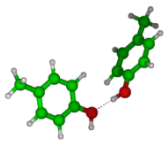
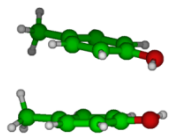
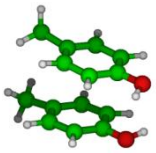
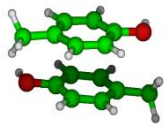
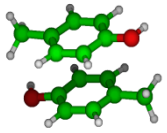
S_0 Optimized geometry	S_0 Relative Energy eV (cm^{-1})	$S_1 \leftarrow S_0$ Vertical Transition eV	Oscillator Strength	S_1 Optimized Geometry	$S_1 \leftarrow S_0$ Adiabatic Transition/(Adiabatic Transition - ΔZPE) eV
	0.00 (0.00)	4.50	0.02		3.95 / 3.76
	0.06 (484)	4.60	0.05		3.88 / 3.69
	0.12 (968)	4.46	0.03		3.92 / 3.73
	0.14 (1129)	4.54	0.08		4.24 / 4.05
	0.16 (1291)	4.47	0.06		4.19 / 4.00
	0.18 (1452)	4.43	0.03		3.93 / 3.74
	0.28 (2258)	4.44	0.06		3.93 / 3.74

Table S2: Optimized structures of the isomers of (*p*-CreOH)$_2$ dimer in the S_0 and S_1 states, relative energies, vertical and adiabatic energies and oscillator strengths for the $S_1 \leftarrow S_0$ transition, calculated at the RI-CC2/cc-pVDZ level of theory.

S_0 Optimized geometry	**S_0 Relative Energy eV (cm^{-1})**	**$S_1 \leftarrow S_0$ Vertical Transition eV**	**Oscillator Strength**	**S_1 Optimized Geometry**	**$S_1 \leftarrow S_0$ Adiabatic Transition/(Adiabatic Transition - ΔZPE) eV**
	0.00 (0.00)	4.87	0.04		4.65 / 4.46
	0.02 (161)	4.79	0.002		4.11 / 3.92
	0.04 (322)	4.81	0.001		4.12 / 3.93