Density functional theory applied to excited state intramolecular proton transfer in imidazole-, oxazole- and thiazole-based systems

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Table S1: Comparison between structural parameters of S_E and HBT from Purkayastha [5] and crystallographic data [78]. Bond length (Å) and angle formed (^{o}) in ground state

Structural parameters	Calculated	Purkayastha	Cryst. data
$C_8 - O$	1.342	1.366	1.305
$C_3 - N_1$	1.315	1.327	1.280
$C_2 - N_1$	1.379	1.400	1.404
$C_3 - S$	1.751	1.751	1.749
$C_4 - S$	1.747	1.687	1.757
$C_2 - N - C_3$	113.3	110.3	110.8
$C_3 - S - C_4$	90.1	91.0	88.6

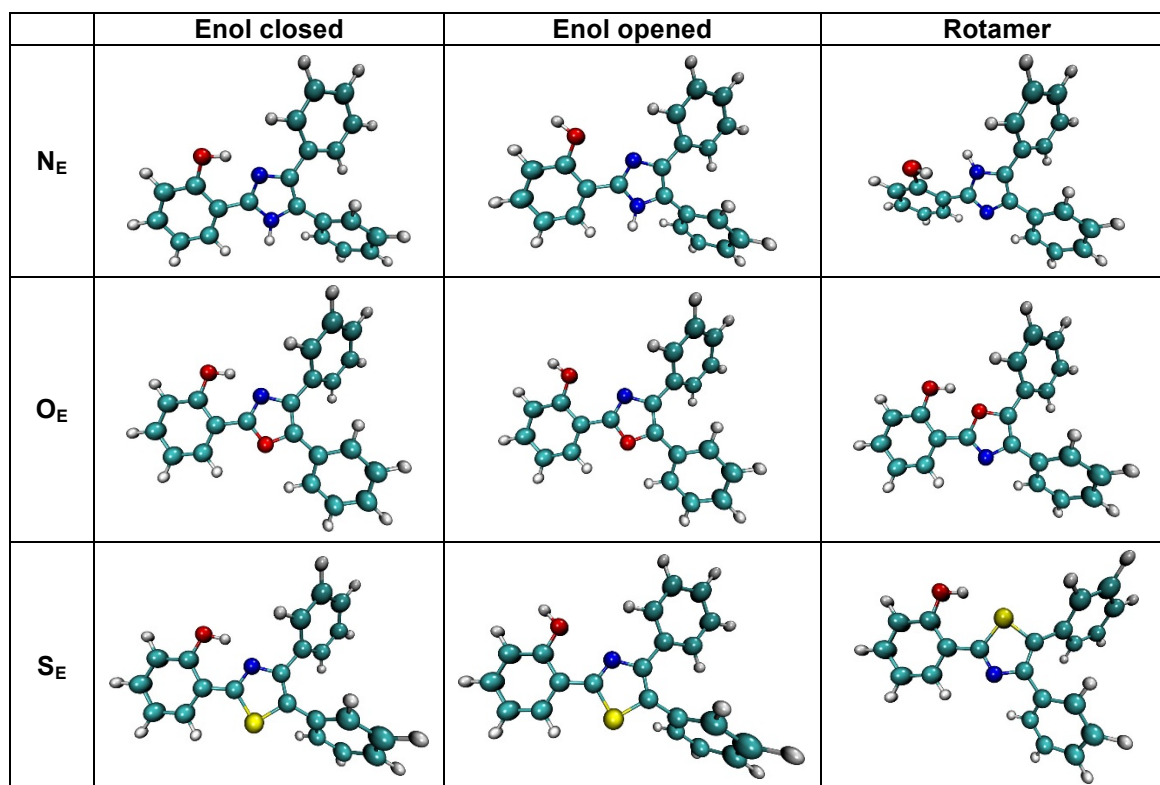|	Enol closed	Enol opened	Rotamer
N_E			
O_E			
S_E			

Figure S1: Optimized structure of N_E, O_E and S_E in enol closed forms, enol opened forms and their rotamers.
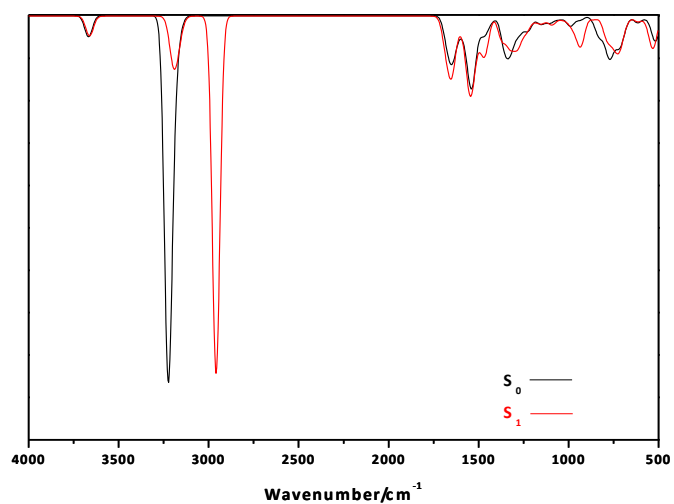
Figure S2: Vibrational spectrum of N_E in the ground and excited state in gas phase.
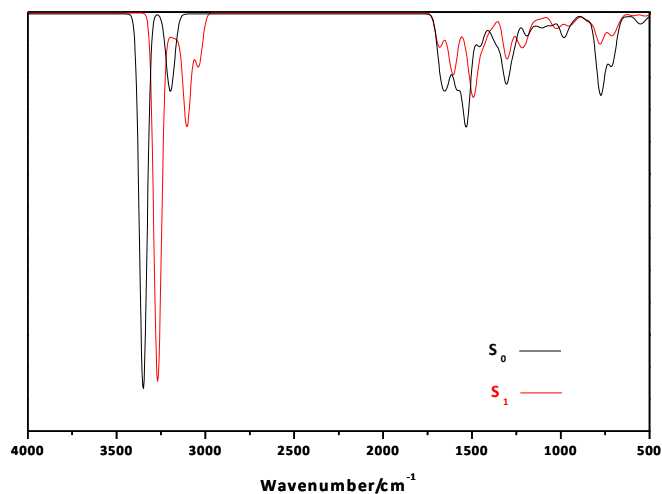

Figure S3: Vibrational spectrum of O_E in the ground and excited state in gas phase.
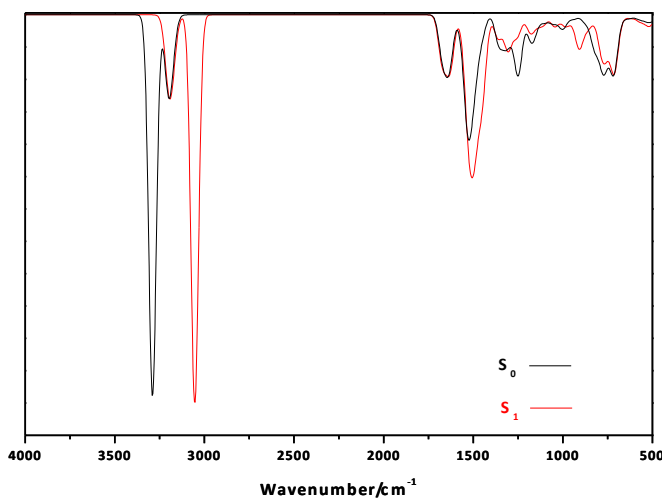

Figure S4: Vibrational spectrum of S_E in the ground and excited state in gas phase.

Table S2: HOMO → LUMO transition calculated with different functionals: theoretical absorption wavelength (λ_{abs}) and oscillator strength (f) calculated for N_E compound

Functional	% HF exchange	λ_{abs} (nm)	f
B3LYP	20	337.5	0.3850
M06	27	329.4	0.2948
wB97X-D3	22*	283.7	0.6434
M06-2X	54	274.6	0.4458

* Range separated hybrid functional with 22% short-range HF exchange, Grimme´s dispersion correction and range-separation parameter γ = 0.2
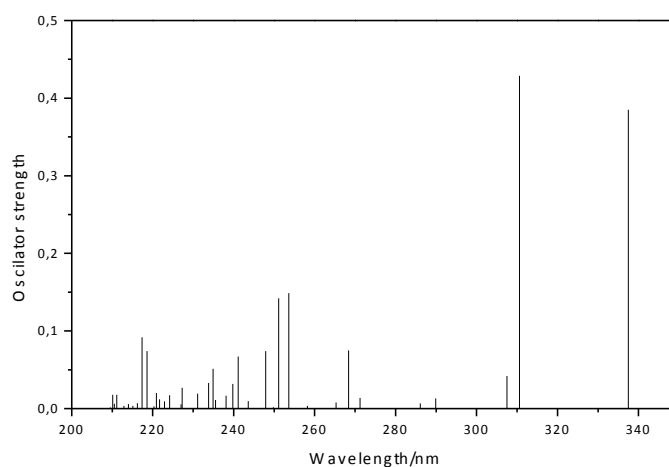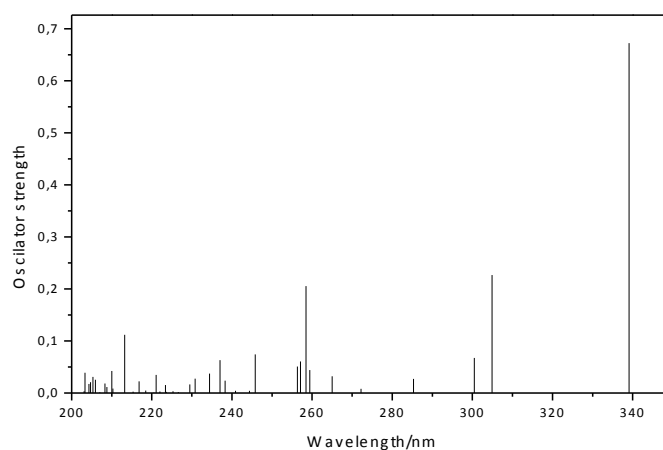

Figure S5: Absorption spectrum of N_E in gas phase.
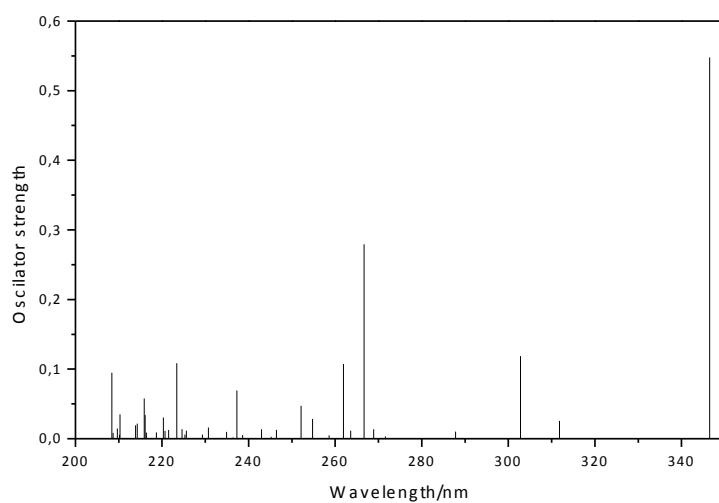

Figure S6: Absorption spectrum of O_E in gas phase.
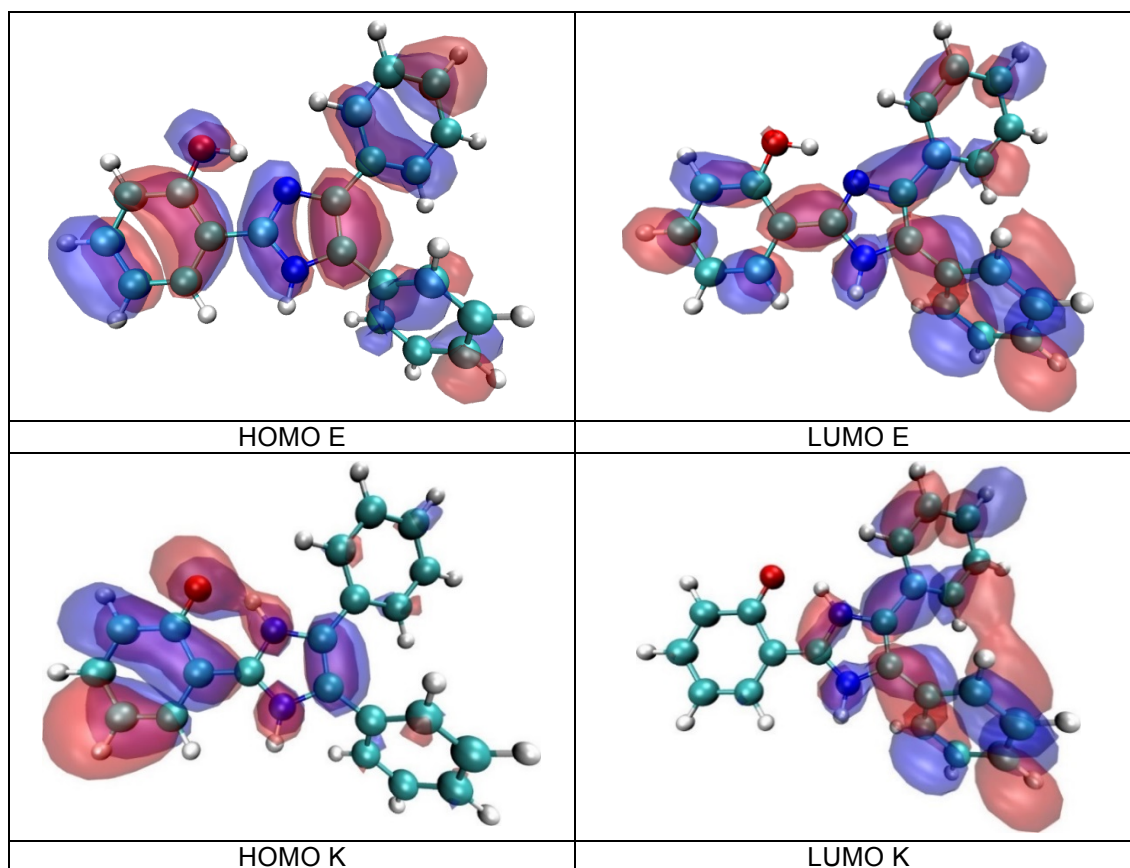
Figure S7: Absorption spectrum of S_E in gas phase.

HOMO E	LUMO E
HOMO K	LUMO K

Figure S8: HOMO and LUMO orbitals of enolic (E) and ketonic (K) forms of triphenylimidazolic species.

HOMO E	LUMO E
HOMO K	LUMO K

Figure S9: HOMO and LUMO orbitals of enolic (E) and ketonic (K) forms of triphenyloxazolic species.

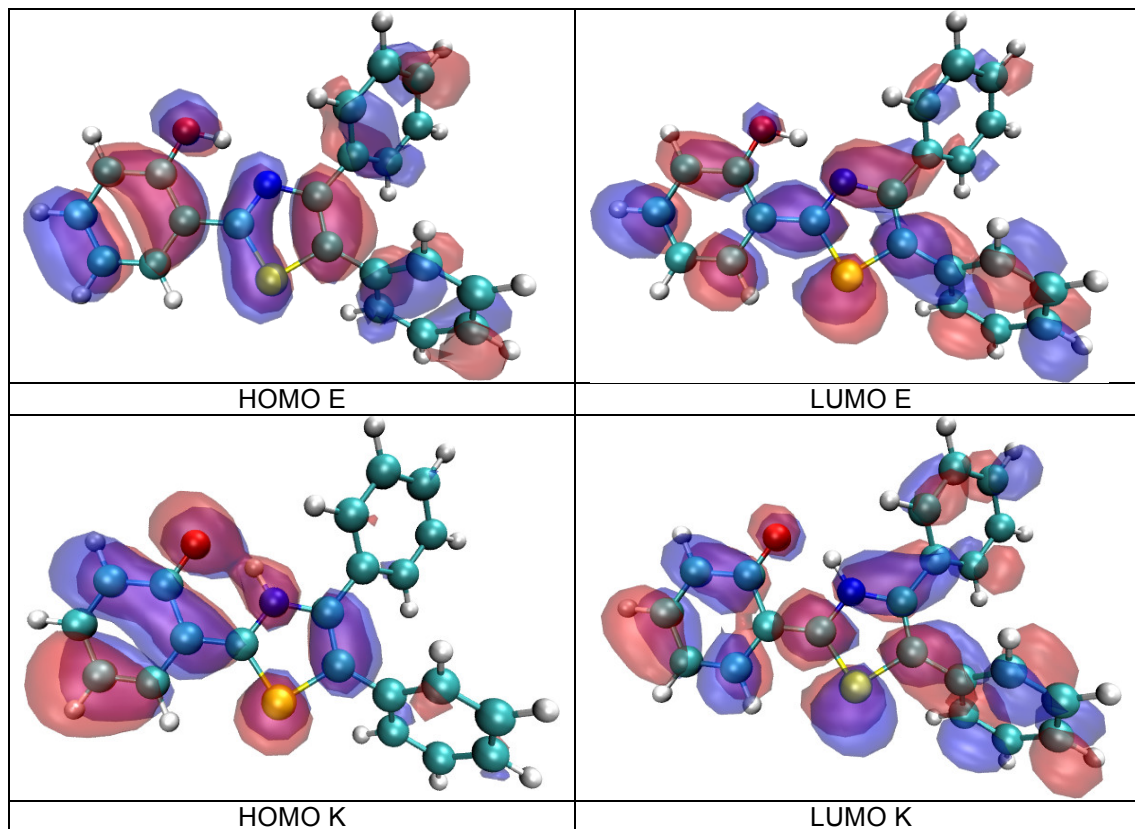|	
HOMO E	LUMO E
HOMO K	LUMO K

Figure S10: HOMO and LUMO orbitals of enolic (E) and ketonic (K) forms of triphenylthiazolic species.