Electronic Supplementary Material (ESI) for New Journal of Chemistry.
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Supporting Information

For

Time-Dependent Density Functional Theory Study on the tetrasubstituted imidazole compounds（TIC）: A special high Excited-State Intramolecular Proton Transfer (ESIPT) process

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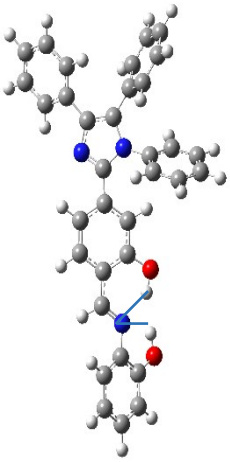
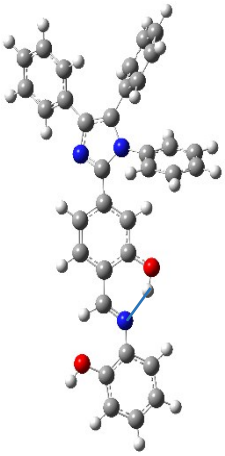
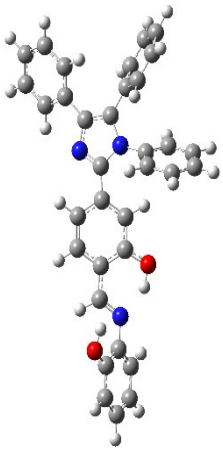
1. The structure of TIC isomers



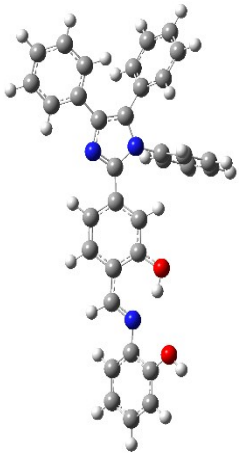
1 Δ *E*=-0.1796 eV



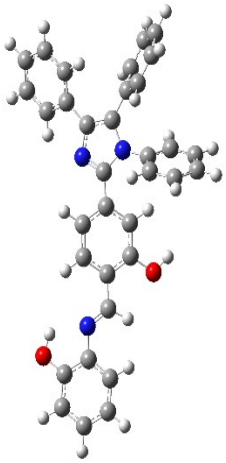
2 Δ *E*=0.0000 eV



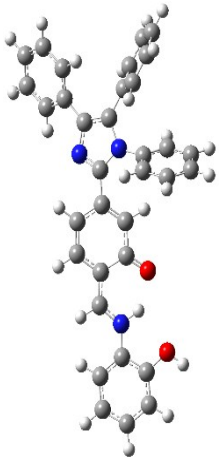
3 Δ *E*=0.0109 eV



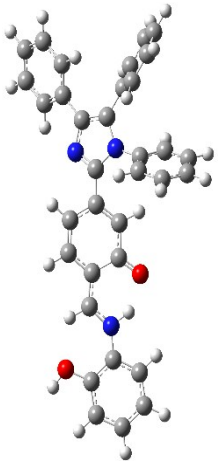
4 Δ *E*=0.0327 eV



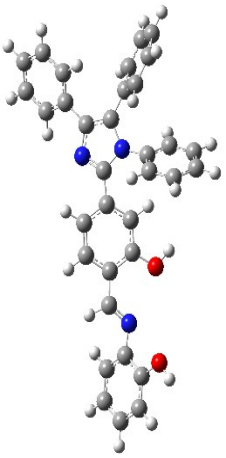
5 Δ *E*=0.1306 eV



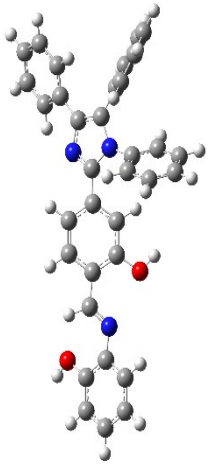
6 Δ *E*=0.1333 eV



7 Δ *E*=0.1361 eV



8 Δ *E*=0.6313 eV



9 Δ *E*=0.6411 eV

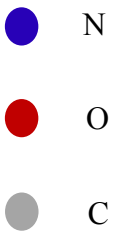


Figure 1S. A series of optimized conformations of TIC and their calculated relative energies (Δ*E* in eV) in the ground state. Gray: C, azury: H, red: O, blue: N.

2. Additional Data

Table 1S. Calculated IR, ^{1}HNMR, ^{13}CNMR and UV-VIS spectra (cal) and the experimental values (exp).

	exp	cal	
		Conformation 1	Conformation 2
$\nu(O_{13}–H_{14})/cm^{-1}$	3430	3525	3591
$\nu(O_2–H_1)$ /cm^{-1}	3061	3149	3064
$\nu(C_5 \quad N_6)$ /cm^{-1}	1615	1607	1608
δ(–OH, H_1)/ppm	13.97	11.25	12.56
δ(–OH, H_{14})/ppm	9.71	6.47	10.18
δ(– HC N,H)/ppm	8.89	9.26	8.31
δ(C)/ppm	160.75, 116.27	158.22, 111.06	160.62, 112.60
UV–VIS/nm	376, 435	417, 308	401