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LIST OF ABBREVIATIONS

ESPT	Excited state proton transfer
ESIntraPT	Excited state intramolecular proton transfer
ESInterPT	Excited state intermolecular proton transfer
PT	Proton transfer
HBO	2-(2'-hydroxyphenyl)-benzoxazole
HBT	2-(2'-hydroxyphenyl)-benzothiazole
HBI	2-(2'-hydroxyphenyl)–benzimidazole
HBQ	10-hydroxy-benzo[h]quinolone
Tinuvin-P	2-(2'-hydroxy-50-methylphenyl- benzotriazole
3HC	3-hydroxychromone
3HF	3-hydroxyflavoes
E	Enol form
E*	Excited enol form
K	Keto form
K*	Excited keto form
nm	Nanometer
s	Second
fs	Femtosecond
PMMA	Poly methyl methacrylate
MTHF	2-methyltetrahydrofuran
MP	3-methylpentane
MCH	Methylcyclohexane
MeOH	Methanol
DFT	Density functional theory
TD-DFT	Time-dependent density functional theory

B3LYP	Beck's three parameter Lee-Young-Parr
TZVP	Triple zeta valence plus polarization
BOA	Born-Oppenheimer approximation
HF	Hatree-Fock
CI	Configuration Interaction
MPn	Perturbation theory
CC	Coupled-cluster methode
QMC	Quantum Montecarlo
SCF	Self-consistent field
STOs	Slater-type orbitals
GTOs	Gaussian-type orbitals
DZ	Double-zeta
TZ	Triple-zeta
TDSE	Time-dependent Schrödinger equation
PECs	Potential energy curves
NH_3	Ammonia
CH_3OH	Methanol
H_2O	Water
MOs	Molecular orbitals
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital

LIST OF SYMBOLS

S_0	Ground state
S_1	First excited state
S_2	Second excited state
T_1	Triplet state
–OH	Hydroxy group
–C=O	Carbonyl group
$\hat{H}$	Hamiltonian operator
Ψ	Wavefunction
T_n	Kinetic energy of nuclei
T_e	Kinetic energy of electron
V_{en}	Electron-nuclear interaction Coulomb potential
V_{nn}	Repulsive Coulomb potential of nuclear-nuclear
V_{ee}	Repulsive Coulomb potential of electron-electron
ħ	Plank constatnt
M	Mass of nucleus
m	Mass of the electron
R_{AB}	Distance between nuclei A and B
r_{ij}	Distance between electrons *i* and *j*
r_{iA}	Distance between electron *i* and nucleus A
ε_0	Permittivity of free space
Z	Nuclei charge
χ_i	Spin orbitals
α/β	Electron spin up/down
x_i	Coordinates of the electron i
υ^{eff}	Effective potential of each electron
$\rho(r)$	Total electron density of molecule

$E[\rho]$	Electronic energy as a function of electronic density
E_T	Kinetic energy as a function of electronic density
E_V	Interaction energy between electron and nuclei
E_J	Coulomb energy
E_{XC}	Exchange-correlation energy
E_{XC}^{hyb}	Hybrid function energy of a mixture of Hartree-Fock exchange with DFT exchange-correlation
$\rho(r,t)$	Time-dependent potentials and electron densities
P_w	A Wigner distribution
P^i	Momentum associated with the normal coordinate
Q^i	Normal coordinate
ξ_{HO}^n	The harmonic oscillator wavefunction
s	s-orbital
p	p-orbital
d	d-orbital
π	Pi
π-π^*	Pi to Pi* transition (proton transfer)
Å	Angstrom
%	Per cent
f	Oscillator strength