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LIST OF ABBREVIATIONS

IC	Internal conversion
ISC	Intersystem crossing
ESPT	Excited state proton transfer
ESIPT	Excited-state intramolecular proton transfer
N	Normal form
T	Tautomer form
ICT	Intramolecular molecular charge-transfer state
HBI	2-(2'-hydroxyphenyl)benzimidazole
HBO	2-(2'-hydroxyphenyl)benzoxazole
HBT	2-(2′-hydroxyphenyl)benzothiazole
HBQ	10-hydroxybenzo[*h*]quinoline
IMP	2-(iminomethyl)phenol
H-bond	Hydrogen bond
PT	Proton transfer
MCH	Methylcyclohexane
K	Kelvin
nm	Nanometer
DFT	Density functional theory
TD-DFT	Time-dependent density functional theory
EE-MCSI/MM	Electronically embedded multi-configuration shepard interpolation and molecular mechanical
MD	Molecular dynamics
MOs	Molecular orbitals
TRF	Time-resolved fluorescence
PECs	Potential energy curves
d_{DA}	Distance between proton donor and proton acceptor
HBID	9-Hydroxy-3H-benzo[*g*]indole

IPDO	3,4-dihydro indene[1,2-*b*]pyrrole-8-ol
IPRO	H-indeno[1,2-*b*]pyridine-9-ol
PDP	2-(Pyridin-2-yl)phenol
PRP	2-(4*H*-pyrrol-2-yl)phenol
QM	Quantum mechanics
HF	Hartree-Fock calculation
B3LYP	Becke-3-LYP method
AOs	Atomic orbitals
STFs	Slater-type functions
GTFs	Gaussian-type functions
DZ	Double-zeta basis set
TZ	Triple-zeta basis set
TZVP	Triple-ζ valence quality with one set of polarization functions
IR	Infrared spectrum
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
eV	Electron volts
kcal/mol	Kilocalorie per mole
GS-PECs	Ground state potential energy curves
ES-PECs	Excited-state potential energy curves
fs	Femtosecond

LIST OF SYMBOLS

S_0	Ground states
S_1	Excited states
T_1	Triplet states
H	Hamiltonian operator
ψ	Wavefunction
E	Energy
T	Kinetic energy operator
V	Potential energy operator
∇	Spatial differential operator
Z_i	Atomic number
$\hbar$	Planck constant
e	Electron
$P(x,y,z)$	Electron density function
$E(\rho)$	Energy functional
G[n(r)]	Kinetic energy of Hohenberg-Kohn theorems
E_T	Kinetic energy as a function of electron density
E_v	Potential energy as a function of electron density
$E_{coulomb}$	Coulomb self-interaction
E_{xc}	Exchange-correlation energy as a function of electron density
$\rho(r,t)$	Time-dependent potentials and electron densities
χ^0_{HO}	Wavefunction quantum harmonic oscillator for ground state
P_i	Momentum associated with the normal coordinate
Q_i	Normal coordinate
μ^i	Reduced mass of normal mode
ω^i_{HO}	Harmonic frequency of normal mode
ξ^0_{HO}	The harmonic oscillator wavefunction
Å	Angstrom

°	Degree
π	Pi
π*	pi*
π→π*	Pi to pi* transition (proton transfer)
%	Percent
S_1-S_0	Relative energy difference between excited and ground states