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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-hydroxyflavones                            |
| 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                 | Hartree-Fock                          |
| CI                 | Configuration Interaction             |
| MPn                | Perturbation theory                   |
| CC                 | Coupled-cluster method                |
| QMC                | Quantum Monte Carlo                   |
| 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 <sub>3</sub>    | Ammonia                               |
| CH <sub>3</sub> OH | Methanol                              |
| H <sub>2</sub> O   | Water                                 |
| MOs                | Molecular orbitals                    |
| HOMO               | Highest occupied molecular orbital    |
| LUMO               | Lowest unoccupied molecular orbital   |

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## LIST OF SYMBOLS

|                      |  |
|----------------------|--|
| $S_0$                | Ground state                                     |
| $S_1$                | First excited state                              |
| $S_2$                | Second excited state                             |
| $T_1$                | Triplet state                                    |
| $-\text{OH}$         | Hydroxy group                                    |
| $-\text{C}=\text{O}$ | Carbonyl group                                   |
| $\hat{H}$            | Hamiltonian operator                             |
| $\Psi$               | 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 |
| $\hbar$              | Plank constant                                   |
| $M$                  | 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      |
| $\epsilon_0$         | Permittivity of free space                       |
| $Z$                  | Nuclei charge                                    |
| $\chi_i$             | Spin orbitals                                    |
| $\alpha/\beta$       | Electron spin up/down                            |
| $x_i$                | Coordinates of the electron $i$                  |
| $v^{\text{eff}}$     | 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<br>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   |
| $\xi_{HO}^n$   | The harmonic oscillator wavefunction  |
| s              | s-orbital   |
| p              | p-orbital   |
| d              | d-orbital   |
| $\pi$          | Pi  |
| $\pi-\pi^*$    | Pi to Pi* transition (proton transfer)  |
| Å              | Angstrom  |
| %              | Per cent  |
| $f$            | Oscillator strength   |

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