CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

ESPT/HT	Excited-state proton/hydrogen atom transfer
DNA	Deoxyribonucleic acid
PQ	1*H*-pyrrolo[3,2-*h*]quinoline
7HQ	7-hydroxquinoline
7AI	7-azaindole
IC	Internal conversion
ISC	Intersystem crossing
ESInterPT/HT	Excited-state intermolecular proton/hydrogen atom transfer
ESIntraPT/HT	Excited-state intramolecular proton/hydrogen atom transfer
QM	Quantum mechanics
BOA	Born-Oppenheimer approximation
HF	Hatree-Fock
SCF	Self-consistent field
CC	Coupled cluster
CC2	Second-order approximate coupled cluster model
CI	Configuration interaction
RI	Resolution-of-the-identity
ADC(2)	Algebraic diagrammatic construction through second order
RI-ADC(2)	Resolution-of-the-identity with algebraic diagrammatic construction through second order
RI-CC2	Resolution-of-the-identity with second-order approximate coupled cluster model
TDSE	Time-dependent Schrödinger equation
UV	Ultraviolet
AIMD	*Ab initio* molecular dynamics
TDDFT	Time-dependent density functional theory
CASPT2	Complete active space perturbation theory to the second order
HBR	Hydrogen bond rearrangement

REMPI	Resonance-enhanced multiphoton ionization
MRPT2	Multi-reference perturbation theory to second order
N	Normal
T	Tautomer
NT	No tautomerization
ESDPT	Excited-state double proton transfer
ESTPT	Excited-state triple proton transfer
ESQPT	Excited-state quadruple proton transfer
PES	Potential energy surface
SV	Split valence basis set
SVP	Split valence polarized basis set
TZVPP	Triple zeta for valence electrons plus double polarization function
fs	Femtosecond
ns	Nanosecond
$kcal.mol^{-1}$	Kilocalorie per mole

LIST OF SYMBOLS

S_1	First excited singlet state
S_2	Second excited singlet state
S_0	Singlet ground state
T_1	First excited triplet state
T_2	Second excited triplet state
$\hat{H}$	Hamiltonian
Ψ	Wavefunction
E	Total energy
Z_A, Z_B	Nuclear charges
M_A	Mass of nucleus A
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 election i and nuclei A
ε_0	Permittivity of free space
$\hbar$	Plank constant
ψ	Wavefunction associated with solving the electron part
χ	Wavefunction associated with nuclear motion
$\hat{h}^F$	Hartree-Fock operator
α, β	Electron spin
τ_k^c and τ_{kl}^{cd}	Single and double replacement operators
$\mathrm{CIS}(D_\alpha)$	The doubles correlation to CI singles
$\pi\sigma^*$	Excited-state hydrogen atom transfer surface
$\pi\pi^*$	Excited-state proton transfer surface
Å	Angstrom
$\emptyset$	Dihedral angles
°	Degree