CONTENTS

LIST OF TABLES

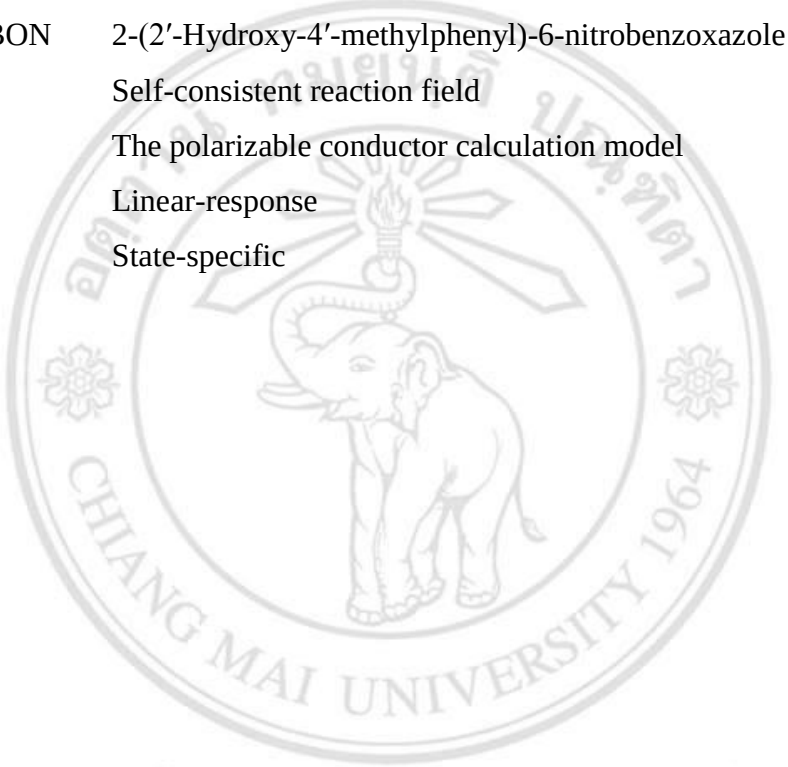
LIST OF FIGURES

LIST OF ABBREVIATIONS

IC	Internal conversion
ISC	Intersystem crossing
s	Second
DNA	Deoxyribonucleic acid
ICT	Intramolecular charge transfer
MLCT	Metal-ligand charge transfer
TICT	Twisted intramolecular charge transfer
BODIPYs	Boron-dipyrromethene
ESIntraPT	Excited-state intramolecular proton transfer
ESPT	Excited-state proton transfer
PT	Proton transfer
ESInterPT	Excited-state intermolecular proton transfer
PQ	1*H*-Pyrrolo[3,2-*h*]quinoline
7HQ	7-Hydroxyquinoline
7AI	7-Azaindole
HBO	2-(2′-Hydroxyphenyl)benzoxazole
HBT	2-(2′-Hydroxyphenyl)benzothiazole
HBI	2-(2′-Hydroxyphenyl)benzimidazole
HBQ	10-Hydroxy-benzo[*h*]quinoline
TIN-H	2-(2′-Hydroxyphenyl)benzotriazole
PPA	Polyphosphoric acid
nm	Nanometer
HF	Hartree-Fock approximation
MP	Møller–Plesset perturbation theory
CI	Configuration interaction calculation
CC	Coupled-cluster method
SCF	Self-consistent filed
MP2	second-order Møller–Plesset perturbation theory

CIS	Single excitation configuration interaction
CISD	Single and double excitation configuration interaction
RI	Resolution-of-the-identity
CC2	Second-order approximate coupled-cluster model
ADC(2)	Algebraic diagrammatic construction through second order
CIS(D_∞)	The iterative variant of the doubles correlation to CI singles
DFT	Density functional theory
B3LYP	Becke, 3-parameter, Lee-Yang-Parr exchange-correlation functional
PBE0	Perdew, Burke, and Ernzerhof exchange-correlation functional
PBE1PBE0	Perdew, Burke, and Ernzerhof exchange-correlation functional
CAM-B3LYP	Handy and coworkers' long-range corrected version of B3LYP using the Coulomb-attenuating method
ωB97XD	Functional from Head-Gordon and coworkers including empirical dispersion
LC-BLYP	The long correction of Hirao and coworkers
TD-DFT	Time-dependent density functional theory
STOs	Slater-type orbitals
GTOs	Gaussian-type orbitals
SV	Split valence
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
fs	Femtosecond
kcal·mol^{-1}	Kilocalorie per mole
UV-vis	Ultraviolet-visible
SVP	Split valence polarized
SV(P)	Split valence
N	Normal form
IS*n*	Intermediary structure for each proton transfer
T	Tautomer
eV	Electron volts

m-MeHBO	2-(2′-Hydroxy-4′-methylphenyl)benzoxazole
MHBO	2-(2′-Hydroxy-4′-methoxyphenyl)benzoxazole
CNHBO	2-(2′-Hydroxy-4′-cyano-phenyl)benzoxazole
HBOM	2-(2′-Hydroxyphenyl)-6-methylbenzoxazole
HBOF	2-(2′-Hydroxy-phenyl)-6-fluoro-benzoxazole
HBOA	2-(2′-Hydroxyphenyl)-6-cabaldehydeben-zoxazole
HBOE	2-(2′-Hydroxyphenyl)benzoxazole-6-carboxylic acid ethyl ester
m-MeHBON	2-(2′-Hydroxy-4′-methylphenyl)-6-nitrobenzoxazole
SCRF	Self-consistent reaction field
C-PCM	The polarizable conductor calculation model
LR	Linear-response
SS	State-specific



LIST OF SYMBOLS

S	Excited singlet state
T	Excited triplet state
$\hbar$	Planck constant
υ	Frequency
S_0	Ground state
S_1	First excited singlet state
S_2	Second excited singlet state
T_1	First excited triplet state
S_n n>1	Second to n excited singlet states
Φ_F	Fluorescence quantum yield
τ	Fluorescence lifetime
°	Degree
o	*ortho*
m	*meta*
R	Substituent
Ψ	Wavefunction
$\hat{H}$	Hamiltonian operator
E	Total energy
ψ	Wavefunction associated with solving the electron part
χ	Wavefunction associated with nuclear motion
T	Kinetic energy
V	Potential energy
$T_N(R)$	Kinetic energy of the nuclei
$T_e(r)$	Kinetic energy of the electrons
$V_{eN}(r,R)$	Electron-nuclei attractive Coulomb potential
$V_{NN}(R)$	Nuclear-nuclear repulsive Coulomb potential and
$V_{ee}(r)$	Electron-electron repulsive Coulomb potential

α and β	Spin α and β of electron
N	Many electron
$\psi_i(N)$	Spin-obital
$\hat{f}$	Fock operator
ε_i	Spin-obital energy
$\hat{H}^{(0)}$	Unperturbed Hamiltonian
$\hat{V}$	Perturbation
$E^{(0)}$	Zeroth-order energy
$E^{(1)}$	First-order energy
$E^{(2)}$	Second-order energy
I	A finite number
C_i	Expansion coefficients
s	State
e^C	Exponential operator
$\boldsymbol{A}$	The Jacobian matrix
∞	Infinity
ρ	Electron probability density
$\rho(r)$	Entire electron density of the molecule
$E[\rho]$	Electronic energy as a function of electron density
$E_T[\rho]$	Kinetic energy as a function of electron density
$E_V[\rho]$	Potential energy as a function of electron density
$E_U[\rho]$	External energy as a function of electron density
$E_{XC}[\rho]$	Exchange-correlation energy as a function of electron density
V_{XC}	Exchange-correlation potential
$\delta\rho$	Integral of electron density
$E_{XC}^{Hybrid}[\rho]$	Hybrid functional energy of a mixture of Hartree-Fock exchange with DFT exchange-correlation
C	Constants determined by Becke
$\rho(r, t)$	Time-dependent potentials and electron densities
ν	Vibration
c_k	A set of first-order differential equation for the amplitudes

k	Electronic state
V_k	Potential energy surface for state k
v	The nuclear velocity
F_{kj}	The nonadiabatic coupling vector between the states k and j
P^W	A Wigner distribution
P^i	Momentum associated with the normal coordinate
Q^i)	Normal coordinate
ξ_{OH}^i	The harmonic oscillator wavefunction
s	*s*-orbital
p	*p*-orbital
d	*d*-orbital
I	*syn*-HBO
II	*anti*-HBO
II	opened HBO
VI	Intramolecular hydrogen-bonded HBO
V	Intermolecular hydrogen-bonded HBO
VI	Intermolecular hydrogen bonding with water or opened-HBO
π	Pi
ππ* and π-π*	Pi to pi* transition (proton transfer)
nπ* and n-π*	n to Pi* transition (intramolecular charge transfer)
πσ*	Pi to sigma* transition (hydrogen-atom transfer)
Å	Angstrom
ΔE	Relative energy
%	Per cent
f	Oscillator strength
Δλ	Deviation between the calculated and experimental wavelength

ข้อความแห่งการริเริ่ม

1) การจำลองพลวัตที่สภาวะกระตุ้นของ 2-(2′-ไฮดรอกซีฟีนิล)เบนซอกซาโซล (HBO) และกลุ่มของน้ำ สามารถให้ข้อมูลทางภาพที่ชัดเจนในระดับโมเลกุลของกระบวนการถ่ายโอนโปรตอน และสามารถใช้เป็นข้อมูลสำหรับการศึกษาเพิ่มเติมในระบบที่คล้ายคลึงที่มีตัวทำละลาย

2) ตัวแทนที่ดีของ HBO ที่มีหมู่แทนที่ซึ่งให้ความเข้มแสงของการคายแสงสูง สโตคส์ชิฟท์มาก และคายแสงในช่วงความยาวคลื่นยาวขึ้นคือ HBO ที่มีหมู่รับอิเล็กตรอนได้ดีแทนที่อยู่บนส่วนของเบนซอกซาโซล

3) การทำนายผลจากการคำนวณด้วยคอมพิวเตอร์เป็นประโยชน์ในการแปลผลการทดลอง และสามารถใช้เป็นเครื่องมือคัดกรองเพื่อแนะนำนักเคมีในการสังเคราะห์อนุพันธ์ HBO ตัวใหม่ได้

STATEMENTS OF ORIGINALITY

1. The excited-state dynamics simulations of 2-(2′-hydroxyphenyl)benzoxazole (HBO) and its hydrated clusters can provide clear pictures in molecular level of proton transfer process and can be used for further studies in the similar systems with solvents.

2. The good candidates of HBO having substituents that provide high intensity of emission, large Stokes shift, and emission in the longer wavelength for use as a fluorescent sensor are HBO having strong electron-withdrawing groups substituted on a benzoxazole moiety.

3. The prediction from the computational calculations is helpful to interpretation of experimental results and can be used as a screening tool to guide chemists for synthesizing new HBO derivatives.