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For Marzena and Julia

Contents

List of Abbreviations

2D	Two-dimensional
ADF	Amsterdam Density Functional program
axial His	Histidine coordinated to Mg^{2+} ion of bacteriochlorophyll *a*
anionic His	Histidine with N_π and N_τ atoms deprotonated
B	Accessory bacteriochlorophyll *a*
B3LYP	Becke 3-Parameter, Lee–Yang–Parr exchange-correlation functional
B800	BChl *a* system in LH2 absorbing at wavelength of 800 nm
B850	BChl *a* system in LH2 absorbing at wavelength of 850 nm
BChl *a*	Bacteriochlorophyll *a*
BChl *a*–His	Bacteriochlorophyll *a*-histidine complex
BLYP	Becke–Lee–Yang–Parr exchange-correlation functional
(B)RC	(Bacterial) Reaction Center
C	Carotenoid
cationic His	Histidine with N_π and N_τ atoms protonated
CIDNP	Chemically Induced Dynamic Nuclear Polarization
CT	Charge Transfer
DFT	Density Funcional Theory
ENDOR	Electron–Nuclear DOuble Resonance
EPR	Electron paramagnetic resonance
φ	Bacteriopheophytin *a*
FT	Fourier Transform
GGA	Generalized Gradient Approximation
GIAO	Gauge-Independent Atomic Orbital
GTF	Gaussian-type Function

H	HOMO
His	Histidine
KS	Kohn-Sham
L	LUMO
LDA	Local Density Approximation
LH1	Light-Harvesting complex I (antenna complex)
LH2	Light-Harvesting complex II (antenna complex)
MeIm	Methylimidazole
neutral$_\tau$ His	Histidine with protonated N_τ and deprotonated N_π
neutral$_\pi$ His	Histidine with protonated N_π and deprotonated N_τ
NICS	Nucleus Independent Chemical Shift
NMR	Nuclear Magnetic Resonance
P	Special Pair
PCET	Proton-Coupled Electron Transfer
PDB	Protein Data Bank
PES	Potential Energy Surface
ppm	parts per million
Q	Ubiquinone-10
QH_2	Ubiquinol
QM/MM	Quantum Mechanics/Molecular Mechanics
Rb.	*Rhodobacter*
RMSD	Root Mean Square Displacement
Rps.	*Rhodopseudomonas*
SOAP	Statistical Averaging of Orbital Potentials potential
SSNMR	Solid-state NMR
STF	Slater-type Function
TMS	Tetramethylsilane
TZP	Triple-Zeta basis set with one set of Polarization functions

Notation

$\widehat{\mathrm{A}}$	Operator A
χ,χ_s	Response function
χ_μ	Basis set function
χ_p	Primitive basis function
δ	Chemical shift [ppm], Chemical Shift Tensor Anisotropy [kHz]
Δ	Laplacian
∇	Nabla
ε_0	Permittivity of vacuum
$\epsilon_{xc}^{uniform}$	Exchange-correlation energy per electron of uniform electron gas
η	Chemical Shift Tensor Asymmetry
e	Electron charge, exponent
E	Energy
$\hbar = \frac{h}{2\pi}$	Planck constant
$\widehat{\mathrm{H}}$	Hamiltonian
J	Coulomb electron–electron repulsion
m	Electron mass
M	Nuclear mass
n	When used in a sum indicates the number of electrons
N	When used in a sum indicates the number of nuclei
ϕ	Kohn-Sham orbital
Ψ	Wavefunction of a system

Q_x	Less intense absorption band of BChl a in the region of 550–600 nm
Q_y	Intense absorption band of BChl a in the region of 750–800 nm
ρ	Electron density
r	Distance
$\mathbf{r}$	Position of the all electrons, vector position is space
$\mathbf{r_i}$	Position of electron i
r_{ij}	Distance between electrons i and j
$\mathbf{R}$	Position of the all nuclei
$\mathbf{R_I}$	Position of nucleus I
R_{IJ}	Distance between nuclei I and J
t	Time
T	Kinetic energy
υ	Potential
V	Potential energy
Y	Spherical harmonic function
Z	Atomic number

Preface

Everything started in 1780 [1] when Joseph Priestley, an English chemist, enclosed a mint plant and a burning candle in a glass jar. Surprisingly, the candle burned without interruption, even though in earlier experiments it was extinguished quickly when no plant was present in the jar. After several more tests he concluded that plants could “restore air which has been injured by the burning of candles” and that “the air would neither extinguish a candle, nor was it all inconvenient to a mouse which I put into it”. His experiments reached a Dutch physician Jan Ingenhousz who then spent a summer near London performing over 500 experiments. He found that only green parts of a plant and only under the sunlight can “correct the bad air” and they make it in a matter of a few hours. Very soon after Jean Senebier, a Swiss pastor and botanist working in Geneva, demonstrated that carbon dioxide is taken up during photosynthesis and a Swiss chemist, Nicolas-Théodore de Saussure, discovered that the other necessary reactant is water. Finally, a German surgeon Julius Robert Mayer completed the basic equation of photosynthesis with the statement that plants convert elusive solar energy into a more rigid form — the chemical energy. It then became evident that in the course of photosynthesis carbon dioxide and water are converted with the use of solar light into glucose and a waste product, oxygen. The “waste” we are highly dependent on...

$$6CO_2 + 6H_2O \xrightarrow{h\nu} C_6H_{12}O_6 + 6O_2$$