

APPENDICES



CONTENTS

<i>A.1</i>	<i>Units</i>	<i>207-208</i>
<i>A.2</i>	<i>Abbreviations</i>	<i>209</i>

SUMMARY

A description is given of the units used in this thesis, and a list of frequently used abbreviations with the corresponding term is given.

A.1

Units

Description of units used in this thesis and conversion factors for transformation into other units

The formulas and properties presented in this thesis are reported in *atomic units* unless explicitly noted otherwise; the exceptions to this rule are energies, which are most frequently reported in kcal/mol, and distances that are normally reported in Å.

In the *atomic units* system, four frequently used quantities (Planck's constant h divided by 2π [\hbar], mass of electron [m_e], electron charge [e], and vacuum permittivity [$4\pi\epsilon_0$]) are set explicitly to 1 in the formulas, making these more simple to read. For instance, the Schrödinger equation for the hydrogen atom is in SI units:

$$\left[\frac{\hbar^2}{2m_e} \right] \nabla^2 \psi - \left[\frac{e^2}{4\pi\epsilon_0 r} \right] \psi = E \psi \quad (1)$$

In atomic units, it looks like:

$$\frac{1}{2} \nabla^2 \psi - \frac{1}{r} \psi = E \psi \quad (2)$$

Before a quantity can be used in the *atomic units* equations, it has to be transformed from SI units into atomic units; the same is true for the quantities obtained from the equations, which can be transformed from atomic units into SI units. For instance, the solution of equation (2) for the ground state of the hydrogen atom gives an energy of -0.5 atomic units (Hartree), which can be converted into other units quite simply by multiplying with the appropriate conversion factor (see table A.1.1).

Not only are the equations easier to comprehend, it is also easier to apply them on atoms and molecules; suppose that, for instance, the electrostatic interaction between two atoms with unit point charge at 100 Bohr distance from each other is needed. In SI units, one would have to multiply $1/4\pi\epsilon_0$ twice with the charge in SI units ($1.602 \cdot 10^{-19}$ C), and then divide by the distance (in m!) to obtain the energy in J, which would have to be transformed into kcal/mol. In atomic units it is simply dividing the unit charges by the distance, leading to 0.01 Hartree, or 6.2751 kcal/mol.

Two other useful factors concerning the conversion from energy (in eV) to wavelength (in nm) and are the following:

– wavelength λ (nm) from energy E (eV) $\lambda = 1239.84/E$ (3)

– electron resonant frequency ν $\nu(\text{cm}^{-1}) = \nu(\text{MHz}) \cdot 0.3335 \cdot 10^4$ (4)

TABLE A.1.1. ATOMIC UNIT SYSTEM AND CONVERSION FACTORS

quantity		value in a.u.		value in SI units
m_e	electron mass	1	$9.10938188(72) \cdot 10^{-31}$	kg
\hbar	angular momentum	1	$1.054571596(82) \cdot 10^{-34}$	Js
h	Planck's constant	2π	$6.62606876(52) \cdot 10^{-34}$	Js
e	charge	1	$1.602176462(63) \cdot 10^{-19}$	C
$4\pi\epsilon_0$	vacuum permittivity	1	$1.112650056 \cdot 10^{-10}$	F/m
a_0	length (Bohr)	1	$5.291772083(19) \cdot 10^{-11}$	m
E_h	energy (Hartree)	1	$4.35974381(34) \cdot 10^{-18}$	J
			627.50947(5)	kcal/mol
			2625.4996(2)	kJ/mol
			27.2113834(11)	eV
c	speed of light	$137.03599976(50)$	$2.99792458 \cdot 10^8$ ^a	m
μ	unit dipole moment	1	$8.47835267365(33) \cdot 10^{-30}$	Cm
			2.54174619(10)	Debye
$\mu'{}^b$	unit polarizability	1	$1.481847093(16) \cdot 10^{-31}$	m ³
			0.1481847093(16)	Å ³
μ_B	Bohr magneton	1/2	$9.27400899(37) \cdot 10^{-24}$	J/T
μ_N	nuclear magneton	$2.72308512(11) \cdot 10^{-4}$	$5.05078317(20) \cdot 10^{-27}$	J/T

a) Exact!

b) In SI units this corresponds to a polarizability volume ($\mu' / 4\pi\epsilon_0$)

A.2

Abbreviations

A list of descriptions for abbreviations that are frequently used in this thesis

<i>Ad</i>	<i>Alcaligenes denitrificans (azurin)</i>
ADF	Amsterdam Density Functional (program)
AMBER	Assisted Model Building with Energy Refinement
<i>az.</i>	<i>azurin</i>
BSSE	Basis Set Superposition Error
CIS	Configuration Interaction using Singles excitations only
CNDO	Complete Neglect of Differential Overlap
DFT	Density Functional Theory
DRF	Direct Reaction Field (approach)
DZV	Double Zeta Valence (basis set)
EPR	Electron Paramagnetic Resonance
ESR	Electron Spin Resonance
F114A	Phe114 Ala114 mutant (<i>azurin</i>)
GROMACS	GRoningen MACHine for Chemical Simulations
GROMOS	GRoningen MOlecular Simulation (package)
H117G	His117 Gly117 mutant (<i>azurin</i>)
HF	Hartree-Fock
IMOMM	Integrated Molecular Orbital and Molecular Mechanics (model)
INDO	Intermediate Neglect of Differential Overlap
M121H	Met121 His121 mutant (<i>azurin</i>)
M121Q	Met121 Gln121 mutant (<i>azurin</i>)
MD	Molecular Dynamics (simulations)
MDC-q	Multipole Derived Charges, reproduced up to quadrupole level
MM	Molecular Mechanics
N42C/H117G	Asn42 Cys42, His117 Gly117 double mutant (<i>azurin</i>)
N47D	Asn47 Asp47 mutant (<i>azurin</i>)
N47L	Asn47 Leu47 mutant (<i>azurin</i>)
ONIOM	Our own N-layered Integrated molecular Orbital + molecular Mechanics (method)
<i>Pa</i>	<i>Pseudomonas aeruginosa (azurin)</i>
QC	Quantum Chemistry
QM	Quantum Mechanics
RHF	Restricted Hartree Fock
ROHF	Restricted Open shell Hartree Fock
TD-DFT	Time-Dependent Density Functional Theory
TZ2P	Triple Zeta valence (basis) including double Polarization functions
TZP	Triple Zeta valence (basis set) including Polarization functions
xc	exchange-correlation (potential)
<i>wt</i>	<i>wildtype (azurin)</i>