Appendix C

Symbols, conversions, and atomic units

This appendix provides a tabulation of all symbols used throughout this thesis, as well as conversion units that may useful for reference while comparing results. Tabel C.6 lists the most common energy units and their conversion factors.

All operators in this thesis are denoted as $\hat{\mathsf{O}}$, all matrices are in bold-face, $\mathbf{M}$, and all vector quantities appear with a vector symbol, $\vec{\mathrm{v}}$. Symbols in each table are listed alphabetically.

Atomic units were used in this thesis during the simulations of rotational wave packets (see Section 4.4.1). Since the eigenvalues of the angular momentum operators are quantized according to $\hbar$, atomic units are convenient in discussions of angular momentum since $\hbar$ receives the numerical value 1. The mass of the electron, m_e, and the charge of the proton, e', and permittivity $4\pi\epsilon_0$ are also set to 1 in atomic units. Table C.7 lists several common physical quantities in atomic units.

QUANTITY	SYMBOL
Energies	
exact ground state nonrelativistic energy	$\mathcal{E}_0$
correlation energy	E_{corr}
exact nonrelativistic electronic energy	$\mathcal{E}_{el}$
Hartree-Fock energy	E_{HF}
ith orbital energy	ε_i
ith exact electronic eigenvalue	$\mathcal{E}_i$
ith eigenvalue of Hamiltonian	E_i
nth order perturbation energy terms	$E_i^{(n)}$
Jth rigid rotor energy	E_J
kth unperturbed wave function energy	$\mathcal{E}_k$
vibrational bound-state eigenenergy	E_v
total energy	$\mathcal{E}_{tot}$
classical kinetic energy	T
discretized kinetic energy	T_k
effective Hartree-Fock potential	V^{HF}
discretized potential energy	$\mathrm{V}(r)$
Angular momenta	
total angular momentum	J
projection of J on body-fixed z axis	K
electronic orbital angular momentum	L
projection of L on body-fixed z axis	Λ
projection of J on space-fixed Z axis	M
$\Lambda + \Sigma$	Ω
nuclear angular momentum	R
spin (intrinsic) angular momentum	S
projection of S on body-fixed z axis	Σ

Table C.1: Symbols of energies and angular momenta

QUANTITY	SYMBOL
Constants	
Bohr radius	a_0
speed of light	c
dielectric constant	ϵ_0
Planck's constant	$\hbar$
Boltzmann constant	k_B

Table C.5: Symbols of constants

QUANTITY	SYMBOL
Functions	
spin-up (↑) function	$\alpha(\varpi)$
spin-down (↓) function	$\beta(\varpi)$
spin orbital	χ
ith canonical Fock spin orbital	χ_i
time-dependent electric field	$\vec{E}(t)$
time-dependent electric field	$f(t)(\equiv E(t))$
frequency-dependent electric field	$\mathcal{F}(\omega)$
basis functions	ϕ
exact wave function for electronic ground state	Φ_0
exact electronic wave function	Φ_{el}
exact time-dependent nuclear wave function	$\Phi_{nuc}(t)$
exact total wave function	$\Phi_{tot}(t)$
sum of exact total time-dependent wave functions	$\Psi_{tot}(t)$
gobbler function	$G(r_i)$
error	$\mathcal{O}(\Delta t)$
kets of momentum space	$\|p\rangle$
rotational partition function	$Q_{\mathrm{rot}}(T)$
kets of coordinate space	$\|r\rangle$
autocorrelation function	$S(t)$
electric field envelope function	$s(t)$
absorption cross-section	$\sigma(\omega)$
integral over Euler angles	$W_{\mathrm{dip}}(\phi, \theta, \chi)$
Boltzmann weighting	$w_J(T)$
spherical harmonic	$Y_J^M(\theta, \phi)$
spatial orbital	ψ
Hartree-Fock wave function	Ψ_0
jth vibrational eigenvector of discretized space	Ψ_j^v

Table C.2: Symbols of functions

QUANTITY	SYMBOL
Operators	
identity operator	$\hat{\mathbf{1}}$
Fock operator	$\hat{\mathbf{f}}$
one-electron Hamiltonian	$\hat{\mathbf{h}}$
Hamiltonian	$\hat{\mathbf{H}}$
perturbation Hamiltonian	$\hat{\mathbf{H}}'$
zeroth-order Hamiltonian	$\hat{\mathbf{H}}_0$
electronic Hamiltonian	$\hat{\mathbf{H}}_{el}$
Hartree-Fock Hamiltonian	$\hat{\mathbf{H}}_{HF}$
nuclear Hamiltonian in effective electronic field	$\hat{\mathbf{H}}^{el}_{nuc}$
rigid rotor Hamiltonian	$\hat{\mathbf{H}}_{rr}$
total angular momentum operator	$\hat{\mathbf{J}}$
one-electron coulomb operator	$\hat{\mathbf{J}}_b$
one-electron exchange operator	$\hat{\mathbf{K}}_b$
Legendrian operator	$\hat{\Lambda}^2$
dipole moment operator	$\vec{\boldsymbol{\mu}}$
Laplacian operator	$\hat{\boldsymbol{\nabla}}^2$
momentum operator	$\hat{\mathbf{p}}$
position operator	$\hat{\mathbf{r}}$
two-electron potential energy operator	$\hat{\mathbf{r}}_{12}^{-1}$
kinetic energy operator	$\hat{\mathbf{T}}$
potential energy operator	$\hat{\mathbf{V}}$
time-dependent potential energy operator	$\hat{\mathbf{V}}(t)$
time-dependent external potential energy	$\hat{\mathbf{V}}^{ext}(t)$
time evolution operator	$\hat{\mathbf{U}}$
Matrices	
polarizability tensor	$\boldsymbol{\alpha}$
expansion coefficients matrix	$\mathbf{C}$
orbital energy matrix	$\boldsymbol{\varepsilon}$
Fock matrix	$\mathbf{F}$
inertia tensor	$\mathbf{I}$
rotation matrix	$\mathbf{R}$
overlap matrix	$\mathbf{S}$

Table C.3: Symbols of operators and matrices

QUANTITY	SYMBOL
Variables	
spin-orbit interaction term	$\mathcal{A}$
rotational constant	B
expansion coefficients	c
rotational wave function expansion coefficients	$C^{J\,\Omega\,M}$
Clebsch-Gordan coefficients	C
expansion coefficients of rotation matrix **R**	$D^{J}_{M'\,M}$
electric field polarization	$\vec{\varepsilon}$
electric field strength	E_0
electric field carrier envelope phase	φ
Euler angles of rotation	ϕ,θ,χ
gobbler parameters	g, g_0
collinear bond angle	γ
maximum intensity	I_{max}
force constant	k
discretized wave number	Δk
number of spatial orbitals	K
grid length	$L = \mathcal{N}\Delta r$
generalized particle mass	m
electron mass	m_e
nuclear mass	m_{nuc}
permanent dipole moment	μ_0
reduced mass	μ
main quantum number	n
generalized rotation axis	$\vec{n}$
number of electrons	N
number of particles	$\mathbb{N}$
number of grid discretizations	$\mathcal{N}$

vibrational frequency	ν
radiation wavelength	λ
electric field carrier frequency	ω
discretized momentum variable	Δp
generalized rotation angle	ξ
charge	Q
spatial coordinate	$\vec{r}$
equilibrium internuclear distance	r_0
discretized position variable	Δr
i–j interelectron distance	r_{ij}
i–A nuclear-electron distance	r_{iA}
A–B internuclear distance	R_{AB}
Gaussian pulse width	σ
rotational period	τ_{rot}
time	t
initial time	t_0
pulse duration	t_p
discretized time variable	Δt
temperature	T
vibrational quantum number	υ
body-fixed Cartesian coordinates	x, y, z
space-fixed Cartesian coordinates	X, Y, Z
spatial and spin coordinate	$\vec{x}$
spin coordinate of α and β spin functions	ϖ
atomic number	Z_A
perturbation	ζ

Table C.4: Symbols of variables

Joule	kJ·mol^{-1}	eV	au	cm^{-1}	Hz
1 Joule =1	6.022×10^{20}	6.242×10^{18}	2.2939×10^{17}	5.035×10^{22}	1.509×10^{33}
1 kJ·mol^{-1} =1.661×10^{-21}	1	1.036×10^{-2}	3.089×10^{-4}	83.60	2.506×10^{12}
1 eV =1.602×10^{-19}	96.48	1	3.675×10^{-2}	8065	2.418×10^{14}
1 au =4.359×10^{-18}	2625	27.21	1	2.195×10^{5}	6.580×10^{15}
1 cm^{-1} =1.986×10^{-23}	1.196×10^{-2}	1.240×10^{-4}	4.556×10^{-6}	1	2.998×10^{10}
1 Hz =6.626×10^{-34}	3.990×10^{-13}	4.136×10^{-15}	1.520×10^{-16}	3.336×10^{-11}	1

Table C.6: Conversion factors for energy units, adapted from Ref. [176]

Quantity	SI units	Atomic Units
mass	$9.109\ 534\times10^{-31}$ kg	$m_e=1$
charge	$1.602\ 189\ 2\times10^{-19}$ C	$\|e\|=1$
angular momentum	$1.054\ 588\times10^{-34}$ J s	$\hbar=1$
permittivity	$1.113\ 65\ \times10^{-10}$	$\kappa=4\pi\varepsilon_0=1$
length	$5.291\ 772\ 49\times10^{-11}$ m	$\kappa\hbar^2/me^2=a_0=1$ (bohr)
energy	27.211 4 eV	$e^2/\kappa a_0=1$ (hartree)
time	$2.418\ 9\times10^{-17}$ s	$\kappa^2\hbar^3/me^4=1$
electric dipole	$8.478\ 36\ \times10^{-30}$ C m(=2.54 Debye)	$ea_0=1$
electric potential	27.11 V	$e/\kappa a_0=1$
electric field strength	$5.142\ 208\ \times10^{11}$ V/m	$e/\kappa {a_0}^2=1$

Table C.7: Conversion from SI units to atomic units, adapted from Ref. [176]