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EXPRESSION OF RESULTS IN QUANTUM CHEMISTRY

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EXPRESSION OF RESULTS IN QUANTUM CHEMISTRY

The end product of a theoretical computation is likely to be a number or a set of numbers that express the value of some computed energy, distance or other quantity. Conversion to the value expressed in SI requires each number to be multiplied by a simple mixture of physical constants, themselves expressed in SI. Since the accepted values of these constants in SI are liable to minor change as new measurements concerning e, $\hbar$, m_e, etc. are available, the conversion to SI is appropriately made by the reader rather than by the author of a publication. Since many readers may not be familiar with the required mixture of constants it is RECOMMENDED that wherever applicable these physical constants be inserted appropriately in the output information of a theoretical paper. Thus, in recording a calculated distance, r, the form might be $= 5.1\ a_o$ or $r/a_o = 5.1$ with the second arrangement being especially suited to tabular matter. Likewise, a magnetic moment would appear as $m = 5.2\ e\ \hbar/m_e$ or $m/\ (e\ \hbar\ /m_e) = 5.2$. (See also the appendix). Of course the values expressed in SI units may also be given where required for discussion; if precise values of the physical constants are required for the conversion to SI the appropriate reference for the values used must be given.

This leaves the question of which physical constants are to be recognized by the reader. The four SI dimensions of length, mass, time and current require four physical constants to be permitted and a sensible minimum choice might be m_e, e, $\hbar$ and $4\pi\varepsilon_o$. Extension beyond these four is not essential, but it is useful to have a separate symbol and name for two, widely used mixtures of these four, namely:

$$(4\pi\varepsilon_o\ \hbar^2\ /\ m_e e^2) = a_o \text{ the Bohr radius}$$

and $$(m_e e^4\ /\ 16\pi^2\varepsilon_o^2\hbar^2) = e^2\ /\ 4\pi\varepsilon_o a_o = \hbar^2\ /a_o^2 m_e = E_h \text{ the Hartree energy}$$

While other constants could be introduced, any quantity not involving nuclear mass, temperature, the velocity of light† or the theory of relativity requires no more than four of the five quantities, m_e, e, $\hbar$, E_h and a_o. Others would be rarely used and unfamiliar and so defeat the object of the recommendation, whose purpose is to make the numerical end results of theoretical work easily transformed to SI by any reader.

The acceptance of this recommendation would circumvent the need for a set of atomic units each with its own symbol and name. It is the traditional use of the phrase "atomic units" in this area which has obscured the real problem.

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†Normally, within calculations retaining relativistic effects, the velocity of light should be given a value equal to the reciprocal of the fine structure constant, namely $\sim$ 137.03604.

Appendix

A table follows with the physical constants or mixtures of physical constants, to be normally used as a factor, to convert into SI the results of theoretical computations of a selected list of physical quantities.

In the first column these physical quantities are listed. The second column shows their usual symbols. The mixture of physical constants X corresponding to each physical quantity is given in the third column; the descriptions of X are not unique (e.g. $E_h = \hbar^2 a_o^{-2} m_e^{-1}$) but the value in SI is naturally unaffected by the form in which X is expressed. For convenience the final column of the table gives values of X to five significant figures. These values are based on CODATA Bulletin No. 11 (December 1973), Committee on Data for Science and Technology of the International Council of Scientific Unions; for higher accuracy the most recent table of physical constants should be used to re-evaluate the numbers.

Calculated physical quantity	Usual symbol	X	Value of X
Length	ℓ	a_o	5.2918×10^{-11} m
Mass	m	m_e	9.1095×10^{-31} kg
Time	t	$\hbar E_h^{-1}$	2.4189×10^{-17} s
Electric current	I	$e E_h \hbar^{-1}$	6.6237×10^{-3} A
Energy	E	E_h	4.3598×10^{-18} J
Charge	Q	e	1.6022×10^{-19} C
Angular momentum	L	$\hbar$	1.0546×10^{-34} J s
Electric dipole moment	p, μ	$e a_o$	8.4784×10^{-30} C m (†)
Electric quadrupole moment	Θ	$e a_o^2$	4.4866×10^{-40} C m^2
Polarizability	α	$e^2 a_o^2 E_h^{-1}$	1.6488×10^{-41} C^{2}m^{2}J^{-1}
Electric field	E	$E_h e^{-1} a_o^{-1}$	5.1423×10^{11} V m^{-1}
Electric field gradient	$-V_{zz}$	$E_h e^{-1} a_o^{-2}$	9.7174×10^{21} V m^{-2}
Magnetic moment*	m, μ	$e \hbar m_e^{-1}$	1.8548×10^{-23} J T^{-1}
Magnetizability	ξ	$e^2 a_o^2 m_e^{-1}$	7.8910×10^{-29} J T^{-2}
Magnetic flux density	B	$\hbar e^{-1} a_o^{-2}$	2.3505×10^{5} T
Magnetic vector potential	A	$\hbar a_o^{-1} e^{-1}$	1.2439×10^{-5} m T
Current density	j	$e E_h \hbar^{-1} a_o^{-2}$	2.3654×10^{18} A m^{-2}
Linear momentum	p	$\hbar a_o^{-1}$	1.9929×10^{-24} kg m s^{-1}
Probability density	$\psi^2(x,y,z)$	a_o^{-3}	6.7483×10^{30} m^{-3}
Note also the molar quantities:-			
Molar energy	E_m		2.6255×10^{6} J mol^{-1}
Molar polarizability	α_m		9.9290×10^{-18} C^2 m^2 J^{-1}mol^{-1}
Molar magnetizability	ξ_m		4.7520×10^{-5} J T^{-2} mol^{-1}

† ea_o also corresponds to ∿2.5418 Debye

* X for magnetic moment is TWICE the value of the Bohr magneton