CHEM2100J Chapter 00-02 RC

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Comments on Homework, Quizzes and Exams

- Homework
  - is designed to prepare you for the quizzes and deepen your understanding of some basic concepts
  - will not be accepted after the closing time and will receive an automatic grading of zero points.
  - only contains multiple choice questions, only retains the last attempt
- Quizzes
  - short examinations of 5 min length on a regular basis, focussing on individual or thematically connected chapters
  - the questions will be different between individuals
  - the grades and answers will be published manually sometimes after the afternoon class
- Exams
  - a 45 minutes midterm exam and a 100 minutes final exam
  - cannot use any form of dictionaries
  - cheating paper may help you a lot, but do not refer to it all the time

Advice

- Attend and listen carefully in lectures and RC.
- Practice your skills on using calculator.
- Carefully finish the homework; refer to exercises in the textbook if you have time.
- Read *Chemical Principle* before and after the lectures. Don't rely too much on Chinese textbooks.
- Ask questions at OH as much as possible. TAs reserve the rights not to answer questions asked via WeChat and Feishu.
- **AI** tools are strictly **PROHIBITED** in this course! Please don't use them to do your homework!

Significant Figures

- **Counting rule**
  Count the number of figures starting from the first non-zero one.
- **Rounding rule**
  - Above 5 - round up
  - Exactly 5 - round to even if no figures behind; round up otherwise
  - Below 5 - round down
- **Operational rule**
  - +-: follow the least decimal place
  - */: follow the least significant figures
  - exponent: decimal place of index = significant figures of answer
  - logarithm: significant figures of antilogarithm = decimal place of answer

Tip: Don't round up in the middle of the calculation!

Significant Figures

Example

1.0080
0.0035
5000
5000.
3.45×10^4
Plank's constant $h = 6.626 \times 10^{-34}$
$(604.01 + 0.53) \times 321.81$

Determine the number of the significant figures!

Significant Figures

Example

A Na_2CO_3 solution has pH=11.61, what's the concentration of H^+?

Significant Figures

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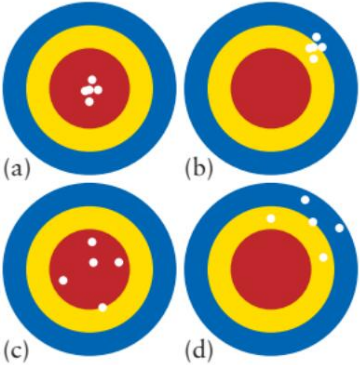
Answer

2.5×10^{-12}

Accuracy & Precision

- Accuracy: how close the average value of a series of measurements to the true value.
- Precision: how close repeated measurements are to one another.



Properties

- Extensive properties: **depends** on the **quantity** of matter
- Intensive properties: **independent** of the **quantity** of matter

Example

pressure

volume

density

temperature

speed

Determine whether the above properties are intensive or extensive!

Properties

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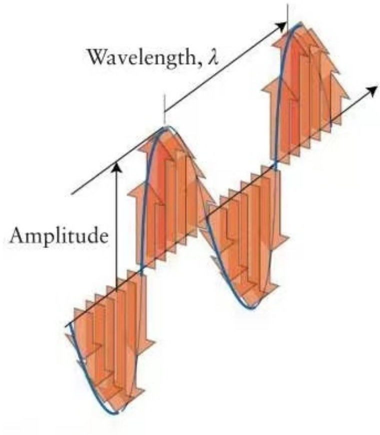
Determine whether the above properties are intensive or extensive!

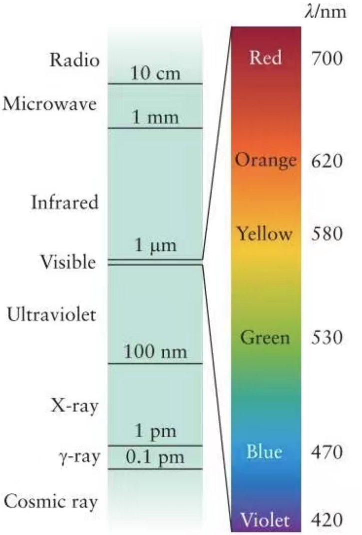
- Remark: Sometimes ratio of two extensive properties will be intensive properties

Electromagnetic Radiation



- Formula: $\lambda \times \nu = c$
- Amplitude
  - the height above the centerline
  - intensity=amplitude^2
- Wavelength
  - distance between peaks

Electromagnetic Spectrum



- Use this diagram to identify the type
- Do copy it onto your cheating paper

Atomic Models

- Democritus
- Dalton
- J.J.Thomson - "Plum-pudding Model"
  - Cathode ray experiment
  - Ratio of an electron's charge to its mass $\frac{e}{m_e}$
- Millikan
  - Oil drop experiment
  - $e = 1.62 \times 10^{-19}\text{C},\ m_e = 9.11 \times 10^{-31}\text{kg}$
- Rutherford - "Nuclear Model"
  - α Scattering Experiment
- Bohr - Bohr atomic model

Black Body

- Stefan-Boltzmann law
  - describes the exponential-like behavior of the total intensity of black body objects
  - Total intensity=$const \times T^4$
  - $const$=5.67×10^{-8} $\mathrm{W \cdot m^{-2} \cdot K^{-4}}$
- Wien's law
  - shows a maximum energy density exists in black body radiation
  - $T\lambda_{max} = const$
  - $const$= 2.898×10^{-3} m/K

Black Body

Exercise

Calculate the temperature of a sun whose maximum intensity of radiation occurs at 490 nm. Use 0.2898 cm/K as constant.

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Solution

According to Wien's law, $T\lambda_{max} = const$, we have

$$T = \frac{0.2898 \times 10^{-2}}{490 \times 10^{-9}} K = 5.91 \times 10^{3} K$$

Photoelectric Effect

$$E_{photon} = KE_{electron} + WorkFunction_{metal}$$

$$h\nu = \frac{1}{2}m_e v^2 + \Phi$$

- illustrates the particle nature of light
- exists a threshold frequency $\nu_0 = \frac{\Phi}{h}$

Exercise

Calculate the velocity of an electron ejected from a metal with a work function of 4.28 eV while being irradiated with light with a wavelength of 140 nm.

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Solution

$$\frac{1}{2}m_e v^2 = h\nu - \Phi$$

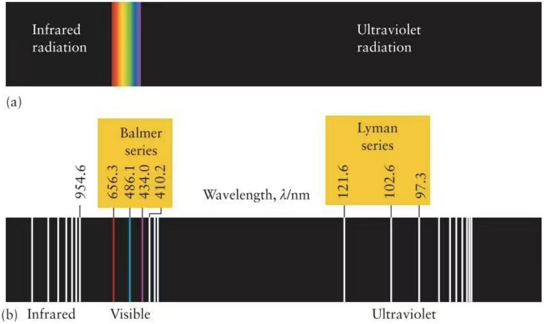
$$\nu = \frac{c}{\lambda}$$

Using the above equations, we can obtain that $v = 1.27 \times 10^6 \mathrm{m/s}$.

(Tip: be careful with the unit conversion! 1 eV=1.60×10^{-19}J)

Emission Spectra of Hydrogen

- **Formulas**
  - $\nu = \mathcal{R}(\frac{1}{n_1^2} - \frac{1}{n_2^2}),\ n_1 = 1, 2, ...; n_2 = n_1 + 1, n_1 + 2, ...$
  - $\frac{1}{\lambda} = \mathcal{R}_\lambda(\frac{1}{n_1^2} - \frac{1}{n_2^2}),\ n_1 = 1, 2, ...; n_2 = n_1 + 1, n_1 + 2, ...$
  - Rydberg constant: $\mathcal{R} = 3.29 \times 10^{15}\mathrm{Hz},\ \mathcal{R}_\lambda = 1.097 \times 10^7 m^{-1}$
- Balmer series - $n_1 = 2,\ n_2 = 3, 4...$
- Lyman series - $n_1 = 1,\ n_2 = 2, 3...$



Emission Spectra of Hydrogen

Exercise

- Use the Rydberg formula for atomic hydrogen to calculate the wavelength of radiation generated by the transition from n $= 2$ to n $= 1$
- What is the name given to the spectroscopic series to which this transition belongs?
- Determine the region of the spectrum in which the transition takes place?

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Solution

122nm; Lyman series; ultraviolet region

Wave-Particle Duality

de Broglie relation

$$\lambda = \frac{h}{p}$$

- matter has both wavelike and particlelike properties
- matter behaves wave properties as it propagates
- matter behaves particle properties when it interacts

Wave-Particle Duality

Exercise

The Gloriana-class battleship Hand of Dorn ($m = 160$ Mt) has engaged its sub-light engines and accelerated to 0.55c. Calculate the deBroglie wavelength.

Wave-Particle Duality

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Solution

According to de Broglie's relation,

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.626\times10^{-34}}{160\times10^{9}\times0.55\times3\times10^{8}}\text{m} = 2.51 \times 10^{-53}\text{m}$$

Heisenberg Uncertainty Principle

- $\Delta x \Delta p \geqslant \frac{1}{2}\hbar$
- $\hbar = \frac{h}{2\pi}$
- Δx is the uncertainty of position and Δp is the uncertainty of momentum

Exercise

Estimate the minimum uncertainty of the position of a 5.0g marble given that its speed is known within $\pm$ 0.20 mm/s.

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Estimate the minimum uncertainty of the position of a 5.0g marble given that its speed is known within $\pm$ 0.20 mm/s.

Solution

$$\Delta p = m\Delta v \leqslant 5.0 \times 10^{-3} \times 0.4 \times 10^{-3} \text{kg}\cdot\text{m/s} = 2.0 \times 10^{-6} \text{ kg}\cdot\text{m/s}$$

$$\Delta x \geqslant \frac{\hbar}{2\Delta p} \geqslant \frac{6.626\times 10^{-34}}{4\times 3.14\times 2.0\times 10^{-6}}\text{m} = 2.6 \times 10^{-29}\text{m}$$

Wave Function and Schrödinger Equation

Wave function

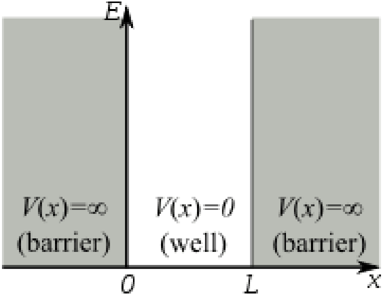
- Ψ - describes the state of microsystem; represents AO or MO in atomic or molecular system
- Ψ^2 - represents the probability density (NOT PROBABILITY!) of electrons in atoms or molecules
- Node - the point where $\Psi = 0$(the probability of finding electrons is 0)

Schrödinger Equation

- the intrinsic form: $-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$
- $-\frac{\hbar^2}{2m}\nabla^2\Psi$ stands for the kinetic energy, $V\Psi$ stands for the potential energy and E stands for the total energy

Particle in 1D Box

The model of 1D box is introduced to help you better understand QM!



Solving the Schrödinger Equation, we obtain the following results:

- when $x \leqslant 0$ or $x \geqslant L$, $\Psi(x) = 0$
- when $0 < x < L$, $\Psi_n(x) = \sqrt{\frac{2}{L}} sin(\frac{n\pi x}{L})$, n=1,2,...

Particle in 1D Box

Exercise

A particle of mass m is confined in a 1D box of length L. Given that the quantum number n, and Plank constant h is known, please verify that $E_n = \frac{n^2 h^2}{8mL^2}$.

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Remarks:

- energy levels are quantized and determined by n
- multiple possibilities of the state of motion
- as m,L increase, the separations between energy levels decrease

Quantum Numbers, Shells and Subshells

TABLE 1D.2 Quantum Numbers for Electrons in Atoms

Name	Symbol	Values	Specifies	Indicates
principal	n	$1, 2, \ldots$	shell	size
orbital angular momentum*	l	$0, 1, \ldots, n-1$	subshell: $l = 0, 1, 2, 3, 4, \ldots$ s, p, d, f, g, . . .	shape
magnetic	m_l	$l, l-1, \ldots, -l$	orbitals of subshell	orientation
spin magnetic	m_s	$+\frac{1}{2}, -\frac{1}{2}$	spin state	spin direction

Remarks:

- n,l determine the energy level of an orbital
- l,m_l determine the shape and orientation of an orbital
- m_s is independent with the other three quantum numbers

The Shape of Orbitals

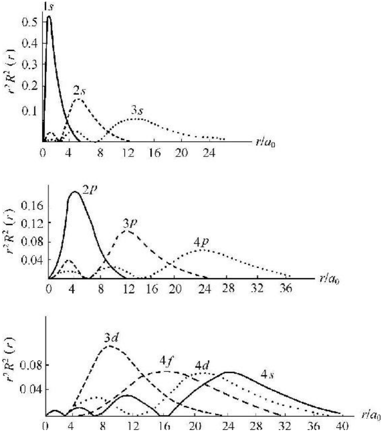
Shape of:

- s orbitals - sphere
- p orbitals - spindle
- d orbitals - petal

Number of:

- total orbitals=n^2
- total nodes=$n-1$
- radial nodes=$n-l-1$
- nodal planes=l

(View the 3D images in file "atomic orbitals.zip" on canvas)



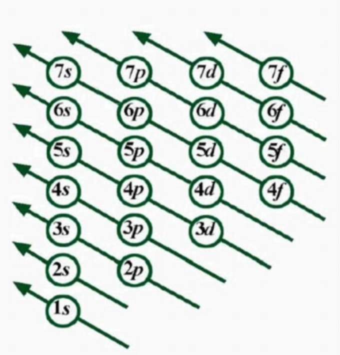
Radial distribution function of AO

Shielding Effect & Penetration Effect

- Shielding effect
  - due to the repulsion of the electrons on inner orbitals, the outer electrons will be shielded from the full attraction of the nucleus.
  - the effective nuclear charge $Z_{eff}e$ is always less than the nuclear charge Ze
  - will cause the energy of electrons $\uparrow$
- Penetration effect
  - the electrons also have the ability to penetrate through the inner cells
  - will cause the energy of the electrons $\downarrow$

Orbital Energies

- $E_n = -\frac{Z_{eff}^2 h\mathcal{R}}{n^2}$, n=1,2,...
- In a many-electron atom, because of penetration effect and shielding effect, the order of orbital energies in a given shell is $s < p < d < f$
- Between different shells, the energy levels may overlap



The Building-Up Principle

- Pauli exclusion principle
  - No more than two electrons may occupy any given orbital
  - When two electrons do occupy one orbital, their spins must be paired($\uparrow$ and $\downarrow$)
  - In other words, no two electrons in an atom can have the same set of four quantum numbers
- Hund's rule
  - If more than one orbital in a subshell is available, add electrons with parallel spins($\uparrow\uparrow$) to different orbitals of that subshell rather than pairing two electrons in one of the orbitals (lowest total energy)
  - Exceptions: half-complete or complete subshell configuration have lower energy

Electron Configuration

- Valence shell - the occupied shell with the largest value of n
- Valence electron - the electrons in the outermost shell
- Ground state - electrons are in the lowest energy state
- Excited state - electrons are in energy states higher than the ground state

Exercise

Write the ground state electron configuration for:

- Fe
- Fe^{3+}
- Cr
- Ag
- Ga

Reference

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Thank you!