2024 Fall Semester Final Examination

For General Chemistry I

[Class C] Prof. Hyunwoo Kim

Date: December 18(Wed), Time Limit: 19:00 ~ 21:00

Write down your information neatly in the space provided below; print your Student ID in the upper right corner of every page.

Professor Name	Class	Student I.D. Number	Name

Problem	points	Problem	points	TOTAL pts
1	/12	**6**	/6	
2	/13	**7**	/8	
3	/8	**8**	/16	/100
4	/10	**9**	/21	
5	/6			

** This paper consists of 20 sheets with 10 problems (***page 18 - 19***: Equation, constants & periodic table, ***page 20***: claim form). Please check all page numbers before taking the exam. Write down your work and answers in the Answer sheet. Please write down the unit of your answer when applicable. You will get 30% deduction for a missing unit.

NOTICE: SCHEDULES on RETURN and CLAIM of the MARKED EXAM PAPER.

(채점 답안지 분배 및 이의신청 일정)

1. Period, Location and Procedure

0 Return and Claim Period: **December 20 (Friday, 12:00 ~ 14:00, 2 hrs)**

The claim is permitted only on this period. Keep that in mind!

0 Location: Each designated room of Creative Learning Bldg. (E11)

Class	Room(E11)
C	405
D	406

0 Procedure

Rule 1: Students cannot bring their writing tools into the rooms (Use a pen only provided by TA)

Rule 2: With or without claim, you must submit the paper back to TA. (Do not go out of the room with it)

If you have any claims on it, write them on the claim form and attach it to the top of the exam paper with a stapler. Give them to your TA.

WARNING!!

If you deliberately alter any original answers or insert something on your marked paper to achieve a better grade, you will get a F grade for this course. Or if you don't keep the rules above, we will regard it as a kind of cheating and give you 0 point. So please don't cheat.

2. Final Confirmation

1) Period: ***December 21(Sat..) ~ 22(Sun)***

2) Procedure: During this period, you can check final score of the examination *on the website* again.

(No additional corrections. If no change in your score after reasoning, the claims were not accepted.)

***** For further information, please visit General Chemistry website at www.gencheminkaist.pe.kr***

1. (12 points)

Answer the following questions:

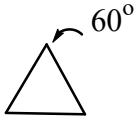
(1) (4 pts) Cyclopropane is 44 kJ/mol less stable than cyclohexane per CH_2 group due to its high strain and reactivity. Identify and describe two major types of strain present in cyclopropane. Explain how these strains contribute to its instability, using chemical structures to support your explanation.

(2) (4 pts) Cyclohexane is significantly more stable compared to cyclopropane. Discuss how the strains observed in cyclopropane are alleviated in cyclohexane. Use chemical structures to illustrate the release of these strains.

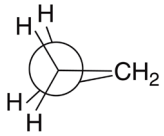
(3) (4 pts) Draw the most stable conformation of cyclohexane, explicitly showing all hydrogens.

(answer)

(1) **Angle Strain**: The bond angles in cyclopropane are constrained to approximately 60°, far from the ideal tetrahedral angle of 109.5°. This significant deviation compresses the sp3-hybridized carbon atoms, resulting in poor orbital overlap and weakened C-C bonds.

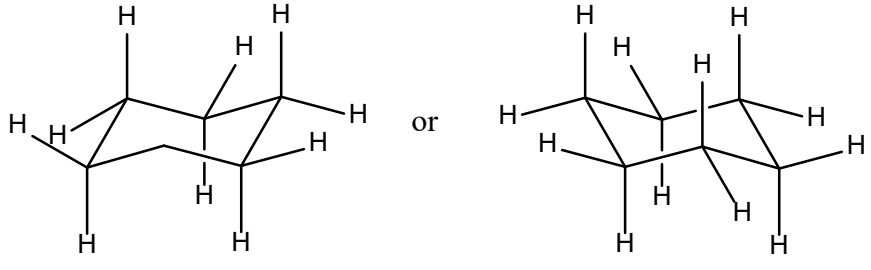


Torsional Strain: All C-H bonds in cyclopropane are eclipsed, leading to increased electron repulsion between adjacent hydrogen atoms. (-1 pts for no mention of "eclipsed", -1 pts for no chemical structure)



(2) The bond angles are close to the ideal tetrahedral angle (109.5°), **releasing angle strain**. The staggered arrangement of C-H bonds eliminates **torsional strain**, as no hydrogens are eclipsed. (-1 pts for no mention of "staggered", -1 pt for no chemical strcuture)

(3)



(-2 pts for non-parallel C-H bonds to C-C bonds)

2. (13 points)

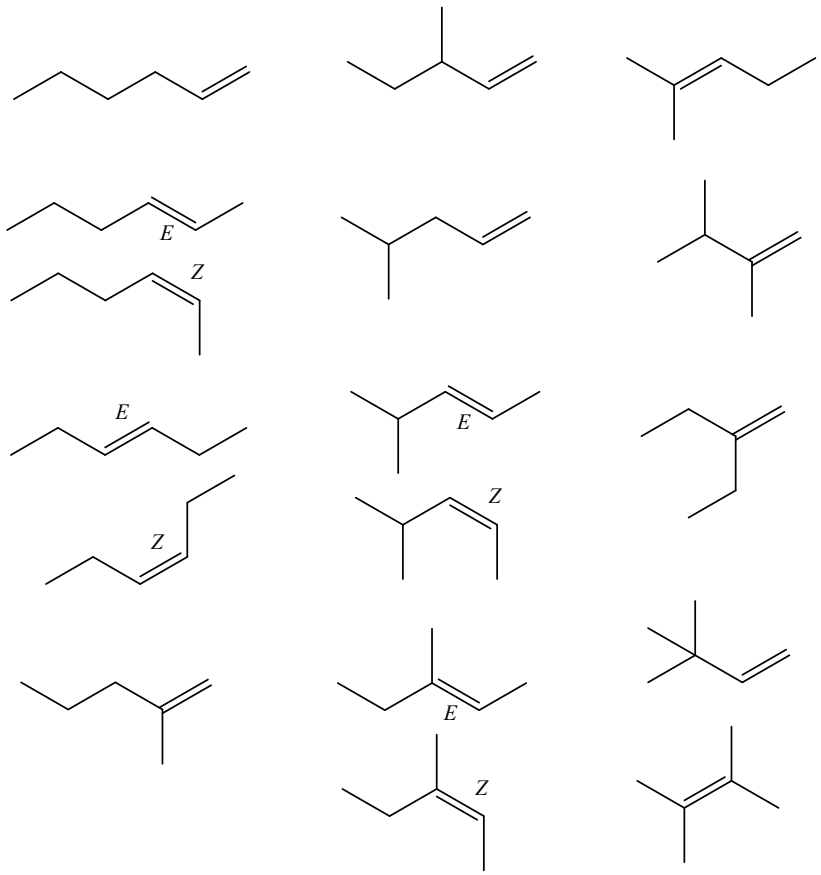
C_6H_{12} represents hydrocarbons with no cyclic carbon structures (acyclic alkenes).

(1) (10 pts) Draw all possible geometrical (structural) isomers of C_6H_{12} including *E*/*Z* isomers. How many pairs of *E*/*Z* isomers are present? Label these *E*/*Z* pairs.

Hint: 1-hexene is one of the isomers

(2) (3 pts) Are any stereoisomers present in the C_6H_{12} isomers? If stereoisomers exist, identify the chiral carbon centers, and draw both enantiomers while labeling each chiral center as *R* or *S*.

(answer)
(1) 17 geometrical isomers (0.5 point for correct structures, maximum 8 points) and 4 pairs of E/Z isomers (0.5 point for a pair of E/Z isomers, maximum 2 points)



(2) 2 pt for identifying the chiral isomer, 1 pt for correct R/S assignment

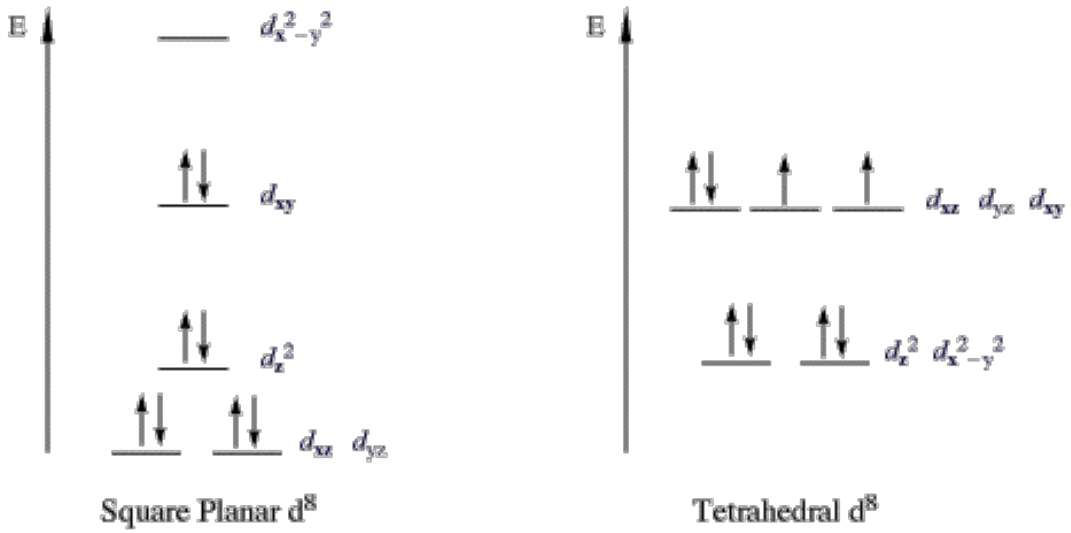
3. (8 points) The first transition metal-catalyzed methane activation was reported using the Shilov catalyst, which has the molecular formula of $PtCl_2(OH_2)_2$.

(a) (6 pts) The given Pt complex could exhibit either tetrahedral or square planar geometry. Provide:

1. The energy level diagram for the 3d orbitals in each geometry.
2. The electronic configuration, specifying the occupancy of each d-orbital.

(b) (2 pts) If the Pt complex is diamagnetic, determine whether it adopts a tetrahedral or square planar geometry. In this case, draw the possible isomeric structures, if any, for the specified geometry.

(answer)
(a)
1. 1.5 point for each



2. 1.5 point for each

Square Planar complex: $d_{xz}^2 d_{yz}^2 d_{z2}^2 d_{xy}^2$
Tetrahedral complex: $d_{z2}^2 d_{x2-y2}^2 d_{xz}^2 d_{yz}^1 d_{xy}^1$

(b) Square planar geometry

4. (10 points)

$[Mn(OH_2)_6]Cl_3$ is an octahedral complex. Answer the following questions to predict the chemical properties of the given transition metal complex.

(a) Determine the oxidation state of the compound.

(b) Determine the number of electrons in the compound's d orbitals.

(c) Considering crystal field theory, draw out the compound's d orbital splitting diagram and label each d orbital. Then, consider the spectrochemical series of ligands, and occupy your d orbitals with the proper numbers of electrons.

(d) Based on your answer above, calculate crystal field stabilization energy in terms of Δ_o.

(e) Is $[Mn(OH_2)_6]Cl_3$ paramagnetic or diamagnetic?

(f) If cyanide ions replace all of the water molecules of the compound, will the wavelength of the absorbed visible light get longer or shorter? And why?

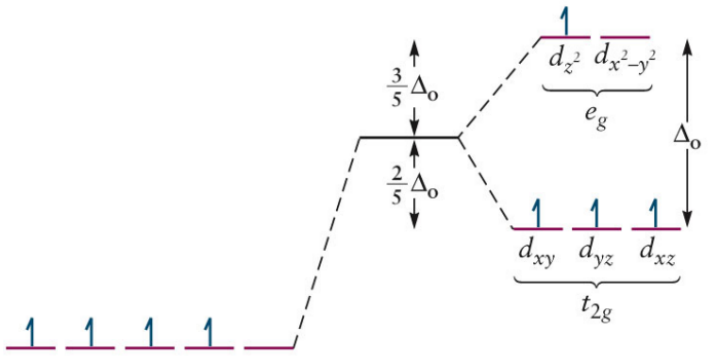
Answer

(a) (1 pt) 3+

(b) (1 pt) Four (4)

(c) (4 pts) draw out the compound's d orbital splitting diagram (1 pt) and label each d orbital (1 pts). Then, consider the spectrochemical series of ligands, and occupy your d orbitals with the proper numbers of electrons (2 pt).

- d^4 octahedral complex



(a) $[Mn(OH_2)_6]^{3+}$ (high spin)

(d) (1 pts)–$(3/5)\Delta_o$

(e) (1 pts) Paramagnetic

(f) (2 pts) longer or shorter? (1pt) And why (1 pt)? Shorter. Given that cyanide is a stronger field ligand than water, Δo is increased, and thus, λ_{max} gets shorter.

5. (6 points)

The equilibrium constant for the "water gas" reaction

$$C(s) + H_2O(g) \rightleftharpoons CO(g) + H_2(g)$$

Is $K = 2.6$ at a temperature of 1000 K. Calculate the reaction quotient Q for each of the following conditions, and state which direction the reaction shifts in coming to equilibrium.

(a) $P_{H2O} = 0.600$ atm; $P_{CO} = 1.525$ atm; $P_{H2} = 0.805$ atm

(b) $P_{H2O} = 0.724$ atm; $P_{CO} = 1.714$ atm; $P_{H2} = 1.383$ atm

Answer: calcualtion of Q: 2 pts, direction: 1 pt

The "water gas" reaction and its associated mass-action expression are

$$C(s) + H_2O(g) \rightleftharpoons CO(g) + H_2(g) \qquad \frac{P_{CO}P_{H_2}}{P_{H_2O}}$$

If the reaction quotient Q is less than K_{1000}, the reaction tends to proceed (to shift) from left to right at 1000 K; if Q is greater than K_{1000}, the reaction tends to proceed from right to left.

a) Substitute the data into the mass-action expression to obtain a Q

$$Q = \frac{P_{CO}P_{H_2}}{P_{H_2O}} = \frac{(1.525)(0.805)}{0.600} = \boxed{2.05}$$

This Q is less than K_{1000} (which is 2.6) so the reaction shifts from $\boxed{\text{left to right}}$ at 1000 K.

b) All three partial pressures are higher than in part **a)**. Use them in the mass-action expression

$$Q = \frac{P_{CO}P_{H_2}}{P_{H_2O}} = \frac{(1.714)(1.383)}{0.724} = \boxed{3.27}$$

Since Q now exceeds K_{1000}, the reaction shifts from $\boxed{\text{right to left}}$ to reach equilibrium at 1000 K.

6. (6 points)

Based on the pKa table below, predict the equilibrium constant K for the following reactions

Acid	HF	Acetic acid	HCO_3^-	NH_4^+	H_2O
pK_a	3.2	4.8	10.3	9.2	14.0

(a) $CH_3CO_2H + NaOH \overset{K_1}{\rightleftharpoons} CH_3COONa + H_2O$

(b) $HF + Na_2CO_3 \overset{K_2}{\rightleftharpoons} NaHCO_3 + NaF$

(c) $CH_3CO_2NH_4 \overset{K_3}{\rightleftharpoons} NH_3 + CH_3CO_2H$

(answer) 2 pts each. Incomplete calculation -1 pt.

(a) $\Delta pK_1 = 14.0 - 4.8 = 9.2$. $K_1 = 10^{9.2} = 1.6 \times 10^9$

(b) $\Delta pK_2 = 10.3 - 3.2 = 7.1$ $K_2 = 10^{7.1} = 1.3 \times 10^7$

(c) $\Delta pK_3 = 4.8 - 9.2 = -4.4$ $K_3 = 10^{-4.4} = 4.0 \times 10^{-5}$

7. (8 points)

For each of the following molecular formulas, there are three possible isomers

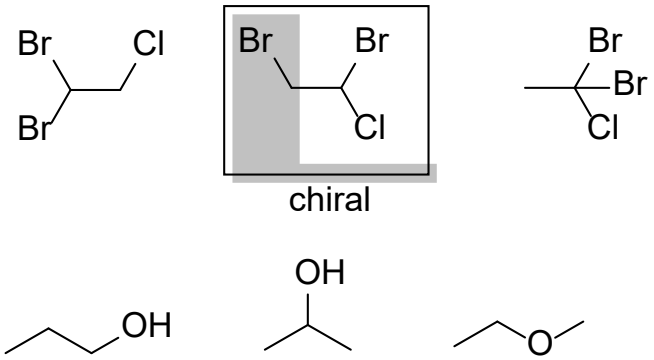
(1) $C_2H_3Br_2Cl$

(2) C_3H_8O

(a) (6 pts) Draw the chemical structures of the three isomers for each formula.

(b) (2 pts) Identify any chiral compounds among the isomers, if present.

(answer)



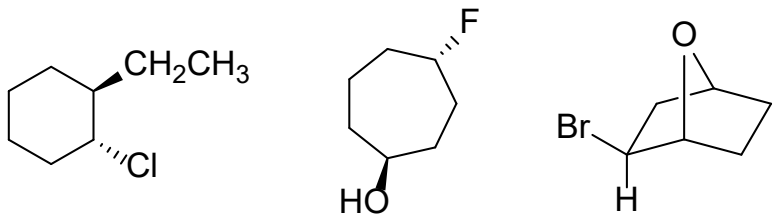
8. (16 points)

Answer the following questions:

(a) (5 pts) What are chiral compounds? How are they defined and identified?

(b) (5 pts) Explain the Kahn-Ingold-Prelog (R/S) system for assigning configurations to stereogenic centers.

(c) (6 pts) Assign the configuration (R or S) of each stereogenic center in the given structures.



(answer)

(1) Chiral compounds are molecules that are **non-superimposable on their mirror images**. These molecules lack an internal plane of symmetry and exist as two enantiomers, which are mirror-image stereoisomers of each other.

Identification:

1. **Presence of a stereogenic center (chiral center)**:
   A stereogenic center is typically a carbon atom bonded to four different groups or atoms. This asymmetry leads to chirality.
2. **Optical Activity**:
   Chiral compounds rotate plane-polarized light, and the two enantiomers rotate light in opposite directions (dextrorotatory, (+), or levorotatory, (−)).

   2 points for correct explanation regarding each keywords

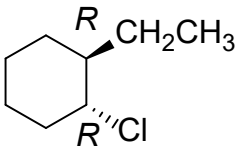
(2) The Kahn-Ingold-Prelog (CIP) system is used to assign the absolute configuration (R or S) to a stereogenic center. The steps are as follows:

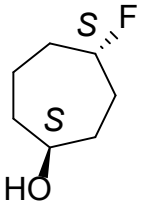
1. **Assign priorities to substituents**:
   Rank the four groups attached to the stereogenic center based on the atomic number of the directly bonded atoms:
   - Higher atomic number → Higher priority.
   - If two atoms are identical, compare the next set of atoms until a difference is found.
   - Double and triple bonds are treated as multiple single bonds for priority determination.

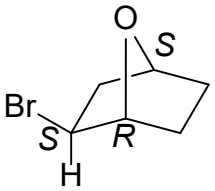
2. **Orient the molecule**:
   Rotate the molecule so that the group with the lowest priority (Priority 4) is positioned **away from the viewer** (into the plane of the page).
3. **Determine the sequence**:
   Observe the sequence of the remaining three groups (Priorities 1, 2, and 3):
   - If the sequence is **clockwise**, the configuration is R.
   - If the sequence is **counterclockwise**, the configuration is S.

(3)

2 points for each molecule

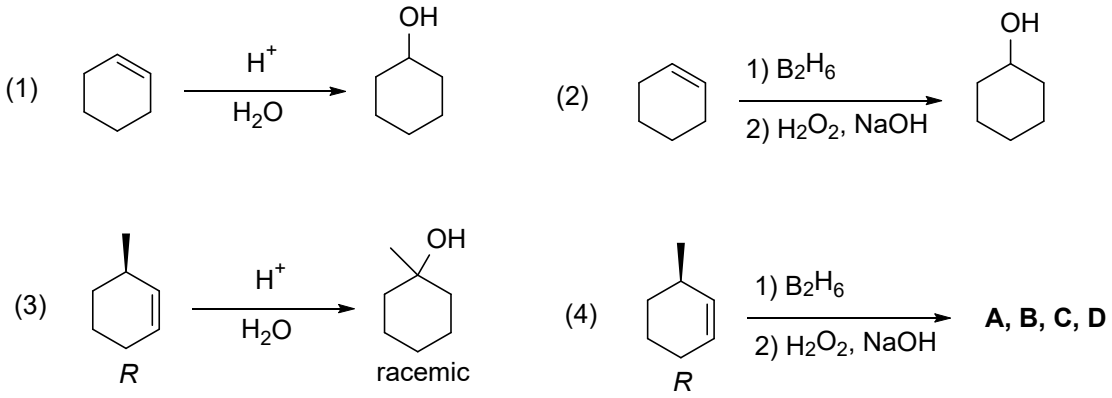






9. (21 points)

Answer the following questions:



(a) (8 pts) Provide a step-by-step reaction mechanism for reactions (1) and (2).

Hint: Treatment with H_2O_2/NaOH converts C-BH_2 bonds to C-OH bonds. This step can be excluded from the mechanism.

(b) (6 pts) For reaction (3), when enantiopure *R*-methylcyclohexene was used, a racemic tertiary alcohol was isolated. Propose a step-by-step reaction mechanism. Additionally, explain why a racemic product was formed.

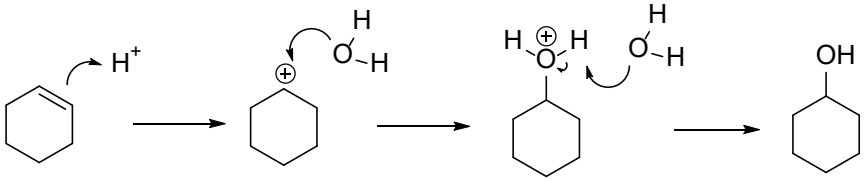
Hint: Carbocations can be migrated via 1,2-hydrogen shift.

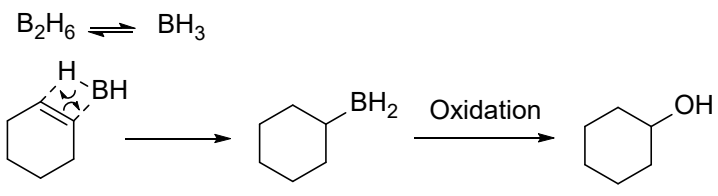
(c) (7 pts) For reaction (4), four alcohol products were isolated, and all are structural isomers.

Determine the structures of the products (**A**, **B**, **C**, and **D**) and assign the configuration (*R* or *S*) to all stereogenic centers in each isomer.

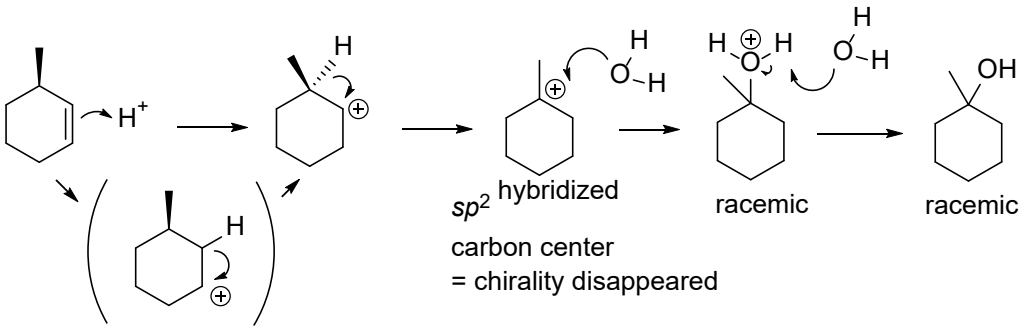
(answer)

(a) each 4 pts

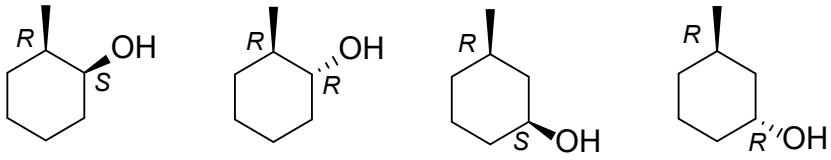




(b) Mechanism 3 pts. Racemization by carbocation: 3 pts



(c) A,B,C,D each 1 pt, Assignment 3 pts



Physical Constants

Avogadro's number	$N_A = 6.02214179 \times 10^{23}$ mol^{-1}
Bohr radius	$a_0 = 0.52917720859$ Å $= 5.2917720859 \times 10^{-11}$ m
Boltzmann's constant	$K_B = 1.3806504 \times 10^{-23}$ J K^{-1}
Electronic charge	$e = 1.602176487 \times 10^{-19}$ C
Faraday constant	$F = 96485.3399$ C mol^{-1}
Masses of fundamental particles:	
Electron	$m_e = 9.10938215 \times 10^{-31}$ kg
Proton	$m_P = 1.672621637 \times 10^{-27}$ kg
Neutron	$m_n = 1.674927211 \times 10^{-27}$ kg
Permittivity of vacuum	$\varepsilon_o = 8.854187817 \times 10^{-12}$ C^{-2} J^{-1} m^{-1}
Planck's constant	$h = 6.62606896 \times 10^{-34}$ J s
Ratio of proton mass to electron mass	$m_P / m_e = 1836.15267247$
Speed of light in a vacuum	$c = 2.99792458 \times 10^8$ m s^{-1} (exactly)
Standard acceleration of terrestrial gravity	$g = 9.80665$ m s^{-2} (exactly)
Universal gas constant	$R = 8.314472$ J mol^{-1} K^{-1} $= 0.0820574$ L atm mol^{-1} K^{-1}

Values are taken from the 2006 CODATA recommended values,
as listed by the National Institute of Standards and Technology.

Conversion factors

Ångström	1 Å $= 10^{-10}$ m
Atomic mass unit	1 u $= 1.660538782 \times 10^{-27}$ kg
	1 u $= 1.492417830 \times 10^{-10}$ J $= 931.494028$ MeV (energy equivalent form $E = mc^2$)
Calorie	1 cal $= 4.184$ J (exactly)
Electron volt	1 eV $= 1.602177 \times 10^{-19}$ J $= 96.485335$ kJ mol^{-1}
Foot	1 ft $= 12$ in $= 0.3048$ m (exactly)
Gallon (U. S.)	1 gallon $= 4$ quarts $= 3.785412$ L (exactly)
Liter	1 L $= 10^{-3}$ m^3 $= 10^3$ cm^3 (exactly)

Liter-atmosphere	1 L atm = 101.325 J (exactly)
Metric ton	1 t = 1000 kg (exactly)
Pound	1 lb = 16 oz = 0.4539237 kg (exactly)
Rydberg	1 Ry = 2.17987197 x 10^{-18}J = 1312.7136 kJ mol^{-1} = 13.60569193 eV
Standard atmosphere	1 atm = 1.01325 x 10^5 Pa = 1.01325 x 10^5 kg m^{-1} s^{-2} (exactly)
Torr	1 torr = 133.3224 Pa

PERIODIC TABLE OF THE ELEMENTS

http://www.ktf-split.hr/periodni/en/

GROUP NUMBERS IUPAC RECOMMENDATION (1985) — GROUP NUMBERS CHEMICAL ABSTRACT SERVICE (1986)

ATOMIC NUMBER — SYMBOL — RELATIVE ATOMIC MASS (1) — ELEMENT NAME

PERIOD	1 IA												13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1	1 1.0079 **H** HYDROGEN	2 IIA																2 4.0026 **He** HELIUM
2	3 6.941 **Li** LITHIUM	4 9.0122 **Be** BERYLLIUM											5 10.811 **B** BORON	6 12.011 **C** CARBON	7 14.007 **N** NITROGEN	8 15.999 **O** OXYGEN	9 18.998 **F** FLUORINE	10 20.180 **Ne** NEON
3	11 22.990 **Na** SODIUM	12 24.305 **Mg** MAGNESIUM	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8	9 VIIIB	10	11 IB	12 IIB	13 26.982 **Al** ALUMINIUM	14 28.086 **Si** SILICON	15 30.974 **P** PHOSPHORUS	16 32.065 **S** SULPHUR	17 35.453 **Cl** CHLORINE	18 39.948 **Ar** ARGON
4	19 39.098 **K** POTASSIUM	20 40.078 **Ca** CALCIUM	21 44.956 **Sc** SCANDIUM	22 47.867 **Ti** TITANIUM	23 50.942 **V** VANADIUM	24 51.996 **Cr** CHROMIUM	25 54.938 **Mn** MANGANESE	26 55.845 **Fe** IRON	27 58.933 **Co** COBALT	28 58.693 **Ni** NICKEL	29 63.546 **Cu** COPPER	30 65.39 **Zn** ZINC	31 69.723 **Ga** GALLIUM	32 72.64 **Ge** GERMANIUM	33 74.922 **As** ARSENIC	34 78.96 **Se** SELENIUM	35 79.904 **Br** BROMINE	36 83.80 **Kr** KRYPTON
5	37 85.468 **Rb** RUBIDIUM	38 87.62 **Sr** STRONTIUM	39 88.906 **Y** YTTRIUM	40 91.224 **Zr** ZIRCONIUM	41 92.906 **Nb** NIOBIUM	42 95.94 **Mo** MOLYBDENUM	43 (98) **Tc** TECHNETIUM	44 101.07 **Ru** RUTHENIUM	45 102.91 **Rh** RHODIUM	46 106.42 **Pd** PALLADIUM	47 107.87 **Ag** SILVER	48 112.41 **Cd** CADMIUM	49 114.82 **In** INDIUM	50 118.71 **Sn** TIN	51 121.76 **Sb** ANTIMONY	52 127.60 **Te** TELLURIUM	53 126.90 **I** IODINE	54 131.29 **Xe** XENON
6	55 132.91 **Cs** CAESIUM	56 137.33 **Ba** BARIUM	57-71 **La-Lu** Lanthanide	72 178.49 **Hf** HAFNIUM	73 180.95 **Ta** TANTALUM	74 183.84 **W** TUNGSTEN	75 186.21 **Re** RHENIUM	76 190.23 **Os** OSMIUM	77 192.22 **Ir** IRIDIUM	78 195.08 **Pt** PLATINUM	79 196.97 **Au** GOLD	80 200.59 **Hg** MERCURY	81 204.38 **Tl** THALLIUM	82 207.2 **Pb** LEAD	83 208.98 **Bi** BISMUTH	84 (209) **Po** POLONIUM	85 (210) **At** ASTATINE	86 (222) **Rn** RADON
7	87 (223) **Fr** FRANCIUM	88 (226) **Ra** RADIUM	89-103 **Ac-Lr** Actinide	104 (261) **Rf** RUTHERFORDIUM	105 (262) **Db** DUBNIUM	106 (266) **Sg** SEABORGIUM	107 (264) **Bh** BOHRIUM	108 (277) **Hs** HASSIUM	109 (268) **Mt** MEITNERIUM	110 (281) **Uun** UNUNNILIUM	111 (272) **Uuu** UNUNUNIUM	112 (285) **Uub** UNUNBIUM		114 (289) **Uuq** UNUNQUADIUM				

LANTHANIDE

57 138.91 **La** LANTHANUM	58 140.12 **Ce** CERIUM	59 140.91 **Pr** PRASEODYMIUM	60 144.24 **Nd** NEODYMIUM	61 (145) **Pm** PROMETHIUM	62 150.36 **Sm** SAMARIUM	63 151.96 **Eu** EUROPIUM	64 157.25 **Gd** GADOLINIUM	65 158.93 **Tb** TERBIUM	66 162.50 **Dy** DYSPROSIUM	67 164.93 **Ho** HOLMIUM	68 167.26 **Er** ERBIUM	69 168.93 **Tm** THULIUM	70 173.04 **Yb** YTTERBIUM	71 174.97 **Lu** LUTETIUM

ACTINIDE

89 (227) **Ac** ACTINIUM	90 232.04 **Th** THORIUM	91 231.04 **Pa** PROTACTINIUM	92 238.03 **U** URANIUM	93 (237) **Np** NEPTUNIUM	94 (244) **Pu** PLUTONIUM	95 (243) **Am** AMERICIUM	96 (247) **Cm** CURIUM	97 (247) **Bk** BERKELIUM	98 (251) **Cf** CALIFORNIUM	99 (252) **Es** EINSTEINIUM	100 (257) **Fm** FERMIUM	101 (258) **Md** MENDELEVIUM	102 (259) **No** NOBELIUM	103 (262) **Lr** LAWRENCIUM

(1) Pure Appl. Chem., **73**, No. 4, 667-683 (2001)

Relative atomic mass is shown with five significant figures. For elements have no stable nuclides, the value enclosed in brackets indicates the mass number of the longest-lived isotope of the element.

However three such elements (Th, Pa, and U) do have a characteristic terrestrial isotopic composition, and for these an atomic weight is tabulated.

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