Inorganic Pharmaceutical Chemistry

Reference text:-
1- Inorganic Medicinal and Pharmaceutical Chemistry by Block, Roche Soine and Wilson
2- Textbook of Organic Medicinal and pharmaceutical Chemistry by Wilson and Gisvold
Course Coverage

Atomic and Molecular Structure

1- Structure of the Atom
2- Atomic Number, Mass Number, & Isotopes
3- Classification of the Elements
4- Quantum Mechanics, Quantum Numbers
5- Electronic Configuration
6- Shielding
7- Atomic Radius, Ionic Radius, Ionization Energy, Electron Affinity, Electronegativity
8- Chemical bond
Course Coverage

Complexes

1- Orbital hybridization
2- Types of hybridization
3- Basic theory
   - Valence bond theory
4- Rules for Naming Coordination Complexes
5- Ligand
Quiz 1/

Write chemical symbol for first 10 elements in proper location on blank periodic table
Atomic Structure

Structure of the Atom
Composed of:
1- Nucleus protons
Neutrons
2- Orbitals electrons
protons
found in nucleus
relative charge of +1 , relative mass of 1.0073 amu
neutrons
found in nucleus
neutral charge , relative mass of 1.0087 amu
electrons
found in electron cloud
relative charge of -1 , relative mass of 0.00055 amu
**Protons** are positively charged and so would be deflected on a curving path towards the negative plate. **Electrons** are negatively charged and so would be deflected on a curving path towards the positive plate. **Neutrons** don't have a charge, and so would continue on in a straight line.

If beams of the three sorts of particles, all with the same speed, are passed between two electrically charged plates:
The nucleus
The nucleus is at the centre of the atom and contains the protons and neutrons. Protons and neutrons are collectively known as *nucleons*. Virtually all the mass of the atom is concentrated in the nucleus, because the electrons weigh so little.

**Working out the numbers of protons and neutrons**

No of protons = ATOMIC NUMBER of the atom  
The atomic number is also given the more descriptive name of *proton number*.  
No of protons + no of neutrons = MASS NUMBER of the atom
The mass number is also called the *nucleon number*. This information can be given simply in the form:

<table>
<thead>
<tr>
<th>Mass number</th>
<th>19</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic number</td>
<td>9</td>
</tr>
</tbody>
</table>

F
Atomic Number, Mass Number, & Isotopes

**Atomic number, Z**
the number of protons in the nucleus
the number of electrons in a neutral atom
the integer on the periodic table for each element

**Mass Number, A**
integer representing the *approximate* mass of an atom
equal to the sum of the number of protons and neutrons in the nucleus

**Isotopes**
atoms of the same element which differ in the number of neutrons in the nucleus
designated by mass number

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Isotopes vs. Allotropes

Isotopes - atoms of the same element with different numbers of neutrons
- different compounds with the same formula
Allotropes - different forms of an element
Carbon exhibits both
Isotopes: C-12, C-13, C-14

Allotropes: graphite, diamond, and fullerenes
**Isotopes** :- The number of neutrons in an atom can vary within small limits. For example, there are three kinds of carbon atom $^{12}$C, $^{13}$C and $^{14}$C. They all have the same number of protons, but the number of neutrons varies

<table>
<thead>
<tr>
<th></th>
<th>Protons</th>
<th>neutrons</th>
<th>mass number</th>
</tr>
</thead>
<tbody>
<tr>
<td>carbon-12</td>
<td>6</td>
<td>6</td>
<td>12</td>
</tr>
<tr>
<td>carbon-13</td>
<td>6</td>
<td>7</td>
<td>13</td>
</tr>
<tr>
<td>carbon-14</td>
<td>6</td>
<td>8</td>
<td>14</td>
</tr>
</tbody>
</table>

These different atoms of carbon are called **isotopes**. The fact that they have varying numbers of neutrons makes no difference whatsoever to the chemical reactions of the carbon.

Isotopes are atoms which have the same atomic number but different mass numbers. They have the same number of protons but different numbers of neutrons.
The electrons

Working out the number of electrons
Atoms are electrically neutral, and the positiveness of the protons is balanced by the negativeness of the electrons. It follows that in a neutral atom:

**no of electrons = no of protons**

So, if an oxygen atom (atomic number = 8) has 8 protons, it must also have 8 electrons; if a chlorine atom (atomic number = 17) has 17 protons, it must also have 17 electrons
In Summary...

For any element:
Number of Protons = Atomic Number
Number of Electrons = Number of Protons = Atomic Number
For krypton:
Number of Protons = Atomic Number = 36
Number of Electrons = Number of Protons = Atomic Number = 36
  Number of Neutrons = Mass Number - Atomic Number
  Number = 84 - 36 = 48
The Origin of the Elements

Nucleosynthesis of light elements
Nucleosynthesis of heavy elements

Hydrogen Burning

Hydrogen Burning (fusion)

$4 \, ^1\text{H} \rightarrow ^4\text{He} + 2 \text{ positrons} + 2 \text{ neutrinos}$

$+ \, 2.5 \times 10^6 \text{ MJ/mol}$

after about 1/10 of hydrogen consumed, changes to helium burning
Classification of the Elements

Metals
• Lustrous, malleable, ductile, electrically conducting solids at room temperature

Nonmetals
• Often gases, liquids, or solids that do not conduct electricity appreciably

Metalloids
• Elements, alloys or compounds that possess some of the characteristics of metals and some of nonmetals
Classification of the Elements

• Metallic elements combine with nonmetallic elements to give compounds that are typically hard, non-volatile solids

• When combined with each other, the nonmetals often form volatile molecular compounds

• When metals combine (or simply mix together) they produce alloys that have most of the physical characteristics of metals
Development of Periodic Table

Dmitri Mendeleev - Russian
1869 - Periodic Law - allowed him to predict properties of unknown elements
<table>
<thead>
<tr>
<th>Row</th>
<th>Group I</th>
<th>Group II</th>
<th>Group III</th>
<th>Group IV</th>
<th>Group V</th>
<th>Group VI</th>
<th>Group VII</th>
<th>Group VIII</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>R₂O</td>
<td>RO</td>
<td>R₂O₃</td>
<td>RH₄</td>
<td>RH₃</td>
<td>RH₅</td>
<td>RH₂O₇</td>
<td>RO₄</td>
</tr>
<tr>
<td>1</td>
<td>H = 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Li = 7</td>
<td>Be = 9.4</td>
<td>B = 11</td>
<td>C = 12</td>
<td>N = 14</td>
<td>O = 16</td>
<td>F = 19</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Na = 23</td>
<td>Mg = 24</td>
<td>Al = 27.3</td>
<td>Si = 28</td>
<td>P = 31</td>
<td>S = 32</td>
<td>Cl = 35.5</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>K = 39</td>
<td>Ca = 40</td>
<td>___ = 44</td>
<td>Ti = 48</td>
<td>V = 51</td>
<td>Cr = 52</td>
<td>Mn = 55</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>(Cu = 63)</td>
<td>Zn = 65</td>
<td>___ = 68</td>
<td>___ = 72</td>
<td>As = 75</td>
<td>Se = 78</td>
<td>Br = 80</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>Rb = 83</td>
<td>Sr = 87</td>
<td>?Yt = 88</td>
<td>Zr = 90</td>
<td>Nb = 94</td>
<td>Mo = 96</td>
<td>___ = 100</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>(Ag = 108)</td>
<td>Cd = 112</td>
<td>In = 113</td>
<td>Sn = 118</td>
<td>Sb = 122</td>
<td>Tc = 125</td>
<td>I = 127</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>Cs = 133</td>
<td>Ba = 137</td>
<td>?Di = 138</td>
<td>?Ce = 140</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>?Er = 178</td>
<td>?La = 180</td>
<td>Ta = 182</td>
<td>W = 184</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>11</td>
<td>(Au = 199)</td>
<td>Hg = 200</td>
<td>Tl = 204</td>
<td>Pb = 207</td>
<td>Bi = 208</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td></td>
<td></td>
<td>Th = 231</td>
<td>U = 240</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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Missing elements: 44, 68, 72, & 100 amu
## Predicted properties of ekasilicon

<table>
<thead>
<tr>
<th>Property</th>
<th>Predicted properties of Ekasilicon</th>
<th>Observed properties of Germanium (Ge)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic weight</td>
<td>72</td>
<td>72.6</td>
</tr>
<tr>
<td>Color of element</td>
<td>Gray</td>
<td>Gray</td>
</tr>
<tr>
<td>Density of element (g/mL)</td>
<td>5.5</td>
<td>5.36</td>
</tr>
<tr>
<td>Formula of oxide</td>
<td>EsO₂</td>
<td>GeO₂</td>
</tr>
<tr>
<td>Density of oxide (g/mL)</td>
<td>4.7</td>
<td>4.228</td>
</tr>
<tr>
<td>Formula of chloride</td>
<td>EsCl₄</td>
<td>GeCl₄</td>
</tr>
<tr>
<td>Density of chloride</td>
<td>1.9</td>
<td>1.884</td>
</tr>
<tr>
<td>Boiling point of chloride (°C)</td>
<td>&lt; 100</td>
<td>84</td>
</tr>
<tr>
<td>Periodic Table of the Elements</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>I A</td>
<td>II A</td>
<td>III B</td>
</tr>
<tr>
<td>-----</td>
<td>------</td>
<td>-------</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>H</td>
<td>He</td>
</tr>
<tr>
<td>1.008</td>
<td>1.008</td>
<td>4.0026</td>
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<tr>
<td>3</td>
<td>4</td>
<td>Be</td>
</tr>
<tr>
<td>Li</td>
<td>Be</td>
<td>B</td>
</tr>
<tr>
<td>6.939</td>
<td>9.0122</td>
<td>4.0026</td>
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<td>Mg</td>
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<tr>
<td>Na</td>
<td>Mg</td>
<td>Al</td>
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<td>22.99</td>
<td>24.312</td>
<td>26.982</td>
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<tr>
<td>19</td>
<td>20</td>
<td>K</td>
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<td>Rb</td>
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<td>85.468</td>
<td>86.62</td>
<td>88.906</td>
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<tr>
<td>55</td>
<td>56</td>
<td>Cs</td>
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<tr>
<td>132.91</td>
<td>137.33</td>
<td>138.91</td>
</tr>
<tr>
<td>87</td>
<td>88</td>
<td>Fr</td>
</tr>
<tr>
<td>227.03</td>
<td>226.03</td>
<td>227.03</td>
</tr>
</tbody>
</table>

Based on symbols used by ACS
S.M. Condren 2007

* Designates that all isotopes are radioactive
**Lanthanum Series 140.12 140.91 144.24 * 145 150.36 151.96 157.25 158.93 162.51 164.93 167.26 168.93 173.04 174.97
*** Actinium Series 232.04 231.04 238.03 237.05 * 244 * 243 * 247 * 247 * 251 * 252 * 257 * 258 * 259 * 260

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Electron configuration and the periodic table

- **s-block elements**
- **p-block elements**
- **d-block elements (transition metals)**
- **f-block elements: lanthanides (4f) and actinides (5f)**

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Quantum Numbers

$n \Rightarrow \text{principal quantum number, quantized energy levels, which energy level}$

$n = 1, 2, 3, 4, 5, 6, 7, \text{ etc.}$
Quantum Numbers

$l \Rightarrow$ secondary quantum number, quantized orbital angular momentum, which sublevel or type of orbital

- $s$ type orbital $l = 0$
- $p$ type orbital $l = 1$
- $d$ type orbital $l = 2$
- $f$ type orbital $l = 3$
- $g$ type orbital $l = 4$
Quantum Numbers

\( m \) = magnetic quantum number, quantized orientation of angular momentum, which orbital within sublevel

- **s type orbital** \( m = 0 \)
- **p type orbital** \( m = +1, 0 \) or \(-1\)
  - one value for each of the three p orbitals
- **d type orbital** \( m = +2, +1, 0, -1 \) or \(-2\)
  - one value for each of the five d orbitals
- **f type orbital** \( m = +3, +2, +1, 0, -1, -2 \) or \(-3\)
  - one value for each of the seven f orbitals
Hydrogenic Energy Levels

\[ E = - \frac{\hbar c Z^2 R}{n^2} \]

where \( n = 1, 2, 3, \ldots \)

\[ R = \text{Rydberg constant} \]

\[ R = \frac{m_e e^4}{8\hbar^3 c \varepsilon_0^2} = 13.6 \text{ eV} \]
s- and p-orbitals
d-orbitals
f-orbitals
Many Electron Atoms

• Electronic Configuration
• Pauli exclusion principle
  – No more than 2 electrons can occupy a single orbital
  – No two electrons can have the exact same four quantum numbers
Electron Filling Order Diagram

Start here

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f
6s 6p 6d
7s 7p
Pauli Exclusion Principle
The Pauli exclusion principle states no two electrons (or other fermions) can have the identical quantum mechanical state in the same atom

Aufbau Principle
Fill from the bottom up

Hund's Rule
If multiple orbitals have the same energy, one electron goes into each of them before they start to double up.