

§ 6-4 Atomic Orbitals, Shapes and Sizes

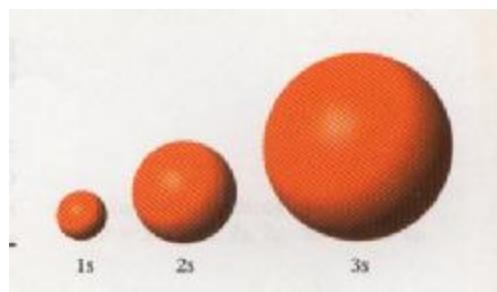


Fig. 6.6: s orbitals.

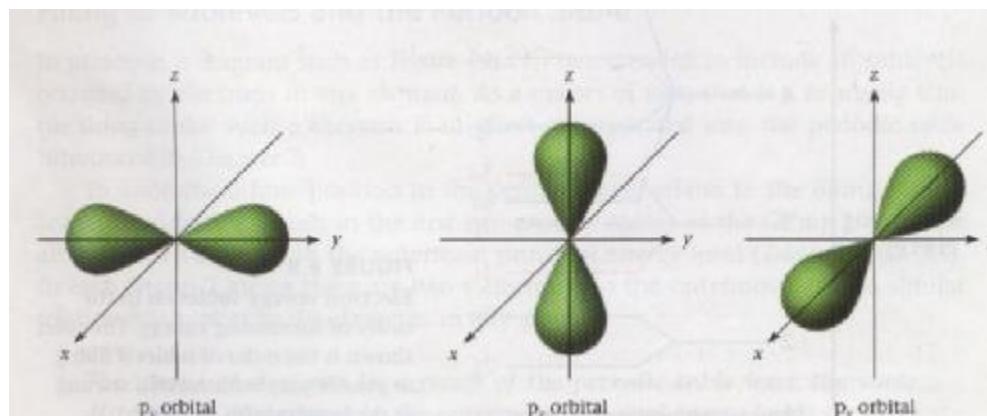


Fig. 6.7: p orbitals. (p_x, p_y, p_z orbit)

§ 6-5 Electron configurations in atoms 原子之電子組態

The simplest way to describe the management of electrons in an atom.

$$F : 1s^2 2s^2 2p^5$$

§ Electron configuration from sublevel energies

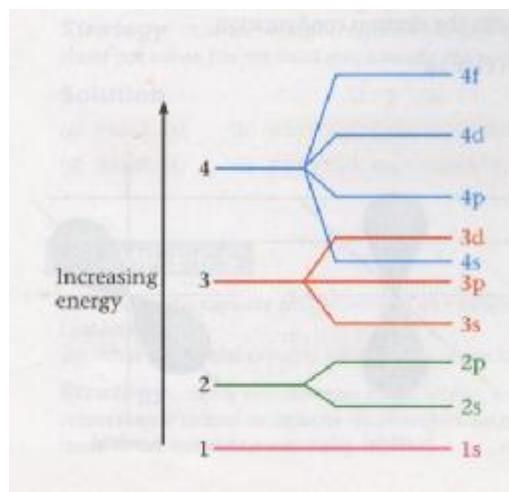
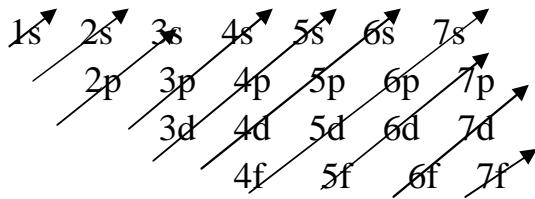


Fig 6.8: Electron energy sublevels in the order of increasing energy.



第一週期	$1s^2$	2
第二週期	$2s^2 2p^6$	8
第三週期	$3s^2 3p^6$	8
第四週期	$4s^2 3d^{10} 4p^6$	18
第五週期	$5s^2 4d^{10} 5p^6$	18
第六週期	$6s^2 4f^{14} 5d^{10} 6p^6$	32
第七週期	$7s^2 5f^{14} 6d^{10} 7p^6$	32

₅B $1s^2 2s^2 2p^1$ ₆C $1s^2 2s^2 2p^2$ ₇N $1s^2 2s^2 2p^3$

₈O $1s^2 2s^2 2p^4$ ₉F $1s^2 2s^2 2p^5$ ₁₀Ne $1s^2 2s^2 2p^6$

₁₂Mg $1s^2 2s^2 2p^6 3s^2$ ₁₈Ar $1s^2 2s^2 2p^6 3s^2 3p^6$

₂₀Ca $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$ [Ar] $4s^2$

₃₀Zn $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$ ₃₆Kr $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$

Ex 6-6 : Find the electron configurations of the sulfur and iron atoms.

Ans : ₁₆S : $1s^2 2s^2 2p^6 3s^2 3p^4$ [Ne] $3s^2 3p^4$ $16 - 2 - 8 = 6$
₂₆Fe : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$ [Ar] $4s^2 3d^6$ $26 - 2 - 8 - 8 = 8$

§ Abbreviated electron configuration

前一週期之鈍氣 + 最後一週期之電子組態

	Electron configuration	Abbreviated electron configuration
₁₆ S	$1s^2 2s^2 2p^6 3s^2 3p^4$	[Ne] $3s^2 3p^4$
₂₈ Ni	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$	[Ar] $4s^2 3d^8$

§ Filling of sublevels and the periodic table

週期表與電子組態是相對照的

1. Group 1, 2 \Rightarrow 填入 s orbital
IA, IIA
2. Group 13 ~ 18 \Rightarrow 填入 p orbital
IIIA ~ VIIIA

3. transition metal Group 3 ~ 12 \Rightarrow 填 d orbital
4. inner transitional element \Rightarrow 填 f orbital

Half-life 半衰期 $t_{1/2}$:

The time for a radioactive element to reduce its weight to half. 一放射性元素，其重量減為原先一半所需之時間。 $t_{1/2} \uparrow \Rightarrow$ 安定性 \uparrow

§ Electron configuration from the periodic table

Ex 6-7: For the iodine atom, write

Ans: ${}_{53}I$: ${}_9F$; ${}_{17}Cl$; ${}_{35}Br$; ${}_{53}I \quad 53 - 2 - 8 - 8 - 18 = 17$

a) electron configuration

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^5$

b) abbreviated electron configuration

[Kr] $5s^2 4d^{10} 5p^5$

		Predicted										observed					
${}_{24}Cr$		[Ar] $4s^2 3d^4$										[Ar] $4s^1 3d^5$					
${}_{29}Cu$		[Ar] $4s^2 3d^9$										[Ar] $4s^1 3d^{10}$					
\Rightarrow 可提高穩定性																	

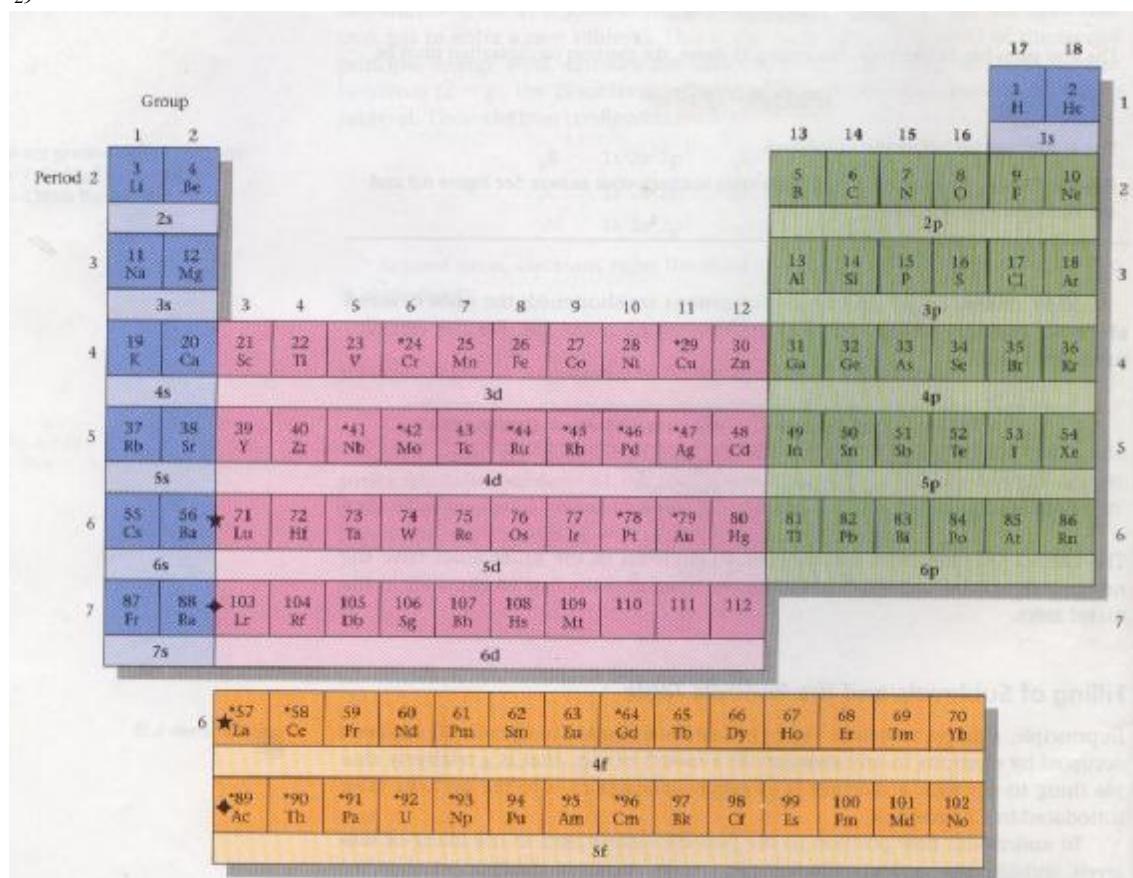


Fig 6-9: 圖中標 * 者 predicted 與 observed 些微不同

§6-6 Orbital diagrams of atoms 原子軌域圖

Show how electrons are distributed among orbitals; orbital 用 () 表示
電子以↑or↓表示

→ 依 spin 方向而異

	1s	2s	2p		
₅ B	(↑↓)	(↑↓)	(↑)	()	()
₆ C	(↑↓)	(↑↓)	(↑)	(↑)	() 最安定

Hund's law :

When several orbitals of equal energy are available, as in a given sublevel, electrons enter singly with parallel spins.

- in all filled orbitals, the two electrons have opposed spins.
- in accordance with Hund's rule, within a given sublevel there are as many half-filled orbitals as possible.

副軌域先各排一個，才排入第二個電子

	1s	2s	2p		
₇ N	(↑↓)	(↑↓)	(↑)	(↑)	(↑)
₈ O	(↑↓)	(↑↓)	(↑↓)	(↑)	(↑)
₉ F	(↑↓)	(↑↓)	(↑↓)	(↑↓)	(↑)
₁₀ Ne	(↑↓)	(↑↓)	(↑↓)	(↑↓)	(↑↓)

paramagnetic 順磁性的 : A solid has unpaired electrons present, it will be attracted by the magnetic field.

diamagnetic 逆磁性的 : A solid contains only paired electrons, it is slightly repelled by the magnetic field.

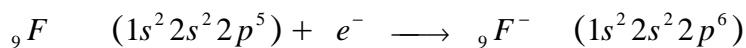
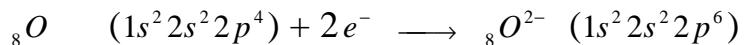
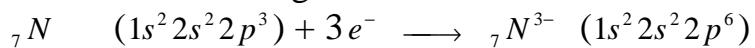
Ex 6-8: Construct orbital diagrams for atoms of sulfur and iron.

Ans: 1s 2s 2p 3s 3p
₁₆S (↑↓) (↑↓) (↑↓) (↑↓) (↑↓) (↑↓) (↑) (↑)

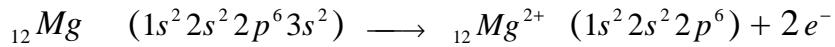
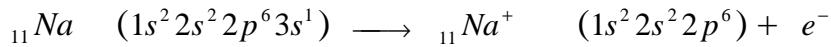
1s 2s 2p 3s 3p
₂₆Fe (↑↓) (↑↓) (↑↓) (↑↓) (↑↓) (↑↓) (↑↓) (↑↓)
4s 3d
(↑↓) (↑↓) (↑) (↑) (↑) (↑) (↑)
4

§ 6-7 Electron arrangements in monatomic ions

Ions with Noble-gas structure



b 相同電子組態



$N^{3-}, O^{2-}, F^-, Na^+, Mg^{2+}, Al^{3+} \Rightarrow$ 等電子 isoelectronic

They have same electron configuration.

Group 1 +1 (IA)

Group 16 -2 (VIA)

Group 2 +2 (IIA)

Group 17 -1 (VIIA)

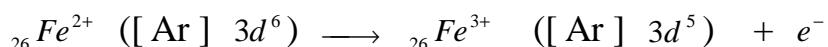
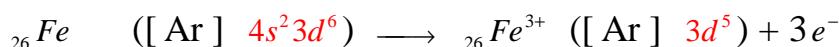
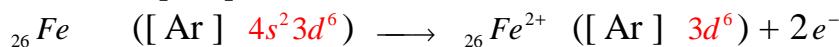
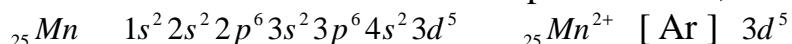
MX M : Li, Na, K, Rb, Cs, Fr X : F, Cl, Br, I, At

MX₂ M : Be, Mg, Ca, Sr, Ba, Ra X : F, Cl, Br, I, At

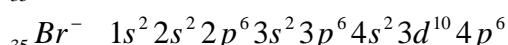
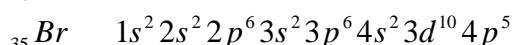
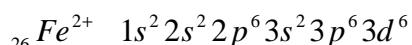
MO M : Be, Mg, Ca, Sr, Ba, Ra X : O

Transition metal cations:

When transition metal atoms form positive ions, the outer s electrons are lost first.



Ex 6-9 : a) Fe^{2+} b) Br^- → electron configuration



§ 6-8 Periodic trends in the properties of atoms.

The chemical and physical properties of elements are a periodic function of atomic number.

討論 :

Atomic radius	
Ionic radius	horizontally or vertically in the periodic table
Ionization energy	
Electronegativity	

§ Atomic radius :

One half the distance of closest approach between atoms in an elemental substance.

Radius : 半徑

- decrease across a period from left to right in the periodic table
同一週期 $Z \uparrow \Rightarrow r \downarrow$
- increase down a group in the periodic table
同一族 $Z \uparrow \Rightarrow r \uparrow$

§ Ionic radius :

Increases moving down a group in the periodic table

$$\text{同一族 } Z \uparrow \Rightarrow \text{ionic } r \uparrow$$

Radii of both cations (left) and anions (right) decrease from left to right across a period.

$$\text{同一週期 } Z \uparrow \Rightarrow r \downarrow \quad Li^+ > Be^{2+} \quad O^{2-} > F^-$$

- positive ions : radius < atom radius
(cations) $Na^+ < Na$
 $r = 0.095\text{nm}$ $r = 0.186\text{nm}$
- negative ions : radius > atom radius
(anions) $Cl^- > Cl$
 $r = 0.181\text{nm}$ $r = 0.099\text{nm}$

Ex 6-10 : Using only the periodic table, arrange each of the following sets of atoms and ions in order of increasing size.

- Ans : a) $_{12}Mg, _{13}Al, _{20}Ca$ $Al < Mg < Ca$
 b) $_{16}S, _{17}Cl, _{16}S^{2-}$ $Cl < S < S^{2-}$ 陰離子 $r^- > r$
 c) $_{26}Fe, _{26}Fe^{2+}, _{26}Fe^{3+}$ $Fe^{3+} < Fe^{2+} < Fe$ 陽離子 $r > r^+$

§ Ionization energy : 游離能

is a measure of how difficult it is to remove an electron from a gaseous atom.
一定 “+” ← ”



ionization energy :

- increase across the periodic table from left to right.

同一週期 $Z \uparrow \Rightarrow \Delta E_1 \uparrow$ 結論與 radius 相反
例外 Be, B; Mg, Al

- decrease moving down the periodic table

同一族 $Z \uparrow \Rightarrow \Delta E_1 \downarrow$

Ex 6-11: Consider the three elements ${}_6 C$, ${}_7 N$, ${}_{14} Si$. Using only the periodic table ,Predict which of the three elements has

- the largest and the smallest atomic radius
- the largest ionization energy and the smallest ionization energy

Ans :

- a) Radius :

${}_{14} Si$ 最大 ${}_7 N$ 最小

- b) ΔE :

${}_7 N$ 最大 ${}_{14} Si$ 最小

§ Electronegativity 負電性

Measures the ability of an atom to attract the electron to itself to form a covalent bond.

F 4.0 最活潑非金屬

Fr (Cs 0.8) 最活潑金屬

背 H(2.2); B(2.0); C(2.5); N(3.0); O(3.5); F(4.0); Si(1.9); P(2.2); S(2.6); Cl(3.2); Br(3.0); I(2.7) 之負電性值。