CHEM110 – Chapter 4
Atomic Energy Levels

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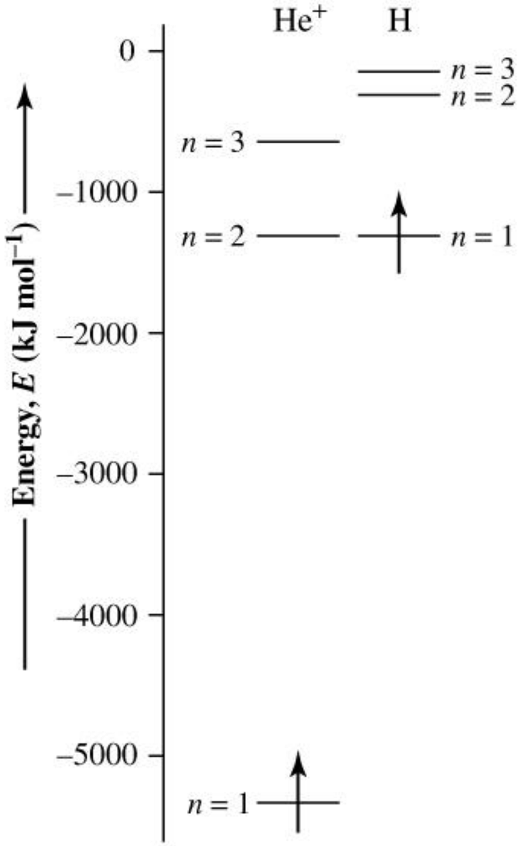
4.5 Atomic Orbital Electron Distributions and Energies

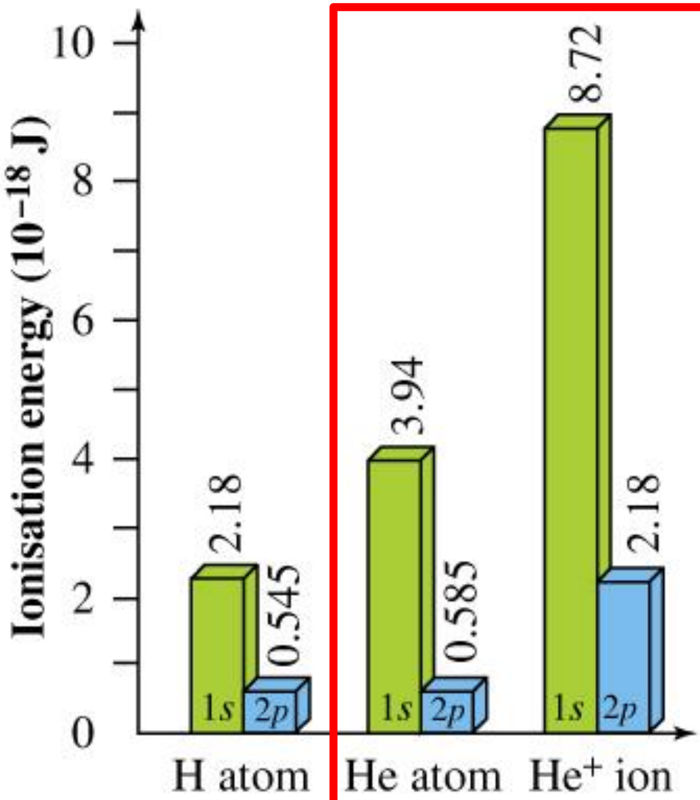
- **The effect of nuclear charge**
  - Energy of an orbital can be determined by measuring the amount of energy required to remove an electron completely
  - Ionisation energy → E_i



$H \rightarrow H^+ + e^-$ $\qquad E_{i\,H} = 2.18 \times 10^{-18}$ J

$He^+ \rightarrow He^{2+} + e^-$ $\qquad E_{i\,He+} = 8.72 \times 10^{-18}$ J

4.5 Atomic Orbital Electron Distributions and Energies



1e$^-$ **Z=1** | **2e$^-$** **Z=2** | **1e$^-$** **Z=2**

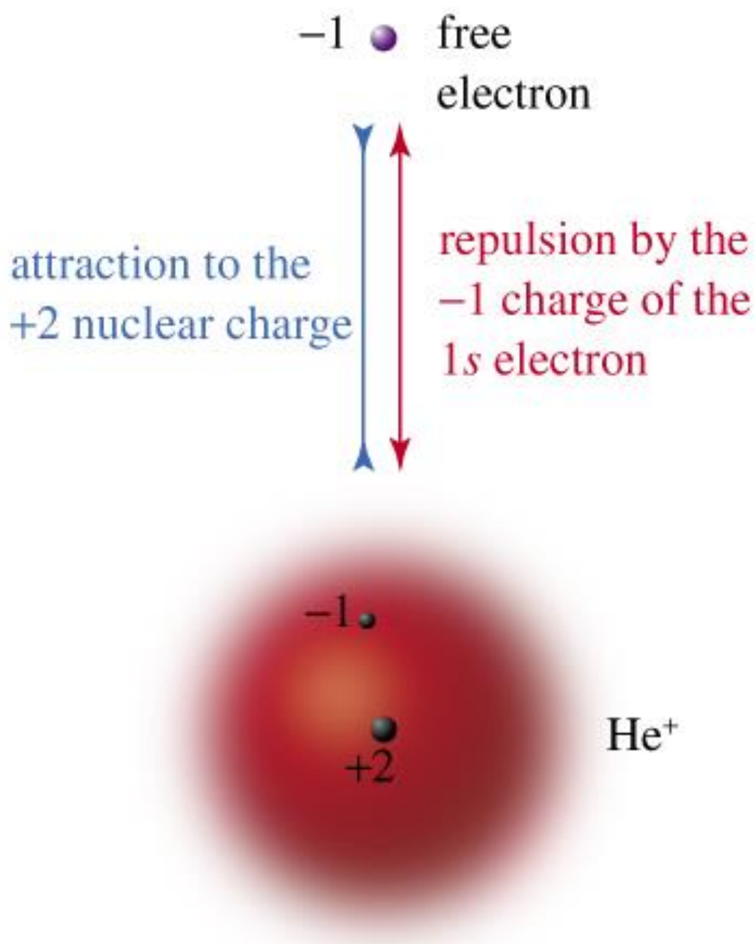
The effect of other electrons

- **Electrons affect each other's properties**
- **A given orbital is of higher energy (easier to remove electron) in a multi-electron atom than it is in a single-electron ion with the same nuclear charge**

4.5 Atomic Orbital Electron Distributions and Energies

- Shielding → Electron-electron repulsion cancels a portion of the attraction between the nucleus and the incoming electron
- A valence electron in a multi-electron atom experiences a charge less than the full nuclear charge
- Effective nuclear charge Z_{eff}

4.5 Atomic Orbital Electron Distributions and Energies



4.6 Structure of the Periodic Table

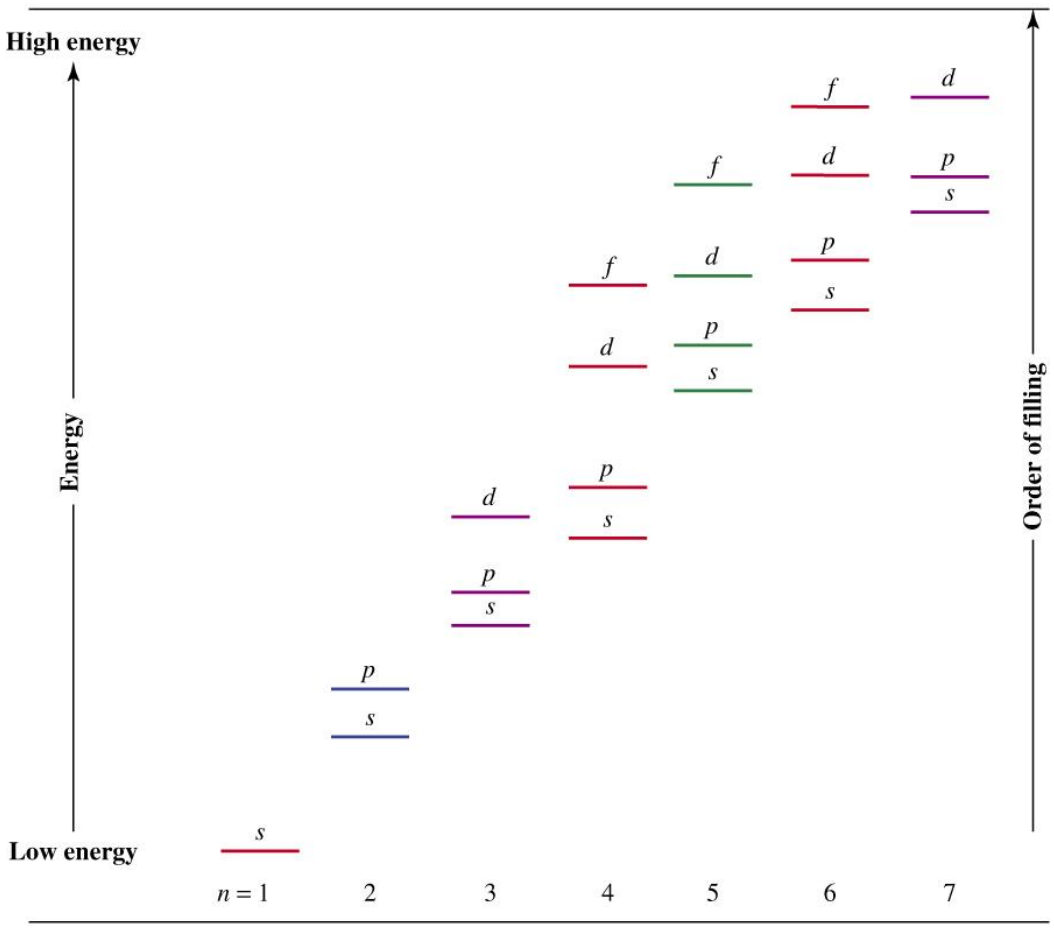
- Elements listed in order of increasing atomic number
- Also in order of increasing number of atomic electrons
- The elements are placed in rows called periods such that the columns are formed with groups of elements that have similar chemical properties

4.6 Structure of the Periodic Table

- **Aufbau principle** → **order of orbital filling**

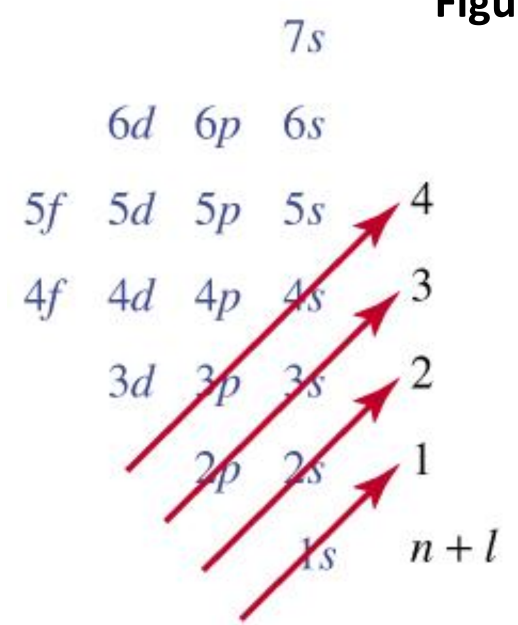
- **Constructed by placing electrons in the orbitals starting with the lowest in energy and moving progressively upward**

4.6 Structure of the Periodic Table



(a)

Figure 4.42



(b)

s **- 2 electrons**
p **set - 6 electrons**
d **set - 10 electrons**
f **set- 14 electrons**

4.6 Structure of the Periodic Table

Figure 4.44

Group number

Row number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** $1s^1$																	2 **He** $1s^2$
	main group (*s* block)												main group (*p* block)					
2	3 **Li** $2s^1$	4 **Be** $2s^2$											5 **B** $2s^22p^1$	6 **C** $2s^22p^2$	7 **N** $2s^22p^3$	8 **O** $2s^22p^4$	9 **F** $2s^22p^5$	10 **Ne** $2s^22p^6$
3	11 **Na** $3s^1$	12 **Mg** $3s^2$	transition metals (*d* block)										13 **Al** $3s^23p^1$	14 **Si** $3s^23p^2$	15 **P** $3s^23p^3$	16 **S** $3s^23p^4$	17 **Cl** $3s^23p^5$	18 **Ar** $3s^23p^6$
4	19 **K** $4s^1$	20 **Ca** $4s^2$	21 **Sc** $4s^23d^1$	22 **Ti** $4s^23d^2$	23 **V** $4s^23d^3$	24 **Cr** $4s^13d^5$	25 **Mn** $4s^23d^5$	26 **Fe** $4s^23d^6$	27 **Co** $4s^23d^7$	28 **Ni** $4s^23d^8$	29 **Cu** $4s^13d^{10}$	30 **Zn** $4s^23d^{10}$	31 **Ga** $4s^24p^1$	32 **Ge** $4s^24p^2$	33 **As** $4s^24p^3$	34 **Se** $4s^24p^4$	35 **Br** $4s^24p^5$	36 **Kr** $4s^24p^6$
5	37 **Rb** $5s^1$	38 **Sr** $5s^2$	39 **Y** $5s^24d^1$	40 **Zr** $5s^24d^2$	41 **Nb** $5s^14d^4$	42 **Mo** $5s^14d^5$	43 **Tc** $5s^24d^5$	44 **Ru** $5s^14d^7$	45 **Rh** $5s^14d^8$	46 **Pd** $4d^{10}$	47 **Ag** $5s^14d^{10}$	48 **Cd** $5s^24d^{10}$	49 **In** $5s^25p^1$	50 **Sn** $5s^25p^2$	51 **Sb** $5s^25p^3$	52 **Te** $5s^25p^4$	53 **I** $5s^25p^5$	54 **Xe** $5s^25p^6$
6	55 **Cs** $6s^1$	56 **Ba** $6s^2$	57–71 *	72 **Hf** $6s^25d^2$	73 **Ta** $6s^25d^3$	74 **W** $6s^25d^4$	75 **Re** $6s^25d^5$	76 **Os** $6s^25d^6$	77 **Ir** $6s^25d^7$	78 **Pt** $6s^15d^9$	79 **Au** $6s^15d^{10}$	80 **Hg** $6s^25d^{10}$	81 **Tl** $6s^26p^1$	82 **Pb** $6s^26p^2$	83 **Bi** $6s^26p^3$	84 **Po** $6s^26p^4$	85 **At** $6s^26p^5$	86 **Rn** $6s^26p^6$
7	87 **Fr** $7s^1$	88 **Ra** $7s^2$	89–103 **	104 **Rf** $7s^26d^2$	105 **Db** $7s^26d^3$	106 **Sg** $7s^26d^4$	107 **Bh** $7s^26d^5$	108 **Hs** $7s^26d^6$	109 **Mt** $7s^26d^7$	110 **Ds** $7s^26d^8$	111 **Rg** $7s^16d^{10}$	112 **Cn** $7s^26d^{10}$	113 **Uut** $7s^27p^1$	114 **Uuq** $7s^27p^2$	115 **Uup** $7s^27p^3$	116 **Uuh** $7s^27p^4$	117 **Uus** $7s^27p^5$	118 **Uuo** $7s^27p^5$

lanthoids and actinoids (*f* block)

6	lanthanoid series *	57 **La** $6s^25d^1$	58 **Ce** $6s^24f^15d^1$	59 **Pr** $6s^24f^3$	60 **Nd** $6s^24f^4$	61 **Pm** $6s^24f^5$	62 **Sm** $6s^24f^6$	63 **Eu** $6s^24f^7$	64 **Gd** $6s^24f^75d^1$	65 **Tb** $6s^24f^9$	66 **Dy** $6s^24f^{10}$	67 **Ho** $6s^24f^{11}$	68 **Er** $6s^24f^{12}$	69 **Tm** $6s^24f^{13}$	70 **Yb** $6s^24f^{14}$	71 **Lu** $6s^24f^{14}5d^1$
7	actinoid series **	89 **Ac** $7s^26d^1$	90 **Th** $7s^26d^2$	91 **Pa** $7s^25f^26d^1$	92 **U** $7s^25f^36d^1$	93 **Np** $7s^25f^46d^1$	94 **Pu** $7s^25f^6$	95 **Am** $7s^25f^7$	96 **Cm** $7s^25f^76d^1$	97 **Bk** $7s^25f^9$	98 **Cf** $7s^25f^{10}$	99 **Es** $7s^25f^{11}$	100 **Fm** $7s^25f^{12}$	101 **Md** $7s^25f^{13}$	102 **No** $7s^25f^{14}$	103 **Lr** $7s^25f^{14}6d^1$

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4.6 Structure of the Periodic Table

- Chemical behaviour of an atom is determined by the electrons that are accessible to an approaching species → valence electrons
- Inaccessible electrons are called core electrons
- Valence electrons participate in chemical reactions → core electrons do not

4.6 Electron Configuration

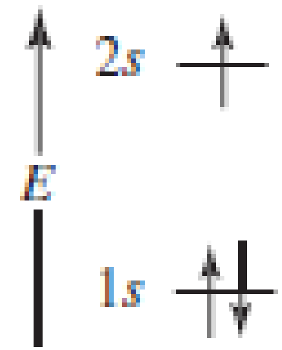
- **Complete specification of how an atom's electrons are distributed in its orbital**
- **There are 3 common ways of representation**
- **H atom → 1 electron**
  - $n = 1, l = 0, m_l = 0, m_s = + \frac{1}{2}$
  - $n = 1, l = 0, m_l = 0, m_s = - \frac{1}{2}$

4.6 Electron Configuration

- Li → 3 electrons

$$n = 2,\ l = 0,\ m_l = 0,\ m_s = +\tfrac{1}{2}$$
$$n = 1,\ l = 0,\ m_l = 0,\ m_s = +\tfrac{1}{2}$$
$$n = 1,\ l = 0,\ m_l = 0,\ m_s = -\tfrac{1}{2}$$

$1s^2 2s^1$



Quantum Numbers

Spectroscopic Notation

Arrow Diagram

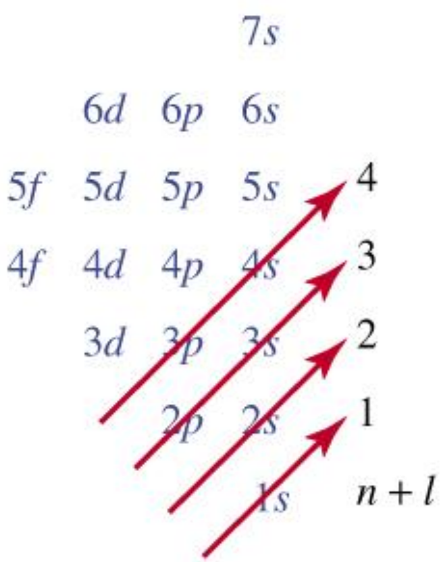
Worked Example 4.11 – page 142

Construct an energy level diagram and the shorthand notation of the ground-state configuration of aluminium. Provide one set of quantum numbers for the highest-energy electron.

Worked Example 4.12 – page 143

Determine the electron configuration of indium.

49 electrons



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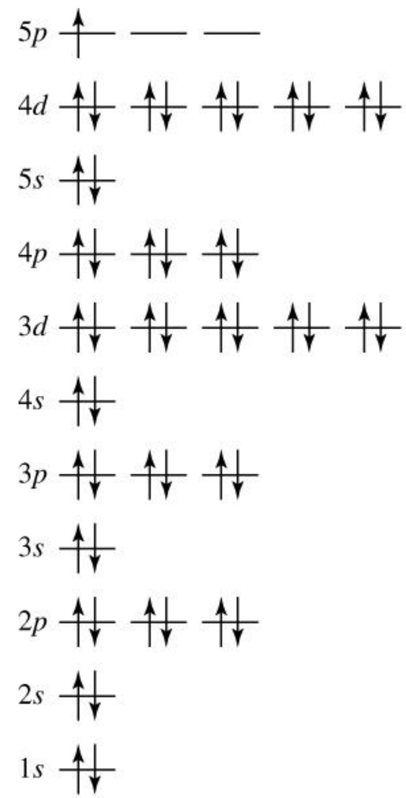
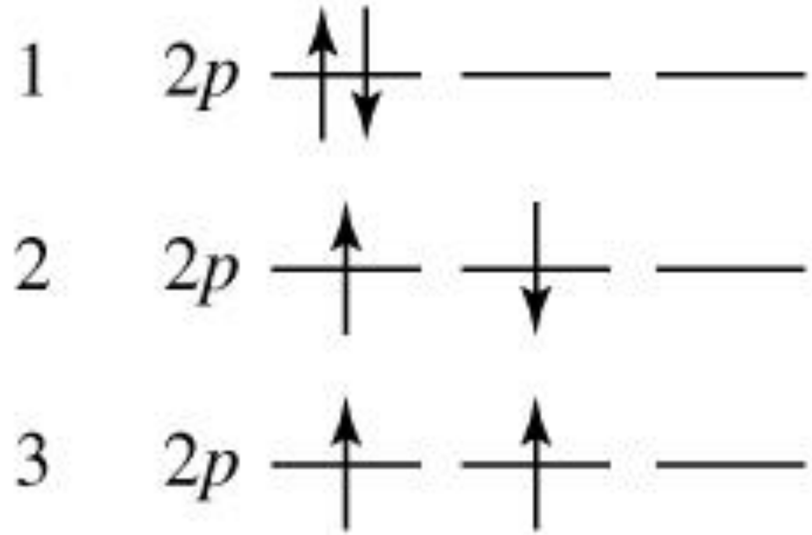


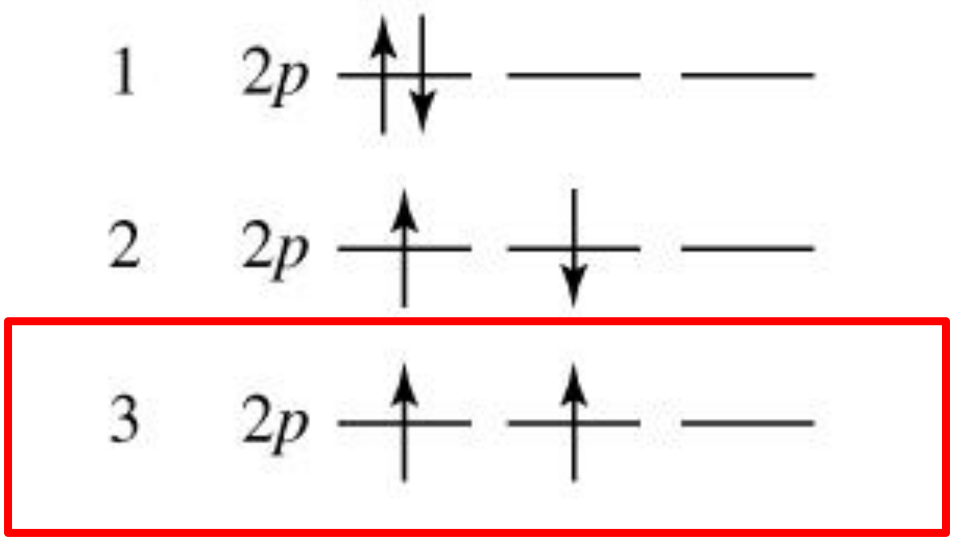
4.6 Electron Configuration



For two or more degenerate orbitals, the lowest energy situation results when electrons occupy the orbitals that keep them furthest apart

4.6 Electron Configuration

Hund's rule → the lowest energy configuration involving orbitals of equal energies is the one with the maximum number of electrons in the same spin orientation



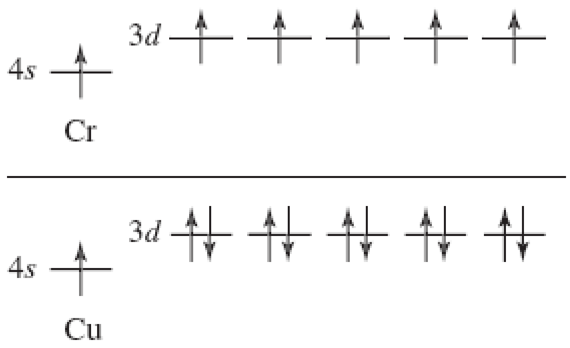
Worked Example 4.13 – page 144

Write the shorthand electron configuration and draw the ground-state orbital energy level diagram for the valence electrons in a sulphur atom.

4.6 Electron Configuration

- **Some elements have ground-state configurations different from the predictions of the regular progression**
- **Orbitals with nearly equal energies**

Orbitals	Atomic numbers affected	Example
$4s$, $3d$	24, 29	Cr: [Ar]$4s^1 3d^5$
$5s$, $4d$	41, 42, 44, 45, 46, 47	Ru: [Kr]$5s^1 4d^7$
$6s$, $5d$, $4f$	57, 58, 64, 78, 79	Au: [Xe]$6s^1 4f^{14} 5d^{10}$
$6d$, $5f$	89, 91–93, 96	U: [Rn]$7s^2 5f^3 6d^1$



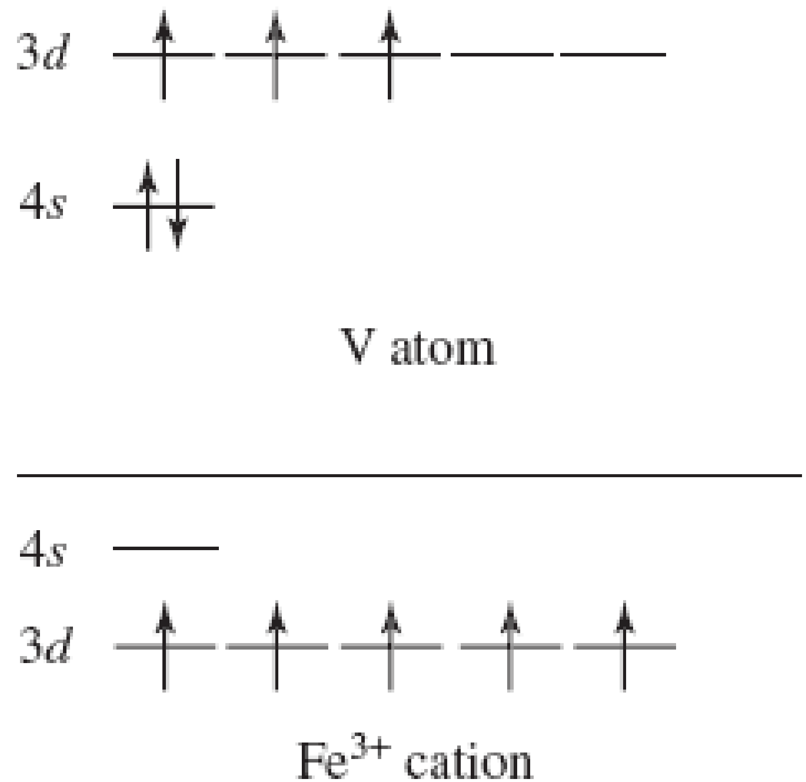
4.6 Electron Configuration

- Configurations of ions → same procedure
- Atoms and ions that have the same number of electrons are said to be isoelectronic
- Na^+, Ne and F^- → 10 electrons $1s^22s^22p^6$
- In general last electron 'added' is first electron lost on ionization
- Na → $1s^22s^22p^63s^1$ Na^+ → $1s^22s^22p^6$

4.6 Electron Configuration

V and Fe^{3+} both have 5 valence electrons

Figure 4.46



V → [Ar]4$s^2$3d^3

Fe^{3+} → [Ar]3d^5

4.6 Electron Configuration

- Magnetic properties of atoms → spins of these electrons cancel each other
- Net spin of zero
- An atom or ion with all electrons paired is termed diamagnetic
- An atom or ion with unpaired electrons is called paramagnetic

Worked Example 4.15 – page 146

Which of these is paramagnetic: F^-, Zn^{2+} or Ti?

$F^- \rightarrow 1s^2 2s^2 2p^6$

$Zn^{2+} \rightarrow [Ar]3d^{10}$

Ti $\rightarrow$ [Ar] $4s^2 3d^2$