Electronic Spectroscopy – Inorganic compounds are strongly colored

Prussian Blue – Ink in Blueprints

$-Fe^{III}-CN-Fe^{II}-N{\equiv}C-Fe^{III}$

CHEMICAL COMPOSITION OF GEMSTONES

THE COLOURS OF GEMSTONES ARE AFFECTED BY DIFFERENCES IN CHEMICAL AND ATOMIC STRUCTURE, LEADING TO THE ABSORPTION OF DIFFERENT WAVELENGTHS OF LIGHT. THEIR HARDNESS IS MEASURED ON THE MOHS SCALE, WHICH RUNS FROM 0-10.

ALEXANDRITE
Al_2BeO_4

Hardness: 8.5

Colour caused by chromium ions replacing aluminium in some sites. Colour varies in different light.

AMETHYST
Cr^{III}

SiO_2

Hardness: 7.0

Their colour is caused by iron 3+ ions replacing silicon in some locations in the structure.

AQUAMARINE
$Be_3Al_2(SiO_3)_6$

Hardness: 7.5-8.0

Colour caused by iron 2+/3+ ions replacing aluminium ions in some locations in the structure.

DIAMOND
C

Hardness: 10

Colourless; can be faintly coloured by the trapping of nitrogen atoms in the crystal.

EMERALD
Cr^{III}

$Be_3Al_2(SiO_3)_6$

Hardness: 7.5-8.0

Colour caused by chromium ions replacing aluminium in some locations in the structure.

GARNET
$Mg_3Al_2(SiO_4)_3$

Hardness: 6.5-7.5

Colour caused by iron 2+ ions replacing magnesium ions in some locations in the structure.

OPAL
$SiO_2.nH_2O$

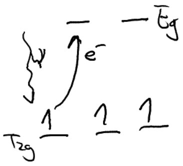
Hardness: 5.5-6.0

Many colours which are caused by interference & diffraction of light passing through the structure.

PEARL
$CaCO_3$

Hardness: 2.5-4.5

Produced in the soft tissue of shelled molluscs. The thinner the layers of the pearl, the finer the lustre.



PERIDOT
Mg_2SiO_4

Hardness: 6.5-7.0

Colour caused by iron 2+ ions replacing magnesium ions in some locations in the structure.

RUBY
Cr^{III}

Al_2O_3

Hardness: 9.0

Colour caused by chromium ions replacing aluminium ions in some locations in the structure.

SAPPHIRE
Fe^{II}

Al_2O_3

Hardness: 9.0

Colour caused by titanium and iron ions replacing aluminium ions in some locations in the structure.

SPINEL
$MgAl_2O_4$

Hardness: 7.5-8.0

A variety of colours are possible, caused by impurities such as iron, chromium and nickel.

TOPAZ
$Al_2SiO_4(F,OH)_2$

Hardness: 8.0

Pure topaz gems are colourless & transparent, but tinted by impurities they can have a variety of colours.

TOURMALINE
$Na_3Li_3Al_6(BO_3)_3(SiO_3)_6F_4$

Hardness: 7.0-7.5

Colour caused by manganese ions replacing lithium and aluminium ions in some sites.

TURQUIOSE
$Al_6(PO_4)_4(OH)_8.4H_2O$

Hardness: 5.0-6.0

Colour caused by the presence of copper ions coordinated to the hydroxide ions and water.

ZIRCON
$ZrSiO_4$

Hardness: 7.5

A range of possible colours that depend on the impurities present. Colourless specimens are popular diamond substitutes.

Quantum Numbers + Microstates

Absorption of $h\nu$ is a quantized process related to e^- promotion

↳ $e^- \leftrightarrow e^-$ interaction perturbs the quantization.

Carbon $C \rightarrow 1s^2 2s^2 2p^2$ $\quad$ ↑ ↑ __ $\quad 2p^2$

Each of the 2p e^- can be described by 4 QN

$n = 2$, $l = 1$

$m_l = 1, 0, -1$

$m_s = \frac{1}{2}, -\frac{1}{2}$

} Interaction of $e^-(1) + e^-(2)$ — Russell Saunders Coupling / LS Coupling

⇓

Creates Atomic States which we call Microstates.

Microstates = New QNs

$M_L = \sum m_l \Rightarrow$ Total Angular Momentum

$M_S = \sum m_s \Rightarrow$ Total Spin Angular Momentum (Related to Multiplicity)

A microstate = An individual description of an electronic config

$C = 1s^2 2s^2 2p^2$ $\quad$ ↑ ↓ __ $\quad$ $l = 1$ (2p)

m_l: 1 $\quad$ 0 $\quad$ −1

$[1^+ \; 0^-]$ (e_1^-, e_2^-)

First e^- $\quad m_l = 1 \quad m_s = \frac{1}{2}$

Second e^- $\quad m_l = 0 \quad m_s = -\frac{1}{2}$

In determining microstates for a given atomic species

① No 2 e^- in the same microstate can have identical QN

② Only unique microstates

i.e. 1^+0^- and 0^-1^+ are duplicates

③ Total # of microstates $= N = \frac{i!}{j!(i-j)!}$

i = # of $(m_l)(m_s)$ combinations

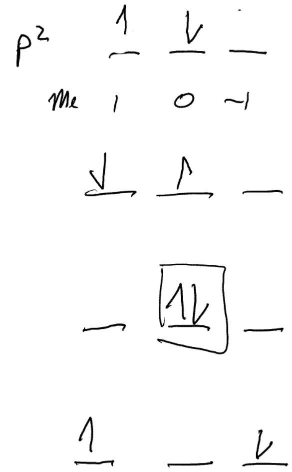
j = # of e^- in system

For the case of Carbon (p^2)

$m_l = 1, 0, -1$ 3 possibilities
$m_s = +1/2, -1/2$ 2 possibilities

$$N = \frac{(3)(2)!}{2!(6-2)!} = \frac{6!}{2!(4!)} = 15$$

M_L \ M_S	1	0	-1
2	X	1^+1^-	X
1	1^+0^+	1^+0^-, 1^-0^+	1^-0^-
0	1^+-1^+	0^+0^-, 1^+-1^-, 1^--1^+	1^--1^-
-1	-1^+0^+	-1^+0^-, -1^-0^+	-1^-0^-
-2	X	-1^+-1^-	X



L = Total Orbital Angular Momentum QN
S = Total Spin Angular Momentum QN } Describe collections of Microstates
J = Total Angular Momentum QN ⇒ Mixing of L and S

$M_L = 0, \pm1, \pm2 \ldots \pm L$ $\qquad$ $m_l = 0, \pm1, \pm2 \ldots \pm l$

$M_S = S, S-1, S-2 \ldots -S$ $\qquad$ $m_s = \pm 1/2$

$L = 0, 1, 2, 3, 4$ — S, P, D, F, G $\qquad$ $l = 0, 1, 2, 3, 4$ — s, p, d, f, g

The distribution of microstates in the microstate Table that allows us to determine the term symbols for an electronic config.

$p^2 \Rightarrow {}^3P, {}^1D, {}^1S$ $\qquad$ ${}^{(2S+1)}L$

${}^3P \Rightarrow L = 1$ $\quad m_l = 1$ $\quad m_l = 0$ $\quad \therefore S = 1$

${}^1D \Rightarrow L = 2$ $\quad m_l = 1$ $\quad m_l = 1$ $\quad \therefore S = 0$

${}^1S \Rightarrow L = 0$ $\quad m_l = 0$ $\quad m_l = 0$ $\quad \therefore S = 0$

	-1	0	1
2	0	1	0
1	1	2	1
0	1	3	1
-1	1	2	1
-2	0	1	0

	-1	0	1
2		~~x~~	
1	⊗	⊗ ~~x~~	⊗
0	⊗	⊗ △ ~~x~~	⊗
-1	⊗	⊗ ~~x~~	⊗
2		~~x~~	

^1D

	-1	0	1
2		x	
1		x	
0		x	
-1		x	
-2		x	

1 column is consistent w/ singlet
Five Rows ⇒ 5 M_L ⇒ D

^3P

	-1	0	1
2			
1	⊗	⊗	⊗
0	⊗	⊗	⊗
-1	⊗	⊗	⊗
-2			

3 Columns consistent w/ triplet
3 Rows $M_L = \pm 1, 0$ ⇒ P

^1S

	-1	0	1
2			
1			
0		△x	
-1			
-2			

1 column + 1 row consistent w/ singlet S