



Causes Of Colour In Gems

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A substantially rare, durable and beautiful, solid substance can be defined as a gemstone. It could be a mineral, rock aggregate or an organic substance which possess above mentioned characteristics. Colour is the dominant character with regard to its beauty apart from various other factors such as luster, transparency, brilliance, etc.

In order to generate vision proper coordination between object, light and human eye is necessary. When light waves hit an object, some energy is absorbed and some is reflected. The constructive result of the reflected energy within the visible range will be seen and identified by human eye, as the perception of colour relevant to the particular object.

There are certain phenomena or mechanisms that cause energy absorption in visible wavelength range (around 380-750nm) by gems (Fritsch and Rossman, 1987). They are dispersed metal ions, colour centers, charge transfer phenomena, band theory, and physical optics.

Effect of Dispersed Metal Ions

In 1987, Fritsch and Rossman have emphasized that the ions which are sufficiently isolated from one another as 'dispersed ions'. Effect of transition metal ions on formation of colour can be explained by Crystal field theory. Depending on the strength and nature of the bonding in a lattice and the valence state of the transition metal ion, a 'crystal field' is generated around the metal ion which determines the orbiting energy level of the unpaired d-shell electrons.

Gems which include transition metal ions (ions of Ti, V, Cr, Mn, Fe, Co, Ni, and Cu) either as idiochromatic (as a major constituent) or allochromatic (as an impurity) absorb specific energy from visual radiation, as electrons get excited and jump into a quantized and specific energy level by the crystal field. They emit back the absorbed energy either as heat or luminescence because the excited electrons are unstable in higher energy levels.

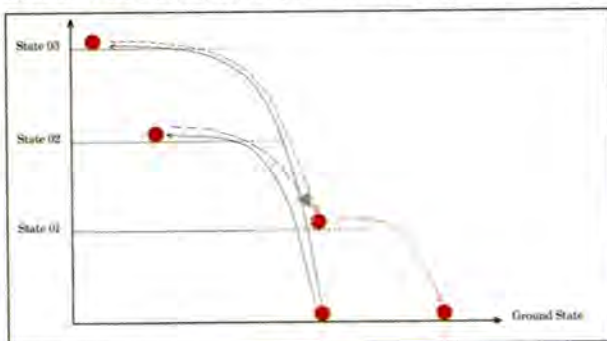


Figure 01:

Excited electrons jump into higher energy states and emit back energy as heat (state 03, 02 to state 01) and luminescence (state 01 to ground state)

For instance, Cr^{3+} ions that are substituted for Al^{3+} ions as an impurity in ruby, give the characteristic red colour. This occurs as a result of emitted residual colours after absorbing energy by electrons which jump into the higher energy levels that are created by the crystal field around the chromium ions. In the other hand, characteristic greenish colour of emerald is also due to Cr^{3+} ion impurities. This colour variation is due to the difference in energy of quantized levels around Cr^{3+} ions in ruby and emerald lattices.

Colour Centers

Colour centers can form due to misplacement of an ion or displacement of an electron in gemstones. Either any of these situations can generate an unpaired electron which can absorb energy and moves up to higher energy levels in non transition metal ions, similar as in transition metal ions. Here, if an electron is present at a vacancy, it is called an 'electron' colour center while if an electron is missing from a location where there should usually be a pair of electrons, it is called a 'hole' colour center (Nassau, 1978).

For an example, electron trapped in a vacancy created by misplacement of an F^- ion in fluorite form an electron colour center which causes the purple colour.

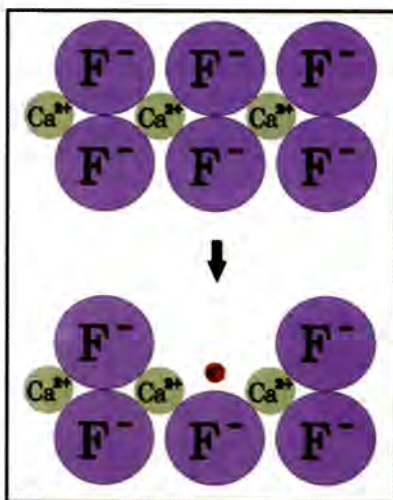


Figure 02:
Electron colour center in fluorite

In the other hand, characteristic colour of smoky quartz is due to a hole colour center formed due to a missing electron in oxygen ion. Here, substituted Al^{3+} ions in place of Si^{4+} ions in SiO_2 disturb the electro-neutrality, losing weaker valence electrons in oxygen ions if exposed to a radiation. As a result of this, the remaining unpaired electron can raise the smoky colour according to the crystal field theory.

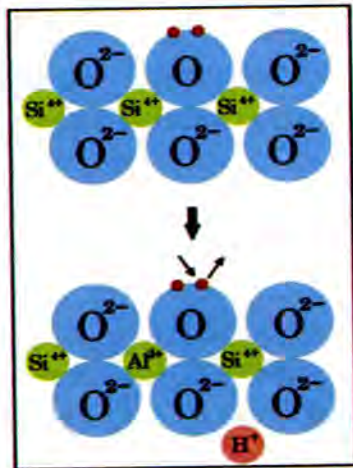


Figure 03:
Hole colour center in smoky quartz

Charge Transfer Phenomena

Particular phenomena could be explained using the molecular orbital theory that describes the orbit in which electrons travel when multiple atoms combine together chemically. When two transition metal elements of the same type or other, present in two valence states in a covalent bond some electrons in the outer shell can orbit among two ions. The required energy for particular transition will be absorbed by energy of visual radiation transmitting residual colour.

Blue sapphire is considered to be coloured by the inter-valance charge transfer between Fe^{2+} and Ti^{4+} ions as noted below:



Charge transfer between Fe^{2+} and Fe^{3+} ions are considered to raise blue colour of codierite.

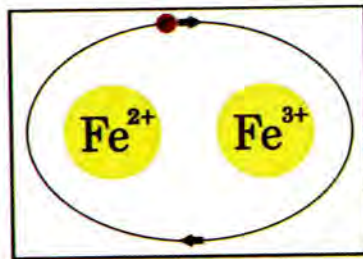
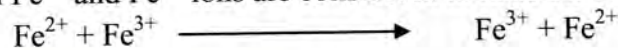


Figure 04:
Charge transfer in codierite

In contrary, metal-nonmetal charge transfers can be occur if no unpaired electrons available in metal ions as in crocoites ($PbCrO_4$). The charge transfer between Cr^{6+} and O^{2-} ions cause orangish colour in particular gemstone (Nassau, 1978).

The Band Theory

Valance electrons actively participate in bonding between atoms and relatively they are weakly bonded. In case of a crystal there is large number of valance electrons. If those valance electrons are considered in a pool, it is named as a Valance Band. On the other hand, the mobile electrons

cause conductivity in together, is named as Conduction Band. The barrier of an electron to moves from Valance Band to Conduction Band is called a Band Gap.

In case of pure diamond, comprising lattice structures with large band gaps, no electrons move in to conduction band absorbing no energy from visual radiation. If nitrogen impurity is present, one excess valance electron is added and then some electrons can be excited into the conduction band absorbing energy in visual radiation causing residual yellow colour. On the contrary, if boron impurity is present vacancy will be created in the valance band, and hence other electron from the valance band could excite to fill the vacancy by absorbing energy causing the blue color.

Physical optics

Colours that occur Based on the physical phenomena, are listed bellow as described by Nassau, 1978.

- Dispersion: 'Fire' effect in high dispersion gem stones; ex: diamond, zircon
- Scattering:
 - Chatoyancy; ex: cats eye effect in corundum, tigers eye
 - Asterrism; ex: star corundum, quartz
 - Aventurescence; ex: sunstone, aventurine albite , aventurine quartz , schiller spar
 - Adularescence; ex: moonstone, milky opal
 - Luster as in pearl, gypsum
- Interference: Interference effect within the cracks of iris quartz
- Diffraction: Diffraction grating produced by periodic spacing; ex: opal, labradorite

References

Emmanuel Fritsch and George R. Rossman,(1987), AN UPDATE ON COLOR IN GEMS. PART 1: INTRODUCTION AND COLORS CAUSED BY DISPERSED METAL IONS, GEMS & GEMOLOGY, pages 126-139, 1987

Emmanuel Fritsch and George R. Rossman,(1988), AN UPDATE ON COLOR IN GEMS. PART 2: COLORS INVOLVING MULTIPLE ATOMS AND COLOR CENTERS, GEMS & GEMOLOGY, pages 3-15, 1988

Kurt Nassau, (1978), The origins of color in minerals, American Mineralogist, Volume 63, pages 219-229, 1978

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