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Crystallography and mineralogy

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Mineralogy science studies the homogeneous materials occurs in nature and formed by it like gold, copper.

The main objective of this science is to identify minerals and their chemical and physical prosperities, formation, and place of occurrences.

The term mineral refers to an inorganic naturally occurring solid material, which has a specific "not fixed" chemical composition and unique crystal structure (e.g., quartz, hematite, and calcite).

a question here is any material can be termed as mineral?

Certainly, no there some conditions should be met in the material to be considered a mineral;

1- Solid

Where non-solid material (Liquid or gaseous liquids lack regular atomic structure, i.e., they are amorphous such as hydrocarbon and or glass.

2- Naturally occurring (non-organic)

Minerals were not living organisms, but some minerals that contain carbon are an exception to this, such as diamonds, which may have previously been of organic origin, as well as graphite. Calcite, which is the component of the shells of some marine animals, such as snails and oysters, is a product of organic processes. However, if these minerals crystallize and harden, they fall within the framework of the mineral definition.

3- Have a well-defined chemical composition

Each mineral constituted one chemical element or more than one for example quartz Si+o2= sio2, The chemical makeup of most minerals is not fixed as a pure substance.

4- Have Specific crystal structure

It must have a well-defined crystallographic structure; or, more generally, an ordered atomic arrangement. This property implies several macroscopic physical properties, such as crystal form, hardness, and

cleavage.

اناتاس TiO2



البروكيت TiO2



الروتيل TiO2



Chemical composition of earth crust

In the form of elements		In the form of oxides	
Elements	%	Oxide name	%
Oxygen (o)	46.71	-	-
Silicon (si)	27.69	sio2	59.08
Aluminum (Al)	8.07	Al2o3	15.23
Iron (Fe)	5.05	Feo Fe2o3	6.81
Calcium (Ca)	3.65	Сао	5.10
Sodium (Na)	2.75	Na2o	3.71
Potassium (K)	2.58	К2о	3.11
Magnesium (mg)	2.08	Mgo	3.45
Total	98.58		96.48

Based on these information we can conclude these two facts

1-8 elements are forming nearly 99 % in weight from earth crust and the other elements including gold, copper, leads, zinc are forming 1 %.

2- oxygen is the most common element occurs in earth crust, but it is not mean oxygen is free but chemically connected to rocks.

The previous chemical studies refer to that the elements are metals except oxygen. Silicon can be considered metal but also can be between metals and non- metals. The 7 elements act with oxygen to form oxides

Mgo +sio2 = mgsio3 (enstatite)

K2o+al2o3+6sio2= 2KALsi3o8 (orthoclase)

Physical prosperities of minerals

1- Optical properties : rely on light like color – streak – luster – luminescence – transparency

<u>Color</u>

The color of the mineral results from its ability to reflect a certain type of light waves and absorb other waves that make up normal white light.- The color of the metal appears red if it reflects red waves- Metal appears black if it does not reflect light A mineral appears white if it reflects all light waves.

Some minerals have constant color and called idiochromatic such as sulfur has yellow color, malachite "green color", azurite "blue color "







Quartz mineral



Sulfur





malachite

Sometimes the color change in the different types of one mineral and called allochromatic this due to pigments or inclusions such as quartz which is colorless but sometimes there some colored types as rose quartz due to red iron oxides and purple quartz (amethyst) due to manganese oxide also smoky quartz. Sometimes inclusions spread irregularly in mineral or as spots such as Saphir and purple quartz. Also, occur as layers , ring, or belts such as Agate and tourmaline. Sometime the change in color of one minerals is due to change in chemical composition such as sphalerite ZnS (yellow brown to black).

Play of colors







This feature depend on the ability of mineral in spread of light "dispersion"

This property is attributed to the splitting of ordinary white light rays into their colored components as they enter and exit the mineral. Such as diamond.

Change of color

This feature is like property play of color. However, it results from the interference of light rays reflected from the surfaces of parallel planes containing thin sheets of other minerals such as labradorite which gives blue, green, yellow colors from different sides or moving it.

Opalescence

Pearly or milky appearance of some minerals such as opal . It results from light reflections from within the mineral , where there are still molecules in different arrangements, giving different optical properties. And appear pearly such as moonstone.



Iridescence

Some minerals are colored in bright spectrum colors because of the interference of light rays in tiny cracks bounded by air or liquid membranes inside the metal like some types of quartz, calcite and mica.

Chatoyancy

The property of the minerals appearing in a bright, eye-catching color that varies depending on how you look at it, like wavy silk (changant) . It results from the difference in light reflections on the surface of fibrous minerals , resembling the sparkle of a cat's eye (as Satinspar mineral) .

Tarnish



It is a superficial change in the color of the mineral because of the decomposition of its outer layer due to various weathering factors, so it appears a color different from its original color such as copper and bornite.

Luminecence

It is a property of mineral to light radiation when exposed to other energy, such as frictional, thermal, electrical, or ultraviolet radiation. Thus, the minerals appears shiny and brightly with a color that may differ from its original color. Such as fluorite mineral when placed on a hot iron disc, also two pieces of quartz when they are friction with each other in darkness , and calcite mineral when exposed to ultraviolet rays. There are two types

A- Fluorescence



The mineral glows only when it is exposed to an external influence, and it disappears when the influence disappears. This feature termed according to fluorite mineral which clearly reflect this property also calcite, scheelite.

B- Phosphorescence

The mineral glows before and after the exposed to an external influence, it can be used to verify the purity of some minerals like diamond.

Streak

Color of the powder of the mineral. Sometimes the streak color differs from the color of mineral for example the color of pyrite mineral is copper yellow while its streak is black. The streak can be identified by scratching it on an unpolished plate.

Luster

It is the appearance of a mineral surface in reflected light. The types of luster as follow

A- Metallic luster

Normal luster of metals such as gold, silver also minerals characterized by dark colors like pyrite – Galena. Also, there are some minerals have weak metallic luster as chromite and usually these mineral are dark and heavy.





B- Non-metallic luster

This luster appears in light and colored minerals, and it include these types

- Vitreous (glassy) luster : like glass luster such as quartz mineral. Or weak vitreous luster called sub-vitreous like calcite.
- Resinous luster : Like glue luster sphalerite and amper minerals as example.
- Pearly luster : Like pearls luster such as talc mineral.
- Silky luster : It appears on the surface of fibrous minerals like Satinspar
- Adamantine luster : It is a stunning brilliance luster resulting from the large index of refraction in minerals such as diamonds. The luster intensity described as splendent based on the amount of reflected light like some hematite minerals.





Transparency

This property depends on the mineral's ability to transmit light. The minerals that allow light to pass through them described as transparent as quartz and described as sub-transparent or semi transparent when a small amount of light pass. There are some minerals allow pass light through them but prevent seeing bodies and called translucent as Mexican onyx mineral. The mineral known as opaque When it is unable to pass light through it even in case of Thin slices.

Cohesive prosperities

This property depends on the type of crystal structure, i.e. the internal atomic arrangement and the strong binding between ions and atoms or molecules that make up the minerals, so these properties vary from one mineral to another. And the most important of these properties

Hardness

Hardness is defined as the resistance of the mineral to scratching, abrasion, crumbling and corrosion, and the hardness of minerals differs from each other and is determined using the Moh scale of hardness.

And used to measure the hardness of the mineral a group of pens called hardness pens, which are holders installed at the end of each of them conical part of one of the group of minerals standard hardness and sometimes prove these pens around a ring known as the wheel of hardness g gemstone sellers sometimes use a solid cooler to differentiate between imitator and real .

Mohs Hardness Scale

	Name	Scale Number	Common Object
A COLOR	Diamond	10	
	Corundum	9	Masonry Drill Bit / 8.5
	Topaz	8	(restruction)
3	Quartz	7	Steel Nail / 6.5
	Orthoclase	6	Knife / 5.5
	Apatite	5	
	Fluorite	4	Penny (Copper) / 3.5
	Calcite	3	
(in	Gypsum	2	Fingernail / 2.5
	Talc	1	

Cleavage

It is the property of crumbling and division of some mineral in the direction of regular parallel levels if lightly knocked and these levels are known as levels of cleavage, and they are closely related to the crystal structure is always parallel to a particular crystalline face or several faces in the cleavage mineral. cleavage results from how to stack atoms and the type of bonds between them in the levels of cleavage the atoms are dense and coherent among themselves strongly while the stacking of atoms is spaced in the vertical direction, meaning that the binding forces are weak and there may be more than one direction for the level of cleavage in one mineral. As for the degree of completion, any extent of ease of cleavage, for example, galena mineral and salt halite crack in levels parallel to the cube family is called cracking cube and there is cleavage in the calcite mineral, where the levels are paralleled to the existing rhombic family.

• Cleavage is also described by the degree of completeness and ease of it is said that the mineral is full or incomplete, or clear cleavage - or good or not clear - weak



Parting

It is the feature of parting the mineral or its division at nonparallel levels of weakness in unstable and unmarked directions. It results from the influence of external factors after the formation of mineral due to exposure to pressure, cracking or other factors.

Fracture

The appearance of mineral surface , being broken in different levels other than the cleavage levels. The minerals which have not level of cleavage, can easily have fracture surface. This appears in non crystalline minerals when subjected to knocking , the types of fracture are, Conchoidal fracture : Where the broken surface curves and appears in the form of arched lines and gradually fade away as they move away from the center, and sometimes the conchoidal fracture appears weak and is described as sub-conchoidal such as quartz and flint.

Even fracture: The broken surface appears almost flat like chert mineral

Uneven fracture: The broken surface appears almost un flatted and rough As a result of the presence of protrusions such as rhodonite mineral.

Hackly fracture: It appears as sharp teeth like copper.

Earthy fracture: The broken surface takes on an uneven appearance, like the surfaces of ground materials such as chalk.



Tenacity

It is the property of mineral when trying to break, cut, pull, hit it by hammer or bend it. It depends on the degrees of tenacity of the constituent particles and the most important types of tenacity are

Brittle: The characteristic of a mineral that breaks or crushes easily and cannot be cut into slices when pressed or knocked, such as pyrite - apatite

- fluorite - quartz.

Sectile : They are minerals that can be easily cut with a knife into slices such as gypsum and graphite.

Malleable : It is a mineral that can be hammered into thin sheets, spread out, and shaped, like gold and copper.

Ductile : Minerals that can be formed into wires, such as copper and silver

Flexible : Where thin layers or sheets of mineral can be bent without breaking and remain twisted even after the pressure is removed, such as talc and selenite.

Elastic : The characteristic of a mineral that can be bent or twisted without breaking but returns to its state immediately after the removal of an influence such as mica.

Sense properties

Taste : When mineral is dissolved in water it has a taste as saline (halite)alkaline (potash and soda)- cooling – astringent (alum)- bitter (epsomite).

Oduor : some minerals have special smile when knocked or scratch or boiled like argillaceous Oduor (kaolin)- bituminous- garlic – sulfurous

Feel or touch : cold like silver or copper- greasy or soapy like talk – rough or harsh like chalk – smooth like sepiollite.

Thermal properties: Minerals tend to be melted (fusibility)

Magnetic properties: Magnetite is characterized by high magnetic properties – hematite and chromite have the property of attraction to magnetics and are called paramagnetic – either metals that repel with the magnets are called diamagnetism such as calcite

Radioactive properties: resulting from the metal containing radioactive elements such as uranium and thorium

Physical prosperities by using special instruments

Optical microscopic prosperities

The microscope magnifies from 20 to 100 magnification powers, depending on the size For the power of ocular and objective lenses

The geology microscope differs from biological one in having stage moves 360 degree around the axis

It is used to identify the properties that can not be

Identified by normal eye such as crystal form -

Cleavage – relief – twinning – Interference colors



Optical prosperities in the Prescence of polarizer only

Polarized light : It is light that oscillates in one direction, and the direction of oscillation is perpendicular to the direction of wave propagation.

Color : is one of the distinctive feature of minerals and the color of hand specimen differ from the color of polished slices as its thickness is 30 microns or 0.03 mm.

Pleochroism : changing mineral color with rotating the stage

Due to unevenness of light absorption in all directions.

Crystal form and habit :

Crystal form is described as euhedral – subhedral – anhedral

Crystal habits described as tabular – prismatic – radial







Euhedral

Idiomorfo



Subhedral

Hipidiomorfo



Anhedral

Xenomorfo

Cleavage : it is a weakness levels related to the internal crystal structure and appears in the form of parallel lines with equal distance between them – the mineral have one set – two sets or three sets of cleavage

Optical properties in the presences of analyzer and polarizer

Interference colors : The colors which appear and described as first order if

it gray or yellow – high order if the color of mineral is blue - green

Twinning : appearance of dark areas alternating with light areas

And described as simple (orthoclase)- lamellar (plagioclase)- crosshatching (microcline)

















Mineral deposits (Formation of minerals)

This study examines the formation of mineral deposits in terms of origin, and presence in nature.

First, in terms of origin and formation

1- From magma or lava

Magma is a molten rock fluid complex composition found at great depths of the earth's surface while lava appears on the surface of the earth flowing from volcanic craters The magma generally consists of

A- Non-volatile components: These components have a melting point more than 1000 consists of 99% seven oxides, one of which is acidic, silicon dioxide (35-75) The rest of the base oxides are aluminum oxides up to 0- 25%, iron oxides and iron up to 0- 20% and magnesium oxide up to 0-45% and calcium oxide up to 20, sodium oxide up to 0- 16% and potassium oxide 0 -12 %

• B- Volatile materials

- Such as fluor chlore boron sulfur water vapor carbon dioxide are found in a small percentage, but they increase in the stage of molten hardening and are important in formation of ore minerals. These components are about 1% with other non-volatile substances.
- When the magma hardens, the base oxides unite with the acidic silica under conditions of pressure and temperature to form silica minerals and the type of minerals depends on the composition of the magma, so it is rich in silica, aluminum and alkali feldspars, form quartz and feldspars, while the ferromagnetic minerals like olivine and pyroxene, amphibole, biotite are formed from magma that is rich in iron, calcium and magnesium oxides. If magma is rich in alkali and poor in silica form felspathoids minerals such as nepheline and leucite

Consolidation of magma

1- Orthomagmatic stage

It begins with the differentiation (segregation) of some metals, oxides and metal sulfides, which are difficult to combined with magma. There is a concentration of metals of economic importance such as gold and platinum iron oxides such as magnetite and these minerals are known as accessory minerals (small portion in comparison to volume of magma), while silicate minerals are called essential minerals because they are form about 99% of the magma. As the magma temperature drops, the essential minerals begin to crystallize – The Bowen Reactive Series



2 - pegmatitic stage

- The magma in this case consists of the liquid part in which the concentration of some economic minerals increases, formed from accessory minerals . The richness of this liquid part by fluxes lead to The growth of crystals in large sizes that allow them to be exploited.
- Pegmatite fluid invades cracks, voids and fractures and seeps into distant places, so its temperature decreases, and its components begin to crystallize slowly, growing crystals of large size such as mica feldspar and ornamental minerals such as topaz or emerald - Aptite and tourmaline

3- Pneumatolytic stage

The stage of the remaining gases after the previous two stages and consists of gases, active hot vapors and strong volatile materials - and leaks looking for an outlet between cracks, separators and faults in the rocks surrounding the magma exposed to cold and interact with each other and with the surrounding rocks or with minerals that have already been formed and be other minerals such as

A- cassiterite mineral

Fluorine reacts with tin, forming tin fluoride SNF4, a volatile substance that is easy to leak, then it reacts with water at a low temperature, and the formation of cassiterite SNO2 and hydrofluoric acid, which interacts with calcareous rocks, forming fluorite mineral.

B-Titanium minerals

Chlorine reacts with titanium and produces titanium chloride TICL4, which in volatile and turn reacts with water and produces hydrochloric acid and titanium oxide tio2 such as rutile, anatase and brookite minerals.

C-phosphorus minerals

Such as apatite, minerals contain boron like tourmaline and mineral contain flour such as topaz.

4- Hydrothermal stage

It is the last stage in the solidification of the magma where the remaining part becomes a hot aqueous solution with chemical activity – so it can dissolve and carry most of the metal compounds of economic value. These solutions seeps into cracks and joints away from its source and begins the process of sedimentation of the minerals they carry because of low pressure and temperature . Based on this the mineral deposits can be divided into
A- hydrothermal mineral

These minerals are deposited from solutions characterized by high temperature 300 – 500 and high pressure as they deposited at far depths like wolframite - topaz – apatite – cassiterite- molybdenite.

B- Mesothermal minerals

These minerals are deposited from solutions characterized by medium temperature 200 – 300 and medium pressure as they deposited at medium depths like galena- chalcopyrite- sphalerite – barite – calcite.

C- Epithermal minerals

These minerals are deposited from solutions characterized by low temperature 200 – 50 and low pressure as they deposited at shallow depths like cinnabar - marcasite – calcite – fluorite – quartz - opal.

Metasomatism

The activity of hydrothermal solution of magma does not only carry or deposit minerals but also react with surrounding rocks. Elements of some hydrothermal solutions can be replaced or replaced, partially or completely, by other elements like them or close to them present in rocks, whereby other new minerals are produced. This change is known in the mineral composition of rocks, as it results from replacing some components of hot solutions with some components of the rocks of the place in which they are located, Passing through it or being present in it, this is known as "metasomatism "

Metasomatism is attributed to that some rocks preferred alkali metal dissolved in hydrothermal solutions if it has high susceptibility to acidic metal. For example, Iron deposits were formed in America, where iron carbonate FeCO3 replaced calcium carbonate CaCO3 because of iron replacing calcium in limestone rocks, which led to the formation of siderite mineral FeCO3. Also, the siliceous wood in the petrified forest in Cairo resulted from the replacement of the cellulose that makes up the wood by silica .

2- From surface solutions

Surface solutions involve dissolved components of seas, oceans, rivers and ground water resulting from rains and seep into joints, cracks , fractures of rocks carrying amount of material that can dissolve it during its seeps. The minerals deposited by it is called sedimentary ore minerals and formed by

A- Evaporation of the solvent

Dissolved salts in the seas are concentrated because of water evaporation to a degree that allows some minerals to crystallize in an order that depends on the degree of solubility of the elements that make up these solutions. Carbonate salts precipitate first, then calcium carbonate such as calcite, then magnesium such as magnesite, then calcium sulphate of gypsum, then chloride such as halite.

B-evaporation of gas helps in dissolution

Carbon dioxide may dissolve in rainwater and give it the property of a weak acid (carbonic), thus dissolving some of the limestone rocks that seep through it and producing calcium bicarbonate (Cah2(CO3)2), which is a compound that is soluble in water and is unstable. Once it loses CO2, it turns into insoluble calcium carbonate. It precipitates, forming the minerals calcite and argentite It occurs in caves and grottoes located in areas with limestone rocks characterized by abundant rainfall, where calcium carbonate is deposited in the form of conical columns hanging from the ceilings of caves, and called stalactites. Drops of limestone solutions also fall on the floor of caves, losing carbon dioxide, and calcium carbonate is deposited in conical columns that rise at the bottom of caves, they are called stalagmites.

3- Formation of minerals from solid rocks (metamorphism)

Some minerals may be formed from solid rock materials under the influence of intense heat or heat accompanied by low pressure, so the minerals change completely or partially. The heat may result from the interference of magma materials or high-temperature solutions in the rocks of the place, and it happens that the rocks melt around contact, transforming the original minerals into other minerals adapting of new conditions. For example, iron minerals are transformed into deposits rich in hematite and magnetite minerals in the contact area and are called contact ore deposits. However, if the heat arises from the interaction of hot solutions, a process of substitution and replacement occurs between them, new minerals are created. This process is called hot liquid and transformation (pyrometasomatism).

Occurrence of mineral deposits

- A- syngenetic mineral deposits
- The minerals of these deposits are formed at the same time as the rocks containing or surrounding it and appear scattered, disseminated in it, for example, the minerals that appear in the stage of differentiation of metals and their oxides in the first stage of the magma solidification at the same time that the crystallization of basic silicate minerals (the appearance of chromite mineral in the ultrabasic rocks of the as well as some bedded mineral deposits that are formed in a contemporary time to form sedimentary rocks)

B- Epigenetic mineral deposits

The minerals of these deposits are formed after the appearance of rocks containing them and are often found in cracks, joints and so they are formed in the form of these spaces. and usually appear in the form of veins that may extend for long distances. sometimes minerals are deposited in the distances between the rocks and these gatherings are called impregnations deposits.

Ore deposits that appear in the same place where they originated are known as primary or in situ deposits, while wind-borne deposits are secondary or placer deposits, such as gold deposits that may exist with magnetite chromite and zircon deposits.

Classification of minerals

There are several methods for minerals classification like chemical classification , crystal chemistry classification , economic chemical classification.

Chemical Classification of minerals

1- Native minerals group

They are metals that exist free elements that are not united with others in nature, and grouped as

Native metals (gold Au-silver Ag – Platine Pt)

Native none metals (sulfur S – Diamond C – graphite C)

2- Oxide Minerals group

None-hydrated metal oxides (magnetite- chromite- hematite- rutile)

Hydrated metal oxides (limonite – goethite – manganite)

3- Sulphates – chromates – molybdates – tungstate minerals

None- hydrated sulphates (barite –anhydrite)

Hydrous sulphates (gypsum - epsomite)

Chromates (crocoisite) – molybdates (wulfenite) – tungstate (wolframite)

4- Phosphates- Vanadates

Phosphates (apatite – turquois – monazite)

Vanadates (vanadinite – carnotite)

5- carbonates – nitrates – borates group minerals

Carbonates (calcite group as calcite – dolomite – magnesite – siderite) and (aragonite group like aragonite – witherite – cerussite) and (malachite group like malachite – azurite)

Nitrate (soda niter) – Borates (kernite – borax)

6- Haloids minerals

- Like halite fluorite cryolite)
- 7- Sulfides and Sulfosalts

Sulfides (argenite – chalcocite – pyrite – chalcopyrite- sphalerite)

Sulfosalts (metal act with nonmetals such as arsenic or antymon with sulfur) such as tetrahedrite

8- Silicate minerals

These minerals formed from $(sio_4)^{-4}$ in form of tetrahedron, oxygen atom surrounded by 4 silicon atoms , with connected this unit with other units produce different types of silicates like

Independent tetrahedral group (topaz, olivine , garnet) , Sorosilicate (hemimorphite) , ring structure or cyclosilicates (Rhodonite), hexagonal ring (tourmaline), chain structure or inosilicates Crystal chemistry of minerals (relation between chemical composition and atomic structure)

Crystals of some minerals overlap during their growth to form zoning crystals despite the difference in the chemical composition of these overlapping crystals in both shape and atomic structure. This means that even though these atoms are structurally different, they are similar in size and in their positions within the crystal, and thus they can replace each other. It indicates a relationship between chemical composition and atomic structure.

Atomic structure of minerals

The atomic structure of minerals means the following three items

1- The geometric arrangement in space of atoms, molecules, and ions that are the building blocks of matter

These structural units are arranged inside the crystal in a geometric system subject to certain symmetrical elements, and the internal arrangement reflects the same on the outside in the form of crystal faces (7 crystal systems which are the highest symmetrical (complete), but there are other systems that are less symmetrical, for a total of 32 crystalline systems).

2- The degree of closeness between these structural units and the way they are arranged and packed into the material: As the crystalline material is characterized by a fixed arrangement of ions or atoms in three dimensions, the spatial arrangement of the ions can be represented by schematic shapes, where the bonds represent the lines between these ions.

3- The type of electrical forces that connect these structural units and their properties



Isomorphism

There are some substances that differ in their chemical composition but are similar in crystal structure. Therefore, they are also similar in their natural, chemical and crystalline properties and have almost the same angles between the two faces. These materials associated with this phenomenon are known as isomorphous substances with similar shapes, an example of this phenomenon,

Isomorphous Substances are similar in their atomic structure, and their crystals overlap with each other. If we analyze a strontachite crystal, we find an amount of calcium and barium that replaced part of the strontium. This is known as isomorphous substitution or replacement.

Replacement either partially or completely and only are in crystals nearly have same size. Example of partial replacement of iron instead of zinc in sphalerite mineral. For complete mineral appear in plagioclase- albite anorthite minerals where sodium and silicon replace calcium – aluminum

Polymorphism

The presence of more than one substance that has the same chemical composition and differs in structure and crystal form. An example of this is diamond and graphite, which have the same chemical composition (carbon), but differ from each other in natural properties such as hardness, specific gravity, and crystal system. Another example is calcium carbonate, which can crystallize under special conditions to give rhombodedrad crystals which belongs to trigonal system (calcite), and under other conditions to give orthorhombic crystals, which are the minerals calcite and argentite, both of which have natural properties different from the other.

Substances that exist in two different crystal forms are called dimorphous, such as carbon and calcium carbonate. However, they are found in three forms known as trimorphous as silicon dioxide, which exists in three forms: quartz (trigonal family), tridymite (rhombic), and cristobalite (tetragonal family).

Pseudomorphism

If a modification occurs to the crystal such that its internal atomic structure changes without any change occurring in the external shape (that is, it maintains its external shape), then in this case it is described as pseudomorph or false form. In a pseudo-shaped crystal, the chemical composition and atomic structure follow a specific mineral, while the external shape follows another mineral. An example of this is the pyrite mineral that changes and gives the mineral goethite, which still maintains the external cubic shape of pyrite (a false form of the mineral goethite resulting from pyrite).

- This Pseudomorphism related to
- 1- A change in form without a change in chemical composition

2- A change in form occurs when a chemical change occurs because of a replacement or substitution process (quartz replaces calcite) or because of decomposition, which is either by adding a new material such as gypsum consisting of anhydrite plus water or removing another material such as hematite from magnetite after removing iron or by adding and removing some materials (Goethite is formed from pyrite by removing sulfur and adding water)

- Crystallography
- ➢Introduction
- ➢Crystal elements
- ➤Crystal habit
- Crystl form
- Crystal symmetry
- ➤Crystal axis
- ➢Crystal systems
- ➤Crystal axis
- Crystal aggregates
- Parameters and indices

Crystal Parts



Crystal Faces = limiting surfaces of growth

Depends in part on shape of building units & physical cond. (T, P, matrix, nature & flow direction of solutions, etc.)

Edges: the edges are intersections of prominent crystal faces

Contact Goniometer



2. Goniometr Mitscherlicha.

Reflection Goniometer

Interfacial angle

Note: "interfacial angle" = the angle between the faces measured like this



Remember, face sizes may vary, but angles can't

Crystallographic Elements

Crystal Axes: generally taken as parallel to the edges (intersections) of prominent crystal faces. Hexagonal a Cubic d b a≠c α=y=90° β=120° a a=b=c $\alpha = \beta = \gamma = 90^{\circ}$ 1 Tetragonal Trigonal b a Golden Rhombus a=b=c $p/q = \phi$ $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$ b a a=b≠c $\alpha = \beta = \gamma = 90^{\circ}$ Orthorhombic Monoclinic a≠b≠c $\alpha = \gamma = 90^{\circ} \neq \beta$ a a≠b≠c $\alpha = \beta = \gamma = 90^{\circ}$ **Crystallographic Axes Axial Angles Triclinic** a a≠b≠c $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$



Rotational Symmetry

The imaginary axis along which the rotation is performed is an element of symmetry referred to as a rotation axis. Rotational symmetry axes possible in crystals are 1,2,3,4,6.

1-Fold Rotation Axis - An object that requires rotation of a full 360° in order to restore it to its original appearance has no rotational symmetry. Since it repeats itself 1 time every 360° it is said to have a 1-fold axis of rotational symmetry.



2-fold Rotation Axis imagine rotation axis perpendicular to the

page

If an object appears identical after a rotation of 180°, that is twice in a 360° rotation, then it is said to have a 2-fold rotation axis (360/180 = 2).







Note: A filled oval shape represents the point where the 2-fold rotation axis intersects the page. **3-Fold Rotation Axis** – An object that repeats itself after a rotation of 120° is said to have a 3-fold axis of rotational symmetry, thus repeating itself 3 times in a 360° rotation (360/120 =3). Note: A filled triangle is used to symbolize the location of 3-fold rotation axis.

4-Fold Rotation Axis - If an object repeats itself

after 90° of rotation, it will repeat 4 times in a

360° rotation, as illustrated. Note: A *filled square*

is used to symbolize the location of 4-fold axis of

rotational symmetry.

4 •

6-Fold Rotation Axis - If rotation of 60° about an axis causes the object to repeat itself, then it has 6-fold axis of rotational symmetry (360/60=6). Note: A filled hexagon is used as the symbol for a 6-fold rotation axis.







Rotation

Is it possible to have 5, 7or 8 -fold rotation symmetry?

Objects with 5, 7and 8 or higher order symmetry do exist in nature, e.g. star fish) 5-fold), flowers with 5 or 8-fold

symmetry.





However, these are not possible in crystallography as they cannot fill the space completely



Mirror Symmetry

A mirror symmetry operation is an imaginary operation that can be performed to reproduce an object. The operation is done by imagining that you cut the object in half, then place a mirror next to one of the halves of the object along the cut. If the reflection in the mirror reproduces the other half of the object, then the object is said to have mirror symmetry. The plane of the mirror is an element of symmetry referred to as a mirror plane. Note: the plane is symbolized with the letter m.



inversion

- Another operation that can be performed through a point is inversion.
- In this operation lines are drawn from all points on the object through a point in the centre of the object, called a
- symmetry centre
- (Note: it is symbolized with the letter "i").
- The lines each have lengths that are equidistant from the original points.



- When the ends of the lines are connected, the original object is reproduced inverted from its original appearance.
- In the diagram shown here, only a few such lines are drawn for the small triangular face. The right hand diagram shows the object without the imaginary lines that reproduced the object.



<u>Crystal Form</u>: It is a group of crystal faces have similar shape and area and display the same physical and chemical properties.

Some characteristic of form:

- 1- It is used to indicates general outward appearance of crystal.
- 2- There is great relation between form and element of symmetry.
- 3- Some crystal construct by one form others by more than one.
- 4- Minimum face in a form is one and maximum are 48 faces.



<u>Type of Crystal:</u> There are two types of crystal depend on the number of form.

1- Simple crystal: The crystal consists one form.





Classification of Form:

- 1- Depend on closing and opening the space:
- A- Close Form. Are those form that constructed a crystal alone.





B- Open Form. Are those form that can not constructed a crystal alone.





2- Depend on relation between form and crystallographic axes:

A- General form. The face of the form intersects all crystal axes at different lengths. Some characteristic of general form:

1- In Orthorhombic, monoclinic and triclinic systems the symbol of the general form is $\{111\}$.

- 2- In tetragonal system the symbol
 - is {121} or {122}.
- 3- In cubic system the symbol

is {123}.

4- In hexagonal and trigonal the symbol

is {1231} or {1231}





B- Special Form. A face of the form is parallel to one or two crystallographic axes



Intersects + c-axis

Parallel to a and b axes

Form No.2



Intersects - a-axis

Parallel to c and b axes

Form No.3

Intersects - b-axis Parallel to a and c axes





- Intersects +a1 and –
 a3 axes
- Parallel to a2 and c axes









Holohedral and Hemihedral Forms



Hemimorphic Form



Enantiomorphic Forms

- a group of faces on a crystal related to the same symmetry functions, the faces of the group are usually the same size and shape on the crystal
- recognition of crystal forms can help determine the symmetry functions present on a crystal and vice versa
- forms related to non isometric classes are quite different than those related to isometric classes
- since more than one form can exist on a crystal, it is more difficult to ascertain each form in the "full form".
CRYSTAL HABIT

The term "crystal habit" is used to identify the shape, size and appearance of a crystal's unique growth characteristics, or "Crystal Forms". A particular mineral may exhibit several different habits, all of which are influenced by the following factors:

- **Crystal Twinning** (two individual crystals share some of the same crystal lattice points)
- Growth Conditions (heat, pressure, and space)
- Trace Impurities (present during crystal formation)

Acicular

slender, needle-like crystals: tourmaline, hornblende, arsenopyrite, rutile, apatite, sillimanite



Capillary and filiform

hair-like or threadlike: native Au, Ag, Cu





Bladed

elongated crystals flattened like a knife blade: kyanite



Dendritic

arborescent, in slender divergent branches, somewhat plantlike--native metals, pyrolusite



Radiating

divergent: zeolite; tremolite; talc pyrolusite, tourmaline



Drusy

surface covered with a layer of small crystals--sugar like: calcite, quartz, sphalerite, pyrite



Dodecahedral

Also commonly seen in Garnets, as in this lab

- 12 sided crystal growth.
- NOTE: Rhombohedral, Cubic, etc. are also geometric habits, i.e. how the crystal grows.





Fibrous

Fibreous tremolite chrysotile asbestos



Globular and colloform

radiating individuals forming small spherical groups

examples include zeolites, quartz, malachite, goethite, pyrolusite, hematite





bunch of grapes, example pyrolusite



Reniform

kidney like, examples hematite, malachite





easily separable into plates or leaves: Micas are the ultimate example



Micaceous

similar to foliated but splits into very thin sheets: muscovite, biotite, chlorite



■ Tabular or lamellar ■ Flat and plate-like: barite, dolomite



Granular

composed of many individual grains of similar size: olivine, garnet



Prismatic or columnar

elongated crystals with identical faces parallel to a common direction: tourmaline, hornblende, apatite





Equant Crystal Habit

Squashed, pinnacoids (terminating face) dominant over prisms



Cubic Crystal Habit





النطاق البلورى

مجموعة من الأوجه تتقابل هي أو امتداداتها عند أحرف متوازية وتوازى في نفس الوقت اتجاها عاما يمر بمركز البلورة ويسمى محور النطاق.







1*0 - 0*1, 0*0 - 1*0, 1*1 - 1*0Zone Symbol = [001]

How to calculate a zone axis [uvw]?

<u>**Crystal zone:**</u> They are a group of faces arranged in such a manner that their intersection edges are parallel. The line pass through the center of the crystal and parallel to these edges is called zone axis.



How the zone axis direction is calculate?

- 1- The zone symbol is put in the bracket [uvw].
- 2- Miller indices of the two faces have to be known, (hkl) and (pqr).
- 3- The indices of each face is written twice.
- 4- Using cross multiplication of determination law.

$$\begin{array}{c|c} h & k & l \\ \hline P & q & r & p & q & r \end{array}$$

$$u = kr - lq$$

$$V = Ip - hr$$

$$W = hq - kp$$

Example-1: The indices of the two faces are (011) and (111), find [uvw].

So the zone axis direction [uvw]= [011]

For determining weather a face has indices (hkl) is locate within the zone [uvw]

The Weiss zone law (Zonal equation) is used as follow:

Uh + vk + wl = 0, if the result equal to zero it means the face is locates, otherwise not.

Example-2: The indices of a face is (012) and the zone axis direction equal to [121]. Find weather this face locates within the zone or not.

Uh + vk + wl = 0

0x1 + 1x2 + 2x1 = 0, yes the face locates within the zone.

Example-2: The indices of a face is (123) and the zone axis direction equal to [022]. Find weather this face locates within the zone or not.

Uh + vk + wl = 0

0x1 + 2x2 + 3x2 = 10, No the face does not locate within the zone.

Example-3: The indices of a faces is (hkl), it locates between the two faces have indices (102) and (211). Find:

- 1- The indices of the face (hkl).
- 2- The zone axis direction.
- 3- Prove weather the face (hkl) locates with in the above zone or not.

h = 1 + 2 = 3

K = 0 + 1 = 1

L = 2 + 1 = 3, The indices equal to (313)

The zone axis direction:

1 0 2 1 0 2 2 1 1 2 1 1 u = 0x1 - 2x1 = -2, v = 2x2 - 1x1 = 3, w = 1x1 - 0x2 = 1So [uvw] = [231] For knowing if (313) locates within [231] uk + vk + wl = 0

2x3 + 3x1 + 1x3 = 0, yes the face locates within the zone.

Individual Crystal Systems and the Axial System

- * The crystal system is a grouping of crystal structures that are categorized according to the axial system used to describe their atomic "lattice" structure.
- * A crystal's lattice is a three dimensional network of atoms that are arranged in a symmetrical pattern.
- * Each crystal system consists of a set of three crystallographic axes (*a*, *b*, and *c*) in a particular geometrical arrangement.
- * The seven unique crystal systems, listed in order of decreasing symmetry, are:
- * 1. Cubic System,
- * 2. Hexagonal System,
- * 3. Tetragonal System,
- * 4. Rhombohedric (Trigonal) System,
- * 5. Orthorhombic System,
- * 6. Monoclinic System,
- * 7. Triclinic System.



CRYSTALLOGRAPHIC AXES AND SYMMETRY SYSTEMS

When relating the 14 Bravais-lattices to Cartesian Principle Axes, intersecting in the center of the space-lattice or crystals formed from the repetitions of them. These crystallographic axes are generally taken parallel to the intersection edges of major crystal faces. They are named as **a-, b-, c-axes**, where c-axis is always vertical. In hexagonal and trigonal systems there are four axes **a1, a2, a3** (horizontal with 120° between them), and **c** (vertical). From the origin the length of the axes are designated as (**+** or **-**).

They are grouped into seven crystal systems based on the following criteria:

- a) relative lengths of the crystallographic axes
- b) number of crystallographic axes
- c) values of the interaxial angles
- d) some essential element of symmetry

The seven crystal systems are:

According to the lengths of crystallographic axes a-, b-, c-axes, and the values of axial angles α , β , γ between them crystals are classified into seven systems as follows:

Symmety Systems	Crystallographic Axes	Axial Angles
1. Cubic (Isometric)	a1 = a2 = a3	$\alpha = \beta = \gamma = 90^{\circ}$
2. Tetragonal	a1 = a2 ≠ c	$\alpha = \beta = \gamma = 90^{\circ}$
3. Hexagonal	a1 = a2 = a3 ≠ c	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$
4. Rhombohedral	a1 = a2 = a3 ≠ c	$\alpha = \beta = 90^\circ, \gamma = 120^\circ$
5. Orthorhombic	a≠b≠c	$\alpha = \beta = \gamma = 90^{\circ}$
6. Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^{\circ} \neq \beta$
7. Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^{\circ}$

The 7 Crystal Systems



The Cubic system:

- Three crystallographic axes, a = b = c, $\alpha = \beta = \gamma = 90^{\circ}$.
- Essential element of symmetry is a three-fold rotary or rotary inversion axis.







The Tetragonal system:

(1) Three crystallographic axes, a = b = c, $\alpha = \beta = \gamma = 90^{\circ}$. (2) Essential element of symmetry is a four-fold rotary or rotary inversion axis.





(4) The Hexagonal system:

Four crystallographic axes, $a1 = a2 = a3 \neq c$, $\alpha = \beta = 90^{\circ}$, $\gamma = I20^{\circ}$ (2) The vertical axis "c" is characterized by being a six fold axis of symmetry.



Hexagonal a1 = a2 = a3 ≠ c, α = β= 90°, γ = I20°



(3) The Trigonal system:

(1) Four crystallographic axes, a1 = a2 = a3 \neq c, $\alpha = \beta$ = 90°, $\gamma = 120^{\circ}$

(2) The vertical axis "c" is characterized by commonly being a three fold axis of symmetry.



(5) <u>The Orthorhombic system</u>:

(1) Three crystallographic axes, $\mathbf{a} \neq \mathbf{b} \neq \mathbf{c}$, $\alpha = \beta = \gamma = \mathbf{90}^{\circ}$ (2) Essential element of symmetry is a two-fold rotary axis.




The Monoclinic system:

(1) Three crystallographic axes, $\mathbf{a} \neq \mathbf{b} \neq \mathbf{c}$, $\alpha = \gamma = 90^{\circ} \neq \beta$ (2) Essential element of symmetry is a two fold rotary axis or a plane. The 2-fold rotational axis is usually taken as the b axis and perpendicular to the mirror plane.

(3) The a axis is inclined to the front ($\beta > 90^{\circ}$), and c is vertical.



(7) The Triclinic system:

(1) Three crystallographic axes, $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$ (2) No essential element of symmetry. <u>Additional criteria:</u> As much as possible, β and α should be both > 90°. The most pronounced zone should be vertical. The axis of this zone is then taken as "c". {001} should slope

forward and to the right.



In the following **Bravais lattices** that belong to each of the 7 symmetry systems:

1. Isometric or Cubic; P, F, I.

3 Bravais lattices



Symmetry elements: Four 3-fold rotation axes along cube diagonals $\mathbf{a} = \mathbf{b} = \mathbf{c}$ $\alpha = \beta = \gamma = 90^{\circ}$

2. Tetragonal; P, I.

Two Bravais lattices



Symmetry element: One 4-fold rotation axis $a = b \neq c$ $\alpha = \beta = \gamma = 90^{\circ}$

3. Hexagonal; P (or C). Only one Bravais lattice



a1 = a2 = a3 \neq c, $\alpha = \beta = 90^{\circ}, \gamma = 120^{\circ}$ Symmetry element: One 6-fold rotation axis

4. Trigonal or Rhombohedral: R.

One Bravais lattice



a1 = a2 = a3 \neq c, $\alpha = \beta = 90^{\circ}, \gamma = 120^{\circ}$ Symmetry element: One 3-fold rotation axis

5. Orthorhombic: P, I, C, F.

Four Bravais lattices



 $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^{\circ}$ α Symmetry element: Three mutually perpendicular 2-fold rotation axes



Two Bravais lattices



a ≠ b ≠ c α = γ = 90° ≠ βαSymmetry element: One 2-fold rotation axis

7. Triclinic: P

One Bravais lattice



 $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$ Symmetry element: None

Subject 8: Axial Ratio & Parameters **Lecturer: Prof. Sayed O. Elkhateeb**

Objective: In crystallography, some time identification of minerals is done through calculating axial ratio, so the students will learn how to calculate axial ratio for different crystal systems? In addition, the students will learn how to measure Weiss Parameters of the crystal faces.

Scientific contents

- **1-Axial ratio.**
- 2- Axial ratio and crystal system.
- **3-** Weiss parameters.
- 4- How to find Parameters?

References

- 1. Introduction to crystallography, 1996, Phillips.
- 2. Mineralogy, 1997, Reynolds, J. M.
- 3. Petrology and mineralogy, 1996, Arabic version,
- 4. www.chem1.com/acad/webtext/states/crystals-ext.html

<u>Axial ratio</u>: It is a ratio between the lengths of crystallographic axes, this ratio is constant for different crystals size and shape of certain mineral.

- Some characteristic of axial ratio:
- 1- The length of b-axis reduce to a unit.
- 2- The ratio expressed as a relative value.
- 3- The unit of measurement is Angstrom, $1A=10^{-8}$ cm.

Axial ratio expressed by the following formula:

a : b : c , Axial Ratio = a/b : b/b : c/b

where a is the actual length of the a crystallographic axis, b, is the actual length

of the b crystallographic axis, and c is the actual length of the c crystallographic axis.

Axial ratio and crystal system:

1-For Triclinic, Monoclinic, and Orthorhombic crystals, where the lengths of the three axes are different, this reduces to:

a/b : 1 : c/b (this is usually shortened to a : 1 : c)

2-For Tetragonal crystals where the length of the a and b axes are equal, this reduces to

1 : 1 : c/b (this is usually shorted to 1 : c)

3-For Isometric crystals where the length of the a, b, and c axes are equal this becomes

1:1:1 (this is usually shorted to 1)

4-For Hexagonal crystals where there are three equal length axes (a1, a2, and a3) perpendicular to the c axis this becomes:

1:1:1:c/a (usually shortened to 1:c)



Example:

For orthorhombic sulfur the unit cell dimensions as measured by x-rays are:

a = 10.47Å b = 12.87Å c = 24.39Å Thus, the axial ratio for orthorhombic sulfur is: 10.47 : 12.87 : 24.39 Divides by b=12.87 Å 10.47/12.87 : 12.87/12.87 : 24.39/12.87 So the axial ratio is: 0.813 : 1 : 1.903



Parameters or (Weiss parameters)

It is also a ratio of crystallographic axes from axial cross to the position at which the face cuts the axes. Or we can say the parameters are the ratio of intercepts.

Some characteristic of parameters:

- 1- It is a relative value and does not indicate an actual length.
- 2- The parameters is independence on the size of crystal.

3- A face intersects all crystallographic axes in a unit distance called a "Unit face"

Parameters of any face is expressed by the following formula:

na : mb : pc Where n, m and p are distances cut off by the a, b and c axes respectively.

The parameters of the blue face is equal to: 1a : 1b : 1c

The parameters of the blue face is equal to:

 $\infty a : \infty b : 1c$

The parameters of the green face is equal to: $\infty a : 1b : \infty c$





Example-1: Find the parameters of the following faces:

- 1- Intersects a-axis and b-axis, running parallel to c-axis.
- 2- Intersects c-axis and b-axis, running parallel to a-axis.
- 3- Intersects a-axis, running parallel to c-axis and b-axis.
- 4- Intersects a1-axis, running parallel to c-axis, a2 and a3-axes.
- 5- Intersects a1-axis and a3-axis, running parallel to c-axis and a2-axis.
 - 1- 1a:1b: ∞ c 2- ∞ a:1b:1c 3- 1a: ∞ b: ∞ c
 - 4- $1a1: \infty a2: \infty a3: \infty c$ 5- $1a1: \infty a2: 1a3: \infty c$

Example-2: Find the parameters of the following faces:

1a:-1b: 1c



 A crystal face intersects only one of the crystallographic axes.

As an example the top crystal face shown here intersects the c axis but does not intersect the a or b axes. If we assume that the face intercepts the c axis at a distance of 1 unit length, then the intercepts, sometimes called Weiss Parameters, are: $\infty a, \infty b, 1c^{-a}$

A crystal face intersects two of the crystallographic axes.

As an example, the darker crystal face shown here intersects the a and b axes, but not the c axis. Assuming the face intercepts the a and c axes at 1 unit cell length on each, the parameters for this face are: 1 a, 1 b, ∞ c

3. A crystal face that intersects all 3 axes.

In this example the darker face is assumed to intersect the a, b, and c crystallographic axes at one unit length on each. Thus, the parameters in this example would be:

1a, 1b, 1c



Example-3: Find the parameters of the following faces:



Crystal Morphology

How do we keep track of the faces of a crystal?

- Remember, face sizes may vary, but angles can't
- Thus it's the orientation & angles that are the best source of our indexing
- Miller Index is the accepted indexing method
- It uses the relative intercepts of the face in question with the crystal axes

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## **Miller Indices**

<u>Miller Indices are a symbolic vector representation for the orientation of an atomic plane in a crystal lattice</u> and are defined as the <u>reciprocals of the fractional intercepts</u> which the plane makes with the crystallographic axes.

To determine Miller indices of a plane, take the following steps;

1) Determine the intercepts or parameters of the plane along each of the three crystallographic directions.

2) Take the reciprocals (invert) of the intercepts.

3) Clear fractions.

#### 3-D Miller Indices (an unusually complex example)

reference face (ABC)	1a	4b	3c
c - unknown face (XYZ) reference face (ABC)	$\frac{2}{1}$	<u>2</u> 4	<u>2</u> 3
C invert	$\frac{1}{2}$	<u>4</u> 2	$\frac{3}{2}$
clear of fractions	(1	4	3)
x A B	N fa	Ailler inde ace XYZ u ABC as the	x of sing he
b			acc

a



Axis	X	Y	Ζ
Parameters	1	8	x
Reciprocals	1/1	1/∞	1/∞
Smallest Ratio	1	0	0
Miller İndices (100)			



Axis	X	Y	Ζ
Parameters	1	1	8
Reciprocals	1/1	1/1	1/∞
Smallest Ratio	1	1	0
Miller İndices (110)			



Axis	X	Y	Z
Parameters	1	1	1
Reciprocals	1/1	1/1	1/1
Smallest Ratio	1	1	1
Miller İndices (111)			



## **Miller Indices**

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- To determine Miller indices of a plane, take the following steps;
- 1) Determine the intercepts or parameters of the plane along each of the three crystallographic directions.
- 2) Take the reciprocals (invert) of the intercepts.
- **3) Clear fractions.**

#### 3-D Miller Indices (an unusually complex example)





Axis	X	Y	Ζ
Parameters	1	8	×
Reciprocals	1/1	1/∞	1/∞
Smallest Ratio	1	0	0
Miller İndices (100)			