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# PROPOSAL OF SOME MATHEMATICAL FORMULAS TO CALCULATE THE NUMBERS, TYPES AND LOCATIONS OF THE SYMMETRY AXES IN CRYSTAL MINERALS SYSTEMS

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## Abstract

The current study included the establishment of relations between the external crystalline properties which are crystalline facets and edges, as well as solid angles between them. So it showed the relation between external and internal crystalline properties such as crystalline axes and axes of symmetry. Fig.1 considers one of study results which appear those relations through concept each of facets, edges and solid angles by the format of crystalline axes in the system. In addition to axes of symmetry relation with all external crystalline properties. Subsequently, the study suggested mathematical formulas for calculating the numbers and types of symmetric axes, as well as sites them in each of seven systems: From the crystalline faces used equation 1 in state of the crystallographic axes are equal in length, and angles which are between them were orthogonal. While employing of equation 2 in state of crystallographic axes are different in length no orthogonal. From the crystalline edges can be used equation 3. From the solid angles is proposed Equation 4. The types of symmetric axes is suggested equation 5. While the locations of symmetric axes is proposed equation 6. These suggestion mathematical formulas can be easily applied to determine number, types, and position of symmetric axes in each crystalline system by quantitative method a better than the descriptive method which is difficult. Consequently, undergraduate studies where studying the natural properties of minerals is essential in geology and soil minerals.

***Key words:*** *Crystalline* systems, Mathematical Formulas, Symmetric axes, Minerals.

## Introduction

The crystalline structure of minerals in the lattice space was determined by several researchers, including Sher (2007), Ladd and Palmer (2013) through XRD. Crystalline metal is an inorganic homogenous solid material formed by natural factors that have a stable internal chemical structure that reflects the external natural properties in the case of crystallization and growth on crystalline axes (Wilson, 2010 and Leslie, 2013). Therefore, crystalline considers one of the physical properties which distinguish minerals. These properties reflect morphological of crystal such as crystal faces, edges and solid angles which are known as the external characteristics of the crystal. Crystal faces are surfaces that determine the crystal from the outside caused regular geometric shape. Edges are straight lines that surround the crystalline faces resulting from the confluence of two crystalline faces. Solid angles are the angles resulting from the intersection of three or more faces in the crystal (Eggleton and Aspander, 2007 and Anwar, 2007).

There are internal characteristics in crystal resulting from the atomic arrangement of elements ions that reflect those external characteristics such as crystallographic axes and crystalline symmetry (Fjellvåg, 2010). Crystallographic axes are imaginary lines that pass and intersect at the center of the crystal, which is three in the most crystalline systems, except hexagonal and trigonal systems consist of four crystal axes. There are angles between them called $\alpha$, $\beta$ and $\gamma$ (Landd and Palmer, 2013). Crystalline symmetry is an expression of the regularity of the crystalline faces, edges and solid angles so that they are repeated in rotation around a specific axis or reflection through a plane or an inversion through the center of the crystal to achieve the conditions of symmetry and similarity calculation of the symmetry axes number, as well as did not indicate clear relationships between the external characteristics and the internal of crystalline minerals, and mathematical formulas which can be used in calculation the numbers of those axes and sites occupied within the crystalline system. As well as

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the type of each of them in that crystalline system of each mineral in nature. The current study came for an investigating the following objectives:

1. Describing the relationships between the external and internal crystalline properties in the seven crystalline systems of metals.
2. Suggesting of mathematical formulas in how to calculate the symmetry axes number of each crystalline system according to those relationships.

## Materials and methods

The current study suggested mathematical formulas according to the relationships shown in table 1 to calculate the axes of symmetry in each system and depending on the lengths of the crystal axes whether they are equal or different, and the angles between them whether they exist or slanted as following:

A. Designation of symmetry axes numbers:

$$N_{sfe}= \Sigma E_{ca}\times 2 / 2 \quad (1)$$

$$N_{sfd} =N_{Dca}\times 2 / 2 \quad (2)$$

Where: Nsfe is the numbers of symmetry axes from crystalline faces for equal crystalline axes in length. $\Sigma E_{ca}$: the sum of crystalline axes numbers which be equal in length for each system. $N_{sfd}$ is the numbers of symmetry axes from crystalline faces for each different crystalline axis in length. $N_{Dca}$ means for each different crystalline axis has two faces. 2: Each of crystalline axis two faces. 2: Each symmetry axis determines through two faces. Equation 1 and 2 suggested according to a theory of the physical properties of solid would be practically regular crystal lattices (Bravais, 2017).

$$Ns_{E} =[\Sigma E_{ca}\times 2\times 4) / 2] /2 \quad (3)$$

$$N_{Sa}=[(\Sigma E_{ca}\times 2\times 4) /3] /2 \quad (4)$$

Where: $Ns_E$ is numbers of symmetry axes from crystalline edges for equal crystalline axes in length. $N_{Sa}$ is the numbers of symmetry axes from crystalline angles for equal crystalline axes in length. 4: Each crystalline face has four edges or angles. 2: Each edge resulted from confluence two faces. 3: Each angle resulted from confluence three faces. 2: Each symmetry axis determines through two edges or angles. Equation 3 and 4 came according to Jacobson (2007) suggestion which relations between angles and axes unit cell.

B. Types and locations of symmetry axes in each system can be determined according to following:

$$TSa = 360°/Tå \quad (5)$$

$$LSa = 360°/TSa \quad (6)$$

Where: TSa is symmetry axis type. Tå: The type of angle that achieves the conditions of crystal symmetry in the solid angles. LSa: location of symmetry axes whether is conformity to the main crystallographic axes or between edges or angles. Equation 5, 6 suggested that the latter is the same as rotation by 0° or any multiple of 360° about the same axis and depending to this rotation would result four simple symmetry operation for each them rotates at a certain angle until it gives the conditions of crystalline symmetry (Pecharsky and Zavalij, 2009).

## Results and discussion

Fig.1 shows the relationship between the external characteristics in crystal of each mineral when it appears as a body in nature to occupy a space in the outer space. The results indicate that each crystalline face has four crystalline edges, and such edges result from the confluence of two crystalline faces. Thus, each crystalline face has four solid angles, and that angle results from a confluence of three or more faces (Nesse, 2000 and Nelson, 2013). Each crystalline system has external characteristics that are related to each other such as Faces and edges crystalline and solid angles, they reflected through the internal atomic arrangement of elements ions according to prevailing environmental conditions, these grow on crystallographic axes and they have elements symmetry, In the present study, they are called internal characteristics. Crystalline systems classify into seven systems depending on lengths of the crystal axes whether they are equal or different, as well as angles confined between them if they are orthogonal or slanted (Bilyeu, 2013). Thus, fig.1 proposed by present study illustrates these relations between external parts and internal characteristics for the application of mathematical formulas in computation of the number of symmetry axes, types and locations of each them in any crystalline system

**Table1:** Formats of crystallographic axes and symmetry elements in crystalline systems (Whittaker, 1981 and Indian Institute of Technology Kanpur, 2015).

| System | Format | Elements of symmetry | | |
|---|---|---|---|---|
| | | Axes | Planes | Center |
| Cubic | $a_1=a_2=a_3$; $\alpha=\beta=\gamma=90°$ | 13 | 9 | 1 |
| Tetragonal | $a_1=a_2\neq c$ ; $\alpha=\beta=\gamma=90°$ | 5 | 5 | 1 |
| Orthorhombic | $a\neq b\neq c$; $\alpha=\beta=\gamma=90°$ | 3 | 3 | 1 |
| Monoclinic | $a\neq b\neq c$; $\alpha=\beta=90°$; $\gamma\neq 90°$ | 1 | 1 | 1 |
| Triclinic | $a\neq b\neq c$; $\alpha\neq\beta\neq\gamma\neq 90°$ | Nil | Nil | Nil |
| Hexagonal | $a_1=a_2= a_3\neq c$; $\alpha=\beta=90°$; $\gamma=120°$ | 7 | 7 | 1 |
| Trigonal | $a_1=a_2=a_3\neq c$ $\alpha=\beta=90°$; $\gamma=120°$ | 4 | 3 | 1 |

of mineral.

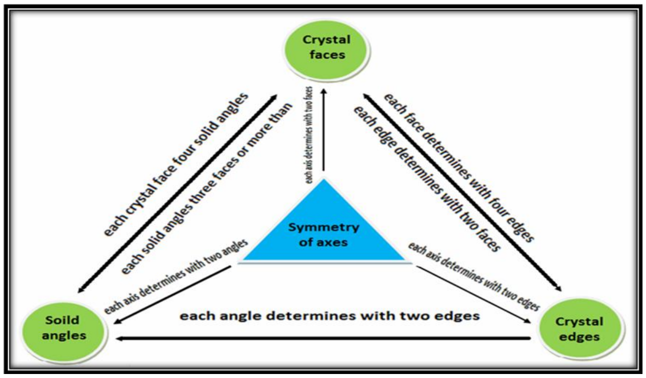


**Fig.1:** Suggestion relations between external and internal crystalline properties.

Depending on the format and table1, the equations proposed by the current study can be applied as following:

In order to calculate the numbers of symmetry axes from the crystal faces, equation 1 can be applied as the case in the cubic system: Numbers of crystallographic axes equal in length are 3 × 2 for each crystalline axis determines in two facets. The result is 6/2 for each symmetry axis determines in two facets, As a result, the numbers of symmetry axes are three (Bravais, 2017). Since the crystallographic axes are perpendicular: $\alpha=\beta=\gamma=90°$, and the full cycle is 360°, therefore, type of these are tetra-symmetry: 360°/90°= 4-folds (Equation 5). While locations of them are applicable to the main crystallographic axes: 360°/4=90° according to Eqution 6.

The numbers of symmetry axes can be calculated from crystalline edges in the same of the cubic system (Equation. 3): The number of crystallographic axes equal to the length are 6×4 for each crystalline face consisting of four edges, the total 24/2 for each edge resulting from the confluence of two crystalline faces =12/2 for each symmetry axis determines by two edges = 6 symmetry axes. Types of these symmetry axes are di-symmetry: 360°/120° = 2-folds, and the locations are 360°/2 = 120° lie between crystalline edges (Eqution 5 and 6).

The numbers of symmetry axes can be calculated from solid angles in the same of the cubic system (Equation.4): The numbers of crystallographic axes equal to the length are 6 × 4 for each crystalline face consisting of four angles, the total 24/3 for each angle resulting from the confluence of three crystalline faces or more than = 8/2 for each symmetry axis determines by two angles = 4 symmetry axes. Types of these symmetry axes are tri-symmetry: 360°/120° = 3-folds, and the locations are 360°/3 = 120° lie between solid angles (Eqution 5 and 6). Thereby, the numbers of analogue axes in the cubic system are 13 (Table1).

Equation 2 can be applied if any different length of the crystallographic axes in that system, as other systems:

Tetragonal system, the numbers of symmetry axes from the crystal faces: The number of crystallographic axes equal to the length are $a_1$ and $a_2$ (horizontal axes): 2×2 = 4/2=2. Since the vertical axis (C) is different from the horizontal crystal axes, it is calculated by itself 1×2 = 2/2= 1. Type of horizontal symmetry axes are bilateral symmetry: 360°/180° = 2-folds. Type of vertical symmetry axis is tetra-symmetry: 360°/90°=4-folds, while locations them applicable to the main crystallographic axes because the angles are perpendicular ($\alpha=\beta=\gamma=90°$). While from crystalline edges are taken the horizontal crystallographic axes equal length because it is the only one that meets the conditions of three symmetry: 2×2 = 4×2 for each crystallin face has two common edges with its counterpart other which fulfills the conditions of symmetry. As a result, the numbers of symmetry axes from the crystalline edges are two (Bilyeu, 2013). As for the solid angles, there are no symmetry axes because they do not meet the three conditions of symmetry. Thus, the numbers of symmetry axes in this system are five.

Orthogonal system has three different crystallographic axes in length (Table1). But perpendicular $\alpha=\beta=\gamma=90°$, So are taken separately according to equation 2: From the crystalline faces, that symmetry axis through the vertical crystallographic axis (C) is one: 1×2 = 2/2 =1, and from front crystalline axis: 1×2 = 2/2 = 1, from the lateral crystalline axis is one too: 1×2 = 2/2 =1. Type of these symmetry axes are 360°/180°=2-folds. The locations of these symmetry axes applicable to the main crystallographic axes: 360°/2 = 180° ($\alpha=\beta=\gamma=90°$) (Eqution 6). While there are no symmetry axes from the crystalline edges and solid angles, they do not achieve symmetry conditions due to lengths of main crystallographic axes are different.

A monoclinic system is characterized that all crystallographic axes are different in length, but only the lateral axis (b) is associated with the frontal (a) and vertical crystalline axis (c) (Table1). Therefore one symmetric axis can be obtained only from crystalline face for the lateral axis (b) because it fulfills crystalline symmetry conditions. From b axis: 1×2 = 2/2=1 (Eqution 2). Type and location of this symmetry axis 360°/180°=2-folds and 360°/2=180° respectively. While the triclinic system does not have symmetry axes because the conditions of crystalline symmetry are not met.

The hexagonal system has four horizontal crystallographic axes of equal length, but they are not orthogonal, while the vertical axis is different in length, but it is bound by an orthogonal relationship with these crystalline axes (Table1). Therefore, Equation. 1 is used to extract the number of symmetry axes from the horizontal crystallographic axes, and equation 2 for numbers of symmetry axes from vertical axis (c): a1=a2=a3, 3×2 = 6/2=3 symmetry axes from crystalline faces fBilyeu, T.Th. (2013) or these horizontal crystallographic axes, and from vertical axis (c): 1×2 = 2/2=1. Type and location of these symmetry axes 360°/ 180°=2-folds and 360°/2 =180° respectively. While Type and location of this symmetry axis: 360°/60° = 6-folds (hexa-symmetry) and 360°/6=60°. Thereby, these are applicable to the main crystallographic axes. From edges: 3×2 = 6×2 = 12/2 = 6/2 = 3 symmetry axes 2-folds, between the horizontal crystallographic axes according to Equtation 5 and 6. From the angles, there are no symmetry axes to the lack of crystalline symmetry conditions.

The trigonal system has the same of formula for hexagonal system (Table 1), but it contents four symmetric axes from only the crystalline faces: 3×2 = 6/2= 3 symmetry axes are 2-folds and applicable to the horizontal crystallographic axes. With one axis tri-symmetry (3-folds) is applicable to the main crystallographic axis (c).

## Conclusion

The current study found relations among the external characteristics which are crystalline faces, edges and solid angles. These characteristics show the natural state of each crystalline minerals as a solid, homogeneous and inorganic body that occupies a certain size in the outer space. Depending on these relations and the crystalline axes formulas in each system, whether they were equal or different in length, and angles which are between them, whether they were orthogonal or slanted, as well as characteristics of crystalline symmetry. Current study proposed mathematical equations to calculate the symmetry axes in each system of minerals crystallized in nature, as well as their types and locations by quantitative and not descriptive methods. This study could be an extension of future researches for calculating the number of symmetric planes in each of system through mathematical formulas.

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