# The need of a structural classification of minerals\*

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ABSTRACT. — Mineralogists have used the chemical classification of minerals for more than one hundred years, and it is now time to change. Several reasons converge to appoint a new classification — a structural classification of minerals (LIMA-DE-FARIA, 1983 a), mainly: the historical analysis of the evolution of the basic criteria of the several mineralogical classifications used throughout the ages, and the need of an appropriate representation, notation and classification of mineral structures in order to deal with the enormous amount of structural data on minerals accumulated during the last seventy years.

#### Introduction

There are still many mineralogists who are little interested in the structural characteristics of minerals, and are very much concerned with their chemical properties. This is possible due to several reasons, and among them we should consider the difficulty in understanding the drawings representing mineral structures, the wide use of a chemical classification and notation instead of structural ones, and the poor development of the relationship between crystal structure and physico-chemical properties. This situation can be improved if mineralogists will give more attention to structural characteristics of minerals, by using appropriate structure representations, a structural notation, and a structural classification of minerals.

On the other hand it is well known that when many scientific data are accumulated there is a need for a systematization of them, in order to take real advantage of the new information. In the case of mineralogy there are hundreds of mineral structures that have been determined and are being determined. The potentiality of this information is certainly enormous, and to deal with it, to use it, we need an appropriate structural classification, not chemical, because it is the structural aspects of minerals that we are considering.

Moreover, historically the classification of minerals has gone through several changes throughout the ages, the criteria of classification always following the advances of mineralogical science, from pratical uses, through physical properties to chemical properties. Mineralogy is now at its structural age, and it is therefore natural to admit that a structural classification can succeed the chemical classification of minerals. Five works in this direction have already appeared, two by the author (1983 a, 1985) and three by HAWTHORNE (1984, 1985 a and b).

Mineralogists have used the chemical classification of minerals for more than one hundred years. It is now time to change, to learn something from the history of science, and to be open to new ideas, to new scientific paths. The great strength of science is creativity, not stagnation.

#### **Representation of crystalline structures**

In what concerns the representation of crystalline structures one of the main difficulties is the existence of several ways of representing structures. The most common ways of representation can be exemplified

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by the structure of olivine (forsterite), Mg<sub>2</sub>SiO<sub>4</sub>. On fig. 1 four different ways of representing this structure are shown: *a*) the projection of the atoms on one side of the unit-cell, *b*) the distribution of the atoms in perspective within the unit-cell, *c*) the coordination polyhedra representation, and *d*) the atomic packing representation. We may add to these the layer description, by using the condensed model (LIMA-DE-FARIA, 1965 a and 1966) of olivine. The layer representation consists of slicing the structure into constructive layers (LIMA-DE-FARIA, ions occupy octahedral voids, and the silicon ions tetrahedral voids. If we start with a standard hexagonal closest packed sheet where the oxygen atoms are represented by large full circles, and the octahedral and tetrahedral voids by small doted circles, fig. 2*a*, we may then paint in black the octahedral and tetrahedral voids and obtain the condensed model sheet of olivine, fig. 2*b*.

Both Mg ions (the large black circles) and Si ions (the small black circles) have zig-zag distribution patterns within the oxygen packed layer. The olivine condensed model



Fig. 1. — Four different ways of representing the structure of olivine (forsterite): a) the projection of the atoms on one side of the unit-cell (after BRAGG and CLARINGBULL, 1965); b) the distribution of the atoms in perspective within the unit-cell (after POVARENNYKH, 1966); c) the coordination polyhedra representation (after POVARENNYKH, 1966), and d) the atomic packing representation (after WYCKOFF, 1965).

1978), represented by plastic sheets. Each constructive layer is formed by a packing layer and the interestitial atoms which are immediately above it, in such a way that the stacking of the constructive layers generates, completely, the crystal structure. In general these layers are all alike, and this is the case of olivine. In olivine the orygens form a hexagonal closest packing, the Mg is formed by only three sheets, because the sequence of the cation distribution is also h, that is, ABAB..., and consequently the third layer repeats the first. The zig-zag of Mg ions is placed over the middle of the two zig-zag of Mg ions on the layer below; that is, the cations on one layer tend to be as distant as possible from the cations on the adjacent layers, for stability reasons

(minimum free energy). The three dimensional condensed model is obtained by placing the transparent plastic sheets on an appropriate supporting rack, which is placed over a viewing screen to improve the visibility of the model. The problem of slicing a certain structure into layers, and the search for the densest layers, which normally corresponds to the simplest description in equal layers, can be very much simplified by the use of computers. A computing program for determining



Fig. 2. — a) Standard sheet for the condensed model of the hexagonal closest packing; b) top sheet of the condensed model of olivine (forsterite).

The transparent sheets can be kept in an envelope and a large collection of models may be organized and kept in a small index box (fig. 3). Another advantage of this kind of model is the possibility of marking, and visualizing easily, the elements of symmetry of the space group. In the case of olivine one can notice the mirror planes, the diagonal glide planes, the screw axes, and the centers of symmetry.

Another example of a structure whose drawings are normally very difficult to interpret, and apparently look very complicate, are those of the corundum structure,  $Al_2O_3$ . However it can be represented by equal simple and very symmetric layers, the oxygens forming an hexagonal closest packing, and the Al atoms being distributed on a honey-comb pattern, in each layer. Many other examples could be given of structures that can be represented by the sequence of equal layers, or by two alternate different layers (LIMA-DE-FARIA, 1978). the densest atomic layers (PRCM), and another for slicing a structure along any direction (bkl), PRSH program, have been already worked out by LANGLET (1975).

In the cases of closest packings (LIMA-DE-FARIA, 1965 a) and of simple loose packings (FIGUEIREDO and LIMA-DE-FARIA,



Fig. 3. — View of a condensed model of olivine placed on a supporting rack, with viewing screen, and also a small index box containing several condensed models of  $\delta$  inorganic structure types.



a)

6)

Fig. 4. — a) Condensed model standard sheet of  $N^{21}$  layers with stacking f (after FIGUEIREDO and LIMA-DE-FARIA, 1977); b) same layer  $N^{21}$ , with stacking f, drawn by a computing plotter as a result of the application of the void program (after LANGLET, FIGUEIREDO and LIMA-DE-FARIA, 1977).

1978) it is relatively easy to calculate the radii of the spheres which will fit into the interstices between two adjacent layers, stacked according to a certain stacking vector, but in more complex cases this calculation becomes very difficult. A program (void program) for the calculation of the sizes of such voids has also been worked out by LANGLET, FIGUEIREDO and LIMA-DE-FARIA (1977). Figure 4 a represents a standard sheet of the condensed model of a N<sup>21</sup><sub>1</sub> layer, that is a layer built of square and triangles, corresponding to the stacking which moves the layer from the origin to the middle of it, called f. The large full circles represent the packing atoms and the doted circles the various voids. On fig. 4 b is shown the same kind of layer but drawn by a computing plotter, as a result of the application of the void program.

The great similarity between figures 4a and b shows clearly the large potentialities of the computing methods to solve such kind of problems.

This representation of the closest packings by layers of spheres was first proposed by KEPLER in 1611 (fig. 5), and it seems probable that he had been inspired by the packing of the cannon-balls which normally exist in old castles (as suggested by HOLSER, 1970). When I started being interested in this type of representation I had the opportunity of seeing these pyramids of packed cannon-balls on a visit to the Saint'Angelo Castle, in Rome, during the International Crystallographic Congress held there in 1963, and this event has strongly influenced the development of my work in this domain.

The problem of slicing a structure into layers is not so easy as we can imagine, and sometimes there are more than one simple layer description, and we have then to find the more appropriate one, the simplest one. Even the halite structure, NaCl, can be represented in two different ways, by layers parallel to the densest layers of the cubic closest packing of the Cl atoms, the (111) planes, or by layers parallel to the cubic faces, the (100) planes (fig. 6). Of these



Fig. 5. — Drawings of close packing layers of spheres to explain the form of snow crystals (after KEPLER, 1611).



Fig. 6. — Packing model of the halite structure, Na°[Cl]°. The large white atoms represent the Cl atoms, and the small black ones the Na atoms. This structure can be sliced along four different closest-packed directions, and along three different plane directions parallel to the cubic faces.

two possible descriptions the one parallel to the cubic faces is the more appropriate because one can mark on it, very easily, the elements of symmetry of the cubic space group. It is curious to notice that there are in this structure four plane directions parallel to the (111) planes, and three parallel to the (100) planes, so that on the whole 7 good plane directions of slicing this structures are available.

On fig. 7 is represented the structure of AuCu, the Au atoms corresponding to the hatched circles and the Cu to the white circles, and, as mentioned before, there are also seven possible plane directions for slicing this structure. However the appropriate one is that parallel to the (100) planes which is perpendicular to the vertical axis of fig. 7, and corresponds to a description of alternate layers of Au and Cu atoms.

On fig. 8 are represented, in an appropriate way, the layer structures of some simple binary compounds  $[X_mY_n]^\circ$ , with mixed cubic closest packings of X and Y atoms, for *m* and  $n \leq 4$ , the corresponding constructive layers necessary for their representations, and also their stacking vectors.

One can notice on fig. 8 that the structures

of ZrSi<sub>2</sub>, ZrGa<sub>2</sub>, and HfGa<sub>2</sub> are very much alike. They are formed by the same sequence of layers, and differ only in the stacking vectores g, (2s)b, and (2s)d (LIMA-DE-FARIA, 1983 b). However, if we search the representation of these same structures in the classical textbooks of BOKII (1954), or of PEARSON (1972), of SCHUBERT (1964), of WELLS (1975), or of WYCKOFF (1963 and 1964), we will find very different representations, difficult to interpret, and they will not appear as parental structures (fig. 9).

# Notation and classification of inorganic crystal structure

When referring to a certain crystal structure the crystallographers still use its chemical formula, and not a structural formula. The reason for this is possibly related to the difficulty of ascribing structural factors to the atoms and their positional distribution, which in many cases can only be qualitative or semiquantitative. The complete description of a structure, indicating the bond strength distribution, and consequently the structural units, the relative size of the various atoms and their corresponding coordination, etc., requires a detailed and difficult study of the structure which the crystallographer is normally not prepared, or even interested.



Fig. 7. — Packing model of the AuCu structure showing that the appropriate description is the one parallel to the cubic faces which is perpendicular to the vertical axis, and that corresponds to alternate layers of Au atoms (*batched circles*) and of Cu atoms (*white circles*).



Fig. 8. — Standard representation of layered inorganic structure types of general formula  $[X_m Y_n]^e$  with m, n < 4 (after J. LIMA-DE-FARIA, Acta Cryst., 1983, B39, p. 320).



Fig. 9. — Representation of the same structures as shown on fig. 8 but found on the classical textbooks of PEARSON (1972), BOKII (1954), and SCHUBERT (1964), and also on an article by A. BROWN, Acta Cryst., 1961, 14, p. 859.

However, this structural information is becoming more and more important, and only with a widely used structural notation we shall be able to take real advantage of it. This classification is mainly based on the bond strength distribution within a structure which defines the «structural units», a concept introduced by LAVES (1930), and



Fig. 10. — Very schematic representation of the bond strength distribution among the five main categories of inorganic structures.

The structural formulae were first introduced by MACHATSCHKI in 1947, for the silicates, and extended by him, in 1953, to the whole domain of minerals. However, this notation has not been widely accepted, possibly due to the reasons appointed above, and today, just a few mineralogists use MACHATSCHKI notation for certain silicates, and for restricted purposes. Liebau, very recently (1985) has developed, for the silicates, a more complete structural notation which includes dimensionality, linkedness, connectedness, branchedness, and multiplicity of the assemblage of silica tetrahedra, but there has not yet been time to test the usefulness of this notation.

Any notation is intimately related to a certain classification. The classification decides what are the important factors to consider, and then the elaboration of the notation is reduced to the finding of the appropriate symbols, as simple and selfexplanatory as possible, to express these factors.

There are several structural classifications of inorganic structures restricted to well defined domains such as the silicates, phosphates, germanates, and aluminosilicates. A general structural classification and notation for the whole domain of inorganic structures has been proposed by LIMA-DE-FARIA and FIGUEIREDO (1976), which is a kind of generalization of the MACHATSCHKI structural classification and notation for the silicates.

developed by NIGGLI (1945). The distribution of the bond strength may be relatively homogeneous, as in many oxides, halogenides, alloys, and intermetallic compounds, where the bonds are predominantly nondirectional, and these structures are formed by the close packing of the larger atoms with the smaller atoms occupying the interstices within the packing. The structural units in this case are isolated atoms, the large packing atoms, normally the anions. However, in structures where the directional forces are dominant the bond strength distribution is heterogeneous, certain atoms being more tightly linked together than the others, forming finite groups, infinite chains, infinite sheets or infinite frameworks (fig. 10). According to this classication there are only five main categories of structural units: isolated atoms, finite groups, infinite chains, infinite sheets, and infinite frameworks, and the corresponding main categories of structures are called atomic, group, chain, sheet and framework structures, respectively.

The structural notation proposed by LIMA-DE-FARIA and FIGUEIREDO (1976) expresses these various structural units, and other structural characteristics. It has its roots in the MACHATSCHKI notation for the silicates, but emphasizes the polymerization process of the structural units, which expresses the condensation of atoms in groups, of certain groups in chains, of chains in sheets, etc. (fig. 11 *a*).

To designate the number of silica tetra-

hedra in a group we use Roman numerals with a superscript to differentiate various different groups with the same number of silica tetrahedra. The symbol of a chain derived from a certain group by polymerization is formed by the symbol of the group plus another superscript to distinguish different chains derived from the same group, and so on (fig. 11 *b*). The notation also expresses the layer description and their packing, whenever possible. Only a very brief description of this notation will be given here.

The atoms which form the structural units are placed within square brackets, and the interstitial atoms on their left. The coordination of the atoms forming the structural units, or of the interstitial atoms, is indicated by as uperscript, either small letters, as t (tetrahedral), o (octahedral), tr



(triangular), or *cb* (cubic), or simply a number for irregular or more complicated coordinations. The category of structural unit is indicated by appropriate symbols following the square brackets:  $\infty$  for group,  $\infty 1$  for chain,  $\infty 2$  for sheet,  $\infty 3$  for framework, the absence of symbol meaning atomic structure.

The group, chain, sheet, or framework structural units are characterized as we said before by a symbol formed by a Roman numeral and an ordering number as a superscript, and in the case of layered structures, which are the most common, the way the structural units pack together is indicated by a capital letter representing the type of layer formed by the structural units, with a sub-indice (small letter) indicating the kind of stacking of the layers, all placed on the top right hand side of the square brackets.

In order to emphasize the importance of the structural notation some structure types of binary compounds are presented on fig. 12 a) without structural notation, as is still widely used, and b) with the structural notation explained here. One can realise immediately the advantage of table b). With table b) it is easy to make structural relationships, while with table a) it is practi-



Fig. 11. — a) Exemplification of the general polymerization process by the condensation of isolated atoms into groups, of groups into chains, of chains or groups into sheets, and of sheets into frameworks; b) examples of three chains deriving from different groups with the corresponding symbology.

cally impossible to relate structures, unless one knows them very well.

An example of a complete structural formula is also given on fig. 13 for the structure of benitoite, with the corresponding explanation of the symbology.

This general structural classification and notation has been applied to 782 inorganic structure types, and presented on a general table of inorganic structure types. Fig. 14 reproduces this table in a very reduced size, just to give an idea of its structure and appearance. This table was published by LIMA-DE-FARIA and FIGUEIREDO in 1976 in microfilm form only, and later, in 1978, republished in an appropriate size.

If we ask how many different structural units are necessary to build these 782 structure types, the answer is 274, and if we ask again how many different polyhedra, « building units », form these 274 structural units, the answer is 20. These results are summarized on a general chart of inorganic structural units and building units (LIMA-DE-FARIA and FIGUEIREDO, 1978) reproduced on fig. 15. These general table and chart correspond to an enormous simplification of the structural description of inorganic structures, which will certainly help to establish relationships among structures, and also to derive the rules governing their stability.

# Structure and properties

Although there are many problems, such as isomorphism, polymorphism, diadochia, phase transformations, cleavage, habit, and twinning, which can only be clearly interpreted if we take into account the structural characteristics of the compounds involved, the problem of the relationship between structure and physico-chemical properties is very little developed. According to Professor HELEN D. MEGAW (1973): « knowledge in this field is still very scanty (except for the very simplest structures) ».

I am convinced than one of the main negative factors in respect to this problem has been the lack of use of a structural classification and notation of inorganic structures, and this constitutes yet another

A	AB	AB <sub>2</sub>		A	AB	AB <sub>2</sub>
Cu	UFb	MoPt,	1	[Cu]°	[UPb]°	[MoPt,] °
Mg	PtCu	CdTi <sub>2</sub>		[Mg] <sup>h</sup>	[PtCu] <sup>c</sup>	[CdTi <sub>2</sub> ] <sup>c</sup>
Pa	AuCu	ZrGa,		[Pa] Tb	[AuCu] <sup>c</sup>	[ZrGa <sub>2</sub> ] <sup>c</sup>
Pu	AuCd	HfGa,		[Pu] Td	[AuCd] <sup>c</sup>	[HfGa,] c
W	LiRh	ZrSi,		[w] <q>f</q>	[LiRh] <sup>h</sup>	[ZrSi] <sup>c</sup>
Po	NaCl	TaPt,		Po] QB	Na <sup>o</sup> [C1] <sup>c</sup>	[TaPt <sub>2</sub> ] <sup>c</sup>
InSn	NiAs	TIO2	*	[InSn.] TS	Ni <sup>o</sup> [As] <sup>h</sup>	Ti°[02]°
	ZnS (c)	CT12			zn <sup>t</sup> [s] <sup>c</sup>	C°[T12] C
	ZnS (h)	CdCl,			zn <sup>t</sup> [s] <sup>h</sup>	cd°[Cl2]°
	FeS	Pb0,			Fe <sup>t</sup> [s] <sup>c</sup>	Fb°[0 <sub>2</sub> ]h
	CuTi	CaCl			[CuTi]Tb	ca <sup>o</sup> [c1 <sub>2</sub> ] <sup>h</sup>
	CW	CdI,			c <sup>p</sup> [w] <sup>Ts</sup>	caº[1]h
	PV	NFe <sub>2</sub>			₽ <sup>₽</sup> [v] <sup>TS</sup>	N°[Fe,]h
	<i>a</i> )		-		<i>b</i> )	

Fig. 12. — Some structure types of inorganic binary compounds of formulae A, AB and  $AB_2$ : a) just the chemical formulae which are the widely used structure type symbols; b) the same structure types as in a) but corresponding to the symbology proposed by LIMA-DE-FARIA (1965) and by LIMA-DE-FARIA and FIGUEIREDO (1976).



Fig. 13. — Example of a complete structural formula (benitoite), with the explanation of the symbology (after LIMA-DE-FARIA and FIGUEIREDO, 1976).

important reason for developing such kind of classification and notation.

# Historical analysis of the basic criteria used in mineralogical classifications

An historical analysis of the basic criteria used in the mineralogical classification through the ages has already been made, and a sketch of its evolution has also been presented (LIMA-DE-FARIA, 1983 a). This historical analysis also contributes to clearly show the need of a new classification — a structural classification of minerals.

From the sketch on figure 16 one can conclude that the ancient classification of minerals was mainly based on their practical uses, minerals being classified as gemstones, pigments, ores, etc., according to THEO-PHRASTOS (372-287 B.C.) and to PLINIUS (77 A.D.). In the MIDDLE AGES GEBER (JABIR IBN HAYYÀN, 721 - c. 803) proposed a classification of minerals based on the external characters and on some physical classification was developed by AVICENNA (IBN SINÁ, 980-1037), AGRICOLA (1546) and WERNER (1774). With WERNER the physical classification attained its maturity, and was generally adopted at the end of the century.

CRONSTEDT (1758) seems to be the first to have outlined a classification whereby the chemical properties were taken first, followed by the physical properties. With the development of chemistry the chemical properties became more and more important, and BERZELIUS (1819) proposed a chemical classification of minerals based on radicals and not on the elements, that is to say, as chlorides, sulfates, silicates, etc., and not

as minerals of zinc, of copper, etc. The main criticism to the chemical classification at that time was that it could not be applied to all minerals because the chemical composition of many of them was not known. However, even WERNER, who so strongly defended the physical classification, modified his classification at the end of his career and elaborated a physical-plus-chemical classification (1817). The chemical classification had been opposed for approximately a century, and only with the advancement of chemistry could it finally be widely adopted, due primarily to the work of DANA (1850, 1954) and of GROTH (1874).

After 1913, when the first structures of minerals were determined, the structural criterium for classification was taken into account, but always with secondary importance. The most striking classification of this type is that of silicates proposed by MA-CHATSCHKI (1928) and developed by BRAGG (1930) and NÁRAY-SZABÓ (1930). The structural classification of silicates was a much better systematics than the old chemical subdivision, and was soon widely adopted. This chemical-plus-structural classification has been applied to may other branches of mineralogy such as fluoaluminates (PABST, 1950), aluminosilicates (LIE-BAU, 1956; ZOLTAI, 1960), and phosphates (LIEBAU, 1966; CORBRIDGE, 1971), and more recently by POVARENNYKH (1956, 1966), who applied it to the whole domain of minerals.

Although the chemical classification of minerals seems to be well established, some dissatisfaction has appeared during the last decades, and other criteria have been proposed for the classification of minerals, some related to particular domains of application, such as geological (LAPPARENT, 1884) or geochemical (UKLONSKII, 1940), others to more theoretical purposes such as the one proposed by MACHATSCHKI (1953) which was based on crystallochemical grounds.

It is apparent from this sketch that the classification of minerals has passed through different stages, from practical, to physical, to physical-plus-chemical, to chemical, to chemical-plus-structural. It seems that it is now time to attribute the primary role to the structural criterium, and to propose a structural classification of minerals.

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Fig. 14. — The general table of inorganic structure types, reproduced in a very reduced size just to give an idea of its organization and appearence (after LIMA-DE-FARIA and FIGUEIREDO, 1976 and 1978).

## J. LIMA-DE-FARIA

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~340 B.C.+	Practical uses - THEOPHRASTOS
77 A.D.+	Practical uses - PLINIUS
~760+	Physical properties - GEBER (Jabir Ibn Hayyân)
~1020	Physical properties - AVICENNA (Ibn Siná)
1546	Physical properties - AGRICOLA (Georg Bauer)
1750- 1758	Chemical + physical properties - CRONSTEDT
1774	Physical properties - WERNER
1784	Chemical + physical properties - BERGMAN
1800- 1801	Chemical + crystallographic properties - HAÜY
1817	Physical + chemical properties - WERNER
1819	Chemical properties - BERZELIUS
1832	Chemical properties - SOKOLOV
1850- 1854	Chemical properties - DANA
1884 1900 -	Paragenetic properties - LAPPARENT
1928 1930 1940 1950 -	Class. silicates based on structural prop MACHATSCHKI Develop. class. silicates b. on st. prop BRAGG Geochemical properties - UKLONSKII
1953	Crystallochemical properties - MACHATSCHKI
1966	Chemical + structural properties - POVARENNYKH

----- well established criterium of classification ----- intermediate criterium of classification

Fig. 16. — Sketch of the evolution of the basic criteria of the mineralogical classification (after LIMA-DE-FARIA, 1983 a).

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## Structural classification of minerals

A structural classification of minerals has to be based on structural factors, and these should pertain not only to mineral structures but to inorganic structures in general, because minerals are a part of them. Therefore the structural classification of inorganic structures already described (LIMA-DE-FARIA and FIGUEIREDO, 1976) may be applied to the mineral kingdom. Such classification has been proposed by LIMA-DE-FARIA (1983 a). On figure 17 most of the important mineral structures are organized according to this structural classification. The main categories of structures are obviously the same as those of the inorganic structures - atomic, group, chain, sheet and framework. However, there are some slight alterations in respect of the general table of inorganic structure types, because the latter was very much influenced by the systematic derivation of structure types, which implies an ordering from the simplest to the more complex structures.

When elaborating a classification of minerals on structural grounds we have to group together the parental mineral structures, those having a similar arrangement although differing by slight distortion or substitution of their atoms. We have also to add the defect and insertion derivatives in the case of more complex structures.

In the case of the elements the principal structure type or aristotype, in the nomenclature of MEGAW (1973), is represented by copper, and includes the other elements with the same atomic arrangement and symmetry such as Pt, and Pd; Hg and In are distortion derivatives; AuCu and AuCu<sub>3</sub> are substitution derivatives, but on the whole they have the same arrangement of atoms. In the case of halite, one should place together with it certain oxides, sulphides, etc., which also have the same atomic arrangement. Certain phosphates and silicates which pertain to the same structure type, like the sheet structures herderite and datolite, have therefore to be placed together.

Compounds pertaining to the same structure type are ordered chemically, the chemical criterium being the same as that normally used for the classical classification. In the case of the halite structure type already mentioned, the halogenides are considered first, followed by the oxides, and

only then by the sulphides, telurides and nitrides. This clearly shows that this classification is not purely structural, but a structural-plus-chemical classification of minerals.

A similar structural classification of minerals, although starting from different roots, has also been proposed by HAWTHORNE (1984, 1985 a and b). This indicates that this problem is ripe, and that there is some hope that mineralogy will soon progress in this direction.

#### **Final remarks**

The structural classification of minerals will certainly face strong opposition from most mineralogists. It is a natural reaction for scientists to try not to change their mental habits. The history of science has clearly revealed the inertia of scientific theories and the stubborn atitude of many scientists, even some of the best, regarding new theories and discoveries. Dana said in his « System of Mineralogy » (1850), « ... chemistry has opened to us a better knowledge of the nature and relation of compounds; and philosophy has throw new light on the principles of classifications. To change is always seeming fickleness. But not to change with the advance of science is worse, it is persistence in error ... ». A similar statement could possibly now be applied to the structural classification. Each stage in the development of a branch of science needs its proper classification, and we are in fact in the structural era of mineralogy. A structural classification will help to use the structural knowledge, which is being accumulated year after year. The many crystallographers and mineralogists who have dedicated and are dedicating most of their time to the determination of mineral structures will get their compensation by knowing that their work was not in vain.

Mineralogists have used the chemical classification of minerals for more than one hundred years. It is now time to change. In the history of science there are always a past and a future; the chemical classification will be the past, the future is the structural classification of minerals.

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#### J. LIMA-DE-FARIA

Fig. 17. (a, b), (c), (d), (e) and (f): sketch of the ordering of minerals in a descriptive mineralogy based on structural grounds (after LIMA-DE-FARIA, 1983 a).

Fig. 17 b)

(Fe,Mn)<sup>6</sup><sub>2</sub>[0<sub>3</sub>]<sup>Q</sup><sup>8</sup> Bixbyite Ia3 (Ca,Mn)<sup>do</sup>Al<sup>o</sup>Si<sup>t</sup><sub>3</sub>[O<sub>12</sub>]\* Calcmanalsilite Ca<sup>do</sup>2r<sup>o</sup><sub>2</sub>(Si,A1)<sup>t</sup><sub>3</sub>[0<sub>12</sub>]\* Kimzeyite T12 03 D S Avicennite (Mg,Fe)30A12Si3012  $\operatorname{Fe_3^{do}Al_2^{o}Si_3^{t}[o_{12}]}$ Pyrope (Mn,Fe)<sup>do</sup>Al<sub>2</sub>Si<sup>†</sup><sub>3</sub>[0<sub>12</sub>]<sup>\*</sup> Spessartite (Na,Ca)<sup>cb</sup>Nb<sup>6</sup><sub>2</sub>0<sub>6</sub>(OH,F) Ca30Fe2Si3[012]\* s Ca<sup>cb</sup>sb<sup>6</sup><sub>2</sub>[0<sub>7</sub>]<sup>c</sup>s Romeite Pb<sup>cb</sup>sb<sup>6</sup><sub>2</sub>[0<sub>7</sub>]<sup>c</sup>s Bindheimite (Ca,Na)2°Ta206(OH,F) Na<sup>do</sup>Ca<sup>do</sup>(Mg,Mn)<sup>o</sup>As<sup>t</sup><sub>3</sub>[0<sub>12</sub>] Mn3<sup>do</sup>Fe2Si3[012]\* Calderine Microlite Berzeliite Bacb Nb2 07-x (H20) D 35 Pandaite Heterogeneous  $\begin{array}{c} \text{Faintaite} \\ \text{Ba}_{2-x}^{\text{cb}}\text{Ta}_{2}^{6} \begin{bmatrix} 0_{7-x}(\text{H}_{2}0)_{x} \end{bmatrix}^{Q_{g}} \\ \text{Rijkeboerite} \end{array}$  $Pb^{8}Bi^{8} \Big\{ \begin{bmatrix} 0_{2} \end{bmatrix} \begin{bmatrix} C1 \end{bmatrix} \Big\}^{(Q^{2}Q^{1})} f \quad \underline{Perite}$  $Cu_2^{cb}Sb_2^6[0_6(H_20)\Box]$ Partzite Bmmb  $Pb^8sb^8\left[ \begin{bmatrix} 0_2 \end{bmatrix} \begin{bmatrix} C1 \end{bmatrix} \right]^{\left(Q^2Q^1\right)} f$  Nadorite Sn2<sup>cb</sup>Ta20,0 Ag<sup>cb</sup>Sb<sup>6</sup><sub>2</sub>[0<sub>6</sub>(H<sub>2</sub>0)□]<sup>Q</sup>s Stefeldtite Sukulaite  $Pb_{2}^{8}Cu^{sq}\left\{\left[(OH)_{4}\right]\left[Cl_{2}\right]\right\}^{(Q^{2}Q^{1})}s \underline{Diabollite} P4mn$ (Ca,U)<sup>cb</sup>(Nb,Ti)<sup>6</sup><sub>2</sub>[0<sub>6</sub>(OH,F)□]<sup>Q</sup><sub>8</sub> Betafite Na<sup>cb</sup>Mg<sup>o</sup>Al<sup>o</sup> [F7] Q<sub>8</sub> Weberite {[0] [Pb]}(Q<sup>2</sup>2Q<sup>1</sup><sub>f</sub>)s Litharge P4/nmm Ibmm  $Pb^{9}[F][c1]^{(q^{2}2Q_{f}^{1})_{s}}$  <u>Watlockite</u> P4/nmm Other packings Al<sup>o</sup>Al<sup>5</sup>Si<sup>t</sup> 050 R<sup>21</sup> Andalusite  $Bi^{9}[0][c1]^{(Q^{2}2Q_{f}^{1})_{s}}$  $Bi^{9}\left[ \left[ 0 \right] \left[ F \right] \right]^{\left(Q^{2}2Q_{f}^{1}\right)_{g}}$ Pnnm  $\begin{array}{c} \operatorname{Cu}^{o}\operatorname{Cu}^{5}\operatorname{Ast}\left[O_{4}\left(\operatorname{OH}\right)\Box\right]^{R}_{by}^{21}\\ \operatorname{Olivenite}\\ \operatorname{2n}^{o}\operatorname{Zn}^{5}\operatorname{Ast}\left[O_{4}\left(\operatorname{OH}\right)\Box\right]^{R}_{by}^{21}\\ \operatorname{Adamite}\end{array}$ Bismoclite Zavaritskite Mn<sup>o</sup>Mn<sup>5</sup>As<sup>t</sup>[0<sub>4</sub>(OH)□]<sup>R</sup>by Eveite GROUP Eveite Cu<sup>o</sup>Cu<sup>5</sup>P<sup>t</sup>[O<sub>4</sub>(OH)D]<sup>R</sup>by Libethenite Homogeneous Simple Betsi2[080](3R01)by Phenakite Linear R3 Zn\_si\_5[0,0](3R\_0^{21})by Willemite Fe<sup>o</sup>[S<sub>2</sub>]<sup>c</sup> Pyrite Pa3 Li<sup>t</sup><sub>2</sub>Al<sup>t</sup><sub>2</sub>Si<sup>t</sup><sub>2</sub>[0<sub>8</sub>D]<sup>(3R<sup>21</sup>)</sup>by Eucryptite Ni<sup>o</sup>[S<sub>2</sub>]<sup>c</sup> Vaesite Pt<sup>o</sup>[AsS]<sup>C</sup><sub>20</sub> Platarssulite R3  $\operatorname{Co}^{\circ}\left[\operatorname{S}_{2}\right]_{\Sigma}^{c}$  Cattierite  $\operatorname{Rh}^{\circ}\left[\operatorname{AsS}\right]_{\Sigma}^{c}$  Hollingworthite Fe<sup>o</sup>[O(OH)]<sup>R</sup>my Lepidocrocite  $\operatorname{Ru}^{O}[S_{2}]_{\Sigma}^{C}$  Laurite  $\operatorname{Ir}^{O}[\operatorname{ABS}]_{\Sigma}^{C}$  Irarsite Amam Al°[O(OH)]<sup>R</sup>my Boehmite Mn<sup>o</sup>[S<sub>2</sub>]<sup>c</sup><sub>2</sub> Hauerite Pt<sup>o</sup>[As<sub>2</sub>]<sup>c</sup> Sperrylite  $(Ni,Cu)^{\circ}[S_{2}]_{\Sigma}^{c}$  Villama-  $(Co,Ni)^{\circ}[SDS]_{\Sigma}^{c}$  Willyamite c<sup>tr</sup>Cu<sub>2</sub><sup>o</sup>[o<sub>3</sub>(OH)<sub>2</sub>]<sup>(2R<sup>41</sup><sub>by</sub>)</sup>oy <u>Malachite</u> F2<sub>1</sub>/a  $Cu_{\mathcal{F}}^{0} e^{\circ} [S_{\mathcal{B}}]_{\mathfrak{D}}^{c}$  Fukuchi- Ni<sup>°</sup>  $[SbS]_{\mathfrak{D}}^{c}$  Ullmannite  $c^{tr}(Zn,Cu)_2^o[0_3(OH)_2]^{(2R_{by}^{41})}$ oy Rosasite Ni<sup>o</sup> Se<sub>2</sub> Penroseite Au<sup>o</sup> Sb<sub>2</sub> Aurostibite Co° Se2 C Trogtalite Pt° Sb2 C Geversite B<sup>tr</sup>Mg<sup>o</sup><sub>3</sub>Mn<sup>o</sup><sub>3</sub>[0<sub>10</sub>]<sup>(2R<sup>41</sup>)</sup>my Pinakiolite P2<sub>1</sub>/m Co<sup>o</sup> [AsS] Cobaltite Pd<sup>0</sup>[Bi<sub>2</sub>]<sup>c</sup><sub>p</sub> Michenerite Ni<sup>o</sup> AsS C Gersdorffite Mg6B2 06(0H)6 R421231 Fluoborite P63/m Fe<sup>0</sup>[S<sub>2</sub><sup><h>]</sup><sup>c</sup> Marcasite Non-layered Pnnm  $\operatorname{Fe}^{\circ}\left[\operatorname{Se}_{2}^{\langle h \rangle}\right]_{\Sigma}^{\circ}$  Ferroselite Ni<sup>o</sup> $\left[\operatorname{As}_{2}^{\langle h \rangle}\right]_{\Sigma}^{\circ}$  Rammelsbergite Zr<sup>do</sup>Si<sup>t</sup>[0<sub>4</sub>]<sup>#</sup> <u>Zircon</u> I4<sub>1</sub>/amd  $\operatorname{Co}^{\circ}\left[\operatorname{Se}_{2}^{\langle h \rangle}\right]_{\Sigma}^{c}$  Hastite  $\operatorname{Fe}^{\circ}\left[\operatorname{As}_{2}^{\langle h \rangle}\right]_{\Sigma}^{c}$  Löllingite  $\mathbb{U}^{do} \operatorname{Sit} \left[ \mathbb{O}_{4-x}(OH)_{x} \right]^{*} \operatorname{Coffin-}_{ite} \mathbb{Y}^{do} \operatorname{Ast} \left[ \mathbb{O}_{4} \right]^{*} \operatorname{Chernovite}_{ite}$ Ni<sup>o</sup> [Se<sup><h></sup>]<sup>c</sup><sub>D</sub> Kulerudite Co<sup>o</sup> [SbS<sup><h></sup>]<sup>c</sup><sub>D</sub> Costibite Y<sup>do</sup>p<sup>t</sup>[0<sub>4</sub>] Xenotime Th<sup>do</sup>Si<sup>t</sup>[04] \* Thorite  $Fe^{O} \left[ Te_{2}^{\langle h \rangle} \right]_{\Sigma}^{c}$  Frohbergite Ni<sup>O</sup>  $\left[ Sb_{2}^{\langle h \rangle} \right]_{\Sigma}^{c}$  Nisbite Ta<sup>do</sup>B<sup>t</sup>[04]\* Behierite CadoCr<sup>t</sup>[0<sub>4</sub>]\* Chromatite Co<sup>o</sup> [AsS<sup><h>]</sup><sup>c</sup> Orthocobaltite  $Y^{do}V^{t}[0_{4}]^{*}$  Wakefieldite Co<sup>O</sup> [As<sub>2</sub><sup><h>]</sup><sup>C</sup> Safflorite Pbma Ca30Al2Si3[012]\* Garnet (Grossular) Ia3d Ni<sup>o</sup> As<sub>2</sub><sup>(h)</sup> Farammelsbergite Pb2,a Ca<sup>do</sup>Cr<sup>o</sup>2Si<sup>t</sup><sub>3</sub>[0<sub>12</sub>]<sup>\*</sup> Uvarovite Ca<sup>do</sup>v<sup>o</sup>2Si<sup>t</sup><sub>3</sub>[0<sub>12</sub>]\* Goldmanite

Fig. 17 c)

2.1				
Polygonal	Al <sup>o</sup> [Si <sup>t</sup> Al <sup>t</sup> 0 <sub>5</sub> ] <sup>2-Il</sup> <sub>by</sub> <u>Sillimanite</u> Pbnm			
Ni <sup><math>\tilde{p}</math></sup> [C <sup>tr</sup> O <sub>3</sub> ] <sup>c</sup> Gaspeite Cd <sup><math>\tilde{p}</math></sup> [C <sup>tr</sup> O <sub>3</sub> ] <sup>c</sup> Otavite	Ca <sup>o</sup> Sn <sup>o</sup> (H <sub>2</sub> O) <sub>2</sub> [Si <sup>t</sup> <sub>3</sub> O <sub>9</sub> ] <sup>I<sup>15</sup><sub>by</sub> <u>Stokesite</u> Pnna</sup>			
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{c} \operatorname{Ca}^{8}\operatorname{Ng}^{o}\left[\operatorname{Si}_{2}^{t}\operatorname{O}_{0}\right]_{\infty 1}^{\operatorname{II}_{cx}^{11}} & \underline{\operatorname{Diopside}} & \operatorname{C2/c} \\ \operatorname{Ca}^{8}\operatorname{Nn}^{o}\left[\operatorname{Si}_{2}^{t}\operatorname{O}_{0}\right]_{\infty 1}^{\operatorname{III}_{cx}^{11}} & \operatorname{Na}^{8}\operatorname{Fe}^{o}\left[\operatorname{Si}_{2}^{t}\operatorname{O}_{0}\right]_{\infty 1}^{\operatorname{III}_{cx}^{11}} \\ \operatorname{Johannsenite} & \operatorname{Aegirine} \end{array}$			
$c_{a}\bar{P}_{kg_{3}}\tilde{p}\left[c_{4}^{tr}o_{12}\right]_{\infty}^{L_{c}^{1}}$ Huntite R32	$\begin{array}{c} \operatorname{Ca}^{\circ}\operatorname{Fe}^{\circ}\left[\operatorname{Si}_{2}^{t}\operatorname{O}_{6}\right]_{\infty 1}^{\operatorname{III}_{\operatorname{Cx}}} & \operatorname{Na}^{\theta}\operatorname{Al}^{\circ}\left[\operatorname{Si}_{2}^{t}\operatorname{O}_{6}\right]_{\infty 1}^{\operatorname{III}_{\operatorname{Cx}}^{1}} \\ \operatorname{Hedenbergite} & \operatorname{Jadeite} \end{array}$			
$Ca^9 [c^{tr}o_3]^{T_s} \xrightarrow{Aragonite} Pacn$ $Sr^9 [c^{tr}o_3]^{T_s} \xrightarrow{S} Strontianite Pb^9 [c^{tr}o_3]^{T_s} Cerussite$	$ \begin{array}{c} \operatorname{Ca}_{4}^{8} \operatorname{Mg}_{3}^{\circ} \operatorname{Al}^{\circ} \begin{bmatrix} \operatorname{si}_{1}^{t} \operatorname{al}^{t} \operatorname{O}_{24} \end{bmatrix}_{\infty 1}^{\operatorname{II}_{cx}^{11}} & \operatorname{Li}_{4}^{8} \operatorname{Al}^{\circ} \begin{bmatrix} \operatorname{si}_{2}^{t} \operatorname{O}_{6} \end{bmatrix}_{\infty 1}^{\operatorname{II}_{cx}^{11}} \\ \operatorname{Augite} & \operatorname{Spodumene} \\ \operatorname{(Na,Ca)}^{8} (\operatorname{Mg,Al})^{\circ} \begin{bmatrix} \operatorname{si}_{2}^{t} \operatorname{O}_{6} \end{bmatrix}^{\operatorname{II}_{cx}^{11}} \end{array} $			
$Ba^{9}Ca^{9} \begin{bmatrix} c^{tr} 0_{3} \end{bmatrix}_{\infty}^{2} \text{ witherite } K^{2} \begin{bmatrix} N^{tr} 0_{3} \end{bmatrix}_{\infty}^{2} \text{ Nitrokalite}$ $Ba^{9}Ca^{9} \begin{bmatrix} c^{tr} 0_{6} \end{bmatrix}_{\infty}^{1} Ba^{1} \text{ Alstonite } Pacn$	Omphacite (Ca,Fe) <sup>7</sup> (Mg,Fe) <sup>9</sup> [Si <sup>t</sup> <sub>2</sub> 0 <sub>6</sub> ] <sup>II<sup>1</sup></sup> Pigeonite P2 <sub>1</sub> /c			
Wg2 [B2r05] <sup>II1</sup> <u>Suanite</u> P21/a	$Mg^{6}Mg^{9} \begin{bmatrix} si_{2}^{t}0_{6} \end{bmatrix}_{\infty}^{II_{cx}^{l1}} Clincenstatite P2_{1}/$			
Tetrahedral	Mg <sup>8</sup> Mg <sup>0</sup> Si <sup>t</sup> <sub>2</sub> 0 <sub>6</sub> H <sup>11</sup> <sub>m</sub> <u>Protoenstatite</u> Fbcn			
$Ca_{3}^{6} \left[ Si_{3}^{t} O_{9} \right]_{\infty}^{III_{c}^{4}} \xrightarrow{Pseudowollastonite} P2_{1}/a$	Ng <sup>8</sup> Mg <sup>0</sup> [si <sup>t</sup> <sub>2</sub> 0 <sub>6</sub> ] <sup>II1</sup> <sub>cbx</sub> <u>Enstatite</u> Pbca			
$Ba^{6}Ti^{0} \begin{bmatrix} Si^{\dagger}_{3} & 0_{g} \end{bmatrix}_{\infty}^{III_{Ta}^{4}} \underline{Benitoite}  P\bar{6}c2$ $Ba^{6}Sn^{0} \begin{bmatrix} Si^{\dagger}_{3}0_{g} \end{bmatrix}_{\infty}^{III_{Ta}^{4}} \underline{Beatite}$	$Ca_{2}^{8}Mg_{5}^{\circ}(OH, \mathbf{F})_{2} \begin{bmatrix} Si_{6}^{t}O_{22} \end{bmatrix}_{\infty 1}^{2-II_{cx}^{11}} \underbrace{\text{Tremolite } C2/m}_{Ca_{2}^{8}Fe_{5}^{\circ}(OH)_{2}} \begin{bmatrix} Si_{6}^{t}O_{22} \end{bmatrix}_{\infty 1}^{2-II_{cx}^{11}} \underbrace{\text{Perroactinolite}}_{Ca_{5}^{8}(Mg, Fe_{5})^{\circ}(OH)_{5}} \begin{bmatrix} Si_{4}^{t}I_{5} \\ Si_{6}^{t}I_{5} \end{bmatrix}_{\infty 1}^{2-II_{cx}^{11}} \underbrace{\text{Tremolite } Si_{6}^{t}I_{5} \end{bmatrix}_{\infty 1}^{2-II_{cx}^{11}} \underbrace{\text{Tremolite } Si_{6}^{t}I_{5} \\ Ca_{5}^{8}(Mg, Fe_{5})^{\circ}(OH)_{5} \begin{bmatrix} Si_{6}^{t}I_{5} \\ Si_{6}^{t}I_{5} \end{bmatrix}_{\infty 1}^{2-II_{cx}^{11}} \underbrace{\text{Tremolite } Si_{6}^{t}I_{5} \\ Ca_{5}^{8}(Mg, Fe_{5})^{\circ}(OH)_{5} \begin{bmatrix} Si_{6}^{t}I_{5} \\ Si_{6}^{t}I_{5} \end{bmatrix}_{\infty 1}^{2-II_{cx}^{11}} \underbrace{\text{Tremolite } Si_{6}^{t}I_{5} \\ Si_{6}^{t}I_{5$			
Cu <sup>°</sup> (H <sub>2</sub> O) [S1 <sup>°O</sup> <sub>3</sub> ] <sup>*</sup> <sub>2</sub> c <u>Dioptase</u> R3 K <sup>CO</sup> (Ca,Na) <sup>O</sup> <sub>2</sub> Th <sup>Cb</sup> [Si <sup>t</sup> <sub>8</sub> O <sub>2O</sub> ] <sup>2-IV<sup>6</sup><sub>2</sub></sup> s <u>Steacyite</u> P4/mcc	$Na_{2}^{8}(Mg, Fe)_{3}^{0}(A1, Fe)_{2}^{0}(OH)_{2} \begin{bmatrix} Si_{8}^{t}O_{22} \end{bmatrix}_{\infty 1}^{2-III_{11}} \text{ makite}$ $Na_{2}^{8}(Mg, Fe)_{3}^{0}(A1, Fe)_{2}^{0}(OH)_{2} \begin{bmatrix} Si_{8}^{t}O_{22} \end{bmatrix}_{\infty 1}^{2-III_{12}} \text{ Glaucophane}$			
Other polyhedra	Na <sup>10</sup> Ca <sup>8</sup> Mg <sup>o</sup> (OH,F) [sitalton] <sup>2-II1</sup> cx			
$\begin{bmatrix} cb_{8} \\ mathbf{s}_{8} \end{bmatrix}_{22}^{T_{d}} \propto -Sulfur$ Fddd	Hornblende C2/m Na <sup>10</sup> Na <sup>9</sup> Pe <sup>o</sup> <sub>2</sub> (OH) <sub>2</sub> [Si <sup>1</sup> <sub>2</sub> O <sub>22</sub> ] <sup>2-II<sup>1</sup></sup> Ka <sup>10</sup> Na <sup>9</sup> Pe <sup>o</sup> <sub>2</sub> (OH) <sub>2</sub> [Si <sup>1</sup> <sub>2</sub> O <sub>22</sub> ] <sup>2-II<sup>1</sup></sup> Karfvedsonite			
CHAIN	2 ) 2 0 2 3 3 1 2 - II <sup>11</sup>			
Homogeneous	Na <sup>10</sup> Na <sup>2</sup> Na <sup>0</sup> Mg <sup>2</sup> Al <sup>0</sup> Fe <sup>0</sup> (OH) <sub>2</sub> [Si <sup>6</sup> <sub>8</sub> 0 <sub>22</sub> ] C <sup>II</sup> Eckermann- ite			
Simple	$Na^{10}Na^{8}_{2}Ma^{0}_{4}(A1,Fe)^{\circ}(OH)_{2}\left[Si^{10}_{80}2_{22}\right]^{2-11}cx$ Kôzulite			
Linear	Na <sup>10</sup> Ca <sup>8</sup> (Mg Pa) <sup>9</sup> (OH) [St <sup>t</sup> 1 <sup>t</sup> 0] <sup>2-II</sup> <sup>11</sup> cx Paramete			
$\begin{bmatrix} Se^2 \end{bmatrix}_{\infty 1}^{T_{by}^{1}} \underline{Selenium}  P_{2}^{3} 2^{21}$ $\begin{bmatrix} Te^2 \end{bmatrix}_{\infty 1}^{T_{by}}  Tellurium$	$\frac{\operatorname{La}_{2}(\operatorname{Mg},\operatorname{Fe})_{5}(\operatorname{III})_{2}}{\operatorname{Na}^{10}\operatorname{Ca}_{2}^{8}(\operatorname{Mg},\operatorname{Fe})_{4}^{\circ}\operatorname{Ti}^{\circ}(\operatorname{OH})_{2}}\left[\operatorname{Si}_{4}^{\circ}\operatorname{Li}_{2}^{\circ}\operatorname{O22}\right]_{\infty 1} \operatorname{II}_{1}^{2-\operatorname{III}_{1}^{11}} \operatorname{Kaersut-}_{1}^{2-\operatorname{III}_{1}^{11}} \right]$			
[Hg <sup>2</sup> s <sup>2</sup> ] <sup>15</sup> <sub>by</sub> <u>Cinnatar</u> P5 <sub>1</sub> 21 Tetrahedral	M6 <sup>2</sup> M6 <sup>0</sup> <sub>2</sub> M6 <sup>0</sup> <sub>2</sub> (OH, P) <sub>2</sub> [Si <sup>6</sup> <sub>8</sub> O <sub>22</sub> ] <sup>conx</sup> Anthophyllite Pnma Li <sup>0</sup> <sub>2</sub> M6 <sup>0</sup> <sub>3</sub> Al <sup>0</sup> <sub>2</sub> (OH) <sub>2</sub> [Si <sup>t</sup> <sub>8</sub> O <sub>22</sub> ] <sup>2-III</sup> <sup>chx</sup> Holmquistite			
Pb <sup>7</sup> Bi <sup>7</sup> [cu <sup>t</sup> S <sub>3</sub> ] <sup>11</sup> <sub>oy</sub> <u>Aikinite</u> Pbnm	Al <sup>o</sup> $\left[ \text{El^t}_{Be^t} \text{O}_4(OH) \right]_{\infty 1}^{2-II_B^{31}} \underline{\text{Buclase}}  P2_1/c$			

Fig. 17 d)

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 $Ca^{o} \left[ si^{t} O_{3} \right]_{\infty 1}^{III_{my}^{61}}$  <u>Wollastonite</u> Pl  $\begin{bmatrix} \pi \\ As \end{bmatrix}_{\infty 2}^{\tilde{H}} \underline{Arsenic} R\bar{3}m$  $Ca^{o}kn^{o}[si_{2}^{t}o_{6}]_{\infty 1}^{III_{my}^{61}}$  Bustamite PĪ  $\begin{bmatrix} \pi & \pi \\ As & Sb \end{bmatrix}_{\infty 2}^{\tilde{H}_{c}} \text{ Allemontite } \begin{bmatrix} \pi \\ Bi \end{bmatrix}_{\infty 2}^{\tilde{H}_{c}} \text{ Bismuth }$ [st] <sup>Ĩ</sup>c, Antimony Na<sup>8</sup>Ca<sup>0</sup><sub>2</sub> [Si<sup>t</sup><sub>3</sub>0<sub>8</sub>(OH)]<sup>III<sup>61</sup></sup><sub>by</sub> <u>Pectolite</u> PĪ Tetrahedral  $Ca_{4}^{p}Ca_{2}^{o}(OH)_{2} \left[ \begin{array}{c} Si_{6}^{t}0_{17} \end{array} \right]_{\infty 1}^{2-III_{S}^{61}} \\ \underline{X}_{onotlite} \quad P2/a \end{array}$  $\mathbf{K}_{6} \mathbf{Al}_{2}^{\circ}(\mathrm{OH})_{2} \left[ \underbrace{\mathrm{Si}_{3}^{\dagger} \mathrm{Al}^{\dagger} \mathrm{O}_{10}}_{\mathbb{O}} \right]_{\infty 2}^{(2\mathrm{II}_{8}^{101})_{c}} \frac{\mathrm{Muscovite}(2\mathrm{M}_{1})}{\mathrm{C2/c}} \right]$  $\operatorname{Na}^{6}\operatorname{Al}_{2}^{0}(OH)_{2}\left[\operatorname{Si}_{3}^{t}\operatorname{Al}^{t}\operatorname{O}_{10}\right]_{\varpi^{2}}^{(2II_{B}^{101})_{c}} \operatorname{Paragonite}(2M_{1})$ Na<sup>7</sup>Na<sup>0</sup>Zr<sup>0</sup>(H<sub>2</sub>0)<sub>3</sub> [Si<sup>t</sup><sub>6</sub>0<sub>15</sub>]<sup>2</sup>-III<sup>61</sup> <sub>∞1</sub> Elpidite Pb2<sub>1</sub>m  $(K,Na)^{6}(Fe,Mg,A1)^{0}_{2}(OH)_{2} \begin{bmatrix} si^{t}_{A1}i^{t}_{0} \\ si^{t}_{A1}i^{t}_{0} \end{bmatrix}_{\infty}^{(2II^{101}_{B})_{c}}$  $\mathtt{Mn}^{7}\mathtt{Mn}_{4}^{o} \begin{bmatrix} \mathtt{si}_{5}^{t} \mathtt{0}_{15} \end{bmatrix}_{\infty 1}^{V_{my}^{11}} \\ \underline{\mathtt{Rhodonite}} \quad \mathtt{P1}$  $Na^{7}Na^{o}Zr^{o} \begin{bmatrix} si_{4}^{t}o_{11} \end{bmatrix}_{\infty 1}^{VIII_{my}^{31}} \underline{Vlasovite}$  C2/c  $\begin{array}{c} \texttt{x}^{6}\texttt{Mg}_{3}^{o}(\texttt{OH})_{2} \begin{bmatrix} \texttt{si}_{3}^{\texttt{t}}\texttt{Al}^{\texttt{t}}\texttt{o}_{10} \end{bmatrix}_{\varpi 2}^{(\texttt{2II}_{g}^{\texttt{101}})_{c}} \\ \underline{\texttt{Phlogopite}}(\texttt{1M}) \end{array}$ C2/m  $\begin{array}{c} \mathbb{K}^{6}(\mathbb{M}_{g}, \mathbb{F}e)_{3}^{0}(\mathrm{OH})_{2} \left[ (\mathrm{Si}, \mathrm{Al})_{4}^{t} \mathrm{O}_{10} \right]_{\infty}^{2} 2 \\ \mathbb{B}iotite(1\mathbb{W}) \\ \mathbb{K}^{6}\mathbb{M}_{3}^{0}(\mathrm{OH})_{2} \left[ \mathrm{Si}_{3}^{t} \mathrm{Al}^{t} \mathrm{O}_{10} \right]_{\infty}^{2} 2 \\ \mathbb{P}hlogopite(2\mathbb{M}_{1}) \\ \mathbb{P}hlogopite(2\mathbb{M}_{1}) \\ (2\mathrm{P}hlog) \\ \mathbb{P}hlogopite(2\mathbb{M}_{1}) \\ \mathbb{P}hhlogopite(2\mathbb{M}_{1}) \\ \mathbb{P}hhlogopite(2$ Pb<sup>T</sup>Pb<sup>4</sup><sub>2</sub>[Si<sup>t</sup><sub>3</sub>09]<sup>XII<sup>11</sup></sup><sub>∞1</sub> <u>Alamosite</u> P2/n Other polyhedra C2/c  $\begin{bmatrix} sb_2s_3 \end{bmatrix}_{\infty 1}^{II_{by}^{41}}$  Stibnite Pbnm  $\begin{array}{c} Fhlogopite(2M_{1}) \\ E^{6}(Mg,Fe)_{3}^{o}(OH)_{2} \left[ (Si,A1)_{4}^{to}_{10} \right]_{\infty 2}^{o} \\ Biotite(2M_{1}) \\ K^{6}Mg_{3}^{o}(OH)_{2} \left[ Si_{3}^{tA1}t_{0}_{10} \right]_{\infty 2}^{o} \\ Phlogopite (3T) \\ F^{6}(Li,A1)_{3}^{o}(OH)_{2} \left[ (Si,A1)_{4}^{to}_{10} \right]_{\infty 2}^{o} \\ Lepidolite(3T) \\ E^{6}(Mg,Fe)_{3}^{o}(OH)_{2} \left[ (Si,A1)_{4}^{to}_{10} \right]_{\infty 2}^{o} \\ Biotite(3T) \\ E^{6}(Mg,Fe)_{3}^{o}(OH)_{2} \left[ (Si,A1)_{4}^{to}_{10} \right]_{\infty 2}^{o} \\ Biotite(3T) \\ F^{6}(Mg,Fe)_{3}^{o}(OH)_{2} \left[ (Si,A1)_{4}^{to}_{10} \right]_{\infty 2}^{o} \\ \end{array}$ Bi2S3 Diby Bismuthinite P3,12 Bi2Se3 Cuanajuatite  $Ca^{do} \left[ Al_{2}^{o} F_{4}(OH)_{4} \right]_{col}^{14}$  Prosopite C2/c Composite  $\begin{array}{c} \texttt{K}^{6}(\texttt{Li},\texttt{Al})^{0}_{2}(\texttt{OH})_{2} \left[(\texttt{Si},\texttt{Al})^{\texttt{t}}_{4}\texttt{0}_{10}\right]^{(\texttt{2III01})}_{\texttt{S}}\texttt{h} \quad \texttt{c2/c} \\ \underline{\texttt{Lepidolite}(\texttt{2M}_{2})} \end{array}$  $Ca_2^7 \left[ Mn^0 As_2^{t} O_8(H_2 O)_2 \right]_{\infty 1}^{III_{bx}^{81}}$  Brandtite  $P_2^{1/c}$ Al2(OH)2 [Si<sup>t</sup><sub>4</sub>0<sub>10</sub>] (2II<sup>101</sup>) Pyrophyllite Cc Ca2 Mn°P208(H20)2 IIImx Fairfieldite PI  $\begin{array}{c} \underline{\texttt{Mg}}_{3}^{\circ}(\text{OH})_{2} \begin{bmatrix} \text{Si}_{4}^{\dagger} \text{O}_{10} \end{bmatrix}_{\text{C2II}}^{(2\text{III}101)} \text{c}} \\ \underline{\texttt{Mg}}_{3}^{\circ}(\text{OH})_{2} \begin{bmatrix} \text{Si}_{4}^{\dagger} \text{O}_{10} \end{bmatrix}_{\text{C2II}}^{(2\text{III}101)} \text{c}} \\ \underline{\texttt{Ni}}_{3}^{\circ}(\text{OH})_{2} \begin{bmatrix} \text{Si}_{4}^{\dagger} \text{O}_{10} \end{bmatrix}_{\text{C2II}}^{(2\text{III}101)} \text{c}} \\ \end{array} \\ \begin{array}{c} \text{Willemsein} \end{bmatrix}$ Ca2 Co<sup>o</sup>As208(H20)2 mi Triclinoroselite Ca2 [B<sup>tr</sup>B<sup>t</sup>04] [V<sup>51</sup> Calciborite-II Fbcn Willemseite  $\begin{array}{c} \text{Al}_{2}^{\circ}(\text{OH})_{4} \begin{bmatrix} \text{si}_{2}^{\circ} \text{o}_{5} \end{bmatrix}_{\substack{\substack{\substack{\alpha \neq 2 \\ \alpha \neq$  $Ca^{7}Na^{o}(H_{2}O)_{3}\left[B_{2}^{tr}B_{3}^{t}O_{7}(OH)_{4}\right]_{\infty1}^{V_{by}^{61}}$  Probertite P21/n  $Ca^{7}(H_{2}O) \left[ B^{tr}B_{2}^{t}O_{4}(OH)_{3} \right]_{\infty 1}^{VI_{my}^{31}} Colemanite P2_{1}/a$ Heterogeneous  $\left\{ \begin{bmatrix} \mathbf{B}_2^{\mathtt{tr}} \mathbf{B}_2^{\mathtt{t}} \mathbf{0}_5(\mathbf{OH})_4 \end{bmatrix}_{\infty}^{\mathtt{IV}^4} \begin{bmatrix} \mathtt{Na}_2^{\mathsf{O}}(\mathtt{H}_2\mathbf{O})_8 \end{bmatrix}_{\infty 1}^{\mathtt{III}^{\mathtt{11}}} \right\}_{\underline{\mathtt{Borax}}} C2/e$  $Ba^{7} \begin{bmatrix} si_{2}^{t}0_{5} \end{bmatrix}_{\infty}^{II_{hx}^{211}}$ Sambornite Pcmn  $x_2^8 zr^o \begin{bmatrix} si_6^t 0_{15} \end{bmatrix}_{\infty 2}^{III_{cx}^{611}} \underline{Dalyite} P\overline{1}$ SHEET Homogeneous  $\mathbf{Ba^{8} Fe^{sq} \left[ si_{4}^{t} \mathbf{0}_{10} \right]_{\infty 2}^{IV_{f}^{602}}}$ Simple Gillespite P4/ncc Linear  $Ca^{8}Cu^{8q} \begin{bmatrix} si_{4}^{t}0_{10} \end{bmatrix} \begin{bmatrix} IV_{f}^{602} \\ m_{2} \end{bmatrix}$  Cuprorivate Ctr]<sup>H</sup>h <sup>∞ 2</sup> Graphite P63/mmc

Fig. 17 e)

#### THE NEED OF A STRUCTURAL CLASSIFICATION OF MINERALS

 $\begin{array}{c} \mathbf{y}_{2}^{cb} \mathbf{F} \mathbf{e}^{o} \begin{bmatrix} \mathbf{B} \mathbf{e}_{2}^{t} \mathbf{S} \mathbf{i}_{2}^{t} \mathbf{0}_{10} \end{bmatrix}_{\infty 2}^{IV_{g}^{301}} \underbrace{\text{Gadolinite}}_{2} \mathbf{F}_{1}^{2} \mathbf{A} \\ \mathbf{C} \mathbf{a}_{2}^{cb} \mathbf{F} \mathbf{e}^{o} \begin{bmatrix} \mathbf{B}_{2}^{t} \mathbf{S} \mathbf{i}_{2}^{t} \mathbf{0}_{10} \end{bmatrix}_{\infty 2}^{IV_{g}^{301}} \underbrace{\text{Homilite}}_{2} \end{array}$ [sito2] m3 Keatite P41212  $Li^{4} \begin{bmatrix} si_{2}^{t}Al0_{6} \end{bmatrix}_{\infty 3}^{III_{Q}^{1}} \beta \underline{-Spodumene} P4_{1}^{2}_{1}^{2}$  $\begin{array}{c} \text{Ca}^{cb} \begin{bmatrix} \texttt{B}^{t} \texttt{Si}^{t} \texttt{O}_{4}(\texttt{OH}) \end{bmatrix}_{\infty 2}^{\texttt{IV}_{g}^{3O1}} & \texttt{Datolite} & \texttt{P2}_{1}/\texttt{a} \\ \text{Ca}^{cb} \begin{bmatrix} \texttt{B}^{t} \texttt{p}^{t} \texttt{O}_{4} \texttt{P} \end{bmatrix}_{g}^{\texttt{IV}_{g}^{3O1}} & \texttt{Yb}^{cb} \begin{bmatrix} \texttt{B}^{t} \texttt{Si}^{t} \texttt{O}_{4}(\texttt{OH}) \end{bmatrix}_{\infty 2}^{\texttt{IV}_{g}^{3O1}} \\ \texttt{Herderite} & \texttt{Yb}^{cb} \begin{bmatrix} \texttt{B}^{t} \texttt{si}^{t} \texttt{O}_{4}(\texttt{OH}) \end{bmatrix}_{\infty 2}^{\texttt{IV}_{g}^{3O1}} \end{array}$  $\begin{bmatrix} 2 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \xrightarrow{(21V_{by})_{g}} \underbrace{\text{Coesite } C2/c} \\ \begin{bmatrix} si^{t} 0_{2} \end{bmatrix}_{co3}^{(21V_{by})_{g}} \underbrace{\text{Sanidine } C2/c} \\ \begin{bmatrix} x^{0} \begin{bmatrix} si^{t} A_{1}^{t} 0_{8} \end{bmatrix}_{co3}^{(21V_{by})_{g}} \\ \begin{bmatrix} si^{t} A_{1}^{t} 0_{8} \end{bmatrix}_{co3}^{(21V_{by})_{g}} \underbrace{\text{Sanidine } C2/m} \\ \begin{bmatrix} x^{0} \begin{bmatrix} si^{t} A_{1}^{t} 0_{8} \end{bmatrix}_{co3}^{(21V_{by})_{g}} \\ \begin{bmatrix} si^{t} A_{1}^{t} 0_{8} \end{bmatrix}_{co3}^{(21V_{by})_{g}} \underbrace{\text{Microcline } FI} \end{bmatrix}$ MngCl(OH)9 Sito15 PJml Other polyhedra  $Ca^{7} \left[ si_{2}^{t} Al_{2}^{t} o_{8} \right]_{\infty 3}^{(2IV_{by}^{1})_{8}}$  Anorthite  $P\bar{I}$  $\begin{bmatrix} \begin{bmatrix} \pi \\ AB_2S_3 \end{bmatrix}_{\infty 2}^{II_{2}^{O1}} \\ \begin{bmatrix} AB_2S_3 \end{bmatrix}_{\infty 2}^{II_{2}^{O1}} \\ \begin{bmatrix} AB_2S_3 \end{bmatrix}_{\infty}^{II_{2}^{O1}} \\ \end{bmatrix}_{\infty}^{II_{2}^{O1}}$ Orpiment P2,/c  $Na^8 \left[ si_{3}^{t} B^{t} 0_8 \right]_{\infty_3}^{(2IV_{by}^{11})_g}$  Reedmergnerite PI Getchellite  $\begin{bmatrix} Te^40_2 \end{bmatrix}_{\infty 2}^{II_f^{111}}$  Tellurite Pbca Ca<sup>7</sup>[Si<sup>t</sup><sub>2</sub>B<sup>t</sup><sub>2</sub>O<sub>8</sub>]<sup>IV101</sup> manual manua manual manu Ca<sup>7</sup> [Be<sup>t</sup><sub>2</sub>P<sup>t</sup><sub>2</sub>0<sub>8</sub>]<sup>IV<sup>201</sup></sup> <sub>m3</sub> Na<sup>cb</sup>Na<sup>6</sup> [Al<sup>o</sup><sub>3</sub>P<sub>14</sub>]<sup>III<sup>201</sup></sup> Chiolite P4/mnc Hurlbutite P2,/c Na<sup>9</sup>C1<sup>4</sup> [A1<sup>t</sup><sub>3</sub>S1<sup>t</sup><sub>9</sub>0<sub>24</sub>]<sup>VIII<sup>201</sup></sup> 3 Composite Scapolite I4/m Ba20 [Si2ti508] [III301 Ba20 [Si2ti508] [mo 2] Presnoite P4bm Ba<sup>10</sup>(H<sub>2</sub>0)<sub>6</sub> [Sitat<sup>t</sup>016]<sup>IV<sup>2</sup></sup><sub>by</sub> <u>Harmotome</u> P2<sub>1</sub>/m K2<sup>11</sup>(H2<sup>0</sup>)3 [v2<sup>5</sup>u2<sup>7</sup>012]<sup>IV<sup>B11</sup> carnotite P21/a</sup> Ba<sup>10</sup>(H<sub>2</sub>0)<sub>4</sub> [Sitalto10]<sub>by</sub> <u>Edingtonite</u> P42<sub>1</sub>m FRAMEWORK  $\begin{bmatrix} cl^{t}Na_{4} \end{bmatrix}_{\infty} \begin{bmatrix} si_{3}^{t}Al_{3}^{t}O_{12} \end{bmatrix}_{\infty 3}^{VI_{c}^{2}} \\ \underline{Sodalite} \\ P\overline{4}\overline{3}n \end{bmatrix}$ Homogeneous [S<sup>t</sup>(Mn,Fe)<sub>4</sub>]<sub>2</sub>[Si<sup>t</sup><sub>3</sub>Be<sup>t</sup><sub>3</sub>O<sub>12</sub>]<sub>203</sub><sup>VI<sup>2</sup></sup> Helvine Simple Linear stzn4 sitBet012 wi Genthelvite [ct]<sup>H</sup>c Diamond Fd3m  $\begin{bmatrix} \mathbf{s}^{\mathsf{T}}\mathbf{p}\mathbf{e}_{4} \end{bmatrix}_{\infty} \begin{bmatrix} \mathbf{s}_{3}^{\mathsf{T}}\mathbf{B}\mathbf{e}_{3}^{\mathsf{T}}\mathbf{0}_{12} \end{bmatrix}_{\infty 3}^{\mathsf{VIC}} \quad \text{Danalite} \\ \begin{bmatrix} \mathbf{s}^{\mathsf{T}}\mathbf{p}\mathbf{e}_{4} \end{bmatrix}_{\infty} \begin{bmatrix} \mathbf{s}_{3}^{\mathsf{T}}\mathbf{B}\mathbf{e}^{\mathsf{T}}\mathbf{0}_{12} \end{bmatrix}_{\infty 3}^{\mathsf{VIC}} \quad \text{Tugtupite} \quad \mathbf{I}\overline{4} \end{bmatrix}$ [ct]<sup>Ĥ</sup>h m3 Lonsdaleite P6z/mmc Tetrahedral  $c_{a,D_{10}(H_2O)_{13}} \left[ s_{16}^{t} s_{14}^{t} s_{24}^{t} \right]_{\infty_3}^{2-VI_c^2} \underline{c_{habazite}} \quad B_{3m}^{3}$ [Si<sup>t</sup>02]<sup>161</sup> m3 Quartz P3,21  $\begin{bmatrix} p^{t}al^{t}0_{4}\end{bmatrix}_{\omega_{3}}^{161}$  Berlinite  $P_{3}^{21}$ Al<sup>o</sup><sub>2</sub>  $\begin{bmatrix} \text{Sit}_{\text{Bet}_{0}}^{\text{t}} \text{Bet}_{0}^{\text{t}} \end{bmatrix}_{\infty^{3}}^{\text{IX}^{201}} \xrightarrow{\text{Beryl}} P6/\text{mcc}$  $Li^{4} [si^{t}ai^{t}o_{4}]^{I_{by}^{161}} \beta - Eucryptite P6_{2}22$ 
$$\begin{split} & \mathtt{Mg}_{2}^{o} \begin{bmatrix} \mathtt{Si}_{5}^{\mathtt{t}} \mathtt{Al}^{\mathtt{t}} \mathtt{Al}_{3}^{\mathtt{t}} \mathtt{O}_{18} \end{bmatrix}_{\varpi 3}^{\mathrm{IX}_{g}^{\mathtt{t}}} & \mathrm{Indialite} \\ & (\mathtt{Mg}, \mathtt{Fe})_{2}^{o} \begin{bmatrix} \mathtt{Si}_{5}^{\mathtt{t}} \mathtt{Al}^{\mathtt{t}} \mathtt{Al}_{3}^{\mathtt{t}} \mathtt{O}_{18} \end{bmatrix}_{\varpi 3}^{\mathrm{IX}_{g}^{2O1}} & \mathrm{Cording} \\ \end{split}$$
P6/mcc [si<sup>t</sup>0<sub>2</sub>]<sup>II<sup>201</sup><sub>c</sub> Cristobalite P4<sub>1</sub>2<sub>1</sub>2</sup> Cordierite Cccm (H20) [Si<sup>t</sup>27n<sup>t</sup>407(OH)<sub>12</sub>] [III<sup>614</sup> Hemimorphite Imm2 Composite  $\begin{bmatrix} 0^{t}H_{2}^{2} \end{bmatrix}_{\infty 3}^{II2Ol} & \underline{Ice} \text{ (antartic) } Pd3m \\ \begin{bmatrix} 0^{t}H_{2}^{2} \end{bmatrix}_{\infty 3}^{II2Ol} & \underline{Ice} \text{ (antartic) } Pd3m \\ \begin{bmatrix} si^{t}o_{2} \end{bmatrix}_{\infty 3}^{II2Ol} & \underline{ridymite} & C222_{1} \\ \hline r^{6} \begin{bmatrix} si^{t}Ai^{t}o_{4} \end{bmatrix}_{\infty 3}^{II2Ol} & \underline{Kalsilite} & P6_{3} \\ \hline r^{9}Na_{3}^{8} \begin{bmatrix} si^{t}_{4}Ai^{t}o_{16} \end{bmatrix}_{\infty 3}^{II2Ol} & \underline{Nepheline} & P6_{3} \\ \hline 0^{t}H_{2}^{2} \end{bmatrix}_{\infty 3}^{II2Ol} & \underline{Ice} \text{ (normal) } P6_{3}/mmc \\ \end{bmatrix}$ Na<sup>8</sup><sub>2</sub> Ti<sup>o</sup>Si<sup>t</sup><sub>4</sub>0<sub>11</sub> v<sup>901</sup><sub>f</sub> <u>Narsarsukite</u> I4/m BetBtrog(OH) VI0 Hambergite Fbca Ba<sup>10</sup>Na<sup>7</sup><sub>4</sub> [Ti<sup>o</sup><sub>2</sub>Si<sup>t</sup><sub>10</sub>B<sup>t</sup><sub>2030</sub>] <sup>XIV</sup><sup>101</sup><sub>8</sub> <u>Leucosphenite</u> Cm C1 [A1 251 tA1 t0 20 (OH) 18 ] 201 Zunyite P43m

Fig. 17 f)

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