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Mineral classifications re-visited with emphasis on a paragenetic-structural system

Dedicated to Prof. Hugo Strunz
on his 90th anniversary

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Abstract. A fleeting overview is made on the classifications of minerals in order to put accent on a more natural system based on a dual geochemical-paragenetic and crystal chemical-structural principle. Morphology of minerals is wholesomely interpreted in terms of this principle. Paragenetic cationic subdivisions (metallic assemblages) within the traditionally accepted, only slightly rearranged anionic subdivisions (classes), are further subdivided into salient structure types, viz. chain-like or axial A-type, sheet-like or planar P-type and framework or pseudoisometric (I)-type respectively isometric I-type. For evolving of these three structure types only the bulk anisometricity is used expressed by the axial ratios of the unit cells or sub-cells of the minerals. Such a classification is deemed better fitting the minerals as geoobjects displaying variable crystal habits which depend on predominant strong bonds in their structure and on the conditions of their growth under diverse geological environments. Sulphate minerals are worked out as an example.

Key words: mineral classification, paragenesis, crystal structure, anisometricity of unit cell, morphology
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Резюме. Направен е кратък преглед на класификациите на минерали с оглед да се наблегне върху една по-рационална система, базирана на двоен геохимично-парагенетичен и кристалохимично-структурен принцип. Морфологията на минералите е изцяло интерпретирана въз основа на този принцип. Парагенетичните катионни подразделения (метални асоциации) в традиционно възприетите само леко прередени анионни подразделения, са по-нататък разделени в специфични структурни типове, а именно верижни или аксиален А-тип, слоисти или планарен Р-тип и скелетни или псевдоизометричен (I)-тип, респективно изометричен I-тип. За извеждането на тези три структурни типа е използвана само общата анизометрия, изразена чрез осното отношение на елементарните клетки или субклетки на минералите. Такава класификация се приема за по-добре съответваща на минералите като геообекти, които показват разнообразни кристални хабитуси зависещи главно от условията на техния растеж при различни геоложки обстановки. Като пример са разработени сулфатните минерали.

Ключови думи: минерална класификация, кристална структура, анизометрия на елементарната клетка, морфология
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Introduction

The significance of a classification for science is lucidly outlined by Orcel (1954). In his words: 'une classification est une méthod de travail. Elle ne doit pas être un simple catalogue du faits ou d'événement. Une bon classification est un instrument de recherche; elle est la base fondamentale de tout travail théorique'. As also becomingly put by Hawthorn (1985): 'A scientific classification is distillation of our knowledge concerning the nature of the objects under consideration'. The objects under consideration in the science of mineralogy are geohistorical products and not only chemical elements and compounds. They are products which bear the impact of geological processes active throughout the evolution of the Earth's crust and mantle. Their growth in nature, their manner and trend of crystallization, and their 'social' links (parageneses) should therefore not be overlooked when a rational system for them is ventured.

To write this article impetus the author got from a statement of the Commission on Classification of Minerals of the International Mineralogical Association (IMA), laid down during the Second Business Session of the 16th General Meeting of IMA in Piza, viz. 'to improve or extend existing models of classifications, trying to evaluate strength and weaknesses of each of them'. In a series of papers and monographs (Kostov, 1964; 1968; 1975; 1981; 1986; Kostov, Minčeva-Stefanova, 1982) the present author extended a classification (sometime misquoted) in which an attempt is made to cover the requirements of mineralogists and geochemists as a whole. A reduced classification of sulphate minerals is worked out as a model for this, here finally improved, paragenetic-structural system.

On the existing classifications

A scrupulous persual of the classification of minerals known so far reveals gaps in the arrangemant and misplacement of mineral species due largely to available knowledge or personal interests. Comprehensive historical reviews are presented by Povarennykh (1972), Lima-de-Faria (1983) and Strunz (1984). Chemical and crystal chemical classifications predominate following the tradition of the earliest such scheme of Berzelius since 1815. The tendency in these classifications is to arrange the minerals in classes according to their anionic constituents (sulphides, oxides, silicates, etc. plus native elements) and then according to type of compounds, ratio of metal/non-metal, respectively anhydrous and hydrated minerals. Modernized such versions are presented by the classic Dana's System of Mineralogy (Palache et al., 1944; 1951) and Klockmanns Lehrbuch der Mineralogie (Ramdohr, Strunz, 1980).

The basic criteria used for classification of minerals are suitably summarized by Lima-de-Faria (1983), Strunz (1978, 1984) and Godovikov (1997). As tabulated by the first author, usefulness, physical properties, chemical and structural properties and geochemical peculiarities are nuslei of corresponding classifications, his own being purely structural (Lima-de-Faria, 1986; 1994). In the structural classification structural patterns of minerals are systematically arranged but not the minerals *per se*. The crystal chemical classification of Povarennykh (1972) tends to be allied to the structural classifications but in it chemistry is not overlooked. Structural with stressed morphological aspect is the system of Niggli (1926) in which cubic respectively hypocubic, tetragonal respectively hypotetragonal and hexagonal respectively hypohexagonal types are recognized with axial, hypocubic and planar subtypes for the latter two types. Bond type as prime subdivisions is used by Barsanov (1964) and Godovikov (1997), their classifications termed crystal-chemical, respectively structural-chemical. Structure types of salient minerals as subdivisions prevail in the handbook '*Minerals*' (1960-1992). In the so-called genetic classifications minerals are considered according to origin in corresponding geological setting (magmatic, metamorphic, sedimentary) so in them not the minerals *per se* but geological processes are classified.

Geochemical accent within divisions based on M:S ratio, couple in some of them with coordination number of principal metals provides an improved classification of sulphides offered by Strunz (1993). Hey's 'Index of Mineral Species' (1950; 1963; 1974), allready a classic, is essentially a geochemical classification, while the 'Lists of New Mineral Names' initiated by L. J. Spencer since 1892 in the Mineralogical Magazine, compiled by Embrey and Fuller (1980), as well as 'Fleischer's Glossary of Mineral Species' (Mandarino, 1999) together with the 'Handbook of Mineralogy' (Anthony et al., 1990) are alphabetical manuals perfectly well serving their purpose.

The paragenetic classification defended by A. de Lapparent in 1900 takes into account the evolution of the earth's crust and the minerals in their mode of occurrence, viz. magmatic, metamorphic from metalliferous and non-metalliferous ore deposits, and combustible ores, so it is in fact genetic and not properly paragenetic (s. Orcel, 1954).

All classifications briefly touched above, as well as their manifold variants, have of course merits because, as put by Liebau (1985), 'the best classification which can be chosen is the one that is best able to serve the particular purpose under consideration'.

Proposed classification

The classification offered is based on geochemical-paragenetic and crystal chemical-structural criteria. Its trends run as follows:

1. Paragenetic trend:
1.1. Native elements and anionic subdivisions as **classes**. These subdivisions are universally accepted with slight rearrangements.
1.2. Cationic (metallic) subdivisions as **mineral assemblages**, based on geochemically associated metals in the composition of the minerals, becomingly presented as triads.
2. Structural trend;
2.1. Structural subdivisions based on anisometricity of unit-cell or sub-cell and strong bonds in the structure, viz. chain-like or **axial A-type**, sheet-like or **planar P-type**, **pseudoisometric (I)-type**, and **isometric I-type**. These subdivisions roughly correspond to the generally accepted structural patterns in the pure structural classifications of minerals but exclude subdivisions with isolated coordination polyhedra, finite clusters of polymerized polyhedra of one or different kinds, as well as framework structures which by unit cell or sub-cell anisometricity fall either into the isometric and pseudoisometric structure types (most of them) or within axial or planar types.
2.2. **Groups** and **sub-groups** of minerals, based on identity or similarity of crystal structure and space group.

The trend of the classes could be envisaged as running upward in accordance with a general tendency of increasing Eh values and change of bonds from predominant metallic and covalent (native elements, sulphides et al.) to ionic isodesmic (oxides, halides), mesodesmic (silicates, borates) and anisodesmic (the remaining classes). The carbon group of diamond and graphite occupies an off-side position, linking at the base inorganic and organic minerals. Within each of the inorganic classes for the next subdivisions are picked up triads, eventually plus other chemical elements geochemically and paragenetically making up the composition of the minerals. On the one side are distinctly sulphophile, selenophile and tellurophile metals with affinities also toward As, Sb and Bi, while on the other side are oxiphile metals with affinities towards F, Cl, CO_3, BO_3, BO_4, SiO_4 and other anionic groups and elements.

The anisometricity of the unit cell or sub-cell is expressed in terms of axial retios c/a, respectively $2c/(a+b)$, $2b/(a+c)$ and $2a/(b+c)$ for structures of minerals with spindle symmetry respectively lower symmetries. A reciprocal relationship between shape of unit cell and tendency of development of a crystal form is discerned. When the corresponding ratios are less than 1.0 the structures tend to be chain-like, becomingly called by Niggli axial here denoted as A-type, respectively A^c, A^b or A^a types; when the corresponding ratios are larger than 1.0 the bulk structural patterns tend to be sheet-like, planar, denoted as P-type, respectively P^c, P^b and P^a types; with ratios approximately 1.0 the bulk structures tend to be pseudoisometric, denoted as (I)-type for the minerals with spindle symmetry and $(I)^c$, $(I)^b$ and $(I)^a$ types for those of lower symmetry depending on the axis of close pseudoisome-tricity. Isometric, I-type, are all cubic minerals.

Sub-cells ratios are used when structural patterns permit such ratios as demonstrated by chalcopyrite $CuFeS_2$, space group $I\bar{4}2d$, cell dimencions a 5.24 and c 10.32 Å, c/a formal ratio ~2.0 coresponding to a planar P-type mineral but in fact pseudoisometric (I)-type, made up of doubled sphalerite unit cell. Thaumasite $Ca_3Si(OH)_4(SO_4)(CO_3).12H_2O$, is another example with formal pseudoisometric ratio 0.94, but its exclusive fibrous development requires a halved sub-cell ratio of 0.46, fitting an axial A-type mineral (s. also Kostov, Kostov, 1999).

In addition to space group symmetry for proper differentiation of the bulk structure type attention should be also paid to cleavage and striations, twinning, tendency of crystal growth in nature and laboratory, as well as to optical properties (e.g. birefringence). In the pure structural classification this procedure is overlooked leading to misplacement of minerals. Such is for instance the case with barite, considered in the structural classifications of Sabelli and Trosti-Ferroni (1985), and Rastzvetaeva and Pushcharovskii (1989) a sheet-like mineral in spite of its perfect (001) and (210) cleavages.

The significance of the notation offered for the bulk structure types is crystallogenetically enhanced through adding as subscripts indices (hkl) for predominent crystal habit forms, and/or zone symbol [uvw] for direction of elongation. Thus and A-type mineral may develop as tabular $A_{(001)}$ or prismatic $A_{[uvw]}$ crystal habits, intermediate pseudoisometric crystal habit suitably denoted as A_i type. For the low symmetry minerals the tendency may be flattented on a face and elongated along a direction, e.g. $A^c_{(hkl)[uvw]}$ respectively $A^c_{[uvw](hkl)}$, in addition to the principal $A^c_{(hkl)}$, A^c_i and $A^c_{[uvw]}$ crystal habits. For fibrous crystal habits subscript 'f' is proposed, for twinned crystals subscript 't' following the indications of the habit form (Kostov, Kostov, 1999).

The crystal habits of minerals with their outer and inner peculiarities are of prime importance for deciphering the conditions under which they had grown in nature. Factors such as supersaturation, rate of crystallization, impurities, temperature, pressure, pH, Eh and position of nucleated mineral, are which influence the development of its crystal habit. Accepted growth mechanisms are through screw dislocations and layer-by-layer (BCF respectively VKS mechanisms), which follow each other with increased supersaturation of the solutions or supercooling of the melts from which the mineral crystallize. Autoepitaxial accretion and skeletal growth is achieved at still higher rates of crystallization. Growth terraces down to one or even one half unit cell have been observed on crystal faces when they grow according to the spiral and layer-by-layer mechanisms, while for proper autoepitaxial growth macro-, micro- and submicroscopic crystallites are considered responsible.

The classification trend improved up to the end shown above is considered much more natural and rational for the minerals *per se* then that of the other classifications. Its significance is properly quoted by Liebau (1985) refering to a paper by the present author on the classification of silicate minerals. He writes: 'The extended Bragg classification is based soleley on crystal chemical principles and therefore suitable for finding relations between the chemical composition and crystal structure... On the other hand the classification of silicate minerals developed by Kostov (1975) is designed to fulfill the need of mineralogists and geologists. To this end Kostov based his classification partly on crystal structure and partly on other equally essential properties of chemical composition and crystal morphology… The morphology of a crystal depends primarily on the relative strength and number of bonds per volume parallel in the various directions in the crystals…Since all bonds contribute to this ratio [refering to the present author's axial ratio, N.B.] the Kostov classification avoids those shortcomings of the crystal chemical classifications (pp. 137; 138)'.

To illustrate the 'strength' of the proposed paragenetic-structural classification of minerals in Table 1 is presented a newly worked concise model for the more important and representative sulphate minerals. Use is made mostly of mineral species included in the detailed classifications of sulphate minerals by Sabelli and Trosti-Ferroni (1983), and Rastzvetaeva and Pushcharovskii (1989). There are about 300 sulphate minerals known up till now of which 57 species are tabulated by the first authors as with unknown structures. In the proposed classification all sulphate minerals can find their proper sites within the subdivisions by using cell or sub-cell anisometricity as well as physical properties.

Table 1. *Paragenetic-structural classification of the sulphate minerals*
Таблица 1. *Парагенетично-структурна класификация на сулфатните минерали*

1. Al-Mg-Fe Assemblages

1.1. Axial (Chain–like) Structures
1.1.1. Alumininite $Al_2SO_4(OH)_4.7H_2O$
1.1.2. Pickeringite $MgAl_2(SO_4)_4.22H_2O$
Halotrichite $FeAl_2(SO_4)_4.22H_2O$
1.1.3. Kalinite $KAlSO_4.11H_2O$
Mendosite $NaAlSO_4.11H_2O$
Ettringite $Ca_6Al_2(SO_4)_3(OH)_{16}.26H_2O$
1.1.4a. Epsomite $MgSO_4.7H_2O$
Tauriscite $FeSO_4.7H_2O$
Morenosite $NiSO_4.7H_2O$
1.1.4b. Melanterite $FeSO_4.7H_2O$
Hexahydrite $MgSO_4.6H_2O$
Ferrohexahydrite $FeSO_4.6H_2O$
1.1.5. Sideronatrite $Na_2Fe(SO_4)_2(OH).3H_2O$
1.2. Planar (Sheet–like) Structures
1.2.1. Alunogen $Al_2(SO_4)_3.17H_2O$
1.2.2. Alunite $KAl_3(SO_4)_2(OH)_6$
Jarosite $KFe_3(SO_4)_2(OH)_6$
1.2.3a. Starkeyite $MgSO_4.4H_2O$
Rozenite $FeSO_4.4H_2O$
Coquimbite $Fe_2(SO_4)_3.9H_2O$
Römeite $Fe_2Fe(SO_4)_4.14H_2O$
1.3. (Pseudo-) Isometric (Framework) Structures
1.3.1. Soda alum $NaAl(SO_4)_2.12H_2O$
Potash alum $KAl(SO_4)_2.12H_2O$
1.3.2a. Langbeinite $K_2Mg_2(SO_4)_3$
D'Ansite $Na_{21}Mg(SO_4)_{10}Cl_3$
1.2.3b. Vanthoffite $Na_6Mg(SO_4)_4$
Polynalite $K_2Ca_2Mg(SO_4)_4.2H_2O$
1.3.3. Kieserite $MgSO_4.H_2O$
Szomolnokite $FeSO_4.H_2O$
1.3.4. Kainite $KMgSO_4Cl.3H_2O$

2. Na(K)-Ca-Ba Assemblages

2.1. Axial (Chain–like) Structures
2.1.1. Mirabilite $Na_2SO_4.10H_2O$
2.1.2. Syngenite $K_2Ca(SO_4)_2.H_2O$
2.2. Planar (Sheet–like) Structures
2.2.1. Gypsum $CaSO_4.2H_2O$
2.3. (Pseudo-) Isometric (Framework) Structures
2.3.1. Thenardite Na_2SO_4
Arcanite K_2SO_4
Glaserite $K_3Na(SO_4)_2$
Glauberite $CaNa_2(SO_4)_2$
2.3.2. Anhydrite $CaSO_4$
Celestite $SrSO_4$
Barite $BaSO_4$
2.3.3. Kogarkoite $Na_3(SO_4)F$
Galeite $Na_3(SO_4)(F,Cl)$
Sulfohalite $Na_6(SO_4)_2(F,Cl)$
Schairerite $Na_{21}(SO_4)_7F_6Cl$

3. Zn-Cu-Pb(U) Assemblages

3.1. Axial (Chain–like) Structures
3.1.1. Zincosite $ZnSO_4$
Goslarite $ZnSO_4.7H_2O$
3.1.2. Chalcocyanite $CuSO_4$
3.1.3. Cyanotrychite $Cu_4Al_2SO_4(OH)_{12}.2H_2O$
Ransomite $CuFe_2SO_4.6H_2O$
3.1.4. Chlorothionite $K_2CuSO_4Cl_2$
3.1.5. Linarite $PbCuSO_4(OH)_2$
Fleischerite $Pb_3Ge(SO_4)_2(OH)_2$
Elyite $Pb_4CuSO_4(OH)_8$
3.2. Planar(Sheet–like) Structures
3.2.1. Zincbotryogen $ZnFe(SO_4)_2(OH).7H_2O$
Zinccopiapite $ZnFe_4(SO_4)_6(OH)_2.2H_2O$
3.2.2. Antlerite $Cu_3SO_4(OH)_4$

Langite $Cu_3SO_4(OH)_4.H_2O$
Brochantite $Cu_4SO_4(OH)_6$
Posnjakite $Cu_4SO_4(OH)_6.H_2O$
Wroewolfeite $Cu_4SO_4(OH)_8.2H_2O$
3.2.3. Kröhnkite $CuNa_2(SO_4)_2.2H_2O$
3.2.4. Plumbojarosite $PbFe_6(SO_4)_4(OH)_{12}$

3.3. (Pseudo)-Isometric (Framework) Structures

3.3.1. Bonatite $CuSO_4.3H_2O$
Chalcanthite $CuSO_4.5H_2O$
Boothite $CuSO_4.7H_2O$
3.3.2. Dolerophanite $Cu_2(SO_4)O$
Connellite $Cu_{19}SO_4(OH)_{32}Cl_4.3H_2O$
3.3.3. Anglesite $PbSO_4$
3.3.4. Caracolite $Pb_2Na_3(SO_4)_3Cl$

4. Sulphates with Other Cations

4.1. Axial (Chain–like) Structures

4.1.1. Bentorite $Ca_6Cr_2(SO_4)_3(OH)_{12}.26H_2O$

4.2. Planar (Sheet–like) Structures

4.2.1. Klebelsbergite $Sb_4FeSO_4(OH)O$
Peretaite $CaSb_4(SO_4)_2(OH)_2O_4.2H_2O$

4.3. (Pseudo-) Isometric (Framework) Structures

4.3.1. Zircosulphate $Zr(SO_4)_2.4H_2O$
4.3.2. Schuetteite $Hg_3(SO_4)O_2$
Gianellite $(Hg_2N)_2SO_4$

5. Sulphates with Other Anions

Mixed-anion sulphate minerals (F- and Cl-bearing excluded) can also be subdivided into axial, planar and (pseudo-)isometric, when (SO_4) anion prevail over the other anions; otherwise they should be transferred to corresponding other classes.

Conclusion

Paraphrazing a Chinese wisdom it can be said that systematics of minerals 'is like an empty vessel, that never dries'. The manifold classifications of minerals so far known prove this wisdom. For geoscientists a system based on geochemically paragenetic links plus generalized crystal structures seem more recommendable. Thus evolved the system proposed may need certain final touches but its trend is considered logical, unifying salient features of the minerals. Projected on a wider frame of geological setting (magmatic, volcanic, metamorphic, pegmatitic, hydrothermal, sedimentary, etc.) as 'superclasses', the paragenetic-structural classification *sensu stricto* may fruitfully turn into a paragenetic-structural classification *sensu lato*.

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