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REPORT OF THE INTERNATIONAL MINERALOGICAL ASSOCIATION (IMA) – INTERNATIONAL UNION OF CRYSTALLOGRAPHY (IUCr) JOINT COMMITTEE ON NOMENCLATURE*

S. W. BAILEY (Chairman), *Department of Geology and Geophysics, University of Wisconsin, Madison, Wisconsin 53706, USA,* V. A. FRANK-KAMENETSKII, *Department of Geology, Leningrad State University (LGU), University Embankment 7/9, Leningrad, USSR,* S. GOLDSZTAUB, *Laboratoire de Minéralogie, 1 rue Blessig, Université de Strasbourg, Strasbourg, France,* A. KATO, *Department of Geology, National Science Museum, 3-23-1, Hyakunin-cho, Shinjuko, Tokyo 160, Japan,* A. PABST, *Department of Geology, University of California, Berkeley, California 94720, USA,* H. SCHULZ, *Max-Planck-Institut für Festkörperforschung, Postfach 1099, Heilbronner Strasse 69, 7000 Stuttgart 1, Germany (BRD),* H. F. W. TAYLOR, *Department of Chemistry, University of Aberdeen, Aberdeen, Scotland,* M. FLEISCHER, *(ex officio* IMA*), US Geological Survey, 958 National Center, Reston, Virginia 22092, USA* and A. J. C. WILSON, (*ex officio* IUCr), *Department of Physics, University of Birmingham, PO Box 363, Birmingham B15 2TT, England*

Abstract

This report lists nomenclature recommendations from a six-year study of problems common to the disciplines of mineralogy and crystallography. The recommendations include definitions of polytypism, topotaxy, syntaxy, and epitaxy, certain criteria for mineral names, preferred format for chemical formulae, and preferred symbols for crystallographic axes and repeat distances. Two recommended systems of structural symbols to be used to differentiate polytypes are presented.

Sommaire

Ce rapport présente les recommandations découlant d'une étude de six ans portant sur des problèmes de nomenclature communs à la minéralogie et à la cristallographie. Les recommandations couvrent la définition des termes polytypisme, topotaxie, syntaxie et épitaxie, certains critères pour l'appellation des minéraux, la forme préférée des formules chimiques et les symboles préférés pour les axes cristallographiques et pour leurs périodes. Deux systèmes de symboles structuraux servent à différencier les polytypes.

(Traduit par la Rédaction)

Introduction

This Joint Committee was set up to consider problems of nomenclature that are common to the disciplines of mineralogy and crystallography. In particular, the committee was asked to consider problems resulting from the phenomenon of polytypism in layered structures and to recommend a system of notation for polytypic structures. In addition, solicitation of other problems for consideration was made through both organizations and by each committee member in his own country. All business of the committee was conducted by correspondence, and after discussion of issues the votes taken were considered final only if there was a substantial majority on one side. The final report presented here has received official approval of both the International Mineralogical Association and the International Union of Crystallography. Due account has been taken of all comments and criticisms presented by the Nomenclature Committees and Councils of both societies.

The report will be divided into three parts. Part I includes definitions of terms and general recommendations. Part II describes a system of polytype notation based on symmetry and unit-cell repeats that can be used even if the structure is unknown. Part III describes a more complex system of polytype notation that specifies the exact sequence of sheets and layers in the structure. Most of Part III will be published separately as an original contribution by the authors of the system.

Part I. Definitions and General Recommendations

A. "*Polytypism* is the phenomenon of the existence of an element or compound in two or more layer-like crystal structures that differ in layer stacking sequences. The layers need

*This report has also been published in other mineralogical and crystallographic journals.

not be crystallographically identical, but should be similar. Polytypism differs from polymorphism (in the present and strict definition of the latter term) in permitting small differences in chemical composition between structures, not to exceed 0.25 atoms per formula unit of any constituent element. Layer structures that differ from one another by more than this amount are to be called *polytypoids* rather than *polytypes.*"
(Vote = 6-1 in favor)

Comment: The definition above is designed to create enough leniency to make polytypism a useful concept. There is increasing evidence that some polytypes are characterized either by small deviations from stoichiometry of the major elements or by small amounts of impurities. Likewise, the layers may be distorted slightly differently from one polytype to another so that they are non-equivalent in a strict crystallographic sense. The committee has not considered a redefinition of *polymorphism* but it is evident that a similar argument as to small chemical differences could be made for that term as well. The true distinction is that the unit cells of polytypes are simply related (by stacking differences), whereas those of polymorphs (that are not polytypic) are not simply related.

B. "In general, polytypes should not receive individual mineral names. Instead, a set of related polytypes should be designated by a single name followed by a structural symbol suffix that defines the layer stacking differences."
(Vote 7-0 in favor)

C. "Polytype mineral names already in existence that have international acceptance and serve a useful function need not be discarded. Decision on retention of individual names should be the responsibility of the I.M.A. Commission on New Minerals and Mineral Names."
(Vote 7-0 in favor)

D. "In general, mineral names should not be given to compounds that differ only by minor isomorphous substitutions. Instead, a single name should be used along with an adjectival modifier to indicate the chemical variant (such as those given by Schaller 1930)."
(Vote = 7-0 in favor)

E. "Mineral names already in existence for minor chemical variants need not be discarded if the name has international acceptance and serves a useful function. Decision on retention of individual names should be the responsibility of the I.M.A. Commission on New Minerals and Mineral Names."
(Vote = 7-0 in favor)

F. "In general, chemical formulas for compounds should be written as structural formulas rather than as combinations of oxides, unless such usage is clearly confusing or inappropriate in context."
(Vote = 7-0 in favor)

G. "Minerals that exhibit minor deviations in symmetry, crystal form, or optical and physical properties should not be given individual names unless it can be demonstrated that such deviations are due to significant underlying structural reasons."
(Vote = 6-1 in favor)

H. "It is recommended that *X, Y, Z* or [100], [010], [001] be used for directions of crystallographic axes and *a, b, c* for the repeat distances along these axes."
(Vote = 6-0 in favor)

Comment: At the present time, *a, b, c* often are used both for axial directions and for repeat distances. A previous objection that *X, Y, Z* might be confused with optical directions has been nullified by wide acceptance of α, β, and γ for the latter usage.

I. "*Topotaxy* is the phenomenon of mutual orientation of two or more crystals of different species resulting from a solid state transformation or a chemical reaction."
(Vote = 7-0 in favor)

J. "*Syntaxy* is the phenomenon of mutual orientation of two crystals of different species, with three-dimensional lattice control (cell in common), usually, though not necessarily, resulting in an intergrowth."
(Vote = 7-0 in favor)

Comment: Examples of syntactic intergrowths are those between bastnaesite–röntgenite, bastnaesite–synchysite, parisite–röntgenite, parisite–synchysite, röntgenite–synchysite, coquimbite–paracoquimbite, galeite–schairerite, *etc.*

K. "*Epitaxy* is the phenomenon of mutual orientation of two crystals of different species, with two-dimensional lattice control (mesh in common), usually, though not necessarily, resulting in an overgrowth."
(Vote = 7-0 in favor)

Comment: Examples of epitactic overgrowths are $NaNO_3$ on calcite, alkali halides on muscovite, bixbyite on topaz, arsenolite on fluorite, boehmite on albite, Ni on periclase, uraninite on columbite, *etc.*

L. "*Monotaxy* is the phenomenon of mutual orientation of two crystals of different species, with one-dimensional lattice control (line in common)."
(Vote = 5-1 in favor)

Comment: No examples of monotaxy are known to the committee, but this is a desirable term that could be used for such cases if they are recognized in the future.

M. "Adjectival forms of the terms defined under I through L above may end in -tactic or -taxic, but not in -axial. For example, epitactic and epitaxic are acceptable, but epitaxial is not acceptable."
(Vote = 7-0 in favor)

N. No agreement was reached by the committee on a definition for *polycrystal*, nor on the necessity for such a term.

PART II. MODIFIED GARD NOTATION SYSTEM

The Committee has examined systems of structural symbols already in the literature for polytypic structures. These notation systems can be divided into two categories. The first category includes systems that can be used without knowledge of the crystal structures, *i.e.*, the exact stacking sequence of layers. Such systems necessarily make use of observable characteristics, such as symmetry, periodicity of layers, interchange of axes, *etc*. The second category includes notation systems that specify in some manner the exact stacking sequence of layers.

Most notation systems in the literature have been designed specifically for certain types of structures and, in the opinion of the committee, cannot be applied universally to polytypes with quite different structures. Several notation systems that showed promise were examined in more detail and modified as needed. The committee recommends adoption of one such notation system for each of the two categories mentioned above, as described in detail in the remainder of Part II and in Part III of this report, respectively.

J. A. Gard (1966) has described a nomenclature system for fibrous calcium silicates that has been modified by A. Kato and H. Schulz of this committee. The modified Gard system is recommended here (Vote = 6-0 in favor) because it takes into account multiple periods along all three axes as well as the interchange of axes relative to a standard subcell. For polytypes with no interchange of axes and with multiple periods only normal to the layers, a simplified version of the notation is similar to that introduced by Ramsdell (1947) for SiC and in common usage for phyllosilicates. Although this modified notation system has been adapted here to describe polytypes, it is evident from the examples considered below that it also can be useful in other non-polytypic cases involving permutations of axes or superlattices in one or more directions.

In this system the symbol to describe polytypic phases is composed of a mineral name and an italicized suffix, combined by a hyphen. The suffix contains four positions, with a few additive marks when necessary. The first position in the symbol is filled by one or more capital letters to indicate the crystal system of the compound:

cubic	= *C*
hexagonal	= *H*
trigonal	= *T*
rhombohedral	= *R*
tetragonal	= *Q* (quadratic) or *TT*
orthorhombic	= *OR* or *O*
monoclinic	= *M*
triclinic	= *A* (anorthic) or *TC*

Three lower case letters, accompanied by numbers when necessary, following the symmetry symbol indicate the periodicities of the three unit-cell edges (in the order *a, b, c*) of the compound relative to those of the smallest parental subcell of the polytypic system. Thus, molybdenite-2*H* is written as molybdenite-*Haa*2*c* and molybdenite-3*R* as molybdenite-*Raa*3*c*. In cases where the true symmetry is unknown or where the pseudosymmetry is of special interest, the letter *P* (abbreviation of pseudo-) is added before the symmetry symbol. For example, *PH* means pseudohexagonal. Thus, pearceite could be written as pearceite-*PHabc* and arsenopolybasite as pearceite-*PH*2*a*2*b*2*c*. If desired, a space can be used between each of the four positions within the symbol.

Permutations of axes relative to the parental subcell are easily indicated by permuting the appropriate symbols. For example, bayerite = gibbsite-*PORabc*, hydrargillite = gibbsite-*Mbac*, and gibbsite = gibbsite-*PM*2*b*2*ac*, respectively. The definitions of these species are as given in Strunz (1966).

In order to distinguish the polytypes of xonotlite described by Gard, such as *P*121 and *P*∞21, both of which are given as *Ma*2*bc* or *PORa*2*bc* according to the proposed system, an additional symbol *d* (abbreviation of disordered) is written as a subscript to the letter involved. That is, *P*∞21 is written as Ma_d2bc or $PORa_d2bc$.

In order to reconcile the present notation with that of Ramsdell, the following simplification can be made. If the four-position notation expresses a tetragonal or hexagonal compound, the first two cell edges are the same, as in graphite–*Haa*2*c*. In this case, it is permissible to delete the first two cell edges and to place the periodicity of the third cell edge in front of the capital letter(s) symbolizing the crystal system.

Table 1. Examples of application of the modified Gard nomenclature to some representative mineral groups, followed by traditional names in parentheses. Not all examples are strict polytypes.

ELEMENTS
graphite-2*H* (graphite-2*H*)
graphite-3*R* (graphite-3*R*)
lonsdaleite-2*H* (lonsdaleite)
lonsdaleite-3*R* (diamond)
. . . . . .

SULFIDES
wurtzite-2*H* (wurtzite)
wurtzite-3*R* (matraite or wurtzite-3*R*)
wurtzite-4*H* (wurtzite-4*H*)
. . . . . .
sternbergite-*ORab*2*c* (sternbergite)
sternbergite-*ORabc* (argentopyrite)
pyrrhotite-*Hbb*2*c* (troilite)
pyrrhotite-*H*2*a*2*a*6*c* (6*C* type pyrrhotite)
pyrrhotite-*OR*2*a*2*b*11*c* (11*C* type pyrrhotite)
pyrrhotite-*H*2*a*2*a*5*c* (5*C* type pyrrhotite)
pyrrhotite-*M*2*b*2*a*4*c* (4*C* type pyrrhotite)
molybdenite-2*H* (molybdenite-2*H*)
molybdenite-3*R* (molybdenite-3*R*)
berndtite-2*T* (berndtite or *C*6 type berndtite)
berndtite-4*H* (*C*27 type berndtite)
pearceite-*PHaac* (pearceite)
pearceite-*PH*2*a*2*a*2*c* (arsenpolybasite)
polybasite-*PHaac* (antimonpearceite)
polybasite-*PH*2*a*2*a*2*c* (polybasite)
. . . . . .
andorite-*ORab*2*c* (fizelyite)
andorite-*ORab*4*c* (sundtite)
andorite-*ORab*6*c* (ramdohrite)
andorite-*ORab*12*c* (andorite)
andorite-*PORab*24*c* (nakaseite)

HALOGENIDES
atacamite-*R*2*a*2*a*3*c* (paratacamite)
atacamite-$PH\ \frac{b}{2}\ 2ca$ (atacamite)
boleite-3*Q* (cumengeite)
boleite-4*Q* (pseudoboleite)
boleite-8*Q* (boleite)
laurionite-*ORabc* (laurionite)
laurionite-$PH\frac{2a}{\sqrt{3}}\ bc$ (paralaurionite)

OXIDES
taaffeite-4*H* (taaffeite)
taaffeite-9*R*
högbomite-4*H* (högbomite-4*H*)
högbomite-5*H* (högbomite-5*H*)
. . . . . .
tridymite-2*PH*
tridymite-10*PH*
. . . . . .
gibbsite-*PORabc* (bayerite)
gibbsite-*Mba*2*c* (hydrargillite)
gibbsite-*PM*2*b*2*ac* (gibbsite)
gibbsite-*Aba*2*c* (nordstrandite)

CARBONATES
hydrotalcite-2*H* (manasseite)
hydrotalcite-3*R* (hydrotalcite)
stichtite-2*H* (barbertonite)
stichtite-3*R* (stichtite)
pyroaurite-2*H* (sjögrenite)
pyroaurite-3*R* (pyroaurite)

BORATES
veatchite-*Ma*2*bc* (veatchite)
veatchite-*Mbac* (p-veatchite)
hilgardite-*PORabc* (hilgardite)
hilgardite-*PMa*2*bc* (parahilgardite, after Hurlbut's cell)

SULFATES
coquimbite-1*T* (coquimbite)
coquimbite-3*R* (paracoquimbite)

PHOSPHATES, ARSENATES, and VANADATES
variscite-*PORabc* (metavariscite)
variscite-*OR*2*abc* (variscite)
strengite-*PORabc* (phosphosiderite)
strengite-*OR*2*abc* (strengite)
laueite-*Aabc* (laueite)
laueite-*A*2*abc* (stewartite)

SILICATES
chloritoid-*Aabc* (chloritoid-1*A*)
chloritoid-*Mab*2*c* (chloritoid-2*M*)
zoisite-*Mabc* (clinozoisite)
zoisite-*OR*2*abc* (zoisite)
tschevkinite-*Mabc* (perrierite)
tschevkinite-*Mab*2*c* (tschevkinite)
cordierite-1*H* (indialite)
cordierite-1*PH* (cordierite)
enstatite-*Mabc* (clinoenstatite)
enstatite-*OR*2*abc* (enstatite)
anthophyllite-*Mabc* (cummingtonite)
anthophyllite-*OR*2*abc* (anthophyllite)
wollastonite-*Aabc* (wollastonite)
wollastonite-*M*2*abc* (parawollastonite)
pectolite-*Aabc* (pectolite)
pectolite-*A*2*abc*
foshagite-*PMa*2*b*2*c*
foshagite-*PM*2*a*2*b*2*c*
. . . . .
xonotlite-*POR*2*a*2*bc*
xonotlite-*PORa*2*b*2*c*
. . . . .
prehnite-*ORabc* (prehnite)
prehnite-*Mabc*
. . . . .
muscovite-1*M* (muscovite-1*M*)
muscovite-2*M* (muscovite-2M_1)
muscovite-*Mba*2*c* (muscovite-2M_2)
muscovite-3*T* (muscovite-3*T*)
muscovite-6*H* (muscovite-6*H*)
kaolinite-*Aabc* (kaolinite)
kaolinite-*Mab*2*c* (dickite)
kaolinite-*Mba*2*c* (nacrite)
talc-1*A* (talc-1*A*)
pyrophyllite-1*A* (pyrophyllite-1*A*)
. . . . . There are many other phyllosilicates with polytype derivatives for which the present system is applicable.
gyrolite-1*T*
gyrolite-6*H*
manganpyrosmalite-1*T* (manganpyrosmalite)
manganpyrosmalite-3*R* (friedelite)
kalsilite-1*H* (kalsilite)
kalsilite-*H*3*a*3*ac* (tri-kalsilite)
kalsilite-*H*3*b*3*bc* (kaliophilite)
cancrinite-1*H* (cancrinite)
cancrinite-*Hbbc* (microsommite)
cancrinite-4*H* (afghanite)
erionite-1*H* (offretite)
erionite-2*H* (erionite)
erionite-3*R* (levyne)
chabazite-2*H* (gmelinite)
chabazite-3*R* or -3*PH* (chabazite)

Then graphite–*Haa2c* becomes graphite–2*H*. This rule also is applicable to the case of pseudo-hexagonal symmetry. In this case, the deleted letters are not always *aa* but may be *ab, ba, etc.* where $b=a\sqrt{3}$. Thus, indialite may be given as cordierite–1*H* and cordierite (*s.str.*) as cordierite–1*OR* or cordierite–1*PH*.

In the case of the mica polytypes, $2M_1$ and $2M_2$ require different treatment. Thus, muscovite–$2M_1$ = muscovite–*Mab*2*c* or –*PHab*2*c* can be shortened to muscovite–2*M* or –2*PH*. But muscovite–$2M_2$ = muscovite–*Mba*2*c* or *PH ba*2*c* should retain the long symbol if it is desired to express the reversal of axes. But this system is not intended to replace symbols, such as $2M_1$ and $2M_2$, that are useful and have international acceptance.

Examples of the proposed nomenclature system are given in Table 1 for a representative number of mineral groups. The mineral names tabulated here were chosen in the order of familiarity and are intended to be illustrative, rather than definitive, and to cover related phases by the least number of names. It should be recalled also (Part I) that the committee does not necessarily recommend that all traditional names be dropped.

Part III. Dornberger-Schiff, Ďurovič, and Zvyagin Symbols

In certain polytypic systems it is quite possible to have a large number of different polytypes that would have identical modified Gard symbols. For such cases it is desirable to have available a more detailed symbolism that would allow specification of the exact stacking sequences of layers involved, where known. Such detailed systems are necessarily complex, and the ideal goal is a system that gives the necessary information in an understandable format. Too complex a system will tend not to be used, except perhaps by a few experts in the field.

The Joint Committee is aware of only two nomenclature systems that are both generalized and detailed enough to allow universal application. One is the system of Zvyagin (1967) which has been modified for the benefit of the committee in order to be of more general application. The other is unpublished and was submitted to the committee by K. Dornberger-Schiff and S. Ďurovič. The Zvyagin system makes use of structural units, such as the component sheets and layers in the structure. An origin is specified within each structural unit, and the displacement or rotation of these origins and units relative to one another and to the resultant crystallographic axes is given by a sequence of symbols with attached subscripts and superscripts. The Dornberger-Schiff and Ďurovič system incorporates several features of the Zvyagin system relating to the displacement and orientation vectors. The major difference is that the Dornberger-Schiff and Ďurovič system uses asymmetric units, which may not be the most obvious structural units in the Zvyagin scheme, and emphasizes the symmetry relationships between these. The system is based on O–D theory (O–D = order–disorder), but a detailed knowledge of the theory is not necessary for application. It is shown that the symbols of Hägg and Zhdanov are special cases of the proposed general system.

In recognition of the features that are common to the Zvyagin system and to the Dornberger-Schiff and Ďurovič system, the respective authors have agreed to combine their separate proposals into a single unified system so far as possible. Preparation of the generalized system is still in progress at the time of this report, but it is anticipated that the authors will publish their results jointly at a later date and will indicate their areas of agreement as well as any unresolved problems. The Joint Committee recommends usage of this generalized notation system for those cases in which specification of the exact stacking sequence of layers is important.

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