

THE USE OF CHEMICAL-ELEMENT ADJECTIVAL MODIFIERS IN MINERAL NOMENCLATURE

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ABSTRACT

Chemical-element adjectival modifiers are not part of the name of a mineral species. Schaller-type adjectival modifiers, which have the endings -oan or -ian, formerly recommended by the CNMMN of the IMA, in many cases give erroneous information about the valence of an ion, and are therefore inappropriate. Instead of such modifiers, the CNMMN has now approved a proposal that chemical-element adjectival modifiers employing the chemical-element symbol or the name of the chemical element together with a descriptive term should be used. The valence (nominal numerical charge plus sign) or the numerical oxidation state may be added, if required. Authors should therefore feel free to use chemical-element adjectival modifiers that are chemically correct and that meet their particular requirements. For example, chemical-element adjectival modifiers such as “Mg-rich”, “Mg-Fe-rich”, “Fe²⁺-poor”, “iron(2+)-enriched”, “iron(II)-bearing”, “alkali-deficient”, “sodium-exchanged”, “Cr-doped”, or “H₂O-saturated” may be used. Synthetic or hypothetical analogues of mineral species or natural analogues of mineral species unapproved by the CNMMN could be written with a chemical-element(s) suffix. The synthetic product “topaz-OH” is the OH-dominant analogue of topaz, Al₂SiO₄F₂. The use of quotation marks around “topaz-OH” is essential to show that the name is not approved by the CNMMN and to avoid confusion with names of real mineral species, such as chabazite-Ba. A chemical-element symbol should not be used as a prefix to a name of a mineral species. However, if used in a diagram, table, or running heading owing to space limitations, then a correct version must be used in the text together with the short version in quotation marks to show that the name is not approved by the CNMMN. For example, “Al-goethite” used in a table owing to space limitations should be shown as Al-rich goethite in the text.

Keywords: Schaller modifier, adjectival modifier, chemical suffix, chemical prefix, mineral nomenclature, Commission on New Minerals and Mineral Names.

SOMMAIRE

Les qualificatifs indicateurs d'un élément chimique ne font pas partie du nom d'un minéral. Ceux qui ont été proposés par Schaller, se terminant en anglais par -oan ou -ian, et recommandés déjà par la Commission des Nouveaux Minéraux et des Noms de Minéraux, donnent une indication erronée à propos de la valence d'un élément, et sont donc inappropriés. A leur place, la Commission vient d'approuver l'utilisation de qualificatifs utilisant le symbole d'un élément ou le nom de l'élément avec un terme descriptif. La valence (valeur numérique nominale avec un signe) ou l'état d'oxydation numérique pourrait être ajouté si nécessaire. Les auteurs ont entière liberté de se servir de qualificatifs indiquant la composition qui sont chimiquement corrects et qui satisfont leurs propres exigences. A titre d'exemples de qualificatifs approuvés, on peut se servir de “magnésien”, “riche en Mg-Fe”, “pauvre en Fe²⁺”, “enrichi en fer(2+)”, “porteur de fer(II)”, “déficientaire en alcalins”, “échangé en sodium”, “dopé au Cr”, ou “saturé en H₂O”. Pour les produits synthétiques, les analogues hypothétiques d'espèces minérales ou les analogues naturels d'espèces minérales pas encore approuvées par la Commission, on peut les écrire avec le symbole d'un élément comme suffixe. Par exemple, le produit de synthèse “topaze-OH” est l'analogue à dominance de OH de la topaze, Al₂SiO₄F₂. L'utilisation de guillemets est essentielle pour souligner l'absence de l'approbation de la Commission et pour éviter toute confusion avec les

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noms d'espèces véritables comme la chabazite-Ba, où le suffixe est légitime et officiel. Le symbole d'un élément ne doit pas être utilisé comme préfixe d'un nom de minéral. Toutefois, dans le cas d'une utilisation rendue nécessaire pour conserver l'espace, dans un tableau ou un diagramme, ou dans un titre courant, par exemple, il est nécessaire d'utiliser la version correcte dans le texte et la version courte entre guillemets, afin de démontrer que ce dernier n'est pas approuvé. Par exemple, l'utilisation de "Al-goethite" dans un tableau devrait être présentée comme goethite alumineuse dans le texte.

(Traduit par la Rédaction)

Mots-clés: qualificatif de Schaller, adjectif qualificatif, suffixe chimique, préfixe chimique, nomenclature des minéraux, Commission des Nouveaux Minéraux et des Noms de Minéraux.

INTRODUCTION

During the last century, the science of chemistry has significantly progressed. The number of different valences of many chemical elements has significantly increased. Therefore, the chemical-element adjectival modifier system of the 1930s is no longer adequate to represent the present state of knowledge. A chemically correct system is introduced to overcome these problems.

HISTORICAL BACKGROUND

Chemical composition is one of the main determinants of a mineral species, and in defining a mineral species, the predominant chemical element in each structural site must be specified. Partial replacement of the predominant chemical element by a minor chemical element does not affect the species status of the mineral and, where appropriate, is indicated by some chemical-element adjectival modifier.

Dana (1892) used eight variants of chemical-element adjectival modifiers to indicate chemical varieties of mineral species, with suffixes such as -iferous, -ian, -al, -eous, and -ic. In an attempt to standardize the chemical-element adjectival modifiers, Schaller (1930) proposed a simple system of chemical-element adjectival modifiers, which will be referred to here as "Schaller modifiers". The valency of the substituting ion in a Schaller modifier is indicated by the suffix "-oan" (for the lower valency) or "-ian" (for the higher valency). These served a similar purpose as the chemical-element adjectival modifiers of Dana (1892), but had the advantage of being briefer.

Initially, the Commission on New Minerals and Mineral Names (CNMMN) of the International Mineralogical Association (IMA) expressed disinterest in promoting the proper use of chemical-element adjectival modifiers (Hey & Gottardi 1980). However, the use of Schaller modifiers was later advocated, and a list of Schaller modifiers was extended (Nickel & Mandarino 1987), and subsequently restated (Nickel & Grice 1998). The chief purpose in advocating the Schaller modifiers was not to exclude the use of other chemical-element adjectival modifiers, but rather to prevent the

substituting minor chemical element becoming incorporated in the name of a mineral species.

In the mineralogical literature, in addition to Schaller modifiers, various chemical-element adjectival modifiers have been used, for example "Mg-rich", "Mg-Fe-rich", "Fe²⁺-poor", "iron(2+)-enriched", "iron(II)-bearing", "alkali-deficient", "sodium-exchanged", "Cr-doped", and "H₂O-saturated". In the published CNMMN subcommittee reports, chemical-element adjectival modifiers are used, such as titanium-rich and yttrium-rich by Hogarth (1977), sodium-rich, sodium-bearing, *manganreich*, and *manganhaltiger* by Hey & Gottardi (1980), iron-rich and magnesium-rich by Morimoto (1989), Mg-rich by Coombs *et al.* (1997), and Al-rich by Rieder *et al.* (1998).

The symbol for the chemical element together with a superscript consisting of an Arabic numeral followed by the charge sign indicates the valency, *i.e.*, Fe²⁺, or Fe³⁺. The word for the chemical element should be followed by the Arabic numeral and charge, all in parentheses, and on the line, *e.g.*, iron(2+), iron(3+), iron(II), or iron(III). Both the valency (nominal Arabic numerical charge plus sign) and the Roman numerical oxidation state together are not allowed, *e.g.*, Mg²⁺-iron(II)-rich.

SHORTCOMINGS OF THE SCHALLER MODIFIERS

There are two main shortcomings of the Schaller modifiers: firstly, some chemical elements have only one stable valence state, and some have more than two valences; secondly, the concept of ionic valences is meaningless in compounds with a substantial component of covalent or metallic bonding.

The Schaller modifiers implicitly specify valence states by the use of the suffixes "-oan" (for the lower valency) or "-ian" (for the higher valency). These suffixes are inappropriate for chemical elements with only one stable valence state, such as the alkalis and alkaline earths. On the other hand, chemical elements with more than two different valences, such as manganese, create an insoluble problem. Thrush (1968) listed six valences for manganese (hexavalent), and recently a seventh valency, Mn⁵⁺, has been reported (Reiche *et al.* 2001). The problem becomes progressively worse as additional valences are found for the other chemical

elements. In an attempt to deal with some of these uncertainties, Nickel & Grice (1998) made the scientifically dubious statement that "If the valency of an element in a particular mineral is not known, the adjectival modifier derived from the more likely, or more common, valence state of the element should be used."

The valence of chemical elements in ionic structures is self-evident, but only about two percent of mineral species are purely ionic. The bonding in most mineral species has an appreciable covalent component. For example, the nominal numerical charge of silicon is 4+, but the actual charge usually varies between 3+ and 1½+. The actual charge of silicon is about 2.3+ for quartz and about 2.5+ for olivine (Tossell 1977). Lake & Craven (2001) recorded the actual charge of Mg, PO₄ and (OH) in kovdorskite as 1.2+, 2.0- and 0.5-, respectively. Mineral species where silicon is not 4+ include gupceite, Fe₃Si, and native silicon.

Schaller modifiers also are inappropriate for native chemical elements, as the actual charge of native chemical elements such as antimony is zero. The suffixes "-oan" or "-ian" for an As-rich or Bi-rich variety of antimony would indicate 3+ or 5+, respectively, which is chemically misleading. Malitch & Thalhammer (2002) used the term "ferroan platinum", yet the actual charge of the iron is zero. Therefore, the use of "ferroan" is incorrect. About 15% of mineral species, mainly sulfides and sulfoxysalts, have metallic bonding, which makes the concept of ionic charge meaningless for such mineral species. For example, the nominal numerical charge of iron in pyrite is 2+, but the actual charge is 0.08+. Therefore, the use of the Schaller modifiers "nickeloan" or "cobaltian" for a Ni-Co-rich variety of pyrite would imply 2+ or 3+, respectively, which is chemically misleading. Similarly, the use of the term "cobaltian arsenopyrite" by Wagner & Lorenz (2002) is misleading, because the actual charge of cobalt in arsenopyrite is near zero. As Schaller modifiers imply nominal ionic valences of the substituting chemical elements, their use in describing mineral species with covalent or metallic bonding is incorrect.

Nickel & Mandarino (1987) stated that CNMMN generally recommends that the Latin version of the chemical element is preferred to the English version (*e.g.*, kalian to potassian, natrian to sodian, stiboan to antimonoan, and wolframian to tungstenian). If the use of Schaller modifiers is abandoned, this choice disappears.

RECOMMENDATIONS ON THE USE OF CHEMICAL-ELEMENT ADJECTIVAL MODIFIERS

We submitted a proposal on Schaller modifiers to the CNMMN (Voting Proposal 03-A), and it was subsequently approved, with 13 agree, 2 disagree, and 1 abstain. It stated: "It is proposed that the general CNMMN advocacy of Schaller modifiers be dropped. When it is desired to indicate the presence of subordi-

nate chemical components in a mineral, Schaller modifiers may be used in unambiguous cases, namely those in which the element has two, and only two, valence states. In the more general case, adjectival modifiers such as "-bearing" or "-rich" should be used together with the specified element(s), and with the numerical oxidation state, if required, *e.g.*, "Mn²⁺-rich", "V(III)-deficient", "Mg-bearing", *etc.*"

Members of the CNMMN requested that a list of unambiguous cases be furnished. The list of Schaller modifiers in Nickel & Mandarino (1987) contains 21 chemical elements with two valence states; however, the Handbook of Chemistry and Physics (Lide 1999) and Pearson's Handbook of Crystallographic Data for Intermetallic Phases (Villars & Calvert 1991) show that all of these chemical elements have three to five valence states. Therefore, there appears to be no chemical element that meets this criterion.

If it is necessary to indicate the valence or oxidation state of a chemical element in a mineral species with a strong ionic bonding component, it can be done in several ways. Taking iron as an example, divalent iron can be shown a Fe²⁺, iron(2+), or as iron(II). This symbolism can be incorporated into the chemical-element adjectival modifier as "Fe²⁺-bearing forsterite", for example.

Chemical-element adjectival modifiers are not regarded as part of the name of a mineral species, and their use is not regulated by the CNMMN. Authors should therefore feel free to use chemical-element adjectival modifiers that are chemically correct and that meet their particular requirements. For example, "Mg-rich", "Mg-Fe-rich", "Mn-enriched", "Fe²⁺-poor", "iron(2+)-enriched", "iron(II)-bearing", "alkali-deficient", "sodium-exchanged", "Cr-doped", or "H₂O-saturated" may be used.

The Commission on the Nomenclature of Inorganic Chemistry of the International Union of Pure and Applied Chemistry (CNIC of IUPAC) very strongly disapproves of the "-oan" and "-ian" chemical-element adjectival modifiers (Leigh 1990). CNIC of IUPAC strongly recommends that chemists use the CNMMN-approved mineralogical nomenclature, and therefore mineralogists should also use the chemical nomenclature approved by the CNIC of IUPAC, so that chemists and mineralogists can communicate effectively with each other.

CHEMICAL-ELEMENT SUFFIXES FOR CHEMICAL ANALOGUES

A chemical-element suffix is part of a mineral species name. The system of using chemical-element suffixes for rare-earth mineral species was introduced by Levinson (1966), with mineral species names such as aeschynite-(Ce), aeschynite-(Nd) and aeschynite-(Y). The system was revised and extended by Bayliss & Levinson (1988). Versions of this system have been

applied to other mineral groups, such as the pumpellyite-group minerals (Passaglia & Gottardi 1973), zeolites (Coombs *et al.* 1997), and labuntsovite-group minerals (Raade *et al.* 2004), all of which have the approval of the CNMMN. It has also been applied to synthetic phases, such as “topaz-OH” (Schmidt *et al.* 1998) for the synthetic OH analogue of topaz, $\text{Al}_2\text{SiO}_4\text{F}_2$. Synthetic analogues of existing mineral species are not regarded as real mineral species, and therefore do not come within the jurisdiction of the CNMMN (Nickel 1995). The authors suggest that such analogues can be given names with chemical suffixes, like that of “topaz-OH”, with care being taken to put this name in quotation marks to show that it is not a CNMMN-approved name and to avoid confusion with names of real mineral species such as chabazite-Ba.

CHEMICAL-ELEMENT SYMBOL PREFIXES

Over 1,300 names with chemical-element symbol prefixes have been published, and this unfortunate tendency appears to be increasing. The percentage distribution of these chemical-element symbol prefixes, as taken from Bayliss (2000), is as follows:

39% chemical-element symbol prefix of mineral species, *e.g.* Al-goethite for Al-rich goethite,

21% chemical-element symbol prefix of mineral group, *e.g.* K-feldspar for the orthoclase, microcline and sanidine group,

9% exchangeable cation, *e.g.*, Na-montmorillonite for Na-rich montmorillonite,

7% non-mineral name, *e.g.*, Al-kohl for stibnite,

11% mineral species analogues, *e.g.*, Al-pumpellyite for the Al analogue of pumpellyite-(Mg), and

13% synthetic compounds or analogues of hypothetical species, *e.g.*, Al-ludwigite for the hypothetical $\text{Mg}_2\text{AlBO}_3\text{O}_2$.

This breakdown demonstrates the ambiguity of such names, and is a strong argument for abandoning the practice. Nickel & Grice (1998) stated that “In some papers, an adjectival modifier is given in the form of a hyphenated chemical prefix, *e.g.*, Li-tosudite, rather than lithian tosudite or lithium-bearing tosudite. Such usage is *incorrect and should be avoided*.” The use of chemical-element adjectival modifiers such as -rich, -enriched, -poor, -bearing, -deficient, -exchanged, -doped, or -saturated is more informative than a simple chemical-element symbol prefix.

The present situation is unsatisfactory, because the use of chemical-element symbol prefixes is ignored by some members of the mineralogical community,

although CNMMN considers such usage as incorrect and to be avoided. Why do mineralogists use chemical-element symbol prefixes? Lithium-bearing is 15 characters long, lithian and Li-rich are seven characters long, whereas Li- is short, at only three characters long. Such chemical-element symbol prefixes generally occur in a diagram, table, or running heading (*e.g.*, Cr-mullite by Fischer & Schneider 2000), where there is a space limitation. In such cases, a correct version must be used in the text together with the short version in quotation marks, to show that the name is not approved by the CNMMN. “K-feldspar” is tolerated because it applies to a group of minerals, rather than to a species; it has historically been used and is still in common usage.

CONCLUSION

To quote James Dwight Dana (1850), “To change is always seeming fickleness. But not to change with advancement of science is worse; it is persistence in error.”

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REFERENCES

- BAYLISS, P. (2000): *Glossary of Obsolete Mineral Names*. Mineralogical Record, Tucson, Arizona 85749, USA.
- _____ & LEVINSON, A.A. (1988): A system of nomenclature for rare-earth mineral species: revision and extension. *Am. Mineral.* **73**, 422-423.
- COOMBS, D.S., ALBERTI, A., ARMBRUSTER, T., ARTIOLI, G., COLELLA, C., GALLI, E., GRICE, J.D., LIEBAU, F., MANDARINO, J.A., MINATO, H., NICKEL, E.H., PASSAGLIA, E., PEACOR, D.R., QUARTIERI, S., RINALDI, R., ROSS, M., SHEPPARD, R.A., TILLMANN, E. & VEZZALINI, G. (1997): Recommended nomenclature for zeolite minerals: report of the Subcommittee on Zeolites of the International Mineralogical Association, Commission on New Minerals and Mineral Names. *Can. Mineral.* **35**, 1571-1606.
- DANA, E.S. (1892): *System of Mineralogy* (6th ed.). J. Wiley & Sons, New York, N.Y.
- DANA, J.D. (1850): *System of Mineralogy* (3rd ed.). J. Wiley & Sons, New York, N.Y.
- FISCHER, R.X. & SCHNEIDER, H. (2000): Crystal structure of Cr-mullite. *Am. Mineral.* **85**, 1175-1179.
- HEY, M.H. & GOTTARDI, G. (1980): On the use of names, prefixes and suffixes, and adjectival modifiers in the mineralogical nomenclature. *Can. Mineral.* **18**, 261-262.

- HOGARTH, D.D. (1977): Classification and nomenclature of the pyrochlore group. *Am. Mineral.* **62**, 403-410.
- LAKE, C.H. & CRAVEN, B.M. (2001): The crystal structure and charge density analysis of kovdorskite ($Mg_2(PO_4)(OH) \cdot 3H_2O$). *Mineral. Rec.* **32**, 43 (abstr.).
- LEIGH, G.J., ed. (1990): *Nomenclature of Inorganic Chemistry, Recommendations 1990* [issued by the Commission on the Nomenclature of Inorganic Chemistry]. Blackwell Scientific Publications, Oxford, U.K.
- LEVINSON, A.A. (1966): A system of nomenclature for rare-earth minerals. *Am. Mineral.* **51**, 152-158.
- LIDE, D.R., ed. (1999): *Handbook of Chemistry and Physics* (79th ed.). Chemical Rubber Co., Boca Raton, Florida.
- MALITCH, K.N. & THALHAMMER, O.A.R. (2002): Pt-Fe nuggets derived from clinopyroxenite-dunite massifs, Russia: a structural, compositional and osmium-isotope study. *Can. Mineral.* **40**, 395-418.
- MORIMOTO, N. (1989): Nomenclature of pyroxenes. *Can. Mineral.* **27**, 143-156.
- NICKEL, E.H. (1995): Mineral names applied to synthetic substances. *Can. Mineral.* **33**, 1335.
- _____ & GRICE, J.D. (1998): The IMA Commission on New Minerals and Mineral Names: procedures and guidelines on mineral nomenclature, 1998. *Can. Mineral.* **36**, 913-926.
- _____ & MANDARINO, J.A. (1987): Procedures involving the IMA Commission on New Minerals and Mineral Names, and guidelines on mineral nomenclature. *Can. Mineral.* **25**, 353-377.
- PASSAGLIA, E. & GOTTARDI, G. (1973): Crystal chemistry and nomenclature of pumpellyites and julgoldites. *Can. Mineral.* **12**, 219-223.
- RAADE, G., CHUKANOV, N.V., KOLITSCH, U., MÖCKEL, S., ZADOV, A.E. & PEKOV, I.V. (2004): Gjerdingenite-Mn from Norway – a new mineral species in the labuntsovite group; descriptive data and crystal structure. *Eur. J. Mineral.* **16**, 979-987.
- REICHE, I., VIGNAUD, C., CHAMPAGNON, B., PANCZER, G., BROUDER, C., MORIN, G., SOLÉ, V.A., CHARLET, L. & MENU, M. (2001): From mastodon ivory to gemstone: the origin of turquoise color in odontolite. *Am. Mineral.* **86**, 1519-1524.
- RIEDER, M., CAVAZZINI, G., D'YAKONOV, YU.S., FRANK-KAMENETSKII, V.A., GOTTARDI, G., GUGGENHEIM, S., KOVAL, P.V., MÜLLER, G., NEIVA, A.M.R., RADOSLOVICH, E.W., ROBERT, J.-L., SASSI, F.P., TAKEDA, H., WEISS, Z. & WONES, D.R. (1998): Nomenclature of the micas. *Can. Mineral.* **36**, 905-912.
- SCHALLER, W.T. (1930): Adjectival ending of chemical elements used as modifiers to mineral names. *Am. Mineral.* **15**, 566-574.
- SCHMIDT, M.W., FINGER, L.W., ANGEL, R.J. & DINNEBIER, R.E. (1998): Synthesis, crystal structure, and phase relations of $AlSiO_3OH$, a high-pressure hydrous phase. *Am. Mineral.* **83**, 881-888.
- THRUSH, P.W., ed. (1968): *A Dictionary of Mining, Mineral and Related Terms*. U.S. Department of the Interior, Washington D.C.
- TOSSELL, J.A. (1977): A comparison of silicon-oxygen bonding in quartz and magnesian olivine from X-ray spectra and molecular orbital calculations. *Am. Mineral.* **62**, 136-141.
- VILLARS, P. & CALVERT, L.D. (1991): *Pearson's Handbook of Crystallographic Data for Intermetallic Phases*. American Society for Metals, Metals Park, Ohio.
- WAGNER, T. & LORENZ, J. (2002): Mineralogy of complex Co-Ni-Bi vein mineralization, Bieber deposit, Spessart, Germany. *Mineral. Mag.* **66**, 385-407.

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