Nomenclature of pyroxenes

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Abstract

This is the final report on the nomenclature of pyroxenes by the Subcommittee on Pyroxenes established by the Commission on New Minerals and Mineral Names of the International Mineralogical Association. The recommendations of the Subcommittee as put forward in this report have been formally accepted by the Commission. Accepted and widely used names have been chemically defined, by combining new and conventional methods, to agree as far as possible with the consensus of present use. Twenty names are formally accepted, among which thirteen are used to represent the end-members of definite chemical compositions. In common binary solid-solution series, species names are given to the two end-members by the '50% rule'. Adjectival modifiers for pyroxene mineral names are defined to indicate unusual amounts of chemical constituents. This report includes a list of 105 previously used pyroxene names that have been formally discarded by the Commission.

KEYWORDS: nomenclature, pyroxenes, IMA.

Introduction

THE subcommittee on pyroxenes has, after a thorough evaluation of the group of pyroxene minerals, presented its recommendations for a new classification and nomenclature to the Commission on New Minerals and Mineral Names (hereafter abbreviated as CNMMN). These recommendations have been approved by the Commission by a formal vote (20th May, 1987).

The classification and nomenclature of the pyroxenes have been largely based on their crystal chemistry. In practice the chemical content of the pyroxene formula unit calculated to six oxygens, or to four cations (Vieten and Hamm, 1978), is essential for the classification. This formula unit corresponds to one quarter of the unit cell for the monoclinic pyroxenes and to one eighth of the unit cell for the orthorhombic pyroxenes. The basic principle adopted for amphibole nomenclature (Leake and Winchell, 1978) is to denote principal stoichiometries by generally well-established names, with adjectival modifiers to indicate the presence of substantial substitutions that are not essential constituents of the end-members; this has

been followed as far as possible in the pyroxene nomenclature.

No new names have been introduced in the proposed nomenclature. Accepted and widely used names have been chemically defined by combining new and conventional methods to agree as far as possible with the consensus of present use. Two kinds of adjectival modifiers are used: one to specify a part of the compositional range shown by a mineral that forms a wide solid solution (e.g. magnesium-rich augite and iron-rich augite); the other to specify elemental substitutions that are not essential constituents (e.g. titanian augite). 105 previously used pyroxene names, mostly synonyms, obsolete or almost unused, recommended for rejection, have formally been discredited by the CNMMN.

General publications dealing with the pyroxene group include Rock-Forming Minerals (Deer et al., 1978) (hereafter DHZ), the Special Papers (ed. Papike, 1969) and Reviews in Mineralogy (ed. Prewitt, 1980) of the Mineralogical Society of America, which provide references to the voluminous literature.

Crystal chemistry of the pyroxenes

Pyroxenes are silicates that, in their simplest form, contain single SiO_3 chains of linked SiO_4 tetrahedra. Generally, small amounts of Si are replaced by Al and other small cations. The repeat along the chain (c axis) comprises two tetrahedra and is approximately 0.52 nm in length. The general chemical formula (formula unit) for all pyroxenes is $M2M1T_2O_6$, where M2 refers to cations in a generally distorted octahedral coordination, M1 to cations in a regular octahedral coordination, and T to tetrahedrally coordinated cations.*

Any pyroxene belongs to either the orthorhombic or the monoclinic crystal system. There are two orthorhombic pyroxene types: orthopyroxene (Pbca) and orthopyroxene (Pbca). Only the former has been found in nature. Monoclinic pyroxenes are called clinopyroxenes. Their space groups are C2/c, $P2_1/c$ and P2/n, depending on their chemical composition and genetic history.

Throughout this report, the standard pyroxene formula is used with superscripted Arabic numerals (e.g. Fe²⁺) referring to charges, and subscripted numerals (e.g. Mg₂) to numbers of atoms.

In order to derive a pyroxene formula from a chemical analysis, the calculation should be based on six oxygen atoms, when Fe^{2+} and Fe^{3+} are both determined. In microprobe analyses, only total Fe is determined and the option of calculating to four cations should at least be permitted if not actually preferred. Vieten and Hamm (1978) show that calculation to four cations will be more reliable for microprobe analyses of the majority of pyroxenes. Therefore, for microprobe analyses it is recommended that the components be totalled to six oxygens and four cations by adjusting the ratios Fe^{2+}/Fe^{3+} , Ti^{4+}/Ti^{3+} , etc.

The standard pyroxene formula $M2M1T_2O_6$ contains two tetrahedral sites. In the allocation of the cations to obtain a pyroxene formula, the following procedure is recommended:

- (1) Sum T to 2.000 using Si^{4+} , then Al^{3+} , then Fe^{3+} .
- (2) Sum M1 to 1.000 using all $A1^{3+}$ and Fe^{3+} in excess of that used to fill the T sites. If there is insufficient $A1^{3+}$ and Fe^{3+} to sum to 1.000, then add Ti^{4+} , Cr^{3+} , V^{3+} , Ti^{3+} , Zr^{4+} , Sc^{3+} , Zn^{2+} , Mg^{2+} , Fe^{2+} and finally Mn^{2+} until the sum is 1.000.
- (3) Sum M2 using all Mg²⁺, Fe²⁺ and Mn²⁺ in excess of that used to fill the M1 sites. Then add Li⁺, Ca²⁺ and Na⁺ so that the sum becomes 1.000 or close to it. If the sum is far from 1.000, one must be suspicious about the results of the analysis.
- * Footnotes, indicated by superscript numbers, are to be found at the end of the paper.

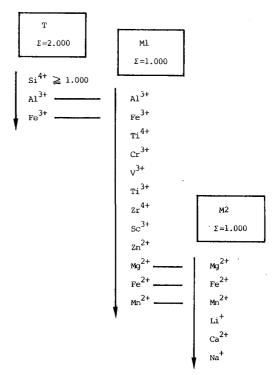


FIG. 1. Flow chart for ideal site occupancy of cations between the T, M1 and M2 sites of pyroxenes. Only representative cations are included. Arrows indicate order of filling of sites. Real site occupancy is usually slightly different from the ideal site occupancy.

A flow chart (Fig. 1) gives a diagrammatic representation of the site allocation of the principal cations in pyroxenes. However, because the distribution of cations among the M1, M2 and T sites in a given pyroxene is partly a function of temperature, the accurate site occupancy must be determined by structure determination. The site occupancy given in Fig. 1 is called ideal site occupancy to distinguish it from real occupancy. A method for classifying pyroxenes by their ideal site occupancies has been proposed by Bokij and Ginzburg (1985). In the present classification of pyroxenes, the M1 and M2 sites are considered together as a single M site in order to avoid the difference between the real and ideal site occupancies.

Starting from the most common pyroxene formula, $M2(R^{2+})M1(R^{2+})T_2(2R^{4+})O_6$, four coupled substitutions are possible if one assumes more than one R^{4+} in the T site. They are listed in Table 1, where the elements in parentheses are coupled substitutions.

Substitution site	M2	м1	Т	examples
standard	R ²⁺	R ²⁺	2R ⁴⁺	
substitution(1)	(R ⁺)	(R ³⁺)	2R4+	Na-Al Na-Fe3+ Na-Cr3+ Na-Sc3+
substitution(2)	(R ⁺)	$R_{0.5}^{2+}(R_{0.5}^{4+})$	2R4+	Na-(Ti ⁴⁺ /2)
substitution(3)	R ²⁺	(R ³⁺)	(R ³⁺)R ⁴⁺	A1-A1 Fe3+-A1 Cr3+-A1
Substitution(4)	R ²⁺	$R_{0.5}^{2+}(R_{0.5}^{4+})$	(R ³⁺)R ⁴⁺	(Ti ⁴⁺ /2)-Al

Table 1. Four coupled substitutions of pyroxenes in the standard chemical fourmula $R^{2} {}^+R^{2} {}^+R^4_3 {}^+O_6$.

Substitution (1) encompasses the end-members jadeite (NaAlSi₂O₆), aegirine³ (NaFe³⁺Si₂O₆), kosmochlor⁴ (NaCr³⁺Si₂O₆), and jervisite (NaSc Si₂O₆). Substitution (2) results in components such as NaFe²⁺ $_{0.5}$ Ti⁴⁺ $_{0.5}$ Si₂O₆, but is less important than the other substitutions.

In substitution (3) the Al-Al couple is often referred to as 'Tschermak's component'; CaAlAl SiO₆, in particular, is called 'calcium Tschermak's component'. Substitution in esseneite⁵, CaFe³⁺Al SiO₆, is obtained by this type of substitution. This substitution is also important in 'fassaite'⁶. Substitution resulting in CaTi³⁺AlSiO₆ was reported by Dowty and Clark (1973) and Mason (1974) in pyroxenes from the Allende meteorite (Table 3, No. 4). In substitution (4) the component CaMg_{0.5}Ti_{0.5} AlSiO₆ is found in some pyroxenes. There are a few instances of the component of substitution (2) or (4) amounting to nearly 50%, as described later (Table 3). However, no particular names are given for the end-member components of substitutions (2) and (4).

Mineral names of the pyroxenes

Twenty (20) mineral names and their grouping. The pyroxenes form extensive solid solutions by various types of ionic substitutions, some of which are described above. To cope with the problem of pyroxene nomenclature, it is necessary to subdivide the solid-solution series into ranges with specified compositions and names. Whenever there is a complete solid-solution series between two end members, it is customary in mineral nomenclature to use only two names, and the division between them should be at $A_{50}B_{50}$ (the '50% rule'). However, this '50% rule' cannot be applied rigorously to the large groups of pyroxenes which show wide ranges

of coupled substitutions. This is particularly so when the minerals concerned are abundant and widespread, and have a historically-established nomenclature in mineralogical and petrological circles. Taking this situation into consideration, 20 accepted and widely used names have been adopted as mineral species names of the pyroxenes (Table 2).

The definition of the pyroxene species has been based on thirteen end-members, or chemical components, listed in Table 2, and the component $Ca_2Si_2O_6$ (Wo)⁷. These end-members are given the names of the minerals whose compositions they most closely approximate. The 20 pyroxene species are grouped into six chemical subdivisions on the basis of the cation occupancy of the M2 sites and crystal chemical similarity. This classification is a slight modification of the widely used scheme proposed by DHZ (1978).

For the precise classification of the pyroxenes into 20 mineral species, however, the following characteristics of the pyroxenes must be considered. First of all, the Mg-Fe pyroxenes and some of the Ca pyroxenes are the most common rockforming pyroxenes and form wide solid solutions which cover the pyroxene quadrilateral of the ternary Ca₂Si₂O₆ (Wo)-Mg₂Si₂O₆ (En)-Fe₂Si₂O₆ (Fs) system. Therefore, these pyroxenes are better treated together as the Ca-Mg-Fe or 'quadrilateral' pyroxenes. Secondly, Na pyroxenes form continuous solid-solution series with the Ca-Mg-Fe pyroxenes, forming the Na-Ca pyroxenes. Thirdly, donpeacorite and kanoite in the Mn-Mg pyroxenes, johannsenite, petedunnite and esseneite in the Ca pyroxenes, and spodumene, are rare in occurrence and unique in chemistry. For simplicity they are treated together as 'other' pyroxenes8.

All the pyroxenes are thus divided into four

Table 2. Accepted pyroxene mineral names and their chemical subdivisions. Name, abbreviation and composition are given for any pyroxene that is used as an end-member of a pyroxene solid solution; such end-members are numbered between parentheses from 1 to 13. Main compositions are given for solid solutions. Space groups are also given.

mineral names	composition as end-member	main composition as solid solution	space group
I. Mg-Fe pyroxenes			
1. enstatite (En)	(1) Mg ₂ Si ₂ O ₆	(Mg,Fe) ₂ Si ₂ O ₆	Pbca
ferrosilite(Fs)(2) Fe ₂ ²⁺ Si ₂ O ₆	3 (1137-17,201206	1200
clinoenstatite		(Mg,Fe)2Si2O6	<u>P</u> 2 ₁ / <u>c</u>
4. clinoferrosili	te	3	
pigeonite		$(Mg,Fe,Ca)_2Si_2O_6$	<u>P</u> 2 ₁ / <u>c</u>
6. donpeacorite		(Mn,Mg)MgSi ₂ O ₆	Pbca
· -) MnMcSiaOs	2 0	
7. kanoite (Ka)(3) MnMgSi ₂ O ₆	(Mn, Mg) MgSi ₂ O ₆	<u>P</u> 2 ₁ / <u>c</u>
· •		(Mn, Mg) MgSi ₂ O ₆	<u>P</u> 2 ₁ / <u>9</u>
7. kanoite (Ka)(3		2 0	
7. kanoite (Ka)(3 III. Ca pyroxenes 8. diopside (Di)((Mn, Mg) MgSi ₂ O ₆	<u>P</u> 2 ₁ / <u>9</u>
7. kanoite (Ka)(3 III. Ca pyroxenes 8. diopside (Di)(9. hedenbergite(H	4) CamgSi ₂ O ₆	(Mn, Mg) MgSi ₂ O ₆	<u>P</u> 2 ₁ / <u>c</u>
7. kanoite (Ka)(3 III. Ca pyroxenes 8. diopside (Di)(9. hedenbergite(H 10. augite	4) CaMgSi ₂ O ₆ d)(5) CaFe ²⁺ Si ₂ O ₆ c)(6) CaMnSi ₂ O ₆	(Mn, Mg) MgSi ₂ O ₆	<u>P</u> 2 ₁ / <u>9</u> <u>C</u> 2/ <u>c</u>

14. omphacite15. aegirine-augite		(Ca,Na)(R^{2+} ,Al)Si ₂ O ₆ (Ca,Na)(R^{2+} ,Fe ³⁺)Si ₂ O ₆	<u>C</u> 2/ <u>c</u> , <u>P</u> 2/ <u>n</u> <u>C</u> 2/ <u>c</u>
V. Na pyroxenes			
16. jadeite (Jd)(9)	NaAlSi ₂ 06	No.(3) Fo3+)Si O	<u>C</u> 2/c
17. aegirine (Ae)(10)	NaFe ³⁺ Si ₂ O ₆	Na(Al,Fe ³⁺)Si ₂ O ₆	<u>u</u> 2/ <u>u</u>
18. kosmochlor(Ko)(11)	NaCr ³⁺ Si ₂ O ₆		<u>c</u> 2/ <u>c</u>
19. jervisite (Je)(12)*3	NaSc ³⁺ Si ₂ O ₆		<u>C</u> 2/ <u>c</u>
VI. Li pyroxene			
20. spodumene (Sp)(13)	LiAlSi206		<u>c</u> 2/ <u>c</u>

- *1 Petedunnite has been determined by Essene and Peacor (1987) to have the composition $(Ca_{0.92}Na_{0.06}Mn_{0.02})(Zn_{0.37}Mn_{0.19}Fe_{0.19}^{2+})$ $Fe_{0.12}^{3+}Mg_{0.14})$ (Si_{1.94}Al_{0.06})O₆ by means of an electron microprobe. This mineral was approved as a valid species CNMMN, IMA, in 1983.
- *2 Esseneite has been determined by Cosca and Peacor (1987) to have the composition $(Ca_{1.01}Na_{0.01})(Fe_{0.72}^{3+}Mg_{0.16}Al_{0.04}^{Ti}o_{0.03}Fe_{0.02}^{2+})$ $(Si_{1.19}Al_{0.81})o_{6.00}$ by means of an electron microprobe. This mineral was approved as a valid species by the CNMMN, IMA, in 1985.
- *3 Jervisite has been determined by M. Mellini et al. (1982) to have the composition $(Na_{0.43}Ca_{0.31}Fe_{0.14}^{2+} 0.12)(Sc_{0.66}Fe_{0.15}^{2+}I_{5M}g_{0.19})Si_{2}O_{6}$ by means of an electron microprobe. This mineral was approved as a valid species by the CNMMN, IMA, in 1982.

chemical groups for the purpose of broad classification: Ca-Mg-Fe pyroxenes (Quad, 8); Ca-Na pyroxenes (Ca-Na, 2); Na pyroxenes (Na, 2) and 'other' pyroxenes (Others, 8). The abbreviations of the groups and the numbers of the accepted species are given between parentheses. Quad represents 'quadrilateral' for the Ca-Mg-Fe pyroxenes. The four chemical groups are further divided into 20 mineral species by using 12 components (using the Wo component for Di and Hd components). The composition ranges for the accepted names will be given later.

The pyroxene names may be qualified by one or more adjectival modifiers according to definite rules described later to specify important (though relatively minor) departures from the composition ranges. When the composition range of the mineral species is large, as in augite, one or more adjectival modifiers are used to specify the composition more clearly (e.g. subcalcic augite, Fe-rich augite).

Application of 50% rule. The 50% rule has been applied to complete solid-solution series between two end members as far as possible. They are the Mg-Fe pyroxene series (enstatite-ferrosilite and clinoenstatite-clinoferrosilite series), Ca pyroxene series (diopside-hedenbergite series) and Na pyroxene series (jadeite-aegirine series). Subdivision names of the intermediate solid solution ranges, such as bronzite, hypersthene and eulite of the enstatite-ferrosilite series and salite and ferrosalite of the diopside-hedenbergite series, have been discarded. However, the 50% rule was not applied rigorously to the Ca-Mg-Fe pyroxenes and Na-Ca pyroxenes. The widely accepted terms such as augite, pigeonite, omphacite and aegirineaugite9 have been retained.

Gem names of spodumene. Two names, 'hiddenite' and 'kunzite', are often used respectively for (pale) emerald-green and lilac coloured spodumene of gem quality. They are not accepted as formal pyroxene names, but can be used as varietal gem names.

Relationships with the pyroxenoids. Pyroxenoids are closely related to pyroxenes in that they have a similar type of chemical composition and a structure that also consists of SiO₃ single chains. However, the repeat of the chains, which is two SiO₄ tetrahedra in the pyroxenes, is three or more SiO₄ tetrahedra in the pyroxenoids. Though the tetrahedral sites are mostly occupied by Si ions, the large cations are mostly Ca, Mn and Fe²⁺ ions in the pyroxenoids. The classification and nomenclature of the pyroxenoids are beyond the scope of this report. However, the following two points may be noted. Firstly, there is a polymorphic relationship with some pyroxenes such as ferrosilite, heden-

bergite and johannsenite. These show pyroxenoid structures at high temperatures or pressures. Secondly, the wollastonite chemical component (Ca₂Si₂O₆) is used to express the composition of the Ca-Mg-Fe pyroxenes, though wollastonite belongs to the pyroxenoid structural group.

Classification and nomenclature of the pyroxenes

Preliminary classifications—construction of the Q-J diagram and application of pyroxene data. Before classifying the pyroxenes into the 20 mineral species listed in Table 2, the following procedure is recommended to divide them into four chemical groups: Ca-Mg-Fe pyroxenes (Quad), Na-Ca pyroxenes (Na-Ca), Na-pyroxenes (Na), and other pyroxenes (Others) (Morimoto and Kitamura, 1983).

In this procedure the pyroxenes are classified by using the total numbers of specified cations at the M (M1 and M2) sites on the basis of six oxygens. The M1 and M2 sites are considered together as M sites, without considering the site preference of atoms between the two sites.

The numbers of Ca, Mg, Fe²⁺ and Na cations in the M sites are plotted in the Q-J diagram (Fig. 2) as $Q = \text{Ca} + \text{Mg} + \text{Fe}^{2+}$ and J = 2Na. The lines representing the following equations are used to subdivide the Q-J diagram:

- (1) Q + J = 2.0
- (2) Q + J = 1.5
- (3) J/(Q+J) = 0.2
- (4) J/(Q+J) = 0.8

The areas corresponding to the Ca-Mg-Fe pyroxenes, Ca-Na pyroxenes, Na pyroxenes and other pyroxenes are labelled (Fig. 2) Quad, Ca-Na, Na, and Others, respectively.

In this diagram, J is meant to include the total number of Na and R³⁺, usually Al, Fe³⁺, Cr³⁺ and Sc³⁺, that couple with Na in substitution (1) mentioned in Table 1. When the coupling substitution in the pyroxene is not of type (1), but of type (2) or (3), the J value apparently does not represent the real numbers of Na and R^{3+} at the M sites. However, substitution (3) (e.g. Al-Al) works to move the J and Q values closer to the origin of the Q-J diagram, and substitution (2) (e.g. Na-Ti⁴⁺) to move the J value farther away from the O axis of ordinates. Therefore, the effects of substitutions (2) and (3) tend to cancel each other out in and near the Na pyroxenes area. Thus the J (= 2Na) values in the Na-rich pyroxenes represent, to a good approximation, the total number of Na and R^{3+} (Al, Fe³⁺, Cr³⁺ and Sc³⁺) at the M sites.

The boundary Q+J=2.0 represents the upper limit of Q+J at the M sites. The boundary

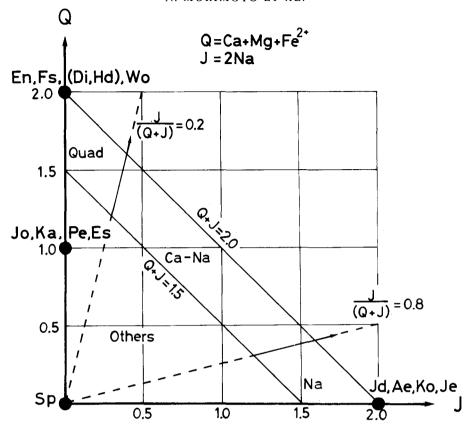


Fig. 2. Q-J diagram for the pyroxenes, on which the positions of the 13 accepted end-members have been indicated. Abbreviations and compositions of the end-members are listed in Table 2.

Q+J=1.5 represents the limit below which more than half of the M1 or M2 sites may be occupied by ions other than Q and J ions. In this case, the pyroxenes are considered as belonging to 'Others', which include the Mn-Mg and Li pyroxenes, johannsenite, petedunnite and esseneite. The third and fourth equations represent the lines dividing the area limited by the two above-mentioned Q+J lines into Ca+Mg+Fe (Quad), Ca-Na and Na pyroxenes. The boundaries defined by J/(Q+J)=0.2 and 0.8 are used by DHZ (1978) and Cameron and Papike (1981).

Because the Mn-Mg pyroxenes and johannsenite (Table 2) have Mn ions occupying more than half of the M2 and M1 sites, respectively, they appear along the Q axis between 1.0 and 1.5 of the Qvalue in the Q-J diagram. Similarly, petedunnite and esseneite appear along the Q axis with its Qvalue between 1.0 and 1.5. Spodumene concentrates at the origin of the Q-J diagram because both Q and J are zero. Thus, the thirteen end-members (Table 2) and Wo are located in the Q–J diagram (Fig. 2).

Application of this classification procedure to 406 pyroxene analyses presented in DHZ has shown that most of the analyses, except those of johannsenite and spodumene, are included in the area between the lines Q + J = 2.0 and 1.5. The 103 DHZ pyroxenes selected by Cameron and Papike (1981), for which the Q values are less than 1.90 and Mn is less than 0.08 atoms per formula unit, are plotted in the Q-J diagram of Fig. 3. The 'CaMg TAL' pyroxene (Cameron and Papike, 1981) is included in the Quad area as described later (Table 3, No. 1). Only twenty analyses among 406 plot slightly over the line Q+J=2.0, and most of these show unusual total numbers of cations. The results of the classification of the pyroxenes into the four chemical groups by this procedure are in almost complete agreement with the results obtained by DHZ (1978) and by Cameron and Papike (1981). A few unusual pyroxenes with Mn less than 0.08

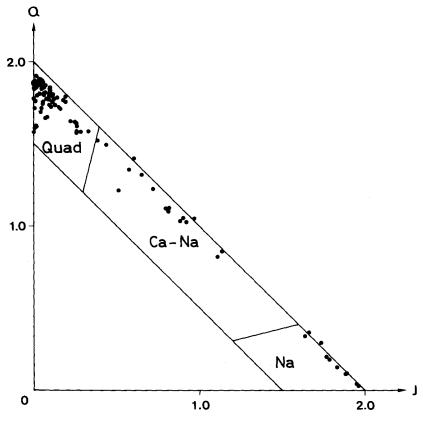


Fig. 3. The 103 DHZ pyroxenes selected by Cameron and Papike (1981) plotted on the Q-J diagram. For these pyroxenes the Q values are less than 1.90, and Mn is less than 0.08 atoms per formula unit.

atoms for the chemical formula unit have been found to lie outside the area between Q+J=2.0 and Q+J=1.5 lines in the Q-J diagram. The classification of these unusual pyroxenes will be discussed later.

The pyroxenes that plot in the area between Q+J=2.0 and 1.5 have components other than Q and J ions at less than 25% of the M sites. Therefore, we can classify such pyroxenes on the basis of the normalized Q and J components, thereby neglecting the effects of the other components. The following procedures are adopted for further classification:

- (1) The pyroxenes in the **Quad** area are classified on the pyroxene quadrilateral Wo-En-Fs diagram with normalized Ca, Mg and Fe (= $Fe^{2+} + Fe^{3+} + Mn$) atoms.
- (2) The pyroxenes in the Na area are jadeite, aegirine, kosmochlor and jervisite. Because kosmochlor and jervisite show little or no solid solution towards other end-members, they play no

role in the classification. Jadeite and aegirine are classified on the Quad-Jd-Ae diagram together with the Ca-Na pyroxenes, aegirine-augite and omphacite.

The classification of the Ca-Mg-Fe 'quadrilateral' pyroxenes. The common rock-forming pyroxenes form wide ranges of solid solutions of the Ca-Mg-Fe pyroxenes and can be expressed by the pyroxene quadrilateral of the $Mg_2Si_2O_6(En)-Fe_2^{2+}Si_2O_6$ (Fs)-Ca $MgSi_2O_6(Di)$ -Ca $Fe^{2+}Si_2O_6$ (Hd) system. The Ca-Mg-Fe pyroxenes include varieties that have orthorhombic symmetry. They consist essentially of a simple chemical series (Mg,Fe)₂Si₂O₆, thus contrasting with the clinopyroxenes which have wide ranges of chemical composition in the Ca-Mg-Fe pyroxenes. Therefore, the Ca-Mg-Fe pyroxenes are defined on the basis of symmetry and relative amounts of Ca₂Si₂O₆(Wo), Mg₂Si₂O₆(En) and Fe₂⁺Si₂O₆(Fs). The composition ranges of the clinopyroxenes and orthopyroxenes are indicated in Figs. 4 and 5, respectively, where the

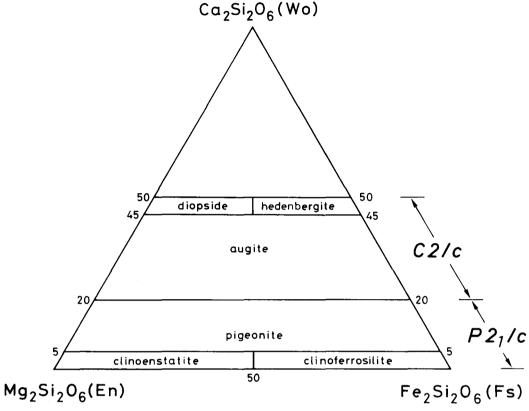


Fig. 4. Composition ranges of the Ca-Mg-Fe clinopyroxenes with accepted names.

composition is normalized to $Ca + Mg + \Sigma Fe = 100$ with $\Sigma Fe = Fe^{2+} + Fe^{3+} + Mn^{2+(10)}$.

The distinction between augite and pigeonite in the Ca-Mg-Fe pyroxenes is primarily structural, their space groups being C2/c and $P2_1/c$ respectively. There is a miscibility gap between augite and pigeonite, and many pyroxenes with 15-25% Wo have proved to be mixtures of the two. Augite with less than about 25% Wo is often called subcalcic augite. On heating, pigeonite undergoes a rapid displacive transformation to a C2/c structure

which cannot be quenched. Augite does not show this type of transformation.

The most calcium-rich orthopyroxene contains approximately 5% Wo. The high-temperature form of enstatite has the space group *Pbcn* and can be expressed as 'enstatite-*Pbcn*'. This form is not quenchable and has not been found in nature. 'Protoenstatite' has been used conventionally to describe this form, but this name is not adopted as a mineral name. The Wo value of 'enstatite-*Pbcn*' does not exceed 2% and the En value commonly

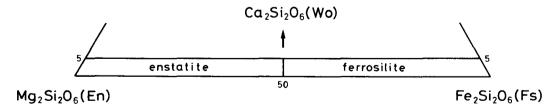


Fig. 5. Composition ranges of orthopyroxenes with accepted names.

exceeds 90%. Thus the composition field of 'enstatite-Pbcn' is different from that of enstatite-Pbca

The classification of the Na and Ca-Na pyroxenes. The Na pyroxenes, jadeite and aegirine, commonly contain more than 90% of the NaAlSi₂O₆ or NaFe3+Si2O6 component, respectively, but contain neither the Ko nor the Je component. Because kosmochlor is a rare accessory constituent of some iron meteorites and only one terrestrial locality is known for each of kosmochlor and jervisite, these two species are separately treated in the classification of the Na pyroxenes. Both jadeite and aegirine, however, show extensive solid solution with the Ca-Mg-Fe pyroxenes, especially with the diopside-hedenbergite series and augite, leading to the Ca-Na pyroxenes. The Na and Ca-Na pyroxenes are classified on the Quad-Jd-Ae diagram (Fig. 6) with normalized Q (Wo + En + Fs),

accepted as an independent species to keep balance with omphacite, though it is not known to occur with the P2/n structure. The classification of the Ca-Na pyroxenes by Essene and Fyfe (1967) is not followed in this report.

The classification of other pyroxenes. Most naturally occurring pyroxenes in the 'Others' area are johannsenite (CaMnSi₂O₆), petedunnite (CaZn Si₂O₆) and spodumene (LiAlSi₂O₆) (Fig. 2). Recent investigations of natural manganese-bearing pyroxenes have yielded two new minerals, kanoite and its dimorph donpeacorite, (Mn,Mg)MgSi₂O₆, which seem to form a solid solution with En (Petersen et al., 1984). They too occur in the 'Others' area. These results suggest a possible Mn-Mg-Fe pyroxene quadrilateral. Esseneite (CaFe³⁺AlSiO₆) is the first pyroxene with the substitution (3) as described in Table 1.

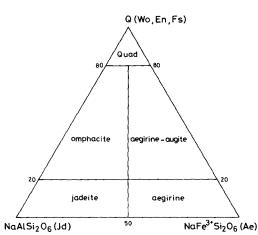


Fig. 6. Ca-Mg-Fe and Na pyroxenes with accepted names. Quad represents the Ca-Mg-Fe pyroxene area (see Fig. 4).

Jd and Ae components¹¹. The arbitrary divisions between the Ca-Mg-Fe pyroxenes, Na-Ca pyroxenes and Na pyroxenes are defined at 20 and 80% of Q = (Wo + En + Fs). Omphacite displays a $C2/c \rightleftharpoons P2/n$ polymorphic transition, and both high-temperature C2/c and low-temperature P2/n polymorphs appear in nature. Omphacite can thus be divided into two subspecies: omphacite-C2/c and omphacite-P2/n. Because omphacite-P2/n shows a unique crystal structure different from that of jadeite and augite, it is accepted as an independent pyroxene species. Aegirine-augite is also

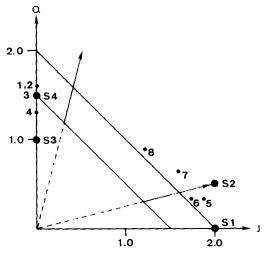


Fig. 7. Q-J diagram for eight unusual pyroxenes with Q-value less than 1.62 and Mn less than 0.08 atoms per formula unit (Table 3). The components formed by the substitutions (1) to (4), as indicated in Table 1, are plotted in the diagram. They represent the following compositions: $S1 = NaR^{3+}Si_2O_6$, $S2 = NaR^{2+}_{0.5}Ti^{4-}_{0.5}Si^{5-}_{0.5}Ti^{4-}_{0.5}AlSiO_6$, $S3 = CaR^{3+}AlSiO_6$ and $S4 = CaR^{2+}_{0.5}Ti^{4-}_{0.5}AlSiO_6$.

The classification of unusual pyroxenes. Several pyroxenes with unusual chemical compositions (Table 3) appear outside the area between the Q+J=2.0 and Q+J=1.5 lines in the Q-J diagram, though they do not belong to the 'other' pyroxenes mentioned above (Fig. 7). They contain large amounts of chemical constituents of substitutions (2), (3) and (4) mentioned in Table 1 in the standard chemical formulae.

Table 3. Chemical composition and classification of eight unusual pyroxenes. Numbers such as 320-8, etc. represent pages and analysis number in DHZ (1978). Other references are in text. With the exception of 320-8 (=406-16), all the DHZ analyses in this table were not included in the 103 selected analyses of Cameron and Papike (1981). All pyroxenes in the table are shown with their numbers in the Q-J diagram (Fig. 7). S2, S3 and S4 represent the following components of substitutions (2), (3) and (4), respectively: $S2=NaR_0^2+5Ti_0^4+5Si_2O_6$, $S3=CaR_0^3+AlSiO_6$, and $S4=CaR_0^2+5Ti_0^4+5AlSiO_6$. To indicate R ions explicitly in these components, the notation S(R), such as S2(Mg) and S3(Al), is used. S3(Fe) is a new pyroxene, esseneite (Es).

No.	1. 320- (406-		2. 403	-3	3. D ar	nd S*1	4. T a	nd R ^{*2}
Si	1.443	2.00	1.506	2.00	1.434	2,00	1.196	2.00
Al	.557	2.00	.494	2.00	.566	2.00	.804	2.00
Al	.091		.171		.306		.186	
Ti 4+	.165		.065		.022	Ti	4+ .111	
Fe ³⁺	.128		.159		.218	Ti	3+ .394	
Mg	.385		.570		.408		.289	
Fe ²⁺	.229	2.00	.063	2.02	.060	2.00		2.00
Mn	.005		.007		.005			
Ca	.992		.975		.979		1.021	
Na	.006		.007		.002			
K	.000		.001		-			
Q	1.61		1.61		1.45		1.31	
J	0.01		0.01		0.00		0.00	
Mineral names	subsilio titanian ferrian diopside	1	subsilic aluminic ferrian diopside	an	subsilio aluminio ferrian diopside	an	subsilic titanoa aluminia pyroxene	n an
Names in litera- ture	titanau (320-8 titanium fassait (406-16 CaMgTAL (C and) n- te 5)	fassaite	9	fassaite	2	titanau	gite

Component ratios;

- 1. $(Wo_{22}En_{12}Fs_{10})_{44}S4(Mg)_{18}S4(Fe)_{16}Es_{13}S3(Al)_{9}$
- 2. $(Wo_{26}En_{25}Fs_2)_{53}S3(Al)_{17}Es_{16}S4(Mg)_{12}S4(Fe)_2$
- 3. $(Wo_{22}En_{20}Fs_2)_{44}S3(Al)_{31}Es_{21}S4(Mg)_4$
- 4. $S3(Ti)_{39}S4(Mg)_{22}(Wo_{11}Fs_9)_{20}S3(Al)_{19}$

These pyroxenes can be divided into two groups: firstly Ca-rich pyroxenes with the S3 (Ca R^{3} +Al SiO₆) and S4 (Ca $R_{0.5}^{2}$ -Ti $_{0.5}^{4}$ -AlSiO₆) components representing substitutions (3) and (4), respectively, and secondly Na-rich pyroxenes with the S2 component (Na $R_{0.5}^{2}$ -Ti $_{0.5}^{4}$ -Si $_{2}$ O₆) representing substitu-

tion (2). The former shows a significant deficiency of Si atoms such as Si < 1.60 in the standard formula resulting in the Q-value close to or less than 1.5 (point S4 in Fig. 7). The latter appears outside the line Q + J = 2.0 approaching point S2 in Fig. 7. All these unusual pyroxenes are classified by using

b)	Na-rich	group	related	to S	32
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No.	5. 488-	9	6. 491-	14	7. 492- (C and	-19 1 G*4)	8. C ar	nd G*4
Si	1.994	2 00	2.024	2.02	2.026	2.03	2.009	2.01
Al	.032	2.00	.000	2.02	.000	2.03	.000	2.01
Al	.000		.021		.098		.348	
Ti 4+	.265		.023		.227		.104	
Fe ³⁺	.458		.728		.192		.031	
Mg	.150		.070		.070		.168	
Fe ²⁺	.107	2.00	.113	2.00	.420	1.98	.356	2.00
Mn	.003		.006		.021		.011	
Na	.933		.872		.794		.610	
Ca	.083		.155		.152		.361	
к	-		.009		-		.006	
Q	0.34		0.34		0.64		0.89	
J	1.87		1.74		1.59		1.22	
Mineral names	titanian magnesian ferroan aegirine		calcian ferroan aegirine		titaniar aegirine augite		titaniar ferroan omphacit	
Names in litera- ture	titanian aegirine		aegirine augite	-	titaniar aegirine augite (492-19 titaniar aegirine (C and	9) 1	titaniar ferro-om	

Component ratios;

- 5. $Ae_{46}S2(Mg)_{28}S2(Fe)_{20}^{\Delta_6}*5$
- 6. $(Ae_{73}Jd_2Wo_8Fs_6En_3)_{92}S2_4\Delta_4$
- 7. $(Ae_{19}Jd_{10}Fs_{12}Wo_8En_2)_{51}S2(Fe)_{42}S2(Mg)_4\Delta_3$
- 8. $(Jd_{35}Ae_3Wo_{18}Fs_{15}En_7)_{78}S2(Fe)_{14}S2(Mg)_6\Delta_2$
- *1 Devine and Sigurdsson (1980), Table 1 for fassaite.
- *2 Tracy and Robinson (1977), Table 3, Analysis I for pyroxene from the Allende meteorite (Mason, 1974).
- *3 Cameron and Papike (1981), Table A3, Analysis 320-8 and 406-16.
- *4 Curtis and Gittins (1979), Table 2, Analysis 5 for No.7 and Table 5, Analysis 5 for No.8.
- *5 Δ represents minor components, some of which have unusual metal ratios for the pyroxene structure.

the accepted pyroxene names and the adjectival modifiers mentioned below, except the Allende pyroxene (Table 3, No. 4) which is called subsilicic titanoan aluminian pyroxene.

The Allende pyroxene (No. 4) contains 39% of the S3(Ti) component and can be considered as a new mineral. However, we have decided only to use the accepted names in this report and if a species has not yet been approved, we use *pyroxene* as for No. 4 in Table 3. The names used in literature for the unusual pyroxenes are listed in Table 3 in com-

parison with those in this report. The 'CaMgTAL' pyroxene (No. 1) is diopside in this classification.

Adjectival modifiers

Adjectival modifiers for mineral names are used to indicate unusual amounts of chemical constituents. In order to define the unusual amounts for the pyroxene mineral group quantitatively, extreme compositions of pyroxenes have been listed in Table 4, where the values for the main

Table 4 Extreme chemical compositions of pyroxenes in DHZ (1978). Number of cations per formula unit, minimum values for Si and maximum values for other cations. Bold numbers are for the main constituent elements. Numbers in the parentheses such as 42-9, etc. indicate pages and analysis numbers in DHZ (1978). Other references are in text.

	Mg-Fe pyroxenes	Ca pyroxenes	Na pyroxenes
si	1.76 (42-9)	1.44 (320-8)*1	1.94 (488-9)
A13+	0.24 (42-9)	0.56 (320-8)	0.07 (488-8)
Fe ³⁺	0.04 (49-8)	0.09 (320-11)	0.02 (488-9)
A1 ³⁺	0.15 (49-6)	0.35 (320-11)	0.98 (464-1)
Ti 4+	0.04 (40-30)	0.17 (320-8)*2	0.27 (488-9)*3
Fe ³⁺	0.12 (170-8)	0.37 (321-5)*4	0.97 (487-1)
Mg ²⁺	1.99 (41-1)	1.27 (208-4)	0.15 (488-9)
Fe ²⁺	1.72 (47-33)*5	1.09 (220-13)	0.11 (488-9)
Mn ²⁺	0.27 (45-21)*6	0.36 (217-5)*7	0.03 (487-4)
Cr ²⁺	0.02 (36-9)	0.06 (207-11)	_ *8
Ni ²⁺	-	0.003 (317-1)	-
zn ²⁺	-	0.21 (216-11)*9	-
Ca ²⁺	0.26 (169-2)	1.03 (202-4)	0.16 (466-14)
Na+	0.10 (169-2)	0.31 (323-7)	0.98 (464-1)

^{*1} Table 3, No. 1. Table 3, No. 4: Pyroxene from the Allende meteorite 1.20 (Mason, 1974; Tracy and Robinson, 1977).

cations are shown as well as those for the accessory cations. The table was constructed using data from DHZ (1978) and Robinson (1980).

An element specified as a modifier should be present as a general rule in a quantity larger than 0.1 or 0.01 atoms in the standard chemical formula of 6 O or 4 metal atoms (Table 5) depending on the maximum content in Table 4.

The suffixes are those proposed by Schaller (1930) and adapted by CNMMN (Nickel and

Mandarino, 1988). The suffix -ian is used for the higher valence state (e.g. ferrian) or for an element with a non-variable state (e.g. lithian). The suffix -oan implies the lower valence state (e.g. ferroan). It is recommended that such modifiers never be used for main cations normally contained in the named mineral, for example, in terms like calcian augite, aluminian omphacite, and sodian aegirine-augite, in which the modifiers are obviously superfluous.

^{*2} Probe analysis 0.252 & 0.282, half of $Car_{0.5}^{2+}Ti_{0.5}^{4+}AlSio_{6}$ (S4) (Tracy and Robinson, 1977; Robinson, 1980).

^{*3} Table 3, No. 5. Half of NaR²⁺_{0.5}Ti⁴⁺_{0.5}Si₂O₆ (S2).

^{*4 406-15 0.67,} omitted because of possible errors in chemical analysis.

^{*5} Probe analysis 1.880 (Jaffe et al., 1978).

^{*6} Probe analysis 0.301 (Robinson, 1980), Kanoite 1.04 (Kobayashi, 1977).

^{*7} Johannsenite 0.963 (417-2).

^{*8} Kosmochlor 0.90 (522-1).

^{*9} Petedunnite 0.37 (Table 2, remark *1).

If there is less than the amount necessary for the assignment of the modifiers such as 'aluminian' in Table 5, or 0.1 Al, but if the increased content of the element must be stressed, a modifier 'aluminiumbearing' may be used. This second type of modifier should be used also (1) if only an incomplete analysis is available preventing the calculation of a full chemical formula or (2) for pyroxenes where the valence state of a cation is unknown. With regard to the Si content in pyroxenes, it is suggested that Si < 1.75 is a suitable limit for use of the term 'subsilicic', though one should bear in mind that the Si < 5.75 limit for 'subsilicic' in amphiboles corresponds to Si < 1.5 for pyroxenes.

Table 5. List of adjectival modifiers to be used for pyroxene mineral names. The limit of the content is determined based on the values listed in Table 4.

cation	content*1	name
A13+	>0.10	aluminian
Ca 2+	>0.10	calcian
Cr3+	>0.01	chromian
Fe ²⁺	>0.10	ferroan
Fe ³⁺	>0.10	ferrian
Li ⁺	>0.01	lithian
Mg ²⁺	>0.10	magnesian
_{Mn} 2+	>0.10	manganoan
Mn ³⁺	>0.01	manganian
Na+	>0.10	sodian
Ni ²⁺	>0.01	nickeloan
Si ⁴⁺	<1.75	subsilicio
Ti ³⁺	>0.01	titanoan
Ti 4+	>0.10	titanian
zn ²⁺	>0.01	zincian

^{*1} Number of cations per formula unit ${\rm M2M1T}_2{\rm O}_6$. If the mineral name itself implies the presence of certain cations, adjectival modifiers for these cations should not be used ('subsilicic' is an exception).

In certain cases, particularly for the augite series, it is convenient to use the following adjectival modifiers: iron-rich, magnesium-rich, and subcalcic. A prefix actually attached or hyphenated to a mineral name, however, is incorrect and should be avoided (Nickel and Mandarino, 1988), because it would cause the mineral to be indexed alphabetically under the prefix rather than the proper

mineral name. This is why such terms as 'ferropigeonite', 'ferro-augite', etc., should not be used as mineral names.

It is often useful to give the space group of the mineral, particularly when it can occur in two or more forms. For example, we could distinguish between the two forms of omphacite by adding the space group symbol, i.e. omphacite-C2/c, omphacite-P2/n, or by adding the lattice-type symbol, i.e. omphacite-P (Bailey, 1977).

Obsolete pyroxene names

The names of 105 pyroxenes or altered pyroxenes listed in Table 6 have formally been discarded by the CNMMN and are therefore obsolete. The preferred name is underlined in the same table.

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Footnotes

- 1. In omphacite-P2/n, the M1 and M2 sites are further divided into M1a and M1b (for M1) and M2a and M2b (for M2).
- 2. Orthopyroxene (*Pbcn*) is stable only at elevated temperatures for a limited composition near MgSiO₃.
- 3. Aegirine is used in preference to 'acmite' in this report. It is in common usage in the literature, and is consistent with the almost universal use of aegirine-augite for minerals of intermediate compositions, though 'acmite' has priority by 14 years (Dana, 1892). Common practice in experimental petrology has been to use the abbreviation Ac for NaFe³⁺Si₂O₆; Ae should now be used instead.
- 4. The CNMMN, IMA, has recently voted in favour of the name kosmochlor instead of 'ureyite' for the pyroxene of generalized composition NaCrSi₂O₆.
- 5. Essencite is a new pyroxene with the composition CaFe³⁺AlSiO₆ (Table 2, No. 13).
- 6. 'Fassaite' has the general formula Ca(Mg,Fe³⁺,Al) (Si,Al)₂O₆. This name has been rejected as a formal name in this report.
- 7. Ca₂Si₂O₆ exists as wollastonite in nature, which belongs not to the pyroxenes but to the pyroxenoids. To represent the compositions of the Ca-Mg-Fe pyroxenes, the ternary Ca₂Si₂O₆(Wo)-Mg₂Si₂O₆(En)-Fe₂Si₂O₆(Fs) system has been used, e.g. En₂₀Fs₃₈Wo₄₂.
- 8. Definition of the 'Other' pyroxenes is different from that given by Cameron and Papike (1981).
- 9. The name aegirine-augite appears to be in more common usage than 'aegirineaugite' and 'acmite-augite'.

ferrohedenbergite = augite

Table 6. Obsolete pyroxene names. The following pyroxene mineral names, or names which refer to altered pyroxenes, have been formally discarded by the CNMMN. The correct names are underlined. The original form of this table was compiled by Malcolm Ross using the following references:

Dana (1892); Tsehermak (1897); Chester (1886); Ford (1932); Winchell and Winchell (1951);

Deer, Howie, and Zussman (1963, 1978); Strunz (1970); and the unpublished Thesaurus of Mineralogical Terms of the International Mineralogical Association, which has been available since August 1974.

acmite = aegirine ferrohypersthene = ferrosilite aegirite (aegyrite) = aegirine ferro-johannsenite = iron-rich johannsenite aegerine-hedenbergite = augite ferropigeonite = iron-rich pigeonite agalite = probably enstatite partly altered to talc ferrosalite = hedenbergite aglaite = altered spodumene ficinite = enstatite alalite = <u>diopside</u> funkite = hedenbergite alkali augite = aegirine-augite germarite = altered enstatite amblystegite = enstatite hiddenite = spodumene anthochroite = <u>augite</u> hudsonite = hedenbergite asteroite = iron-rich augite hypersthene = enstatite or ferrosilite jadeite-aegirine (jadeite-aegirite) = jadeite or baikalite = diopside bastite = enstatite which has altered to serpentine, aegirine talc, or perhaps anthophyllite jeffersonite = zincian manganoan diopside or augite blanfordite = manganoan aegirine-augite killinite = altered spodumene korea-augite = augite bronzite = enstatite calc-clinobronzite = pigeonite kunzite = spodumene calc-clinoenstatite = pigeonite lavroffite = diopside calc-clinohypersthene = pigeonite lavrovite= <u>diopside</u> calc-pigeonite = subcalcic augite lawrowite = <u>diopside</u> leucaugite = diopside canaanite = diopside chladnite = enstatite lime-bronzite = probably pigeonite or enstatite plus augite, ("inverted" pigeonite) chloromelanite = <u>omphacite</u> or <u>aegirine-augite</u> chrome-acmite = chromian aegirine loganite = diopside + actinolite + talc chromejadeite = chromian jadeite lotalite = hedenbergite clinohypersthene = <u>clinoenstatite</u> or <u>clinoferrosilite</u> malacolite = diopside with good (001) parting, also <u>diopside</u> from Sala, Sweden coccolite (kokkolith) = iron-rich augite cymatolite = altered spodumene mansjoite = augite or diopside or hedenbergite diaclasite = altered enstatite mayaite = omphacite diallage = diopside which has altered or which has good mellcrite = orthopyroxene (100) parting; also used for alteration mondradite =probably an altered pyroxene products of other pyroxenes mussite = diopside diopsidjadeite = omphacite orthobronzite = enstatite endiopside = magnesium-rich augite orthoenstatite = enstatite enstatite-diopside = magnesium-rich <u>augite</u> orthoeulite = ferrosilite eulite = ferrosilite orthoferrosilite = ferrosilite eulysite = ferrosilite orthohypersthene = enstatite or ferrosilite fassaite = ferrian aluminian diopside or augite paulite = enstatite fedorovite = diopside peckhamite = enstatite ferroaugite = augite phastine = altered enstatite

picrophyll = altered pyroxene ?

pigeonite-augite = probably subcalcic augite pitkarantite = pyroxene ? potash-aegirine = synthetic product, probably not properly characterized protheite = augite protobastite = enstatite pyrallolite = altered pyroxene ?, talc ? pyrgom = pyroxene sahlite = diopside salite = diopside schefferite = manganoan diopside schillerspar (schillerspat) = enstatite which is altered to serpentine, talc, or anthophyllite shepardite = enstatite soda-spodumene = sodian spodumene strakonitzite = altered pyroxene, steatite ? szaboite = partly altered enstatite

titanaugite = titanian augite titandiopside = titanian diopside titanpigeonite = titanian pigeonite trachyaugite = augite traversellite = diopside triphane = spodumene tuxtlite = omphacite uralite = pseudomorph of amphibole after pyroxenes urbanite = iron-rich augite or aegirine-augite ureyite = kosmochlor vanadinaugite = vanadium-bearing augite vanadinbronzite = vanadium-bearing enstatite vargasite = altered pyroxene ? victorite = enstatite violaite = augite violan = magnesium-rich augite or diopside

10. For the nomenclature of the Ca-Mg-Fe pyroxenes, normalization must be made to $Ca + Mg + \Sigma Fe = 100$, where $\Sigma Fe = Fe^{2+} + Fe^{3+} + Mn$. Hereafter the mol percent of the end-member components is always used without remark and is represented simply by %. If the mole % quadrilateral components are calculated by the atomic $\frac{9}{10}$ of Ca to the total cations at the M sites, no pyroxenes should contain more than 50% Ca₂Si₂O₆. However, if Ca, Mg and Fe are normalized, or, calculated as $100\text{Ca}/(\text{Ca} + \text{Mg} + \Sigma \text{Fe})$, $100\text{Mg}/(\text{Ca} + \text{Mg} + \Sigma \text{Fe})$ and $100\Sigma Fe/(Ca + Mg + \Sigma Fe)$, respectively, then some augites will plot on a Wo-En-Fs triangular diagram above the 50% Ca₂Si₂O₆ line. Especially, when the plot in the Q-Jdiagram is very close to or outside of the boundary Q+J=1.5, the effect of johannsenite and petedunnite components must be considered. If the effect is negligible, the pyroxene must be considered to have an unusual composition and must be referred to the section of unusual pyroxenes.

11. To normalize Q, Jd and Ae components, Ca+Mg+Fe²⁺+2Na at the M sites must be made to total 100%. Then the normalized 2Na% must be divided to the ratio of Al/Fe³⁺ to give the ratio of Jd/Ae. Thus Q+Jd+Ae must always give 100%. When the plot in the Q-J diagram is significantly outside the boundary Q+J=2.0, the effect of substitution (2) must be considered, as in the section of unusual pyroxenes.

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