

Fluoronyböite from Jianchang (Su-Lu, China) and nyböite from Nybø (Nordfjord, Norway): a petrological and crystal-chemical comparison of these two high-pressure amphiboles

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ABSTRACT

Fluoronyböite, ideally $\text{NaNa}_2(\text{Al}_2\text{Mg}_3)(\text{Si}_7\text{Al})\text{O}_{22}\text{F}_2$, has been found in the Jianchang eclogite pod, Su-Lu coesite-eclogite province, China. It has been approved as a new mineral by the IMA. Single-crystal structure refinement and electron microprobe analysis were used for characterization: $C2/m$, with $a = 9.666(4)$, $b = 17.799(6)$, $c = 5.311(2)$ Å, $\beta = 104.10(3)^\circ$, $V = 886.2(8)$ Å³, $Z = 2$, formula: $^A(\text{Na}_{0.78}\text{K}_{0.06})_{\Sigma 0.84}^B(\text{Na}_{1.53}\text{Ca}_{0.47})_{\Sigma 2.00}^C(\text{Fe}_{0.89}^{2+}\text{Mg}_{2.55}\text{Mn}_{0.01}\text{Zn}_{0.01}\text{Fe}_{0.32}^{3+}\text{Al}_{1.21}\text{Ti}_{0.01})_{\Sigma 5.00}^T(\text{Si}_{7.14}\text{Al}_{0.86})_{\Sigma 8.00}\text{O}_{22}^X(\text{OH}_{0.84}\text{F}_{1.16})_{\Sigma 2.00}$.

Fluoronyböite formed during UHPM conditions, and is preserved in the retrograded kyanite-bearing eclogite sample DJ102 together with clinopyroxene ($\text{Jd}_{70}\text{Ae}_{20}\text{Di}_{10}$), garnet ($\text{Alm}_{60}\text{Prp}_{21}\text{Grs}_{17}\text{Sps}_{02}$), and rutile. Lower-pressure minerals are also present (fluoro-alumino-magnesirotaramite, apatite, paragonite), and symplectitic rims were also developed around clinopyroxene crystals. Cation ordering and the structural and physical properties of fluoronyböite are reported and discussed with reference to those of F-free nyböite from the type locality at Nybø in Norway, for which some as yet unpublished mineral data are also reported. Relations between composition and petrogenetic conditions of these rare high-pressure amphiboles are discussed.

KEYWORDS: fluoronyböite, nyböite, amphibole, structure refinement, UHPM metamorphism.

Nyböite terminology, occurrences, chemistry and petrology

Terminology

HANDLING end-member names in such a complex mineral group as the amphiboles (>50 end-member names: Leake *et al.*, 1997) is sometimes difficult, e.g. in one case a given composition may be characterized and attributed a name by combining the proper root-name and prefixes defined by the International Mineralogical Association (IMA) nomenclature rules in force, and this may be published without realizing that official recognition of the new mineral status has not yet been applied for. In another case, almost

the opposite situation, IMA recognition of the end-member status may indeed be obtained, but complete mineral data are not published, for example because part of the data set is published in the meantime in papers dealing with other topics and not focused on that composition.

This paper describes a new mineral recently approved by the IMA (2002-010), fluoronyböite, and at the same time tries to put some order into the situation concerning nyböitic amphiboles; this necessitates in part a historical approach in this introduction.

The root-name nyböite was proposed by D.C. Smith and L. Ungaretti and was approved by the IMA (in September, 1980); this approval was subsequently cited in diverse indices or reference texts of new mineral species and names, but in the principal scientific publication describing the first nyböite (Ungaretti *et al.*, 1981) the name nyböite

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was mentioned as being under consideration by the IMA, the approval having arrived after the article went to press. Although that article contained much crystallographic and crystal-chemical data, it did not provide the full mineral data desired by the IMA.

The ideal end-member chemical composition, $\text{NaNa}_2(\text{Al}_2\text{Mg}_3)(\text{Si}_7\text{Al})\text{O}_{22}(\text{OH})_2$, had appeared earlier in the literature as a hypothetical composition to which no name, or the unofficial name 'miyashiroite', was attached. When the real mineral was discovered it was preferred to give a name to represent the type locality Nybö in Norway which is a key one in the history of UHPM (Ultra-High Pressure Metamorphism) (e.g. the first reports of pressure up to or exceeding 40 kbar outside of kimberlites and Alpine-type peridotites: Smith, 1976; Lappin and Smith, 1978, 1981).

It is relevant to mention that in 1980 nyböite could not be named according to the existing IMA rules of amphibole nomenclature (Leake, 1978) as those rules imposed the name eckermannite (point 19.6, p. 556) which is quite misleading. This is because that nomenclature system ignored the R^{2+} : R^{3+} relationships in the octahedral site occupancies. Reconsideration of the nomenclature system (Leake *et al.*, 1997) provided a proper place for the nyböite root name and also allowed for possible new species such as "ferronyböite", "ferric-nyböite" and "ferric-ferronyböite" (all three still not recognized by the IMA on the basis of observed natural crystals), as well as a long set of names for potential new species according to the presence of other substitutions, notably of OH by F, e.g. fluoronyböite.

Unit-cell parameters, mean bond lengths and chemical data for nyböite had been provided in Ungaretti *et al.* (1981), in which the petrogenetic evolution of the Nybö eclogite pod was discussed essentially only on the basis of crystal-chemical variations in the amphiboles. However, the complete mineral data have never been published, even though supplementary mineralogical data were given in various abstracts, notably in Kechid and Smith (1982), as well as in Smith (1988) and Oberti *et al.* (1989). A better crystal-chemical formula can now be provided in the light of the present knowledge of amphibole behaviour.

Recently, we realized that the name fluoronyböite had been used in a work discussing Na ordering at the *A* sites (Hawthorne *et al.*, 1996), but that recognition of this new mineral by the IMA had never been sought, an omission which

has now been rectified by IMA-CNMMN approval no. 2002-010. In this paper the complete mineral description of the two end-members is presented, together with revised and updated crystal-chemical formulae.

Chemical particularities and the factor f_{Al}

Nyböite, ideally $\text{NaNa}_2(\text{Al}_2\text{Mg}_3)(\text{Si}_7\text{Al})\text{O}_{22}(\text{OH})_2$, is one of the most extreme compositions with respect to tremolite taken as the origin, which in full is $(\square_1\text{Na}_0)(\text{Na}_0\text{Ca}_2)(\text{Al}_0\text{Mg}_5)(\text{Si}_8\text{Al}_0)\text{O}_{22}(\text{OH})_2$. In the $A_dB_bC_cD_d$ system of amphibole terminology devised by Smith (1988) where $a = R^{1+}$ at the *A* sites (*A*, *Am*), $b = R^{1+}$ at the *B* sites (*M4*, *M4'*), $c = R^{3+}$ at the octahedral sites (*M1*, *M2*, *M3*), $d = R^{3+}$ at the tetrahedral sites (*T1*, *T2*), nyböite has the $\{abcd\}$ formula $\{1221\}$ in comparison to $\{0000\}$ for tremolite. Together with eckermannite and arfvedsonite $\{1210\}$, nyböite has the maximum Na content, i.e. total Na = 3 atoms per formula unit (a.p.f.u.); however, nyböite is also highly aluminous (total Al = 3 a.p.f.u.).

The amphibole which replaces nyböite by eclogite retrogression to amphibolite is aluminomagnesiotaramite; this has the formula $\{1122\}$, hence with lower Na and lower $f_{\text{Al}} = \text{VIAl}/(\text{VIAl} + \text{IVAl}) = c/(c+d)$. As discussed by Smith (1982) and in detail in Smith (1988, p. 59), the factor f_{Al} is a key indicator in metamorphism as in general it tends to increase with increasing pressure (*P*) and decrease with increasing temperature (*T*). Thus f_{Al} is high in blueschist-facies conditions (e.g. eckermannite $\{1210\}$, glaucophane $\{0220\}$ or winchite $\{0110\}$: $f_{\text{Al}} = 1.00$), and decreases with increasing *T* towards eclogite-facies conditions (e.g. aluminobarroisite $\{0121\}$ or nyböite $\{1221\}$: $f_{\text{Al}} = 0.67$), and further decreases with decreasing *P* due to uplift and retrogression towards amphibolite-facies conditions (e.g. aluminomagnesiotaramite $\{1122\}$, aluminotschermakite $\{0022\}$, magnesiohornblende $\{0011\}$ or magnesiokatophorite $\{1111\}$: $f_{\text{Al}} = 0.5$). This trend continues arithmetically to magnesiosadanagaite $\{1023\}$: $f_{\text{Al}} = 0.4$; pargasite, $\{1012\}$: $f_{\text{Al}} = 0.33$, and finally to edenite $\{1001\}$: $f_{\text{Al}} = 0.00$ which is typically found in low-*P* high-*T* rocks. Hence this single simple f_{Al} factor provides a good petrogenetic marker of UHPM before taking into account all of the other petrological features, but on condition that $\text{Mg} \gg \text{Fe}^{2+}$ and $\text{Al} \gg \text{Fe}^{3+}$ since substantial Fe content makes a great difference to

the stability (e.g. glaucophane {0220} in high- P low- T rocks [e.g. blueschists] but riebeckite {0220} in low- P high- T rocks [e.g. granites]). The above list includes all 12 of the 14 sodic, sodic-calcic or calcic clin amphibole root-names (i.e. all except tremolite {0000} and richterite {1100}).

The experimental works most relevant to nyböite are those of Pawley (1992) and Welch and Graham (1992). Pawley (1992) produced 'quaternary' nyböite-glaucophane-katophorite-eckermannite solid-solutions in the T range 600–900°C containing up to 70 mol.% nyböite stable at 32 kbar and unstable below 15 kbar. It had been suggested by Ungaretti *et al.* (1981) that nyböite {1221} was the higher- T equivalent of glaucophane {0220} because of the higher ^{IV}Al content (and hence lower f_{Al}); this was supported experimentally by Pawley (1992, p. 188). Welch and Graham worked on an (OH)-free F-bearing glaucophane starting composition and produced amphiboles with an 'activity' (see their definition, p. 251) of fluoronyböite up to 0.70 in the P - T range 21–24 kbar, 800–850°C. They neatly confirmed (p. 254) that with decreasing pressure the synthesized complex amphibole compositions "sweep.....away from glaucophanic compositions towards nyböite" (i.e. systematically decreasing f_{Al}).

Occurrences and petrological ideas

Nybö

Nyböite was first discovered by one of the authors, DCS, who noticed a pale pink-violet pleochroic colour in a minute crystal in sample C413F, and then larger crystals in a new sample G230F, both collected from the Nybö orthopyroxene-eclogite pod on Nordpollen fjord near Nordfjorden, Vestlandet, Norway. This is an extraordinary chemically-zoned eclogite in which the jadeite (+ minor aegirine) proportion of the clinopyroxene composition, defined by $X_{Na} = Na/(Na + Ca)$, varies continuously from ~21 to 81 mol.% (Smith *et al.*, 1980; Rossi *et al.*, 1983; Smith, 1988, Fig. 1.13). This nyböite was recognized as a new chemical composition from EMP analysis, and X-ray crystal structure refinement clearly confirmed its differences from other amphiboles (Ungaretti *et al.*, 1981). P - T conditions for the stability of amphibole-eclogite (hence including nyböite-eclogite) at the Nybö eclogite pod were initially estimated at 15–25 kbar (Lappin and Smith, 1978, 1981), following an

earlier anhydrous-eclogite paragenesis assigned to 25–45 kbar. These P - T values were slightly adjusted into "best estimates" for coesite-eclogite subfacies conditions at 32 kbar, 800°C and for the subsequent quartz-eclogite subfacies at 23 kbar, 750°C (Fig. 1.6 in Smith, 1988).

Liset

Subsequently, much larger crystals of nyböite were found in the Liset kyanite-eclogite pod near Selje in Møre og Romsdal, also in Vestlandet (Kechid, 1984; Kechid and Smith, 1982, 1985). Lisetite, a new Ca-Al-silicate, was discovered in a retrogressed part of this eclogite and this new mineral was also named by DCS after its locality (Rossi *et al.*, 1986; Smith *et al.*, 1986). At Liset, in addition to nyböite and lisetite, several other unusual mineral compositions occur (e.g. preiswerkite, 'Na-eastonite', 'Na-margarite', Al-F-rich titanite: Kechid, 1984; Smith, 1988), as well as many critical petrographical features such as the first evidence of co-existing jadeite + quartz in Norway (Kechid and Smith, 1985; Smith, 1988) and "deduced coesite" (from radial cracks into the host garnet; Smith 1984, 1988). These discoveries clearly placed the Liset eclogite pod within the "Norwegian coesite-eclogite province" (Smith, 1984) to which the Nybö eclogite pod was also attached. Oberti *et al.* (1989) demonstrated that the trend of variation of amphibole composition with retrogression at Liset followed a sublinear trend subparallel to that of the join nyböite-taramite-sadanagaite, i.e. {1221} to {1122} to {1023} which involves the "plagioclase-type" exchange, i.e. ${}^BNa^+ + {}^T Si^{4+} \rightarrow {}^B Ca^{2+} + {}^T Al^{3+}$ [here the D site of Smith (1988) is replaced by the T symbol used by Leake *et al.* (1997) and by crystallographers].

When reviewing coesite and diamond occurrences in Norway, Smith (1995, p. 316) reiterated his earlier suggestion that the nyböite may have been coeval with the "deduced coesite" at Liset such that nyböite might have been stable in the 25–45 kbar P range rather than the 15–25 kbar range deduced previously (see above). The diamond stability field arrives at only ~5 kbar above the 32 kbar maximum used in the experiments of Pawley (1992), so it is not inconceivable that nyböite could coexist with diamond.

Jianchang

The UHPM studies developed in a similar fashion in China as they had done in Norway a

decade earlier. Thus Yang and Smith (1989) defined the “Su-Lu coesite-eclogite province” on the basis of deduced coesite in the Lanshantou eclogite. Other workers found definite coesite elsewhere in the Su-Lu province (Hirajima *et al.*, 1990). In a paragonite-kyanite-eclogite from the Jianchang kyanite eclogite pod near Donghai (Su-Lu, China) described by Yang (1991), abundant nyböite was found by DCS and this new discovery was reported at the Third International Eclogite Conference when treating related subjects (Oberti *et al.*, 1989; Yang and Smith, 1989). The retrogressive trend towards aluminomagnesirotaramite, similar to those found at Nybö and Liset, was briefly discussed in Smith *et al.* (1990). Hirajima *et al.* (1992) deduced peak *P-T* conditions in the Jianchang eclogite at $\sim 740 \pm 60^\circ\text{C}$ and > 28 kbar. They also recorded evidence of “deduced coesite” at Jianchang.

Zhang *et al.* (1995) provided more comments on the nyböite at Jianchang, in particular that it formed at the peak *P-T* conditions and that these were revised to $T = 700\text{--}890^\circ\text{C}$ and $P > 28$ kbar. These conditions are well within the coesite-eclogite subfacies (cf. Smith *et al.*, 1990; Smith, 1995, see above).

Fluorine

Unlike at Nybö, which has an orthopyroxene-lineage eclogite (Mg-rich, Al-poor bulk-rock composition below the pyrope-wollastonite join on an ACF diagram (see below) and hence contains orthopyroxene in relatively anhydrous samples and phlogopite in hydrous ones), fluorine exists in abundance in the nyböite at Liset which is a kyanite-lineage eclogite (Mg-poor, Al-rich bulk-rock composition above the pyrope-wollastonite join on an ACF diagram and hence contains kyanite in relatively anhydrous samples and phengite, paragonite and/or (clino)zoisite in hydrous ones) (Smith, 1976). The Liset eclogite pod is also famous for the first discovery of Al-F-titanite (Smith, 1977), another phase generally attributed to high-pressure metamorphism (Smith, 1988) as it was shown experimentally to be stable up to at least 40 kbar (Smith, 1981). At Jianchang, F actually exceeds OH in some nyböite crystals, thus giving us the occasion to recognize a new mineral species.

‘Ferronyböite’

Hirajima and Compagnoni (1993) discovered “ferronyböite” in a jadeite-bearing fels of the UHPM Brossasco-Isasca unit (BIU), southern

Dora-Maira Massif, Western Alps, Italy. The “ferronyböite” was deduced to have formed after the peak assemblage of phengite-coesite-eclogite, under low-temperature eclogite-facies conditions at $\sim 500\text{--}570^\circ\text{C}$ and 12–15 kbar prior to further retrogression where “ferronyböite” was partially replaced by aluminomagnesirotaramite (i.e. again the same f_{Al} trend as above, but the whole trend at lower *P* because of the role of Fe mentioned above). Application for the IMA recognition of the new species ferronyböite was never made (T. Hirajima, pers. comm., 2002), partly because the compositions are close to the 50:50 limit along the Mg-Fe²⁺ join. Fluorine was not mentioned in the Italian occurrence.

‘Ferric-nyböite’

Given the occurrence of most Fe³⁺-rich amphibole compositions in lower-*P*, higher-*T* petrologic environments than their Al-rich counterparts (e.g. arfvedsonite, riebeckite), it may be predicted that “ferric-nyböite” should be stable at lower *P* and/or higher *T* conditions than nyböite, such that it is unlikely to be ever found in eclogite.

$F \rightleftharpoons OH$ exchange

It is of particular relevance to examine the influence of the substitution of OH by F in fluoronyböite, i.e. the factor $X_{\text{F}} = F/(F + OH)$, but this is somewhat difficult as few experimental data are available, and even where they are, “a rigorous application....to natural systems is precluded” (Welch and Graham (1992, p. 257). Low-*P* high-*T* amphiboles are often rich in Fe³⁺ (arfvedsonite, riebeckite) and/or Ti (kaersutite); they tend also to have more K and/or F. Deer *et al.* (1992, p. 253) state that “experiments have shown that the substitution of F for OH significantly increases the stability of a hornblende”, apparently meaning stability towards increasing *T*. However, in natural samples with so many minor elements, the crystal-chemical effect of the other elements may well mask the true behaviour of F.

Welch and Graham (1992) extrapolated between the pure (OH) system of Pawley (1992), who showed (p. 187) that the stability field of F-bearing ‘quaternary’ nyböitic amphibole “is shifted to higher *P* with respect to” F-free compositions and their own pure F system and deduced that “reducing water activity destabilises glaucophane relative to more nyböitic amphiboles” (p. 255) on the basis that “analogous field

boundaries in NMAF are displaced to pressures about 4 kbar higher than in NMASH" (p. 255). Thus with X_F and T fixed, all the data fit the initial interpretation (Smith, 1982, 1988) that f_{Al} increases with P thus favouring glaucophane over nyböite towards higher P . Increasing X_F favours nyböite and pushes mineral reactions and specific f_{Al} compositions towards higher P according to Welch and Graham (1992), but their NMAF amphiboles became poorer in nyböite above 24 kbar whereas similarly nyböite-rich compositions in NMASH amphiboles survived to at least 32 kbar (Pawley, 1992). This appears to be contradictory but it may be noted that Welch and Graham (1992) discussed in detail the experimental work of Koons (1982) and Carman and Gilbert (1983) on similar compositions in the same system NMASH as Pawley (1992), and they found numerous discrepancies in the results or in the interpretations of the dataset. In particular, differences in the kind of starting materials, and doubts over the degree of saturation in H_2O in the three other cited studies were mentioned.

One may conclude from this that all is not yet clear, and that it is risky to extrapolate to natural systems where other elements like Ca and Fe are important, and where the coexisting minerals at Liset and Jianchang include kyanite, (clino)zoisite or paragonite rather than the talc or Na-phlogopite of the experiments. It is perhaps useful to emphasize that although the mineral composition nyböite contains 3 Mg a.p.f.u., it also contains 3 Al a.p.f.u. which places it above the garnet join on an ACF diagram (a key boundary in this $[Al^{3+} + Fe^{3+} + Cr^{3+}] - Ca^{2+} - [Fe^{2+} + Mn^{2+} + Mg^{2+}]$ diagram where $\Sigma R^{3+}:\Sigma R^{2+} = 2:3$), hence in the field of kyanite-lineage eclogites. Thus although nyböite is a magnesian mineral (highly magnesian compared to Fe^{2+} and Ca, but not to Al), it occurs inside highly aluminous (and highly sodic) rocks at Liset and Jianchang. At Nybö, although other rock samples are indeed highly magnesian, less sodic and more potassic orthopyroxene-lineage rocks with orthopyroxene and/or phlogopite, the nyböite is only found in the unique rock layer which is effectively a garnet-jadeite and hence also highly aluminous (and highly sodic). Thus nyböite is confined to relatively Na- and Al-rich K- and Mg-poor bulk rock compositions, exactly as is the case for lisetite (Smith *et al.*, 1986).

Robert *et al.* (2000) and Della Ventura *et al.* (2001) showed that the OH-F solid-solution in amphiboles is strongly controlled by the local

bond-valence equilibria around the O3 oxygen, i.e. by the degree of local interaction of the OH group with the NNN O atoms. The OH groups involved in lower hydrogen-bonding with neighbouring oxygen atoms, and characterized by higher frequencies of vibration in IR spectra, are easily exchanged with F. On the contrary, the OH groups involved in higher hydrogen-bonding, characterized by lower frequencies in IR spectra, are not easily exchanged. This kind of behaviour has been well characterized in pargasite (Robert *et al.*, 2000) and in mixed pargasite-richterite amphiboles (Della Ventura *et al.*, 2001), where the OH-F solid-solution is controlled by ordering of cations at the octahedral sites.

Other crystal-structural considerations include the fact that the replacement of OH by F in amphiboles both decreases the volume of the $M1$ and $M3$ sites and eliminates H^-Na hindrance; the consequent decrease of the unit-cell volume strongly favours high- P stability. Moreover, in hydrous minerals such as amphiboles, F increases the thermal stability (no chance of dehydrogenation and crystal collapse); thus F should be ideal under high- P high- T conditions.

As a tentative conclusion one can deduce that increasing X_F may extend the stability of fluoronyböite to higher P and higher T compared to that of nyböite, but the complexities of the effects of other elements such as Ca and Fe render the X_F factor somewhat unreliable.

Formal description of the species

Occurrence of the holotypes

Fluoronyböite

Sample DJ102, which contains the holotype specimen, is a kyanite-bearing eclogite from the Jianchang eclogite pod (Yang, 1991) in the Su-Lu coesite-eclogite province, China (Yang and Smith, 1989; Smith *et al.*, 1990). This is one of the localities in the Jiangsu (Su) and Shandong (Lu) provinces of Eastern China where "deduced coesite" occurs, i.e. particular textures of quartz after coesite (Smith, 1988; Hirajima *et al.*, 1992).

Associated minerals in this sample are "fluoroaluminomagnesiotalc", pargasite, clinopyroxenes ($\sim Jd_{70}Ae_{20}Di_{10}$), garnet ($\sim Alm_{60}Prp_{21}Grs_{17}Sps_{02}$), rutile, apatite, paragonite, plagioclase. Fluoronyböite coexisted with clinopyroxene, garnet and rutile during high- P eclogite-facies conditions, and occurs as a relict phase in the retrograded eclogite sample DJ102 where the lower- P conditions are manifested by

symplectitic rims of plagioclase and taramitic amphiboles around clinopyroxene crystals.

The holotype crystal has been deposited in the Museo di Mineralogia of the Dipartimento di Scienze della Terra, Università di Pavia, under the code 2002-01.

Nyböite

Holotype nyböite occurs as crystal E2 in the rock specimen G230F found in the Nybö eclogite pod, Nordfjord, Vestlandet, Norway (Ungaretti *et al.*, 1981). The thin section is deposited at the Mineralogical Gallery of the Muséum National d'Histoire Naturelle, Paris (no. 181.55).

The Nybö eclogite pod is tectonically enclosed within amphibolite-facies country-rock gneisses. A particular feature of this rock, apparently still unique, is the extreme compositional diversity of clinopyroxenes and amphiboles on a scale of a few centimetres. These variations can be expressed by $X_{\text{Na}} = \text{Na}/(\text{Na}+\text{Ca})$ [total chemical content regardless of which crystallographic site]; X_{Na} varies from 0.21 to 0.81 in clinopyroxenes (Smith *et al.*, 1980; Rossi *et al.*, 1983) and from 0.45 to 0.91 in amphiboles (Ungaretti *et al.*, 1981). Nyböite occurs only in contact with clinopyroxene with $X_{\text{Na}} = 0.65\text{--}0.75$, and it was initially supposed to have formed by hydration of Jd-rich clinopyroxene during decompression from the higher-*P* anhydrous-eclogite-facies (30–45 kbar) to the medium-*P* hydrous-eclogite-facies (~23 kbar; Smith, 1976, 1988). The finding of nyböite at Liset and at Jianchang suggests that nyböite may well have been stable in the coesite-eclogite facies at the highest pressures achieved and hence may have not grown from clinopyroxene but with clinopyroxene (Smith *et al.*, 1990; Smith, 1995; Zhang *et al.*, 1995).

distinctive. Fluoronyböite is bluish-grey in colour, with a translucent lustre, and is very similar to nyböite. Tenacity: brittle. Density (calc.) = 3.18 g/cm³. Biaxial negative, 2V medium. Refractive indices calculated from the empirical formula by means of the linear regression equations of Winchell (1963) are $\alpha = 1.633$ (36), $\beta = 1.624$ (20), and $\gamma = 1.626$ (25); the fact that α is > β and γ is indicative of errors in these equations, perhaps associated with the treatment of fluorine.

Analytical methods

X-ray analysis and structure refinement

Several amphibole crystals from sample DJ102 were mounted on a Philips PW-1100 four-circle diffractometer, and examined with graphite-monochromatized Mo-*K* α X-radiation; the crystal quality was assessed via profile analysis of Bragg diffraction peaks. Unit-cell dimensions were calculated from least-squares refinement of the *d* values obtained from 60 rows of the reciprocal lattice by measuring the centroid of gravity of each reflection and of the corresponding antireflection in the range $-30 < \theta < 30^\circ$. Intensity data were collected for the monoclinic-equivalent pairs (*hkl* and *h-kl*) in the range $2 < \theta < 30^\circ$; they were corrected for absorption, Lorentz and polarization effects, averaged and reduced to structure factors ($R_{\text{int}} \approx 1\%$).

Structure-refinement procedures were as described in Oberti *et al.* (1992) and Hawthorne

TABLE 1. Selected crystal data for holotype fluoronyböite from Jianchang (DJ102-5) and nyböite from Nybö (G230F-E2).

Mineral data

Nyböite is grey-green in colour, with vitreous lustre; cleavage {110}, poor, hardness (Mohs) = 6, density = 3.12 (meas.), 3.13 (calc.) g/cm³. Optically, it is biaxial negative, 2V medium. Refractive indices calculated from the ideal formula after the method of Winchell (1963) are $\alpha = 1.65$ and $\gamma = 1.67$ (no measurement could be made on the holotype pieces because they are embedded in epoxy resin). In thin-section, nyböite is pleochroic, α colourless, β pale brownish-pink, and γ pale bluish-green. The β colour, also called "pale pink-violet" or "lilac", tends towards that characteristic of glaucophane and is quite

	DJ102-5	G230F-E2
<i>a</i> (Å)	9.666 (4)	9.665 (1)
<i>b</i> (Å)	17.799 (6)	17.752 (2)
<i>c</i> (Å)	5.311 (2)	5.303 (1)
β (°)	104.10 (3)	104.11 (1)
<i>V</i> (Å ³)	886.2 (8)	882.4 (2)
<i>d</i> _{calc} g/cm ³	3.18	3.12
<i>N.</i> of measured refl.	2612	2581
<i>N.</i> of unique refl	1348	1335
<i>N.</i> of observed refl. (<i>I</i> >3 σ)	1146	1188
<i>R</i> _{int} (%)	0.9	2.0
<i>R</i> _{all} (%)	2.0	2.8
<i>R</i> _{obs} (%)	1.3	2.3

FLUORONYBÖITE AND NYBÖITE

TABLE 2. Atom coordinates, refined site-scattering values (ss, e.p.f.u.), atomic-displacement parameters (B_{eq} , Å²; $\beta_{ii} \times 10^4$) for holotype fluoronyböite (DJ102-5, first line) and nyböite (G230F-E2, second line).

Atom	ss (e.p.f.u.)	x/a	y/b	z/c	B_{eq}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O1		0.1077 (1)	0.0908 (1)	0.2093 (2)	0.74 (2)	19	7	62	-2	11	-3
		0.1072 (1)	0.0920 (1)	0.2089 (3)	0.69 (3)	20	6	62	-1	10	-2
O2		0.1184 (1)	0.1717 (1)	0.7430 (2)	0.71 (2)	17	6	71	0	4	-1
		0.1180 (1)	0.1724 (1)	0.7446 (3)	0.66 (3)	19	4	72	1	6	-1
O3	17.20 (6)	0.1086 (1)	0	0.7064 (2)	0.90 (3)	25	7	88	-	6	-
	-	0.1109 (2)	0	0.7069 (4)	0.76 (4)	26	4	78	-	7	-
O4		0.3666 (1)	0.2527 (1)	0.8004 (2)	0.84 (2)	31	5	86	-3	23	-2
		0.3676 (1)	0.2528 (1)	0.8011 (3)	0.74 (3)	29	4	78	-3	21	-2
O5		0.3544 (1)	0.1340 (1)	0.0935 (2)	1.03 (2)	20	12	82	1	6	15
		0.3541 (1)	0.1344 (1)	0.0955 (3)	1.00 (3)	23	11	79	0	7	13
O6		0.3425(1)	0.1204 (1)	0.5920 (2)	0.90 (2)	22	8	86	0	9	-10
		0.3417 (1)	0.1197 (1)	0.5945 (3)	0.92 (3)	25	7	94	1	10	-12
O7		0.3390 (1)	0	0.2913 (3)	1.10 (3)	30	6	136	-	15	-
		0.3368 (2)	0	0.2892 (4)	1.04 (4)	31	5	135	-	13	-
T1		0.2825 (1)	0.0869 (1)	0.2966 (1)	0.47 (1)	14	4	41	-1	5	-1
		0.2816 (1)	0.0872 (1)	0.2973 (1)	0.45 (1)	16	3	42	-1	6	-1
T2		0.2917 (1)	0.1732 (1)	0.8095 (1)	0.49 (1)	15	4	41	-1	6	0
		0.2913 (1)	0.1737 (1)	0.8106 (1)	0.45 (1)	17	2	42	-1	7	0
M1	29.65 (8)	0	0.0908 (1)	½	0.55 (1)	19	5	40	-	9	-
	26.86 (12)	0	0.0902 (1)	½	0.55 (2)	21	4	41	-	13	-
M2	33.03 (8)	0	0.1797 (1)	0	0.55 (1)	16	4	53	-	9	-
	29.50 (11)	0	0.1796 (1)	0	0.47 (2)	18	2	50	-	9	-
M3	15.70 (5)	0	0	0	0.55 (1)	21	3	44	-	5	-
	14.96 (6)	0	0	0	0.58 (2)	23	4	42	-	7	-
M4	26.26 (5)	0	0.2780 (1)	½	0.99 (2)	35	6	109	-	37	-
	25.42 (8)	0	0.2782 (1)	½	0.91 (3)	35	5	101	-	37	-
A	0.77 (2)	0	½	0	1.0 (3)	8	15	114	-	29	-
	1.86 (3)	0	½	0	1.8 (3)	20	26	141	-	14	-
Am	6.68 (6)	0.0516(4)	½	0.1107 (8)	2.7 (1)	73	29	236	-	87	-
	2.70 (9)	0.0403 (14)	½	0.0987 (23)	2.5 (3)	98	16	262	-	115	-
A2	1.95 (6)	0	0.4763 (6)	0	3.1 (2)						
	3.98 (8)	0	0.4718 (4)	0	2.3 (2)						
H	0.9 (1)	0.195(8)	0	0.762 (12)	0.7 (1)						
	1.9 (1)	0.188 (5)	0	0.745 (8)	2.0 (1)						

et al. (1995). Reflections with $I > 3\sigma_I$ were considered as observed during unweighted full-matrix least-squares refinement on F . Scattering curves for fully ionized chemical species were used at sites where chemical substitutions occur; neutral vs. ionized scattering curves were used at the T and anion sites (except O3, where the curve of F^- was refined against that of O^-). For the crystal closest to the fluoronyböite end-member composition (sample DJ102-5), refinement information and final R values in the space group $C2/m$ are given in Table 1; atom positions, refined site-scattering values and atom displacement parameters are given in Table 2; and selected

interatomic distances and angles are given in Table 3. Lists of the observed and calculated structure factors have been deposited with the editor. Given the large chemical variability found in each rock sample, powder diffraction data were calculated from the single-crystal refinement; they are reported in Table 4.

Crystallographic and chemical data obtained with similar analytical procedures for the crystal (rock sample G230F, crystal E2) used for the recognition of the new end-member nyböite by D.C. Smith and L. Ungaretti are also reported in the Tables. More experimental details can be found in Ungaretti *et al.* (1981).

TABLE 3. Selected interatomic distances (Å) and angles (°) for holotype fluoronyböite and nyböite.

	DJ102-5	G230F-E2		DJ102-5	G230F-E2
T1-O1	1.641 (1)	1.638 (1)	A-O5	× 4 2.873 (1)	2.878 (1)
-O5	1.647 (1)	1.644 (1)	-O6	× 4 3.162 (1)	3.142 (1)
-O6	1.646 (1)	1.645 (1)	-O7	× 2 2.447 (1)	2.453 (2)
-O7	1.643 (1)	1.642 (1)	<A-O>	2.904	2.899
<T1-O>	1.644	1.642	Am-O5	× 2 3.040 (1)	2.986 (1)
T2-O2	1.626 (1)	1.626 (1)	-O5	× 2 2.858 (1)	2.882 (1)
-O4	1.595 (1)	1.592 (1)	-O6	× 2 2.711 (1)	2.749 (1)
-O5	1.639 (1)	1.640 (1)	-O7	2.470 (1)	2.420 (2)
-O6	1.654 (1)	1.657 (1)	-O7	3.094 (2)	3.173 (2)
<T2-O>	1.628	1.629	-O7	2.603 (1)	2.614 (2)
M1-O1	× 2 2.062 (1)	2.059 (1)	<Am-O>	2.821	2.827
-O2	× 2 2.082 (1)	2.095 (1)	A2-O5	× 2 2.534 (1)	2.480 (2)
-O3	× 2 2.086 (1)	2.085 (1)	-O6	× 2 2.893 (1)	2.828 (1)
<M1-O>	2.077	2.079	-O7	× 2 2.483 (1)	2.504 (1)
M2-O1	× 2 2.064 (1)	2.040 (1)	<A2-O>	2.637	2.604
-O2	× 2 1.988 (1)	1.975 (1)			
-O4	× 2 1.889 (1)	1.879 (1)	O3-H	0.824 (1)	0.725 (2)
<M2-O>	1.980	1.965	T1-T1	3.095 (1)	3.097 (1)
M3-O1	× 2 2.090 (1)	2.099 (1)	T1-T2	3.028 (1)	3.023 (1)
-O3	× 4 2.081 (1)	2.092 (1)	T1-T2	3.110 (1)	3.106 (1)
<M3-O>	2.087	2.097			
M4-O2	× 2 2.415 (1)	2.406 (2)	O5-O6-O5	168.6 (1)	167.7 (1)
-O4	× 2 2.347 (1)	2.342 (1)	Am-O3	3.190 (2)	3.277 (2)
-O5	× 2 2.760 (1)	2.743 (2)	Am-Am	1.343 (1)	1.142 (1)
-O6	× 2 2.488 (1)	2.501 (2)			
<M4-O>	2.502	2.498			

Chemical analysis

The fluoronyböite crystal used for the structure refinement was mounted in epoxy resin, polished, carbon-coated and analysed with a Cameca SX-50 electron microprobe; ten points were analysed in different zones, and then averaged. The following standards and crystals were used for $K\alpha$ X-ray lines: Si, Ca: tremolite, PET; Ti: hornblende, LiF; Fe: arfvedsonite, LiF; Mn: tephroite, LiF; Mg: tremolite, TAP; Na and Al: albite, TAP; K: orthoclase, PET; F: fluororiebeckite, TAP; Zn: willemitte, LiF. Data were processed as discussed in detail in Oberti *et al.* (1992). Details of electron microprobe analysis of holotype nyböite are given in Ungaretti *et al.* (1981).

Unit-formulae were calculated on the basis of 24 (O, OH, F). The good agreement between the group-site scattering values calculated from the unit formulae and those resulting from structure refinement (Table 5) constitutes good evidence for their high accuracy. However, optimization of

these unit formulae may be attempted on the basis of the refinement results. For instance, in nyböite the refined <T2-O> distance rules out the presence of Al at the T2 site, whereas the refined <T1-O> distance suggests a little more tetrahedral Al at the T1 site (~0.78 a.p.f.u.; Oberti *et al.*, 1995). Also, the unit formula in Table 5 would result in a longer <M2-O> distance (1.969 Å; cf. the next section for details) and a lower site scattering at M2 (28.34 e.p.f.u.) than those refined (1.965 Å and 29.50 e.p.f.u., respectively). All these discrepancies can be reduced by increasing the Al content at the T1 site, and considering as trivalent all the Fe at the M2 site. The following crystal-chemical formula can thus be proposed for nyböite G230F-E2: ${}^A(\text{Na}_{0.79}\text{K}_{0.03})_{\Sigma 0.82}{}^B(\text{Na}_{1.65}\text{Ca}_{0.35})_{\Sigma 2.00}{}^C(\text{Mg}_{2.99}\text{Fe}_{0.41}^{2+}\text{Fe}_{0.20}^{3+}\text{Al}_{1.37}\text{Ti}_{0.02}\text{Ni}_{0.01})_{\Sigma 5.00}{}^T(\text{Si}_{7.22}\text{Al}_{0.78})_{\Sigma 8.00}\text{O}_{22}{}^X(\text{OH})_2$. Relevant site populations and calculated vs. refined values of the relevant parameters are provided in Table 6 for fluoronyböite and nyböite.

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 TABLE 4. X-ray (Cu- $K\alpha$) powder diffraction patterns ($I > 15$) calculated from single crystal data; the nine strongest reflections are given in bold*.

Fluoronyböite DJ102-5				Nyböite G230F-E2			
<i>I</i>	2 θ	$d_{\text{calc.}}$	<i>h k l</i>	<i>I</i>	2 θ	$d_{\text{calc.}}$	<i>h k l</i>
64	10.65	8.307	1 1 0	60	10.65	8.307	1 1 0
15	18.20	4.874	-1 1 1	17	18.25	4.861	-1 1 1
18	19.90	4.462	0 2 1	20	19.95	4.450	0 2 1
26	19.95	4.450	0 4 0	31	20.00	4.439	0 4 0
42	26.35	3.382	1 3 1	42	26.40	3.376	1 3 1
24	27.65	3.226	2 4 0	27	27.70	3.220	2 4 0
58	29.00	3.079	3 1 0	55	29.00	3.079	3 1 0
25	30.45	2.936	2 2 1	32	30.50	2.931	2 2 1
100	33.30	2.691	1 5 1	100	33.35	2.687	1 5 1
			-3 3 1				-3 3 1
21	34.85	2.574	0 0 2	16	34.90	2.571	0 0 2
35	34.90	2.571	0 6 1	36	35.00	2.564	0 6 1
47	35.45	2.532	-2 0 2	51	35.50	2.529	-2 0 2
25	39.15	2.301	-3 5 1	26	39.20	2.298	-3 5 1
13	39.50	2.281	-4 2 1	15	39.50	2.281	-4 2 1
18	39.90	2.259	-3 1 2	18	39.95	2.257	-3 1 2
27	42.10	2.146	2 6 1	28	42.15	2.144	2 6 1
22	56.25	1.635	4 6 1	23	56.30	1.634	4 6 1
19	58.30	1.583	-1 5 3	19	58.40	1.580	-1 5 3
23	61.35	1.511	-2 6 3	26	61.45	1.509	-2 6 3
			1 9 2				1 9 2
14	61.45	1.509	-6 0 2	23	61.50	1.508	-6 0 2
			-6 6 1				-6 6 1
23	66.10	1.414	-6 6 1	25	66.15	1.413	-6 6 1

* Tables of observed and calculated structure factors for fluoronyböite and nyböite have been deposited with the Editor and are available from www.minersoc.org/pages/e.journals/dep_mat.htm

Crystal-chemical discussion

The two crystals studied in this work differ mainly in their F content, but also to a minor extent in their octahedral composition, especially $X_{\text{Mg}} = \text{Mg}/(\text{Mg}+\text{Fe}^{2+})$; however, the latter point has no bearing on the terminological distinction of these two mineral species as they are both Mg-dominant.

In fluoronyböite, refinement of H-site occupancy yielded an approximate value of 0.90 a.p.f.u., in agreement with the calculated unit formula and with the absence of dehydrogenation. Fluorine is located at the O3 site, which is bonded to two *M1* and one *M3* sites; therefore, the fluorine content should affect essentially only the *M1*-O3 and *M3*-O3 distances and, hence, also the average $\langle M1-O \rangle$ and $\langle M3-O \rangle$ distances (by -0.013 \AA per F a.p.f.u.; Oberti *et al.*, 1993).

The sizes of the three independent octahedra also depend upon their site population (Table 6),

and the mean distances can be calculated based on regression equations which provide modelling of the amphibole structure constrained by the database available at CNR-IGG-PV (formerly CNR-CSCC). Comparison of the calculated and refined distances results in a fair agreement for the *M2* site, but significant differences at the *M1* and *M3* sites. In nyböite the *M1* site is smaller, but the *M3* site is far larger, than expected on the basis of site population; in fluoronyböite, on the other hand, both the *M1* site and especially the *M3* site are larger than expected on the basis of octahedral site populations and F content. These features show that the exchange $F_1(\text{OH})_{-1}$ at the O3 site cannot be modelled simply on the basis of changes in the ionic radii, but require a strong local relaxation.

Another high-pressure amphibole end-member is glaucophane {0220}, which has the same ideal composition as nyböite {1221} at the *M4* and at the octahedral sites, but has a vacant *A* site and no tetrahedral Al. Relaxation at the *M3* site is also

TABLE 5. EMP analyses and unit formulae for holotype fluoronyböite and nyböite; ss = site scattering; H₂O wt.% calculated to obtain 2 (OH+F) a.p.f.u. at the *X* site.

	DJ102-5	G230F-E2		DJ102-5	G230F-E2
SiO ₂	50.15	52.50	Si	7.14	7.26
TiO ₂	0.13	0.16	Al	0.86	0.74
Al ₂ O ₃	12.35	12.97	Σ <i>T</i> sites	8.00	8.00
Cr ₂ O ₃	0.02	0.00	Al	1.21	1.37
Fe ₂ O ₃	2.94	1.40	Mg	2.55	2.99
FeO	7.47	4.04	Ti	0.01	0.02
MnO	0.09	0.02	Fe ²⁺	0.89	0.46
MgO	12.07	14.50	Fe ³⁺	0.32	0.15
ZnO	0.05	0.00	Mn ²⁺	0.01	0.00
NiO	0.00	0.11	Ni	0.00	0.01
CaO	3.03	2.33	Zn	0.01	0.00
Na ₂ O	8.40	9.26	Σ <i>C</i> sites	5.00	5.00
K ₂ O	0.32	0.14	Ca	0.47	0.35
F	2.58	0.00	Na	1.53	1.65
(H ₂ O)	0.88	2.17	Σ <i>B</i> sites	2.00	2.00
O=F,Cl	1.09	0.00	Na	0.78	0.82
Total	99.39	99.60	K	0.06	0.03
			Σ <i>A</i> sites	0.84	0.85
			F	1.16	0.00
			OH	0.84	2.00
			Σ <i>X</i> site	2.00	2.00
ss values calculated from unit formulae			Refined ss values		
ss <i>C</i> sites	78.56	70.27	ss <i>C</i> sites	78.38	71.32
ss <i>B</i> sites	26.23	25.15	ss <i>B</i> sites	26.26	25.42
ss <i>A</i> sites	9.72	9.59	ss <i>A</i> sites	9.40	8.54
ss <i>A+B+C</i> sites	114.51	105.01	ss <i>A+B+C</i> sites	114.04	105.28
ss <i>X</i> site	17.16	16.00	ss <i>X</i> site	17.20	16.00

TABLE 6. Site populations and agreement parameters in holotype fluoronyböite (first line) and in nyböite (second line); ss = site scattering values; mbl = mean bond length.

Site	Site population (a.p.f.u.)	ss (e.p.f.u.)		mbl (Å)	
		refined	calculated	refined	calculated
T1	0.86 Al + 3.14 Si			1.644	1.645
	0.78 Al + 3.22 Si			1.642	1.642
M1	1.60 Mg + 0.40 Fe ²	29.65	29.60	2.077	2.072
	1.80 Mg + 0.20 Fe ²⁺	26.86	26.80	2.079	2.083
M2	0.21 Mg + 1.21 Al + 0.01 Ti + 0.24 Fe ³⁺ + 0.32 Fe ³⁺ + 0.01 Zn	33.03	33.33	1.980	1.982
	0.40 Mg + 1.37 Al + 0.02 Ti + 0.20 Fe ³⁺ + 0.01 Ni	29.50	28.53	1.965	1.967
M3	0.74 Mg + 0.25 Fe ²⁺ + 0.01 Mn	15.70	15.63	2.087	2.076
	0.79 Mg + 0.21 Fe ²⁺	14.94	14.96	2.097	2.088

present in glaucophane, and has been discussed in detail in Ungaretti *et al.* (1978), who ascribed it to the presence of small trivalent cations at the two adjacent $M2$ sites and to the steric requirements of the double-chain of tetrahedra. The same reasoning holds for nyböite where the need for $M3$ relaxation is even stronger because the $AlSi_{-1}$ exchange increases the size of the $T1$ tetrahedron, which is connected to all the three independent octahedra *via* the $O1$ site. Therefore, both of these high- P amphibole compositions require significant divalent cation contents larger than Mg (i.e. Fe^{2+}), the site preference of which is actually $M3 > M1 > M2$ based on crystal-chemical knowledge and the observed pattern of octahedral distances.

The comparison of nyböite G230F-E2 and a glaucophane with very similar site populations at the $M1$ and $M3$ site but $1.76 Al + 0.24 Fe^{3+}$ a.p.f.u. at the $M2$ site (sample no. 2 in Ungaretti *et al.*, 1978; ss at $M1 = 27.44$ e.p.f.u., ss at $M3 = 15.21$ e.p.f.u.) is particularly interesting in this regard. The $M3-O1$ and $M2-O1$ distances are quite similar in the two samples (2.099 and 2.040 Å in G230F-E2 vs. 2.098 and 2.041 Å in glaucophane no. 2), whereas the $\langle M3-O \rangle$ and $\langle M2-O \rangle$ distances are very different (2.097 and 1.965 Å in G230F-E2 vs. 2.089 and 1.943 Å in glaucophane no. 2). On the contrary, the $\langle M1-O \rangle$ distances are similar (2.079 and 2.081 Å, respectively), whereas $M1-O1$ is much shorter in nyböite (2.059 vs. 2.070 Å). It is thus clear that the further bond strength contribution on $O1$ required by the presence of ^{71}Al in nyböite is provided by the $M1$ site. In terms of deformation of the strip of octahedra, the repetition unit along b and c tends to be maintained at the expense of a shrinking along a sinβ.

Comparison of nyböite and fluoronyböite is somewhat hindered by the different X_{Mg} ; however, it is apparent that the volume contraction in fluoronyböite is obtained by an homogeneous shrinking at the $M3$ site, and by a contraction of $M1-O2$ at the $M1$ site.

In glaucophane, the $^{71}Si-^{72}Si$ distance is very short (e.g. 3.004 Å in sample no. 2 from Ungaretti *et al.*, 1978), even shorter than that observed in coesite (3.016 Å); this distance is 3.023 and 3.028 Å in nyböite and fluoronyböite, respectively. The short intercationic distances and the need for significant Fe^{2+} contents are possible reasons for the well-known thermal instability of glaucophanic amphiboles (beyond 500°C for glaucophane and 400°C for ferroglaucophane), and for the instability of pure ideal glaucophane,

whether with OH or F (Pawley, 1992; Welch and Graham, 1992). Indeed the late L. Ungaretti pointed out that many pure ideal end-member amphiboles could not be stable because they need small amounts of extra (larger) elements to permit necessary geometrical matching. In nyböite, the presence of a larger and less charged cation at $T1$ both increases the $T-T$ distances and decreases repulsive interactions. These features and the filling of the large A cavity increase stability at high T (and P) conditions with respect to glaucophane, and this again explains why glaucophanic amphiboles are found in blueschists and nyböitic amphiboles in eclogites.

Notwithstanding the strong similarity of the A -group site populations, a major difference between nyböite and fluoronyböite is given by the ordering of the A cations. Hawthorne *et al.* (1996) showed that the presence of F at the $O3$ site strongly affects Na partitioning between the $A2$ and Am sites. In keeping with their observations, the shape of the electron density at the A -group sites (Fig. 1) shows that all Na is ordered at the $A2$ site in nyböite (and K is ordered at the Am site), whereas all Na and K are ordered at the Am site in fluoronyböite.

Conclusions

(1) The new mineral species fluoronyböite from Jianchang, China, has been fully characterized and is presented in this paper along with a detailed comparison with nyböite from Nybø, Norway, whose complete mineral description has finally been published.

(2) Major crystal-chemical differences concern the geometry of the octahedral sites and cation ordering at the A sites. Nyböite and especially fluoronyböite have a strong octahedral relaxation, which is also found in the other high- P (but lower- T) amphibole end-member, glaucophane.

(3) Nyböite and fluoronyböite occur in eclogites which share a number of UHPM characteristics (Nybø, Liset, Jianchang) and nowhere else to date (except Brossasco-Isasca for Fe^{2+} -richer compositions). It is possible that they are stable in nature in the coesite-eclogite subfacies (i.e. up to at least 32 kbar at 800°C: Fig. 1.6 in Smith, 1988) but since these rocks evolved along a depressurization path through the quartz-eclogite facies to the amphibolite facies, it is also possible that they may have grown only in the quartz-eclogite-facies (i.e. ~23 kbar at 750°C: Fig. 1.6 in Smith, 1988). However, they are

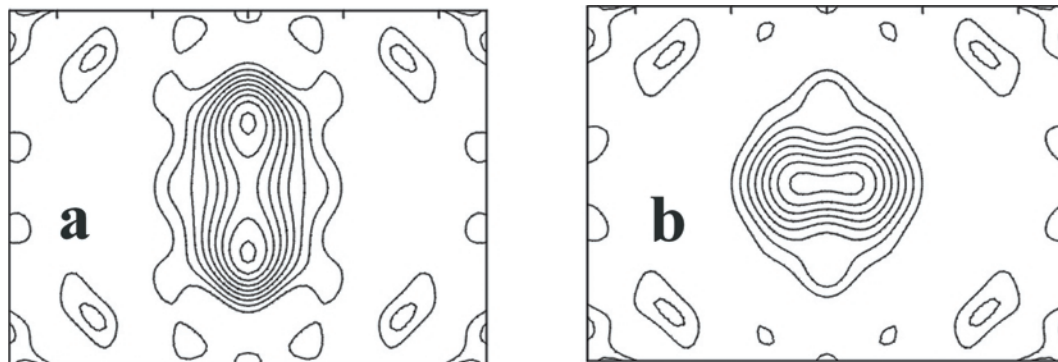


FIG. 1. The electron density at the A-group sites in fluoronyböite DJ102-5 (a) and nyböite G230F-E2 (b). F_o maps are calculated on sections parallel to (-201) ; the b axis is horizontal, and the contours are drawn with steps of $1 \text{ e}/\text{\AA}^3$ starting from 1.

certainly pre-amphibolite-facies minerals because aluminomagnesiotalcarnite replaces them in the amphibolite-facies at the two type localities, Nybö and Jianchang, and also at Liset, Norway (and also in Italy for the Fe^{2+} -rich analogues).

(4) The glaucophanic $\{0220\}$ to nyböitic $\{1221\}$ chemical trend involves principally the ${}^A\text{vacancy} + {}^T\text{Si}^{4+} \rightarrow {}^A\text{Na}^+ + {}^T\text{Al}^{3+}$ exchange which is related mainly to increasing T (decreasing f_{Al} and decreasing P/T ratio concomitant with a shift from blueschist to eclogite), whereas the nyböitic $\{1221\}$ to taramitic $\{1122\}$ chemical trend involves principally the ${}^B\text{Na}^+ + {}^T\text{Si}^{4+} \rightarrow {}^B\text{Ca}^{2+} + {}^T\text{Al}^{3+}$ exchange which is related mainly to decreasing P (decreasing f_{Al} and decreasing P/T ratio concomitant with a shift from eclogite to amphibolite).

(5) It is difficult to establish the petrological role of the $\text{F} \rightleftharpoons \text{OH}$ exchange with respect to P and T conditions, but there are some grounds to believe that in natural rocks fluoronyböite is stable at the same conditions as those of nyböite but also towards higher P and towards higher T .

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References

- Carman, J.H. and Gilbert, M.C. (1983) Experimental studies of glaucophane stability. *American Journal of Science*, **283A**, 414–437.
- Deer, W., Howie, R.A. and Zussman, J. (1992) *An Introduction to the Rock-forming Minerals*, 2nd edition. Longman, Harlow, Essex, UK.
- Della Ventura, G., Robert, J.-L., Sergent, J., Hawthorne, F.C. and Delbove, F. (2001) Constraints for the F-OH substitution in synthetic ${}^{[6]}\text{Al}$ -bearing monoclinic amphiboles. *European Journal of Mineralogy*, **13**, 841–847.
- Hawthorne, F.C., Ungaretti, L. and Oberti, R. (1995) Site populations in minerals: terminology and presentation of results. *The Canadian Mineralogist*, **33**, 907–911.
- Hawthorne, F.C., Oberti, R. and Sardone, N. (1996) Sodium at the A site in clin amphiboles: the effects of composition on patterns of order. *The Canadian Mineralogist*, **34**, 577–593.
- Hirajima, T. and Compagnoni, R. (1993) Petrology of a jadeite-quartz/coesite-almandine-phengite fels with retrograde ferro-nyböite from the Dora-Maira Massif, Western Alps. *European Journal of Mineralogy*, **5**, 943–955.
- Hirajima, T., Ishiwatari, A., Cong, B., Zhang, R., Banno, S., and Nozaka, T. (1990) Coesite from Mengzhong eclogite at Donghai county, northeastern Jiangsu province, China. *Mineralogical Magazine*, **54**, 579–583.
- Hirajima, T., Zhang, R., Li, J. and Cong, B. (1992) Petrology of the nyböite-bearing eclogite in the Donghai area, Jiangsu province, eastern China. *Mineralogical Magazine*, **56**, 37–46.
- Kechid, S.-A. (1984) *Etude pétrologique et minéralogique des éclogites de Liset, Stadlandet, Norvège*. Doctoral thesis, Muséum National d'Histoire Naturelle, Paris.
- Kechid, S.-A. and Smith, D.C. (1982) Nyböite-kataphorite et taramite-pargasite dans la lentille

- d'éclogite de Liset, Région du Gneiss de l'Ouest, Norvège. *9 ème Réunion Annuelle Sciences Terre, Paris, Société Géologique, France*, abstracts vol., p. 333.
- Kechid, S.-A. and Smith, D.C. (1985) The petrological evolution of the Liset eclogite pod, Norway. (Second International Eclogite Conference). *Terra Cognita*, **5**, 422.
- Koons, P.O. (1982) An experimental investigation of the behaviour of amphibole in the system Na₂O-MgO-Al₂O₃-SiO₂-H₂O at high pressures. *Contributions to Mineralogy and Petrology*, **79**, 258–267.
- Lappin, M.A. and Smith, D.C. (1978) Mantle-equilibrated orthopyroxene eclogite pods from the Basal Gneisses in the Selje District, Western Norway. *Journal of Petrology*, **19**, 530–584.
- Lappin, M.A. and Smith, D.C. (1981) Carbonate, silicate and fluid relationships in eclogites, Selje District and environs, SW Norway. *Transactions of the Royal Society of Edinburgh*, **72**, 171–193.
- Leake, B.E. (1978) Nomenclature of amphiboles. *Mineralogical Magazine*, **42**, 533–563.
- Leake, B.E., Woolley, A.R., Arps, C.E.S., Birch, W.D., Gilbert, M.C., Grice, J.D., Hawthorne, F.C., Kato, A., Kisch, H.J., Krivovichev, V.G., Linthout, K., Laird, J., Mandarino, J., Maresch, W.V., Nickel, E.H., Rock, N.M.S., Schumacher, J.C., Smith, D.C., Stephenson, N.C.N., Ungaretti, L., Whittaker, E.J.W. and Youzhi, G. (1997) Nomenclature of Amphiboles: Report of the Subcommittee on Amphiboles of the International Mineralogical Association Commission on New Minerals and Mineral Names. *Mineralogical Magazine*, **61**, 295–321.
- Oberti, R., Previde-Massara, E., Ungaretti, L., Kechid, S.-A. and Smith, D.C. (1989) Nyböite-taramite-sadanagaite trend in amphibole from the Liset eclogite pod, Norway: crystal-chemical and petrogenetical implications. (Third International Eclogite Conference), *Terra Abstracts*, **1**, 17.
- Oberti, R., Ungaretti, L., Cannillo, E. and Hawthorne, F.C. (1992) The behaviour of Ti in amphiboles. I. Four- and six-coordinated Ti in richterite. *European Journal of Mineralogy*, **7**, 1049–1063.
- Oberti, R., Hawthorne, F.C., Ungaretti, L. and Cannillo, E. (1993) The behaviour of Mn in amphiboles: Mn in richterite. *European Journal of Mineralogy*, **5**, 43–51.
- Oberti, R., Ungaretti, L., Cannillo, E., Hawthorne, F.C. and Memmi, I. (1995) Temperature-dependent Al order-disorder in the tetrahedral double-chain of C2/m amphiboles. *European Journal of Mineralogy*, **7**, 1049–1063.
- Pawley, A. (1992) Experimental study of the compositions and stabilities of synthetic nyböite-glaucophane amphiboles. *European Journal of Mineralogy*, **4**, 171–192.
- Raudsepp, M., Turnock, A.C. and Hawthorne, F.C. (1991) Amphibole synthesis at low pressure: what grows and what doesn't. *European Journal of Mineralogy*, **3**, 983–1004.
- Robert, J.-L., Della Ventura, G., Welch, M. and Hawthorne, F.C. (2000) OH-F substitution in synthetic pargasite at 1.5 kbar, 850°C. *American Mineralogist*, **85**, 926–931.
- Rossi, G., Smith, D.C., Ungaretti, L. and Domeneghetti, C. (1983) Crystal-chemistry and cation ordering in the system diopside-jadeite: a detailed study by crystal structure refinement. *Contributions to Mineralogy and Petrology*, **83**, 247–258.
- Rossi, G., Oberti, R. and Smith, D.C. (1986) The crystal structure of lisetite. *American Mineralogist*, **71**, 1378–1383.
- Smith, D.C. (1976) *The geology of the Vartdal Area, Sunnmøre, Norway, and the petrochemistry of the Sunnmøre Eclogite Suite*. PhD thesis, University of Aberdeen, UK, 750 pp.
- Smith, D.C. (1977) Aluminiumholdig titanit i eklogitter fra Sunnmøre. *Geolognytt*, **10**, 32–33.
- Smith, D.C. (1981) The pressure and temperature dependence of Al-solubility in sphene in the system Ti-Al-Ca-Si-O-F. *Progress Report Experimental Petrology*, **5**, NERC Publications Series **D18**, 193–197.
- Smith, D.C. (1982) The essence of an eclogite: Al^{vi}, as exemplified by the crystal-chemistry and petrology of high-pressure minerals in Norwegian eclogites. (First International Eclogite Conference), *Terra Cognita*, **2**, 300.
- Smith, D.C. (1984) Coesite in clinopyroxene in the Caledonides. *Nature*, **310**, 641–644.
- Smith, D.C. (1988) A review of the peculiar mineralogy of the "Norwegian coesite-eclogite province", with crystal-chemical, petrological, geochemical and geodynamical notes and an extensive bibliography. Pp. 1–206 in: *Eclogites and Eclogite-Facies Rocks* (D.C. Smith, editor). Developments in Petrology **12**, Elsevier, Amsterdam.
- Smith, D.C. (1995) Microcoesites and microdiamonds in Norway: an overview. Pp. 299–355 in: *Ultra-High Pressure Metamorphism (UHPM)* (R.G. Coleman and X. Wang, editors). Cambridge University Press, Cambridge, UK 528 pp.
- Smith, D.C., Kechid, S.-A. and Rossi, R. (1986) Occurrence and properties of lisetite, CaNa₂Al₄Si₄O₁₆, a new tektosilicate in the system Ca-Na-Al-Si-O. *American Mineralogist*, **71**, 1372–1377.
- Smith, D.C., Mottana, A. and Rossi, G. (1980) Crystal-chemistry of a unique jadeite-rich acmite-poor omphacite from the Nybö eclogite pod, Sörpollen, Nordfjord, Norway. *Lithos*, **13**, 227–236.

- Smith, D.C., Yang, J., Oberti, R. and Previde-Massara, E. (1990) A new locality of nyböite and taramite, the Jianchang eclogite pod in the "Chinese Su-Lu coesite-eclogite province", compared with the nyböite- and taramite-bearing Liset eclogite pod in the "Norwegian coesite-eclogite province". *15th Meeting of the IMA, Beijing, Abstracts*, vol. **2**, pp. 889–890.
- Ungaretti, L., Mazzi, F., Rossi, G. and Dal Negro, A. (1978) Crystal-chemical characterization of blue amphiboles. *Proceedings of the XI General Meeting of the IMA, Rock-forming minerals*, pp. 82–110.
- Ungaretti, L., Rossi, G. and Smith, D.C. (1981) Crystal chemistry by X-ray structure refinement and electron microprobe analysis of a series of sodic-calcic to alkali amphiboles from the Nybö eclogite pod, Norway. *Bulletin Société Française de Minéralogie et Cristallographie*, **104**, 400–412.
- Welch, M. and Graham, C.M. (1992) An experimental study of glaucophanic amphiboles in the system $\text{Na}_2\text{O}-\text{MgO}-\text{Al}_2\text{O}_3-\text{SiO}_2-\text{SiF}_4$ (NMAF): some implications for glaucophane stability in natural and synthetic systems at high temperatures and pressures. *Contributions to Mineralogy and Petrology*, **111**, 248–259.
- Winchell, H. (1963) Clinoamphibole regression studies. I. Regressions of optical properties and density on composition. *Mineralogical Society of America Special Paper*, **1**, 267–277.
- Yang, J. (1991) *Eclogites, garnet pyroxenites and related ultrabasics in Shandong and North Jiangsu of East China* [in Chinese with a brief summary in English]. Geological Society of China, Geological Publishing House, 99 pp.
- Yang, J. and Smith, D.C. (1989) Evidence for a former sanidine-coesite eclogite at Lanshantou, Eastern China, and the recognition of the Chinese "Su-Lu coesite-eclogite province". Third International Eclogite Conference, *Terra Abstracts*, **1**, 26.
- Zhang, R.-Y., Hirajima, T., Banno, S., Cong, B. and Liou, J.G. (1995) Petrology of ultrahigh-pressure rocks from the southern Su-Lu region, eastern China. *Journal of Metamorphic Petrology*, **13**, 659–675.

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