REVISION 1

Title: Beltrandoite, a new root-name in the högbomite supergroup: the Mg-end member magnesiobeltrandoite-2*N*3*S*

Running title: Magnesiobeltrandoite-2*N*3*S*

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Beltrandoite, a new root-name in the högbomite supergroup: the Mg-end member magnesiobeltrandoite-2*N*3*S*

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Abstract

Magnesiobeltrandoite-2*N*3*S*, ideally $Mg_6Al_{20}Fe^{3+}{}_2O_{38}(OH)_2$, is a new member of the högbomite supergroup of minerals. It occurs in Mg-chloritites of a metamorphosed layered mafic complex in the Etirol-Levaz continental slice of middle Valtournenche, Aosta Valley, Italy. Magnesiobeltrandoite-2*N*3*S* grows in fine-grained chlorite matrix associated as inclusions to relic pre-Alpine hercynite spinels and dolomite in cm- to dm-long darker boudins cut by corundum + clinochlore ± dolomite veins. It occurs as subhedral to black euhedral crystals (~ 50-400 μm), dark reddish-brown in thin section. It shows dark brown streak and vitreous luster. It is brittle, with no cleavage observed and uneven fracture. Mohs hardness ≈ 6-6½. D_{calc} = 3.93 g cm^{-3}. It shows no fluorescence under UV radiation and no cathodoluminescence. The mineral is optically uniaxial (–) with estimated mean refractive index ca. 1.80. Pleochroism is weak with ϵ = deep reddish brown (along *c* axis) and ω = reddish brown (⊥ to *c* axis). Absorption is E > O. The Raman spectrum shows a weak and strongly polarized broad OH-characteristic absorption centred at 3364 cm^{-1}. Electron microprobe analysis combined with Synchrotron Mössbauer source spectrometry yielded the following empirical formula based on 40 anions pfu $[Al_{18.36}Mg_{3.96}Fe^{2+}{}_{2.52}Fe^{3+}{}_{2.08}Ti_{0.56}Cr_{0.40}Zn_{0.06}V^{3+}{}_{0.03}Mn_{0.02}]_{\Sigma 28}O_{38}(OH)_2$. The ideal formula is $Mg_6Al_{20}Fe^{3+}{}_2O_{38}(OH)_2$.The eight strongest lines in the X-ray powder diffraction pattern are [d_{obs}/Å (*I*) (*hkl*)]: 2.858 (42)(110), 2.735 (51)(107), 2.484 (46)(018), 2.427 (100)(115), 1.568(29)(128), 1.514 (30)(0.2.12), 1.438 (42)(2.0.13), and 1.429 (72)(220). The crystal structure of magnesiobeltrandoite-2*N*3*S* [$P\bar{3}m1$, a = 5.7226(3), c = 23.0231(9) Å, V = 652.95(5) Å^3] was refined from X-ray single-crystal data to $R1$ = 0.022, and it is isostructural with magnesiohögbomite-2*N*3*S*.

Keywords: magnesiobeltrandoite-2*N*3*S*, crystal-structure refinement, electron microprobe analysis, chemical formula, högbomite-supergroup minerals, Valtournenche, Aosta Valley, Italy.

1. Introduction

Högbomite-supergroup comprises a series of complex oxide minerals related to the spinel-group minerals. It includes the högbomite, nigerite, and taaffeite groups, which form polysomatic series composed of spinel (S) and nolanite (N) modules (Armbruster 2002). The spinel module has $T_2M_4O_8$ and the nolanite module has $TM_4O_7(OH)$ composition, where T and M represent tetrahedrally and octahedrally coordinated cations. The nolanite module in nigerite and högbomite minerals has the formula $TM_4O_7(OH)$ whereas in taaffeite minerals is modified (*N*') and has the formula $BeTM_4O_8$. The composition and classification of these minerals depend on the composition of the nolanite module (that assigns the root-name), the composition of the spinel module (that determines the prefix) and the polysomatic sequence of *N* and *S* modules (that sets the suffix).

Regarding the root-names, the dominance of the tetravalent cation at the nolanite module, identifies högbomite from nigerite: if Ti-bearing, they are classified with the root-name högbomite; if Sn-bearing they are classified with the root-name nigerite. If Be occupies a tetrahedral position close to the site occupied by hydrogen in the nolanite module of nigerite- and högbomite-group minerals, the root-name is taaffeite and these mineral species are nominally anhydrous.

Regarding the prefix, it depends upon the composition of the spinel module. Up to now, all members of the supergroup have modules of aluminum spinels (spinel, hercynite or gahnite). Therefore, the prefixes magnesio-, ferro- and zinco- are assigned on the basis of the cation defining the spinel module (Mg, Fe and Zn respectively).

Different polysomes constitute different mineral species and thus hyphenated suffix defining the polysome in terms of nolanite and spinel modules are applied. There are 10 known or modelled polysomatic combinations of nolanite and spinel modules (see Table 1c in Shimura *et al*. 2012). Different polytypes of polysomatic sequences have also been described (e.g. magnesiotaaffeite-2*N*'2*S*, Malcherek & Schlüter, 2016).

In the Etirol-Levaz continental slice of middle Valtournenche, Aosta Valley, Mg-chloritite layers occur in a metamorphosed mafic complex. In some chloritites, rare relict mineral aggregates were found that contain, in addition to a green spinel, a brown mineral determined as "högbomite" on the basis of its optical characteristics (Regis *et al*., 2015). However, a deeper and more accurate re-examination based on EMPA

analyses combined with a single-crystal X-ray study allowed identifying this mineral as a new member of the högbomite supergroup isostructural with magnesiohögbomite-2*N*3*S*. Shimura *et al*. (2012) reported that "…*högbomite-group minerals are defined as Ti > Sn. The corresponding Ti-free samples should be classified into a newly defined group in close relation with högbomite and nigerite groups*". The new phase is Ti-poor, Sn-free and has Fe^{3+}-dominant over Ti at the M5 octahedron of nolanite module and for this reason deserved a new root-name, beltrandoite. The proposed root-name honours Marco Beltrando (1978-2015), geologist and petrologist at the Department of Earth Sciences of the University of Torino, for his sound contributions on the evolution of the Alpine orogeny. During his too short but very brilliant career, he got very important scientific results, such as the recognition of hyper-extended margins in the collisional belt of the Western Alps and the heating-cooling cycles in rift systems. He was able to connect structural geology and tectonics with petrology, geochronology and stratigraphy. His great ability to link the observations at the micro-scale to those at the meso- and macro-scale allowed him to shed new light on the evolution of both extensional and collisional systems. His new and original ideas have made him one of the leaders of a new generation of Alpine geologists. It is very sad that Marco's life and brilliant career terminated so suddenly in the place he felt best, in his loved mountains.

The average composition of the spinel modules in this new species has dominant aluminium and has $Mg > Fe^{2+}$ and thus, conforming to the högbomite nomenclature (Armbruster, 2002) the new name "beltrandoite" is prefixed by "magnesio" (as dominant element of the spinel module) and suffixed by "-2*N*3*S*" to represent the alternate spinel (*S*) and nolanite (*N*) modules (c = ~ 23.0 Å). The new mineral and the name was approved in November 2016 (IMA No. 2016-073) by the IMA Commission on New Minerals, Nomenclature and Classification (Cámara *et al*., 2016). The holotype material (a thin section and a 2 mm-thick rock chip) is deposited in the mineralogical collections of the Museo Regionale di Scienze Naturali di Torino, Sezione di Mineralogia, Petrografia e Geologia, via Giovanni Giolitti 36, I-10123 Torino, Italy, catalogue number M/U17182.

2. Occurrence

The sample containing magnesiobeltrandoite-2*N*3*S* was collected by our colleague Marco Gattiglio (University of Torino) along the stream "Marmore" of the middle Valtournenche (Valle d'Aosta, Italy) of (~N 45°49'36"; E 7°34'51") in the debris underneath the Etirol-Levaz slice (Fig. 1).

The Etirol-Levaz slice (ELS; see Fig. 1) is a lens-like continental fragment, sandwiched between the overlying blueschist- to greenschist-facies Combin zone and the underlying eclogite-facies Zermatt-Saas zone, both derived from the Mesozoic Piemonte-Liguria Ocean (Kienast, 1983; Ballèvre *et al.*, 1986; Dal Piaz *et al*., 2015). It was interpreted as an extensional allochthon derived from the Adriatic continental margin and stranded inside the Piemonte-Liguria oceanic domain during Jurassic rifting (Dal Piaz *et al*., 2001; Beltrando *et al*., 2010; Rubatto *et al*., 2011; Regis *et al*., 2015). The slice consists of pre-Alpine, most likely Variscan, amphibolite to granulite-facies gneisses, micaschists and metabasics, locally very well preserved as to both fabric and mineralogy (Kienast, 1983; Ballèvre *et al.*, 1986). During the Early Tertiary subduction, the ELS rocks were overprinted by Alpine eclogite-facies metamorphism and converted to garnet-phengite micaschist ("eclogitic micaschist"), minor fine-grained phengite orthogneiss and paragneiss with small pods of eclogite locally retrogressed to prasinite (Regis, 2007; Fassmer *et al.*, 2016). In the central portion of the ELS, a lens-like body of a layered coronitic metagabbro with cumulus structures has been reported (Kienast, 1983; Ballèvre *et al.*, 1986). The studied rock, containing the högbomite supergroup like minerals, has been proved by two of us (DR and RC) to derive from the layered metagabbro, where it occurs as massive chloritite bands, most likely after primary spinel pyroxenites (Regis *et al*., 2015). The chloritite locally contains cm- to dm-long darker boudins with relict green spinel + a brown högbomite–looking mineral cut by corundum + chlorite ± dolomite veins.

The Alpine reaction coronas developed in the metagabbro around clinopyroxene, orthopyroxene, and spinel were investigated in detail by Kienast (1983). Based on chemical compositions and microstructures of major phases, the author suggested that the layered metagabbro underwent an Alpine high-pressure metamorphic overprint at about 550ºC and 15-16 kbar. More recent thermobarometric studies of the high-pressure Alpine assemblage (garnet + omphacite + phengite + rutile) of ELS eclogites (Regis,

2007; Fassmer *et al.*, 2016) has shown two stages of garnet + omphacite growth during the prograde to peak *P-T* path. The metamorphic H*P* peak was constrained at ~ 560°C and ~ 24 kbar (Regis, 2007; Fassmer *et al.*, 2016).

3. Experimental methods

3.1. Electron-Microprobe analysis (EMPA)

Two thin sections, DB402, and DB321, were obtained from the same rock chip; one includes a corundum vein, and the other the rock matrix. A preliminary study of the chemistry of the minerals present in thin section was carried out by backscattered electron imaging and EDS at the Department of Earth Sciences, University of Turin. The measurements were executed with a Cambridge S-360 SEM equipped with Oxford Instruments Inca Energy 200 EDS spectrometer and X-Act3 SDD detector, operating at an acceleration voltage of 15 kV and beam current of 1 nA. Elemental maps of Kα spectral lines were obtained with SmartMap Option of Inca Energy 200 Oxford Instruments operating at 15 kV and 1 nA.

Chemical analyses were later carried out by WDS with JEOL 8200 Super Probe operating in X-ray wavelength-dispersive mode WDS mode (WDS-EMPA) at the Department of Earth Sciences, University of Milan, operating at an accelerating voltage of 15 kV, a specimen current of 5 nA, and a beam diameter of 1 μm. Minerals and synthetic compounds were used as standards (element, spectral line): olivine (Fe, Kα), rhodonite (Zn and Mn, Kα), NiAs (Ni, Kα), fayalite (Fe, Kα), almandine (Al, Kα), Cr (Kα), V (Kα), ilmenite (Ti, Kα). Corrections to the raw data were made with the ϕρ*Z* procedure (Pouchou and Pichoir, 1985). Representative averages of the minerals present in the sample are reported in Tables 1a-e. The composition of magnesiobeltrandoite-2*N*3*S* corresponds to an average of 55 data points (Table 2). H_2O was calculated on the basis of two OH groups pfu. Sn, Si, P, Ni, Ca, Na, K, were not present in the spectra. The empirical formula of magnesiobeltrandoite-2*N*3*S* calculated on the basis of 40 (O+OH) pfu is $[Al_{18.36}Mg_{3.96}Fe^{2+}_{2.52}Fe^{3+}_{2.08}Ti_{0.56}Cr_{0.40}Zn_{0.06}V^{3+}_{0.03}Mn_{0.02}]_{\Sigma 28}\,O_{38}(OH)_2$. The ideal formula is $Mg_6Al_{20}Fe^{3+}_2O_{38}(OH)_2$, which requires Al_2O_3 = 70.84, MgO = 16.80, Fe_2O_3 = 11.11, H_2O = 1.25, total 100 wt.%.

3.2. Synchrotron Mössbauer source spectroscopy (SMS)

Synchrotron Mössbauer spectroscopy (SMS) was performed at the Nuclear Resonance Beamline ID18 (Rüffer & Chumakov, 1996) using the nuclear monochromator as described by Potapkin *et al*. (2012) at the European Synchrotron Radiation Facility (ESRF), Grenoble. The SMS provides ^{57}Fe resonant radiation at 14.4 keV within a bandwidth of ~ 6 neV, which is tunable in energy over a range of about ± 0.6 μeV. In contrast to radioactive sources, the beam emitted by the SMS can be focused and it is fully resonant and up to 99% polarized. SMS spectra were collected during operation in multibunch mode (7/8 + 1 filling) with the beam focused to a spot size of roughly 15 × 15 μm^2 using Kirkpatrick-Baez bending mirrors. The SMS linewidth was controlled before and after each sample measurement using $K_2Mg^{57}Fe(CN)_6$, whose Mössbauer spectrum consists of a single line, and the velocity scale was calibrated using 25 μm thick natural α-iron foil. The SMS spectrum was collected for ~ 12 hours from a single crystal previously checked using X-Ray single crystal diffraction to exclude the presence of possible inclusions of different species. The spectrum was fitted using the program MossA with the full transmission integral and a Lorentzian-squared source line shape (Prescher *et al*., 2012) and is reported in Figure 2. The spectrum was fitted using four components corresponding to Fe^{3+} and Fe^{2+} in tetrahedral and octahedral composition. Observed hyperfine parameters agree well with observed values for Fe^{2+} and Fe^{3+} in these coordination environments and are reported in Table 3. The refined Fe^{3+}/Fe_{total} ratio is 46(2) %.

3.3. Raman spectroscopy

The Raman spectrum of magnesiobeltrandoite-2*N*3*S* (Fig. 3) was obtained using a micro/macro Jobin Yvon Mod. LabRam HRVIS, equipped with a motorized x-y stage and an Olympus microscope. The backscattered Raman signal was collected with 50× objective for a non-oriented crystal. The 532.11 nm line of a frequency doubled Nd-YAG laser and the 632.81 line of a He-Ne laser was used as excitation; laser power was controlled by means of a series of density filters. The minimum lateral and depth resolution was set to few μm. The system was calibrated using the 520.6 cm^{-1} Raman band of silicon before each experimental session. The spectra were collected with multiple acquisitions (5 to 20) with single counting times ranging between 10 and 20

seconds. The spectrum was recorded using the LabSpec 5 program (Horiba Jobin Yvon, 2004, 2005) from 100 to 4000 cm^{-1} and the results of the spectroscopic analysis are reported below.

3.4. X-ray powder diffraction

X-ray powder diffraction data were calculated from the structure data with XPow (Downs *et al.*, 1993) and are reported in Table 4. Experimental data were obtained on a powdered sample using an Oxford Gemini R Ultra diffractometer equipped with a CCD area detector at CrisDi (Interdepartmental Centre for the Research and Development of Crystallography, Torino, Italy) with graphite-monochromatized Cu*K*α radiation, and are also reported (in Å) in Table 4. Refined cell parameters using GSAS (Larson & Von Dreele, 1994) are a = 5.7164(1), c = 22.9702(8) Å, V = 650.03(2) $Å^3$.

3.5. Single-crystal structural refinement (SREF)

A prismatic crystal was carved with a needle from the chlorite matrix of DB321 rock chip. Single-crystal X-ray studies were carried out on a crystal of 0.080 × 0.060 × 0.020 mm using an Oxford Xcalibur Rubi Gemini Ultra diffractometer equipped with a CCD area detector at CrisDi (Interdepartmental Centre for the Research and Development of Crystallography, Torino, Italy) with graphite-monochromatized Mo*K*α radiation (λ = 0.71073 Å). The sample-to-detector distance was 5.3 cm. A total of 394 exposures (step = 1°, time/step = 63.2 s), covering a full reciprocal sphere with a redundancy of about 8 was used. Data were integrated and corrected for Lorentz and polarization background effects, using the package CrysAlisPro, Agilent Technologies, Version 1.171.37.31 (release 14-01-2014 CrysAlis171.36.24). Refinement of the unit-cell parameters was based on 4873 measured reflections, and gave the following lattice parameters: a = 5.7226(3), c = 23.0231(9) Å, V = 652.95(5) $Å^3$. The c:a ratio calculated from the unit-cell parameters is 4.023. The data were corrected for absorption using the multi-scan method (SCALE3 ABSPACK) with a d_{min} of 0.54 Å. The structure was refined trigonal, space group $P\bar{3}m1$, starting from the atom coordinates of magnesiohögbomite-2*N*3*S* (Hejny & Armbruster, 2002). Ionized atoms scattering curves were used for all atoms, which were refined with anisotropic displacement

parameters. The scattering curve for ionized aluminium was used in all octahedral M sites but M5. For the M5 site the scattering curves of both Mg^{2+} and Fe^{2+} were used with the restrain of complementary full occupancy. The latter approach was adopted for all tetrahedral sites in the structure. Hydrogen was localized as a maximum at ca. 1 Å of the anion site O4 in the Fourier difference maps and it was added to the model fixing the observed atom coordinates and restraining the isotropic displacement using a riding motion model. Twining by reticular merohedry (twin fraction 50.5(1):49.5(1)) was observed as reflection on (001). At convergence *R1* was 0.0222 for 1626 reflections with $F_o > 4\sigma (F_o)$ and 0.0242 for all 1721 data. Parameters for X-ray data collection and crystal-structure refinement are reported in Tables 5. Atom coordinates, anisotropic displacement parameters and main interatomic distances (Å) and geometrical parameters are reported in Tables 6, 7 and 8, respectively. CIF file is provided as supplementary material linked to this article and on the GSW website of the journal: http://eurjmin.geoscienceworld.org

4. Appearance and physical properties

The holotype sample containing magnesiobeltrandoite-2*N*3*S* is a thin section (Fig. 4). The subhedral to euhedral prismatic crystals (~ 50-400 μm), moderately elongated parallel to *c* crystallographic axis, are included in green spinel relics and associated in the matrix together with chlorite and dolomite, and locally show fractures filled with dolomite + clinochlore ± corundum. The mineral is dark reddish-brown in thin section. It shows dark brown streak and vitreous luster. It is brittle, with no cleavage observed and uneven fracture. Mohs hardness is estimated as 6-6½ by analogy to högbomite. Density could not be measured because of small grain size and occasional chlorite and magnesite inclusions. Calculated density using the measured cell volume and empirical formula is = 3.93 g cm^{-3}. Magnesiobeltrandoite-2*N*3*S* is unreactive and insoluble in HCl, HNO_3, and H_2SO_4. It shows no fluorescence under UV radiation and no cathodoluminescence. The mineral is optically uniaxial (–). The mean refractive index (n_{ave} ca. 1.80) was obtained from Gladstone-Dale relationship (Mandarino, 1979, 1981), using the empirical formulae and calculated densities. The estimated values for the refractive indices are well beyond our available experimental range. Dispersion was not determined, but not observed under crossed polarizers and in conoscopic

interference figures. Pleochroism is weak with ϵ = deep reddish brown (along *c* axis) and ω = reddish brown (⊥ to *c* axis). Absorption is E > O.

5. Results and discussion

5.1. Mineral chemistry of the assemblage

The minerals of the hosting chloritite are chlorite group minerals, green spinel, magnesite, dolomite, calcite, Fe-bearing corundum and magnesiobeltrandoite-2*N*3*S* (Fig. 5 and 6a), while in the corundum- and dolomite-bearing veins green spinel and magnesiobeltrandoite-2*N*3*S* are absent. Locally, Cr-rich magnetite, ilmenite with limited pyrophanite *s.s.* and pyrite are also observed in the matrix (type analyses of oxides are reported in Table 1a) and in alteration rims of relic phases (in particular magnesiobeltrandoite-2*N*3*S*) (Fig. 6b and 7a).

Regarding green spinel, core compositions are close to $Sp_{59}Hc_{41}$ with a strong Fe^{2+} zoning (Fig. 7b) that can reach $Sp_{42}Hc_{58}$ in the rim of small grains in the matrix or even $Sp_{30}Hc_{70}$. Rims are also slightly enriched in Cr. Locally, even Cr-richer compositions are observed associated to retrogression of mangesiobeltrandoite-2*N*3*S*, with composition $Sp_{31}Hc_{69}$ (locally up to $Sp_{13}Hc_{87}$) or close to corundum veins, where composition is still more hercynite-rich ($Sp_{20}Hc_{80}$). Cr-rich spinel close to the veins contains also trace amounts of V (Table 1b). Large grains of hercynitic spinel are fractured and cracks are filled by dolomite (Table 1c) and diaspore (Table 1a).

Carbonates in the matrix are dolomite and magnesite with limited Fe substitution (Table 1c). Dolomite in corundum veins may have higher Fe^{2+} (Mn) and trace amounts of V. Calcite was occasionally observed in cracks in spinel and may be secondary.

Chlorites in the matrix show sharp zonation (Fig. 6a, 6b, 7a and 7b) with enrichment of Fe and depletion of Si. The rims correspond to iron aluminian clinochlore (previously classified with the name *corundophilite* and *ripidolite*, now discarded; Bayliss 1975, Table 1d). Charge balance demonstrates that chlorite has no Fe^{3+}.

Magnesiobeltrandoite-2*N*3*S* shows limited zonation with slighter Ti-richer cores but never reaching högbomitic compositions. A chemical profile is reported in Table 1e. Fe^{3+}/Fe_{total} was estimated assuming 2 (OH) pfu and charge balance. The values reported in Table 1e agree fairly well with SMS data (see below). Most of the grains of

magnesiobeltrandoite-2*N*3*S* show incipient alteration to clinochlore even richer in Fe and Al than the rims of crystals in the matrix (Fig. 7a, Table 1d). In Figure 8 the chemical variability of magnesiobeltrandoite-2*N*3*S* of Valtournenche is plotted in a modified version of the (Ti + Sn) – ΣR^{2+} – ΣR^{3+} diagram of högbomite group minerals of Shimura *et al*. (2012). Figure 8 also reports the composition of magnesiohögbomite-2*N*3*S* by Hejny & Armbruster (2002) for comparison. The compositions plotting below the R^{4+} (Ti-Sn) =1 line cannot be classified as högbomite or nigerite because in those compositions neither Ti nor Sn are dominant in the M5 octahedron of the nolanite module.

Regis *et al.* (2015) described that magnesiobeltrandoite-2*N*3*S* grains are included in green spinel relics and associated in the matrix together with chlorite and dolomite, and locally show fractures filled with dolomite + chlorite ± corundum.

The mineral assemblages and microstructural relationships in both the metagabbro and the chloritite indicate that the rocks experienced a complex polymetamorphic evolution. On the basis of microstructures, Regis *et al.* (2015) concluded that the pre-Alpine destabilization of green spinel, beltrandoite and magnesite led to extensive chloritization of the cumulate layers and development of the matrix assemblage Mg-chlorite + dolomite ± corundum ± magnesiobeltrandoite-2*N*3*S*; this stage followed the Permian HT metamorphic evolution. The crystallization of magnesiobeltrandoite-2*N*3*S* predates the formation of the crosscutting Crn + Dol + Mg-Chl veins during the Alpine evolution.

5.2. Raman of magnesiobeltrandoite-2*N*3*S*

The strongest peak positions in the Raman spectrum of magnesiobeltrandoite-2*N*3*S* (Fig. 3a) are observed at 854, 717, 506, and 264 cm^{-1}. Minor bands are also present at 812, 657, 419, 371 and 109 cm^{-1}. Some of the bands are polarized; in particular, the band at 657 cm^{-1} is weaker in the spectrum collected with polarization perpendicular to the length of the crystal.

A weak and polarized band centered at 3364 cm^{-1} (Fig. 3b) corresponds to an O-H bond parallel to *c* axis, indicating that magnesiobeltrandoite-2*N*3*S* is an OH-bearing mineral. A correspondent band was found at 3350 cm^{-1} in magnesiohögbomite-2*N*3S by Hejny & Armbruster (2002) by FTIR.

The Raman spectra of magnesiobeltrandoite-2*N*3*S* present differences with those reported by Shimura *et al*. (2012) for magnesiohögbomite-2*N*4*S*, and the "*Ti-free högbomite*" of Tsunogae & Santosh (2005). For instance, "*Ti-free högbomite*" of Tsunogae & Santosh (2005) has strong and medium bands at 855, 808, 670, 384 and 263 cm^{-1}, not very different from those found in magnesiobeltrandoite-2*N*3*S*. However, "*Ti-free högbomite*" also shows peaks at 764, 556, 447, 421 and 317 cm^{-1}, which are absent in the Raman spectrum of magnesiobeltrandoite-2*N*3*S*. Differences are due perhaps to a different structure, although it is worth noting that the sample reported by Tsunogae & Santosh (2005) is richer in Al and Mg. Magnesiohögbomite-2*N*4*S*, has bands at 872, 780, 709, 659, 489, 419, 302, 263, 217, 142 and 104. Some are coincident with bands present in the spectrum reported in Fig. 3a, some others not.

5.3. Crystal-chemistry of magnesiobeltrandoite-2*N*3*S*

Magnesiobeltrandoite-2*N*3*S* is isostructural with magnesiohögbomite-2*N*3*S*: there are 10 symmetrically independent cation sites and 10 anion sites. Cation sites are 4 tetrahedra and 6 octahedra. Two octahedral sites (M3 and M5) and one tetrahedral site (T4) belong to the nolanite modules, while 4 octahedral sites (M1, M6, M8 and M10) and 3 tetrahedral sites (T2, T7 and T9) correspond to spinel modules (Fig. 9). Following Hejny & Armbruster (2002), the nolanite modules are composed by a $\mathbf{T_1}$-layer of tetrahedrally (T4) and octahedrally (M5) coordinated atoms and a **O**-layer built by octahedrally (M3) coordinated sites; the spinel module is composed by $\mathbf{T_2}$-layers of tetrahedrally (T2 , T7 and T9) and octahedrally (M1 and M8) coordinated atoms and a **O**-layer built by octahedrally (M1 and M10) coordinated sites (Fig. 9).

The largest octahedra and the smaller tetrahedron in the structure are found at the nolanite module, as previously described by Hejny & Armbruster (2002) for magnesiohögbomite-2*N*3*S*. Considering the chemical composition reported in Table 2, the observed sites scattering ($s.s._{obs.}$) and mean bond lengths (values taken from Lavinia *et al.* 2002 and Shannon 1976) site assignment have been calculated and are reported in Table 9. Calculations were done manually changing site occupancies until reaching the minimum delta values reported in last column of Table 9. This site assignment implies that a large amount of Fe^{3+} is dominantly ordered in the M5 site of the nolanite module (0.94 apfu), while some Fe^{3+} is present in the tetrahedral sites of the nolanite module

(T4, 0.16 apfu) and in the T7 and T9 sites of the T_1-layer of the spinel modules (0.12 apfu each site), as well as in octahedral sites of the spinel modules (up to 0.74 apfu). This site distribution implies a total of 0.4 apfu of tetrahedral Fe^{3+} versus 1.68 octahedral Fe^{3+}, i.e. a 24%, which agrees fairly well with the relative areas obtained by SMS spectroscopy (21(1)%) (Table 3). Regarding Fe^{2+}, it is mostly ordered in tetrahedral sites. Only 0.34 Fe^{2+} apfu is ordered in the two octahedral M5 sites pfu of the nolanite modules, which implies a 14% of octahedral Fe^{2+}. This assignment compares also fairly well with the 17% observed by SMS (Table 3). This agreement further supports the site assignment.

The assigned composition of M5 site ($Fe^{3+}_{0.47}Ti_{0.28}Fe^{2+}_{0.17}Mg_{0.07}$) implies that the dominant element of the dominant charge is Fe^{3+}. This is in good agreement with the observed bond-valence incidence per site calculated with structural data (Table 10), which sees a bond valence incidence of 3.063 v.u. at the M5 site. Slight overbonding is observed for anion site O7, which is related to a very distorted environment for T7 and a particularly small M8 site (occupied almost only by Al). Significant underbonding is observed for O3 and O10 that might reflect cation disorder at the bonded sites T4, M5 and T7 (Table 9) that both anions coordinate.

The entrance of Fe^{3+} as dominant species at M5, the site where Ti and Sn are located in högbomite and nigerite, respectively, can be obtained through two charge-balance substitutions:

a) $^{M5}Ti^{4+} + {}^{T4}R^{2+}$ (Fe,Mg,Zn) $\rightarrow {}^{M5}Fe^{3+} + {}^{T4}R^{3+}$ (Fe,Al,Cr)

b) $^{M5}Ti^{4+} + {}^{T4}R^{3+}$ (Fe,Al,Cr) + $^{O4}(O)^{2-} \rightarrow {}^{M5}Fe^{3+} + {}^{T4}R^{3+}$ (Fe,Al,Cr) + $^{O4}(OH)^{-}$

The first substitution assumes complete hydrogenation in the nolanite module and therefore minimum amount of Fe^{3+}; this is the one that has been chosen for formula calculation. The second one assumes that the entrance of Ti^{4+} at the M5 site promotes dehydrogenation, and therefore yields maximum possible oxidation for Fe. However, without a direct estimation of the oxidation state of Fe or the H content is not possible to confirm the presence of the second substitution. In addition, the M5 octahedron is not coordinated with O4 anion, which coordinates M3 octahedron, but both M3 and M5 octahedra share three O3 oxygen sites, and bond strength at the O4 site can be compensated through these shared O sites (Fig. 10). The results of SMS spectrometry thus confirm that the formula assuming full hydration of the O4 sites is the right one.

The ideal formula of magnesiobeltrandoite-2*N*3*S* can be obtained considering the ideal composition of the involved modules, i.e. 2 "*nolanitic*" modules of composition $^{T}Al^{M}(Fe^{3+}Al_3)O_7(OH)$ (since Al^{3+} instead of Fe^{3+} is dominant in T4 site) plus 3 spinel modules ($^{T}Mg_2{}^{M}Al_4O_8$), separating the contribution to tetrahedral and octahedral sites, as $^{T}(Mg_6Al_2)^{M}(Al_{18}Fe^{3+}{}_2)O_{38}(OH)_2$, or in a simplified form as $Mg_6Al_{20}Fe^{3+}{}_2O_{38}(OH)_2$.

6. Relation to other species

Magnesiobeltrandoite-2*N*3*S*, $Mg_6Al_{20}Fe^{3+}{}_2O_{38}(OH)_2$ is a new member of the högbomite supergroup (Mills *et al.*, 2009) and the first "nolanitic" Fe^{3+}-dominant member (Table 6). This magnesiobeltrandoite-2*N*3*S* is very rich in Fe^{2+} (Mg > Fe^{2+} only for 0.10 a.p.f.u.); a "ferrobeltrandoite-2*N*3*S*" most probably occurs in nature. It is worthwhile to note that the amount of Fe^{2+} is the maximum amount calculated on the assumption that there are 2 (OH) per formula unit. The possibility of dehydrogenation (related or not to the Ti content) could only increase the Fe^{3+} and therefore lower further the Fe^{2+} content. Ti-poor högbomite (Grew *et al.*, 1987; Tsunogae & Santosh, 2005) was already found although no indication of the polysome was provided.

The spinel module of magnesiobeltrandoite-2*N*3*S* is basically a spinel, with minor hercynitic molecule. Up to now, all members of the supergroup have modules of aluminum spinels (spinel, hercynite or gahnite). Therefore, the prefix is assigned on the basis of the cation defining the spinel module. The discovering of members with spinel module corresponding to non-aluminic spinels (*i.e.*, Fe or Cr) would probably require a second prefix.

Recently, an official description of the new borate mineral mengxianminite $[(Ca,Na)_2Sn_2(Mg,Fe)_3Al_8[(BO_3)(BeO_4)O_6]_2]$ from Xianghualing skarn, Hunan Province, China, has been approved by IMA-CNMNC (Rao *et al*., 2016). This mineral is supposedly related to the högbomite supergroup of minerals and would be better classified as a taaffeite because the presence of two Sn apfu in the nolanitic module. However, the presence of B at the T sites of the nolanite modules opens new issues in the nomenclature of the högbomite supergroup.

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Captions

Table captions

Table 1a. Chemical analyses and formulae of oxides and hydroxides minerals.

Table 1b. Chemical analyses and formulae of spinel group minerals (on the basis of 4 oxygen atoms per formula unit)

Table 1c. Chemical analyses of carbonates.

Table 1d. Chemical analyses and formulae of chlorite group minerals (on the basis of 18 [O+(OH)] per formula unit)

Table 1e. Chemical profile of one magnesiobeltrandoite-2*N*3*S* grain. Formula on the basis of 40 O+(OH) per formula unit (Sn, Ca, Na, K and F within detection limits)

Table 2. Analytical data (wt.%) for magnesiobeltrandoite-2*N*3*S* (average of 55 spot analyses).

Table 3. Hyperfine parameters derived from the SMS spectrum of magnesiobeltrandoite-2*N*3*S*

Table 4. X-ray powder diffraction data for magnesiobeltrandoite-2*N*3*S**. The eight strongest reflections are reported in bold.

Table 5. Parameters for X-ray data collection and crystal-structure refinement of magnesiobeltrandoite-2*N*3*S* crystal.

Table 6. Atoms, site occupancies, fractional atom coordinates (Å), and equivalent isotropic displacement parameters ($Å^2$) for the studied magnesiobeltrandoite-2*N*3*S* crystal.

Table 7. Anisotropic displacement parameters* for magnesiobeltrandoite-2*N*3*S* (Å).

Table 8. Main interatomic distances (Å) and geometrical parameters for magnesiobeltrandoite-2*N*3*S*.

Table 9. Refined site-scattering and assigned site-populations for magnesiobeltrandoite-2*N*3*S*.

Table 10. Bond-valence values* for structural sites of magnesiobeltrandoite-2*N*3*S*.

Table 11. The högbomite supergroup. (References are given in brackets).

Figure captions

Figure 1. (a) Geotectonic map of the continental Etirol-Levaz slice (ELS), Torgnon, Valtournenche, Valle d'Aosta region**,** Italy and the adjoining units of the Piemonte Zone. (b) Simplified tectonic map of the northwestern Alps with location of the portion enlarged in Fig. 1a. Ivrea Zone (IZ). Sesia Zone (SZ), Dent Blanche Nappe (DBN): in red the Upper Tectonic Units of II DK in SZ and of Valpelline Series of DBN. Gran Paradiso (GP) and Monte Rosa (MR). Mont Blanc Massif (MB)

Figure 2. Room temperature SMS spectrum of magnesiobeltrandoite-2*N*3*S*. Solid circles: experimental data; continuous black line: full transmission integral fit. Four quadrupole doublets were used to fit the spectrum: in blue Fe^{3+} in tetrahedral coordination; cyan Fe^{3+} in octahedral coordination**;** red Fe^{2+} in tetrahedral coordination**;** orange Fe^{2+} in octahedral coordination. Percentage on the left indicates the relative absorption.

Figure 3. Raman spectra of magnesiobeltrandoite-2*N*3*S* in the 100-1200 cm^{-1} region (a) and between 3000 and 4000 cm^{-1} (b).

Figure 4. Relict pre-Alpine H*T* green spinel (Spl) with magnesiobeltrandoite-2*N*3*S* (reddish brown, Bel) in a matrix composed of a fine-grained aggregate of chlorite + dolomite (white, Dol + Chl) + magnesiobeltrandoite-2*N*3*S* (brown, Bel) ± corundum.

Figure 5. Transmitted plane polarized light (a) and composed X-ray fluorescence map (b) obtained by merging the elemental maps of MgKα, AlKα, CaKα and TiKα in the area reported in (a). The red areas indicated as corundum may include diaspore.

Figure 6a. Backscattered image a carbonate-rich zone of the matrix, showing the relation between relic spinel-hercynite grains with a brighter hercynitic rims (hrc) and coeval magnesiobeltrandoite-2*N*3*S* (bel) crystals dispersed in a zoned chlorite matrix. At the center, magnesite cores are included in zoned dolomite. In the lower part of the image, a corundum grain is in contact with hercynite.

Figure 6b. Magnesiobeltrandoite-2*N*3*S* crystal showing incipient alteration to Fe-rich aluminian clinochlore, ilmenite and chromium-rich hercynite. In the matrix, clinochlores show sharp zoning to Fe and Al richer rims.

Figure 7. Backscattered images showing (a) a detail of the incipient alteration of magnesiobeltrandoite-2*N*3*S* (bel) to Fe-Al-rich clinochlore + ilmenite + Cr-rich hercynite, and (b) the Fe-richer zoned rims in spinel grains, cracks filled by dolomite and diaspore.

Figure 8. (Ti + Sn) – ΣR^{2+} – ΣR^{3+} diagram of högbomite supergroup minerals (Shimura et al. 2012); (b) close-up of the area for högbomite-group minerals. Open circles are the analyses of magnesiomeltrandoite-2*N*3*S* from Valtournenche. Black circles are the högbomite analyses of Hejny & Armbruster (2002). Crn = corundum, hem = hematite; spl = spinel; mt = magnetite; usp = ulvöspinel; ilm = ilmenite; gk = geikielite; rt = rutile; nol = nolanite; hgb = högbomite.

Figure 9. Detail of the magnesiobeltrandoite-2*N*3*S* structure showing Al-dominant octahedra in light blue and (Fe+Mg+Ti) dominant tetrahedra and octahedra in orange. Site labels have been reported. Oxygen sites in red. Thermal displacement ellipsoids shown at 95% probability. **O**-Layers of octahedrally coordinated cations (M) and $\mathbf{T_2}$-layers of tetrahedrally (T) and

octahedrally (M) coordinated cations (M) in spinel module as well as **O**-layers and **T$_1$**-layers of nolanite module are also shown. Plot obtained using Vesta 3 (Momma & Izumi, 2011).

Figure 10. Detail of the magnesiobeltrandoite-2*N*3*S* structure showing Al octahedra in light blue and (Fe+Mg+Ti) bearing tetrahedra and octahedra in orange. Plot obtained using Vesta 3 (Momma & Izumi, 2011).

Figure 1

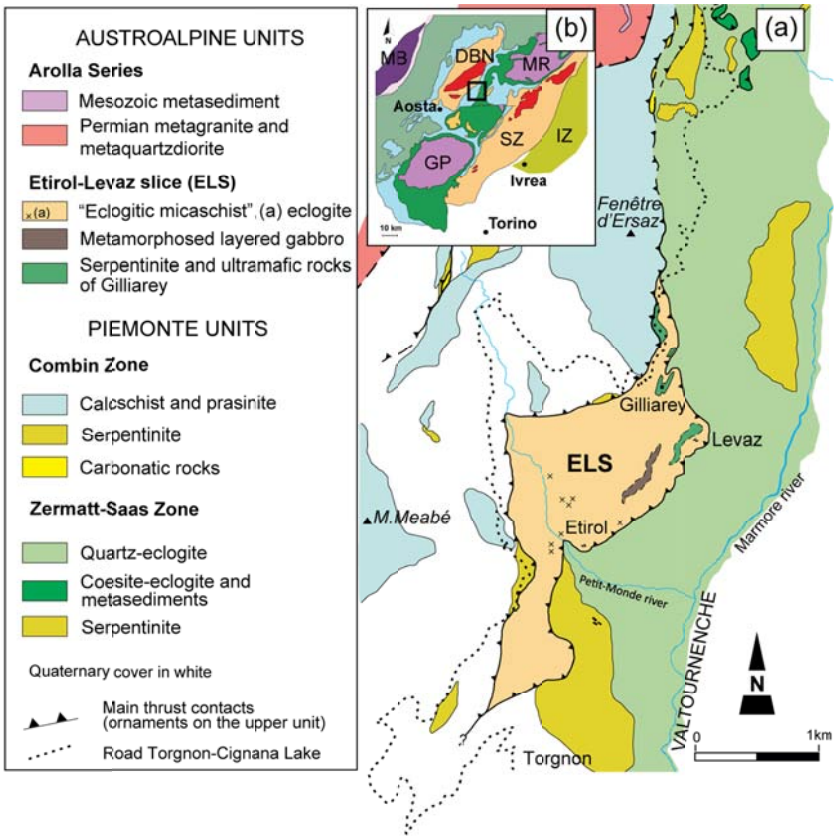

Figure 1. (a) Geotectonic map of the continental Etirol-Levaz slice (ELS), Torgnon, Valtournenche, Valle d'Aosta region**,** Italy and the adjoining units of the Piemonte Zone. (b) Simplified tectonic map of the northwestern Alps with location of the portion enlarged in Fig. 1a. Ivrea Zone (IZ). Sesia Zone (SZ), Dent Blanche Nappe (DBN): in red the Upper Tectonic Units of II DK in SZ and of Valpelline Series of DBN. Gran Paradiso (GP) and Monte Rosa (MR). Mont Blanc Massif (MB)

Figure 2

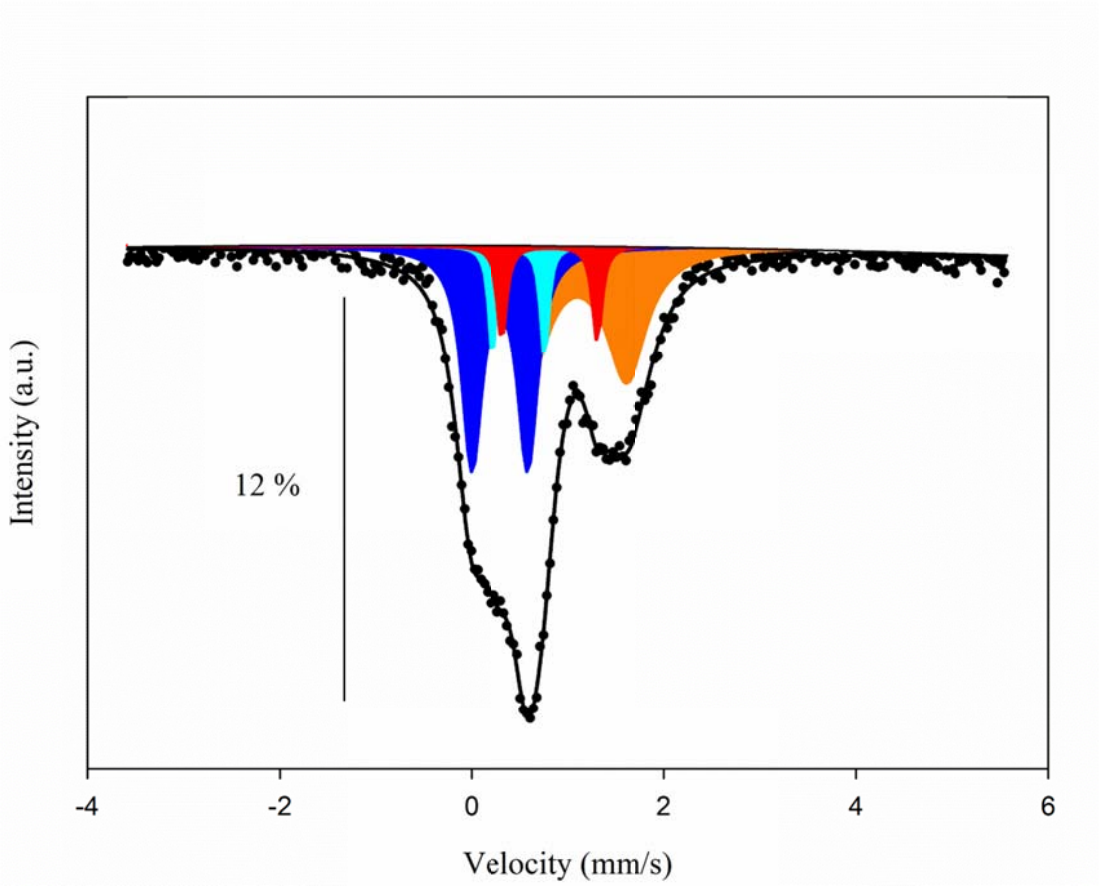

Figure 2. Room temperature SMS spectrum of magnesiobeltrandoite-2*N*3. Solid circles: experimental data; continuous black line: full transmission integral fit. Four quadrupole doublets were used to fit the spectrum: in blue Fe^{3+} in tetrahedral coordination; cyan Fe^{3+} in octahedral coordination**;** red Fe^{2+} in tetrahedral coordination**;** orange Fe^{2+} in octahedral coordination. Percentage on the left indicates the relative absorption.

Figure 3

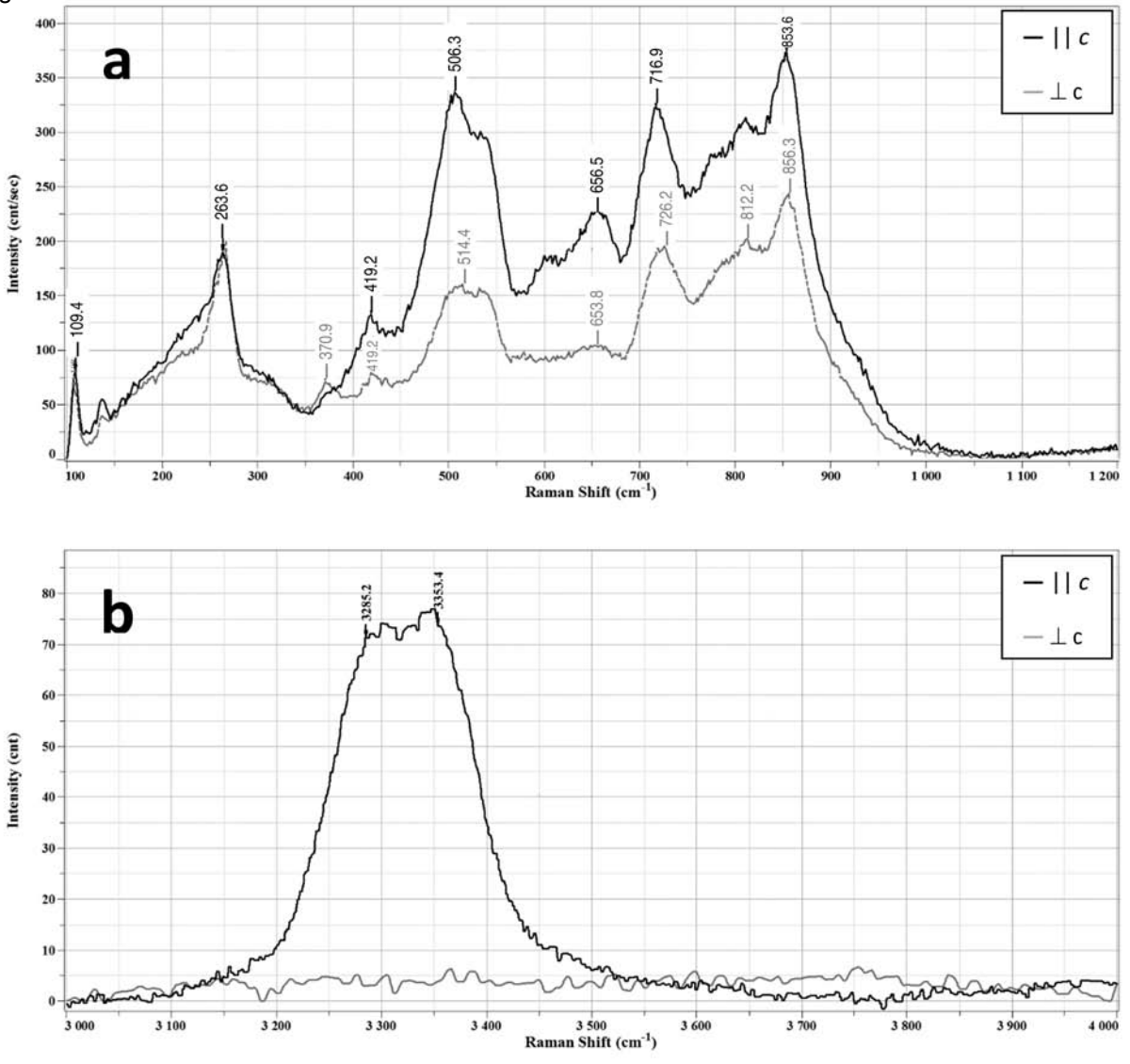

Figure 3. Raman spectra of magnesiobeltrandoite-2*N*3*S* in the 100-1200 cm^{-1} region (a) and between 3000 and 4000 cm^{-1} (b).

Figure 4

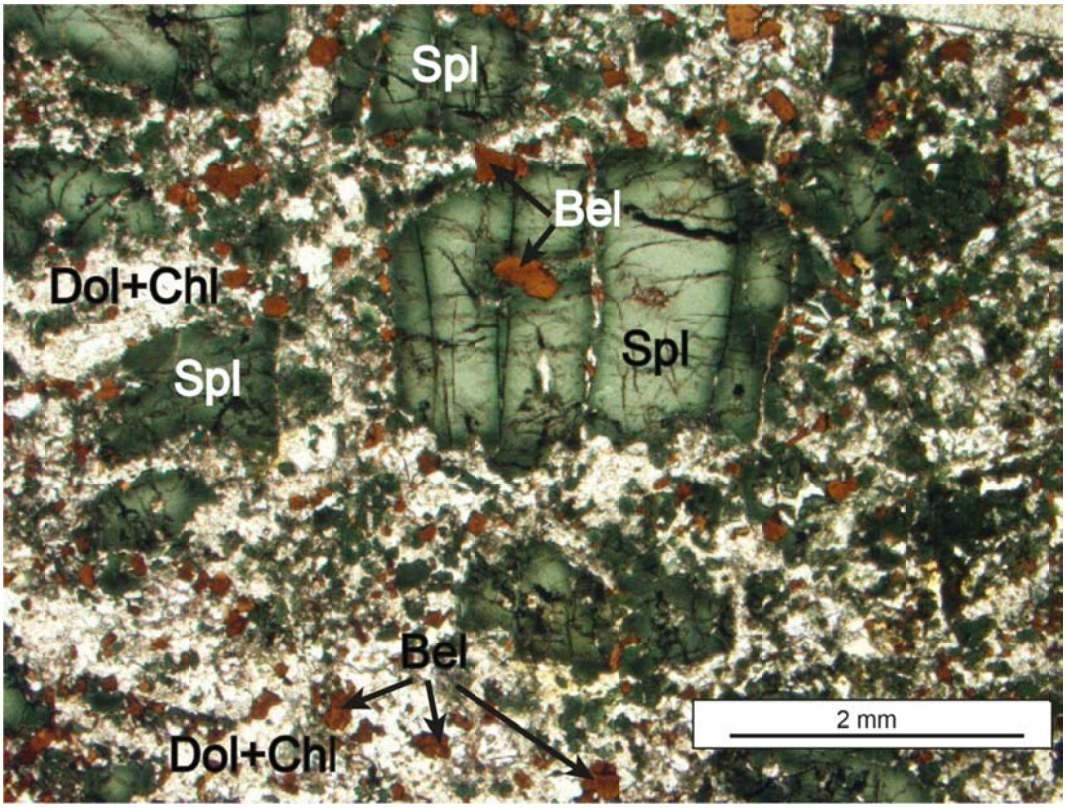

Figure 4. Relict pre-Alpine H*T* green spinel (Spl) with magnesiobeltrandoite-2*N*3*S* (reddish brown, Bel) in a matrix composed by a fine-grained aggregate of chlorite + dolomite (white, Dol + Chl) + magnesiobeltrandoite-2*N*3*S* (brown, Bel) ± corundum.

Figure 5

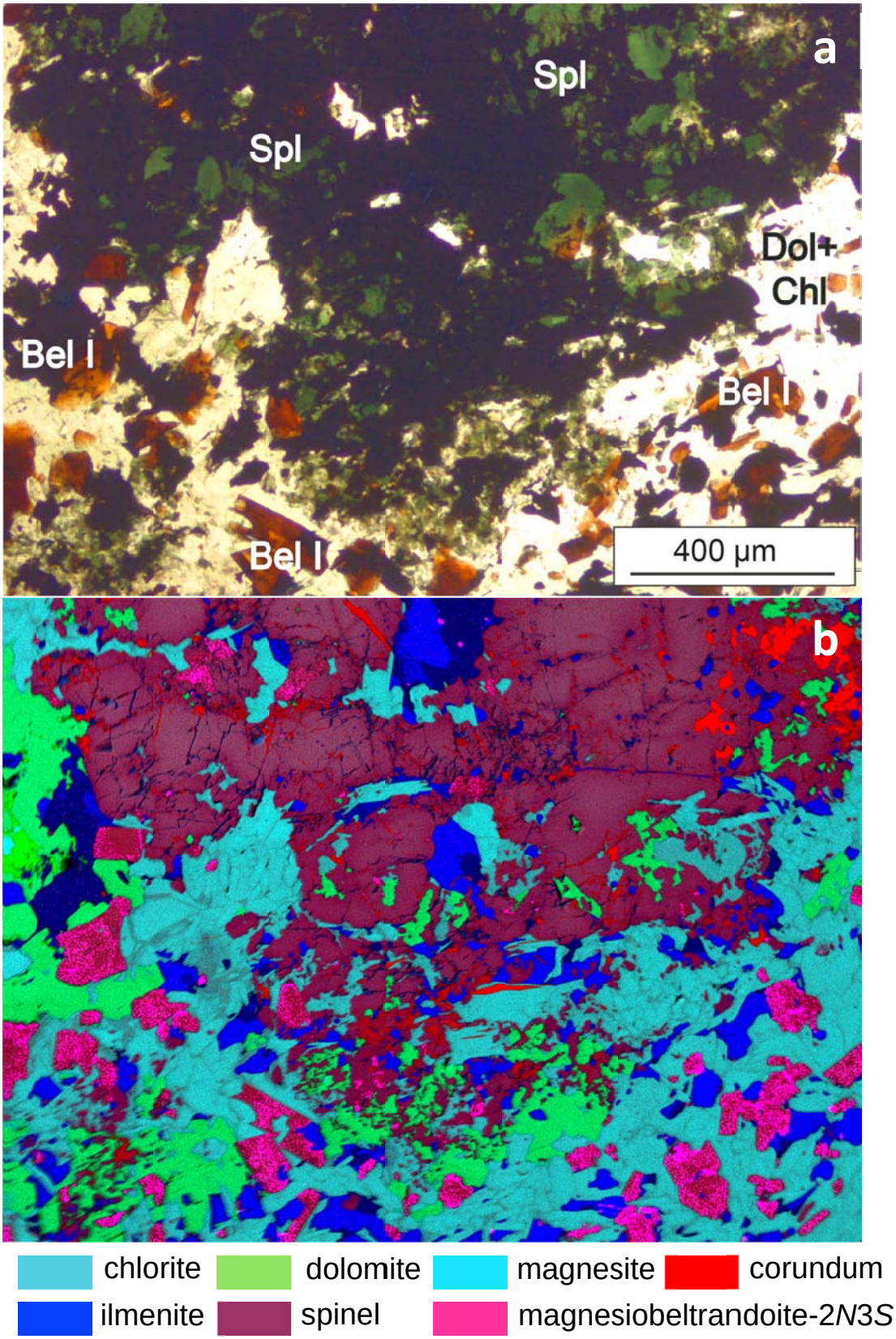

Figure 5. Transmitted plane polarized light (a) and composed X-ray fluorescence map (b) obtained by merging the elemental maps of MgKα, AlKα, CaKα and TiKα in the area reported in (a). The red areas indicated as corundum may include diaspore.

Figure 6

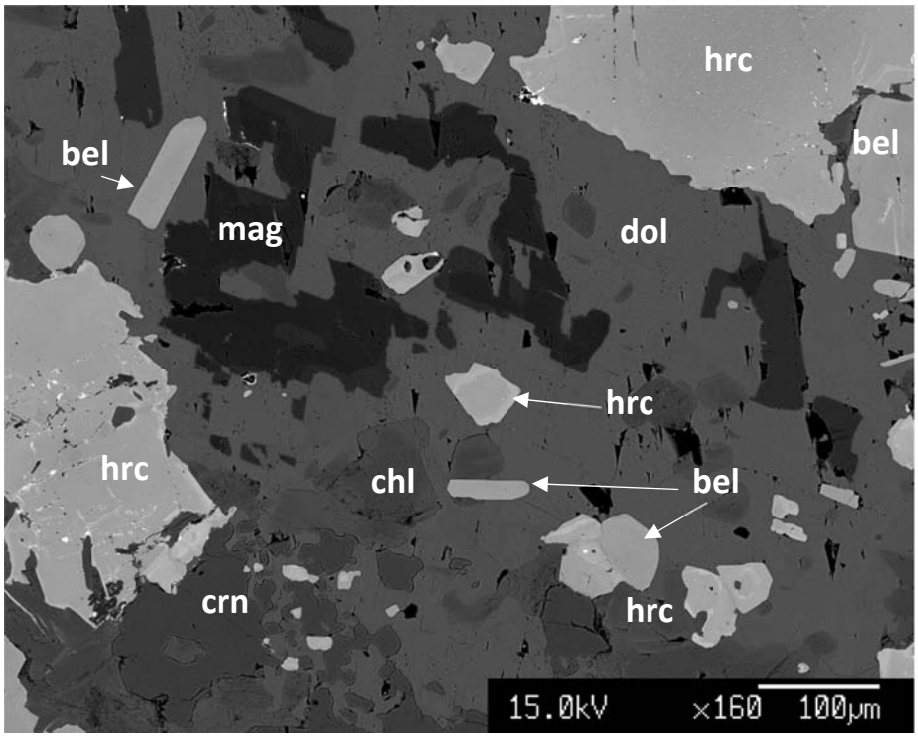

Figure 6a. Backscattered image a carbonate-rich zone of the matrix, showing the relation between relic spinel-hercynite grains with a brighter hercynitic rims (hrc) and coeval magnesiobeltrandoite-2*N*3*S* (bel) crystals dispersed in a zoned chlorite matrix. At the center, magnesite cores are included in zoned dolomite. In the lower part of the image, a corundum grain is in contact with hercynite.

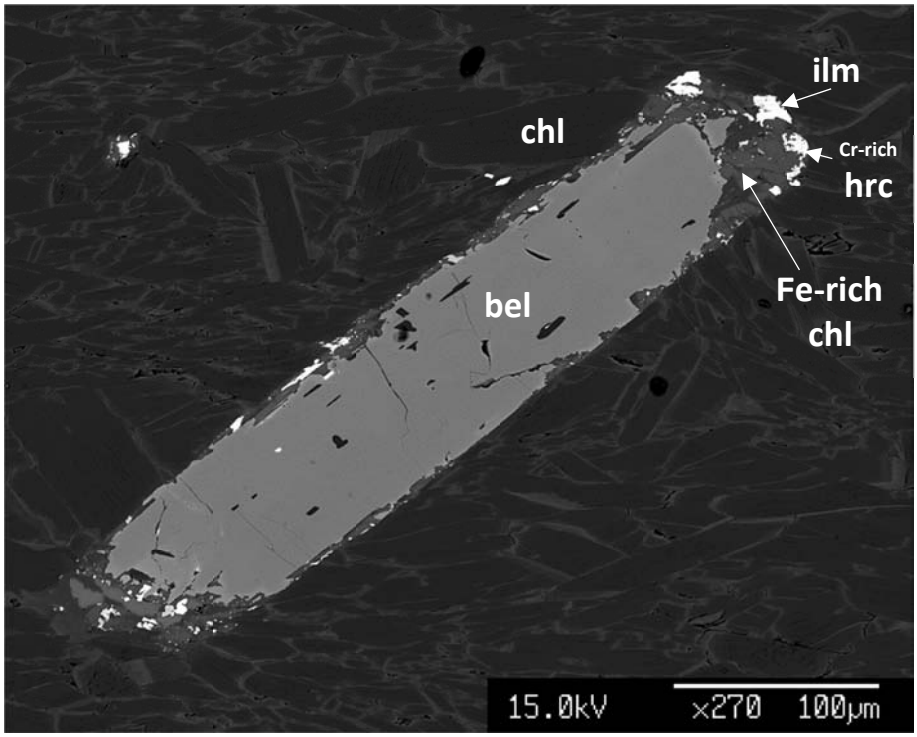

Figure 6b. Magnesiobeltrandoite-2*N*3*S* crystal showing incipient alteration to Fe-rich aluminian clinochlore, ilmenite and chromium-rich hercynite. In the matrix, clinochlores show sharp zoning to Fe and Al richer rims.

Figure 7

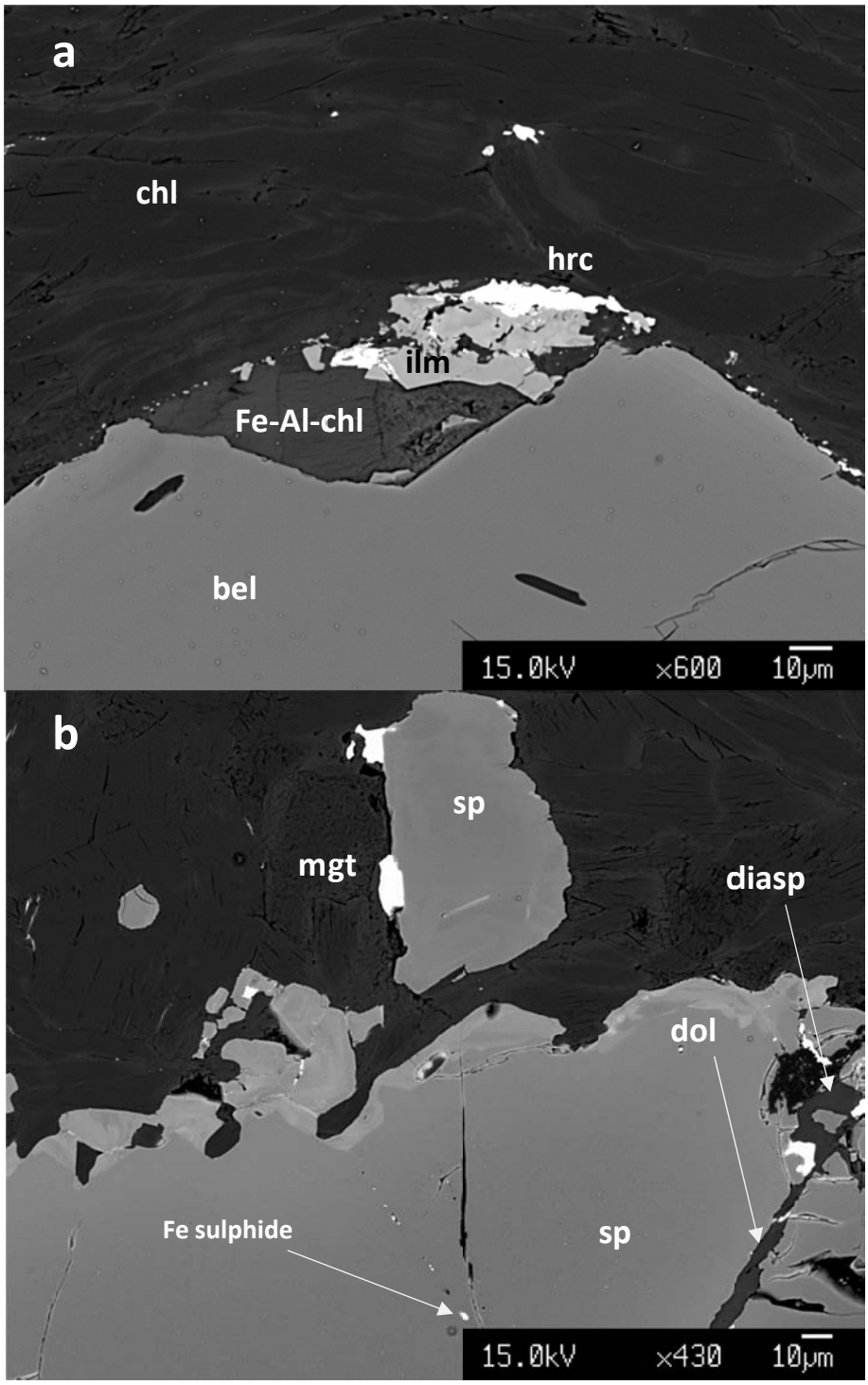

Figure 7. Backscattered images showing (a) a detail of the incipient alteration of magnesiobeltrandoite-2*N*3*S* (bel) to Fe-Al-rich clinochlore + ilmenite + Cr-rich hercynite, and (b) the Fe-richer zoned rims in spinel grains, cracks filled by dolomite and diaspore.

Figure 8

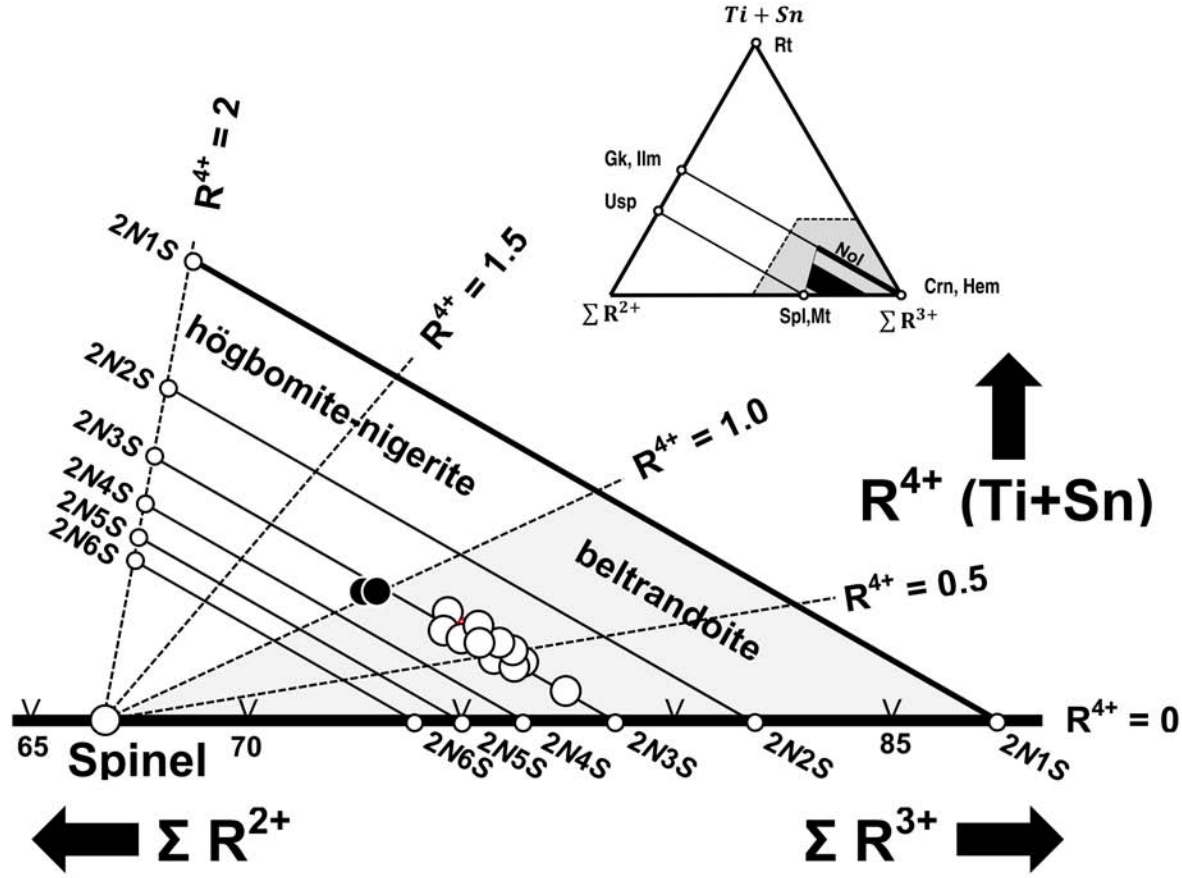

Figure 8. (Ti + Sn) – ΣR^{2+} – ΣR^{3+} diagram of högbomite supergroup minerals (Shimura et al. 2012); (b) close-up of the area for högbomite-group minerals. Open circles are the analyses of magnesiomeltrandoite-2*N*3*S* from Valtournenche. Black circles are the högbomite analyses of Hejny & Armbruster (2002). Crn = corundum, hem = hematite; spl = spinel; mt = magnetite; usp = ulvöspinel; ilm = ilmenite; gk = geikielite; rt = rutile; nol = nolanite; hgb = högbomite.

Figure 9

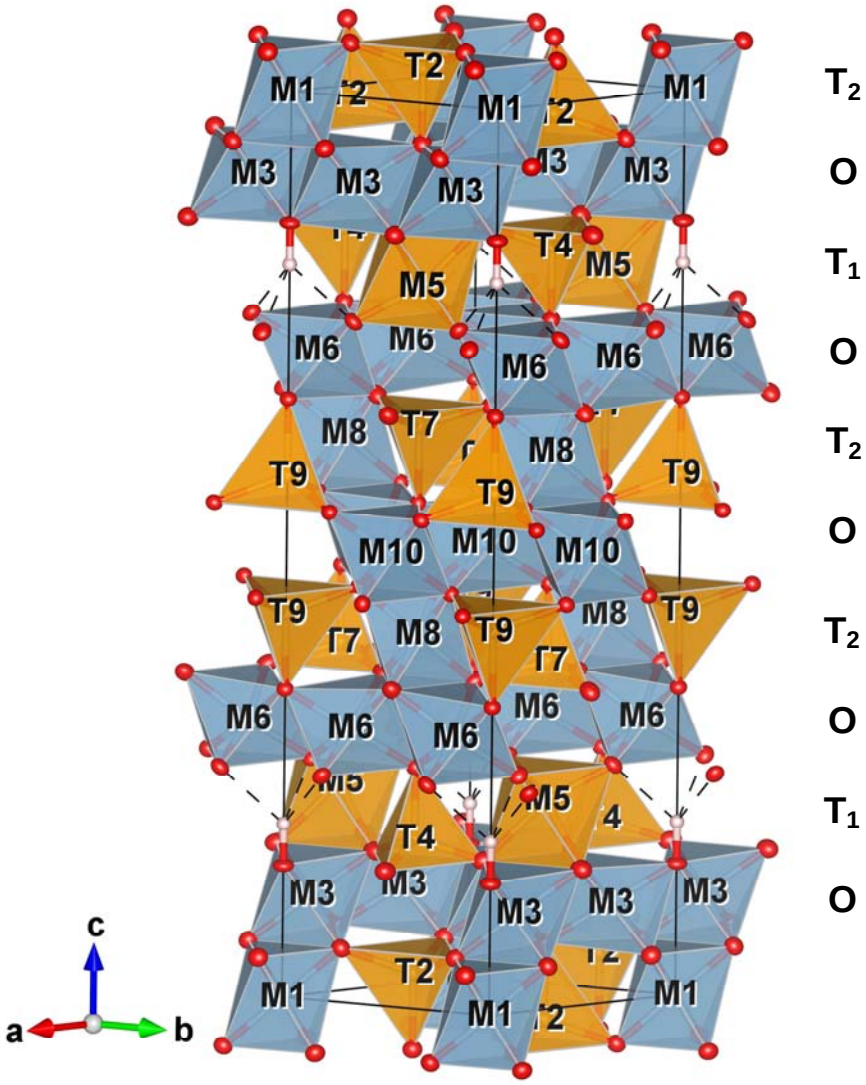

Figure 9. Detail of the magnesiobeltrandoite-2*N*3*S* structure showing Al-dominant octahedra in light blue and (Fe+Mg+Ti) dominant tetrahedra and octahedra in orange. Site labels have been reported. Oxygen sites in red. Thermal displacement ellipsoids shown at 95% probability. **O**-Layers of octahedrally coordinated cations (M) and $\mathbf{T_2}$-layers of tetrahedrally (T) and octahedrally (M) coordinated cations (M) in spinel module as well as **O**-layers and $\mathbf{T_1}$-layers of nolanite module are also shown. Plot obtained using Vesta 3 (Momma & Izumi, 2011).

Figure 10

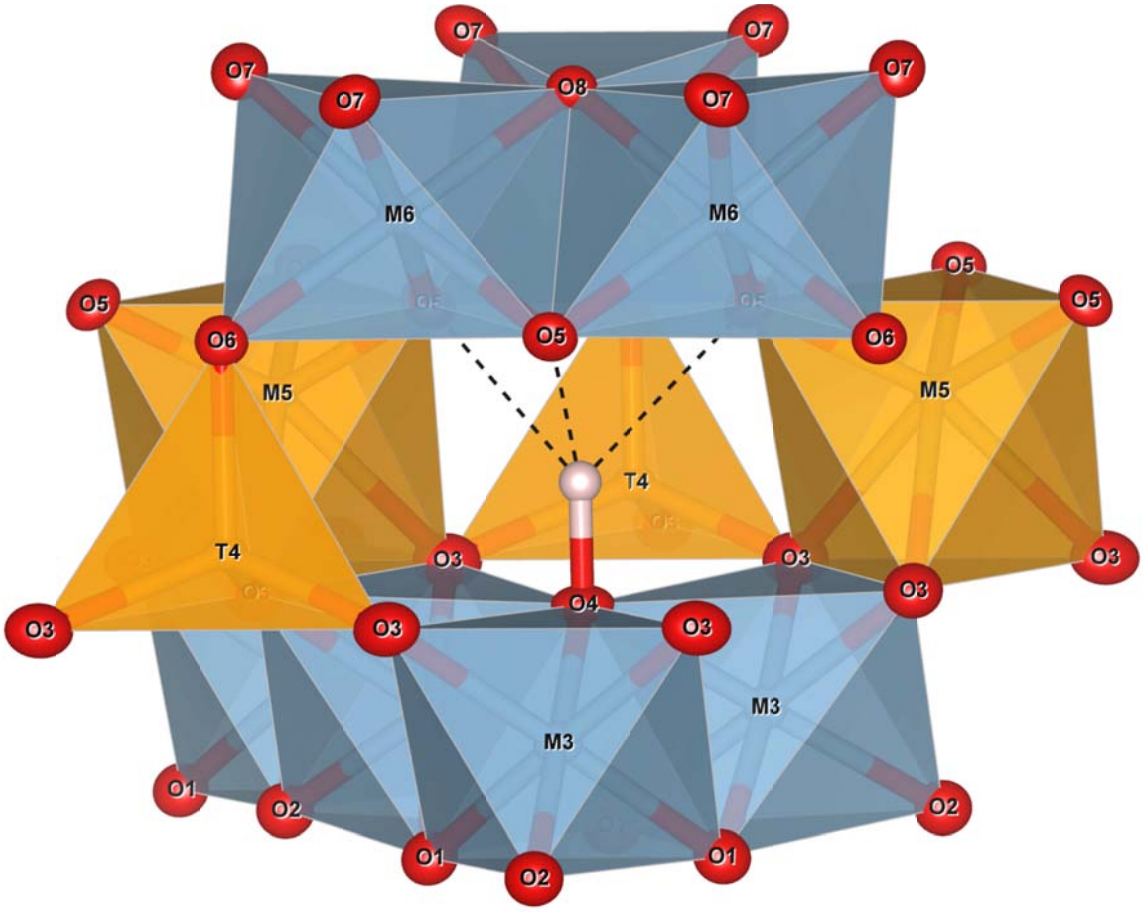

Figure 10. Detail of the magnesiobeltrandoite-2*N*3*S* structure showing Al octahedra in light blue and (Fe+Mg+Ti) bearing tetrahedra and octahedra in orange. Plot obtained using Vesta 3 (Momma & Izumi, 2011).

Table 1a. Chemical analyses and formulae of oxides and hydroxides minerals.

Mineral	ilm DB402-C1-8	ilm DB321-C1-2	ilm DB321-C3-2	mgt DB402-C2-7	crn DB402-C4-1	crn DB402-C5-7	crn DB402-C6-3	Crn DB402-C6-4	diaspore DB402-C3-7
SiO_2	0.07	0.04	0	0.05	0.04	0.02	0.02	0	0
Al_2O_3	1.70	0.10	0.02	0.43	98.90	98.92	98.18	98.14	83.33
TiO_2	50.60	49.98	51.58	0.22	0.05	0	0.09	0.02	0.08
Cr_2O_3	0.49	0.37	0.23	3.11	0.15	0.09	0.10	0.17	1.50
FeO	44.66	45.83	45.39	31.80	0.36	0.34	0.71	0.51	1.15
Fe_2O_3	0	0	1.03	65.63	0	0	0	0	0
MnO	2.50	2.21	2.14	0.08	0.02	0	0	0.00	0
V_2O_3	0.09	0.12	0.09	1.26	0.05	0	0.03	0.01	0.08
NiO	0.05	0	0.07	0.05	0.01	0.01	0	0	0.04
ZnO	0.10	0.19	0.13	0.01	0	0	0	0.04	0
MgO	0.22	0.32	0.39	0.11	0	0.01	0	0	0.10
CaO	0.01	0.01	0.00	0.02	0.01	0.02	0.01	0.03	0.03
Na_2O	0	0	0.00	0.09	0.00	0	0.01	0	0
P_2O_5	0.08	0	0.05	0	0.01	0	0.05	0	0.03
SnO_2	0	0.00	0	0	0.06	0.00	0.03	0.06	0
F	0.03	0	0	0.45	0	0	0	0	0
H_2O*	0	0	0	0	0	0	0	0	15.00
Total	100.58	99.18	101.12	103.12	99.66	99.44	99.23	98.99	101.35
FeO	44.66	45.83	46.32	90.85	0.36	0.34	0.71	0.51	1.15
Fe^{3+}/Fe_{tot}*			0.02	0.65					
No. Oxy	3	3	3	4	3	3	3	3	2
Ti	0.95	0.97	0.97	0.01	0	0	0	0	0
Al	0.05	0	0	0.02	1.99	1.99	1.99	1.99	0.98
Fe^{3+}	0	0	0.02	1.83	0	0	0	0	0
Cr	0.01	0.01	0	0.09	0	0	0	0	0.02
V^{3+}	0	0	0	0.04	0	0	0	0	0
Fe^{2+}	0.93	0.98	0.95	0.98	0.01	0	0.01	0.01	0
Mn^{2+}	0.05	0.05	0.05	0	0	0	0	0	0
Mg	0.01	0.01	0.01	0.01	0	0	0	0	0
Σ	2.00	2.02	2.00	2.98	2.00	1.99	2.00	2.00	1.00
OH									1.00

Notes: * Calculated; ilm = ilmenite; crn = corundum.

Table 1b. Chemical analyses and formulae of spinel group minerals (on the basis of 4 oxygen atoms per formula unit)

	hrc	hrc	spl	spl	spl	spl	spl	spl	spl	spl	spl	spl	spl	spl	spl
	DB321	DB321	DB402	DB321	DB321	DB321	DB402	DB402	DB402	DB402	DB402	DB402	DB402	DB402	DB402
	-C1-3	-C3-1	-C1-7	-C5-11	-C5-12	-C5-13	-C3-1	-C3-2	-C3-3	-C3-4	-C3-5	-C5-9	-C7-1	-C7-2	-C7-3
Comment	alt.^ bel	alt. bel	alt. bel	core	rim	rim	core	core	core	rim	rim	matrix	vein	vein	vein
SiO_2	0.04	0.15	0.02	0	0	0.01	0.02	0.06	0	0	0	0.01	0.02	0.00	0.03
Al_2O_3	31.57	45.64	48.93	59.87	53.98	52.31	61.67	62.00	60.84	57.18	57.24	60.89	47.01	46.85	47.74
TiO_2	0.49	2.18	0.12	0.05	0	0	0	0.03	0.03	0.01	0	0	0.07	0.10	0.01
Cr_2O_3	23.88	12.65	10.84	1.20	6.21	7.51	1.10	1.20	1.19	4.29	4.00	0.79	12.10	12.06	10.93
FeO	32.19	30.47	28.27	27.22	29.99	29.28	18.24	18.90	22.43	25.25	24.24	26.53	31.33	31.57	30.27
Fe_2O_3	7.85	1.78	4.69	1.59	1.75	2.83	4.45	3.71	3.40	3.83	4.39	0	3.44	3.90	4.16
MnO	0.58	0.44	0.33	0.24	0.34	0.30	0.34	0.32	0.27	0.32	0.28	0.34	0.48	0.47	0.45
V_2O_3	0.37	0.19	0.37	0.10	0.08	0.08	0.18	0.11	0.09	0.11	0.07	0.14	1.49	1.53	1.33
NiO	0.06	0.04	0.08	0.17	0.12	0.13	0.20	0.09	0.17	0.14	0.03	0.16	0.05	0.05	0.05
ZnO	1.57	1.92	1.01	1.14	0.82	0.88	0.54	0.59	0.77	0.86	0.83	0.71	1.98	1.93	2.17
MgO	2.63	5.77	6.96	9.32	7.17	7.27	14.63	14.75	12.01	10.05	10.25	11.15	4.47	4.34	4.80
CaO	0	0.01	0.02	0.30	0.49	0.40	0.01	0.03	0.01	0.02	0.01	0.13	0.01	0	0.01
Na_2O	0.09	0.08	0.09	0.04	0.09	0	0	0.03	0.01	0.08	0.03	0.05	0.06	0.10	0.12
K_2O	0	0	0	0.01	0	0	0	0.01	0	0.01	0	0.01	0	0.01	0.01
P_2O_5	0	0.04	0.04	0.03	0.03	0	0.03	0.10	0.06	0	0.02	0.01	0.03	0.04	0
Total	101.32	101.36	101.77	101.28	101.07	101.00	101.41	101.93	101.28	102.15	101.39	100.92	102.54	102.95	102.08
FeO_{EMPA}	39.26	32.07	32.49	28.65	31.57	31.83	22.24	22.23	25.49	28.69	28.19	26.53	34.43	35.08	34.01
$Fe^{3+}/Fe_{tot}{}^{*}$	0.18	0.05	0.13	0.05	0.05	0.08	0.18	0.15	0.12	0.12	0.14	0	0.09	0.10	0.11
Ti	0.01	0.05	0	0	0	0	0	0	0	0	0	0	0	0	0
Al	1.17	1.56	1.64	1.91	1.79	1.74	1.89	1.89	1.90	1.82	1.83	1.93	1.60	1.60	1.63
Fe^{3+}	0.19	0.04	0.10	0.03	0.04	0.06	0.09	0.07	0.07	0.08	0.09	0	0.07	0.08	0.09
Cr	0.60	0.29	0.24	0.03	0.14	0.17	0.02	0.02	0.03	0.09	0.09	0.02	0.28	0.28	0.25
V^{3+}	0.01	0	0.01	0	0	0	0	0	0	0	0	0	0.03	0.04	0.03
Fe^{2+}	0.85	0.74	0.67	0.62	0.70	0.69	0.40	0.41	0.50	0.57	0.55	0.60	0.76	0.76	0.73
Mn^{2+}	0.02	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Mg	0.12	0.25	0.30	0.38	0.3	0.31	0.57	0.57	0.47	0.41	0.41	0.45	0.19	0.19	0.21
Ni^{2+}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Zn^{2+}	0.04	0.04	0.02	0.02	0.02	0.02	0.01	0.01	0.02	0.02	0.02	0.01	0.04	0.04	0.05
Σ cat	3.01	2.98	2.99	3.00	3.00	3.00	2.99	2.98	3.00	3.00	3.00	3.02	2.98	3.00	3.00

Notes: * Calculated; ^ alt. = alteration; hrc = hercynite; spl = spinel.

Table 1c. Chemical analyses of carbonates.

mineral	dol DB402-C3-6	dol DB402-C4-7	dol DB402-C5-4	dol DB402-C6-1	dol DB402-C6-2	dol DB321-C5-14	magnes DB402-C5-1	magnes DB402-C5-2	magnes DB402-C5-3	calcite DB321-C3-3
comment	crack in sp	matrix	matrix	vein	vein	matrix	matrix	matrix	matrix	inc in bel
CaO	28.47	28.54	28.89	28.91	27.17	26.87	0.38	0.17	0.34	55.61
MgO	17.09	16.91	18.46	19.87	18.09	17.89	44.00	42.56	41.37	1.79
FeO	3.93	4.33	4.78	7.16	3.17	3.63	8.49	10.53	11.86	1.86
MnO	0.46	0.44	0.50	0.82	0.34	0.45	0.76	0.77	0.84	0.47
NiO	0	0.03	0	0.05	0.04	0	0.04	0	0	0.02
ZnO	0	0.06	0	0	0	0.02	0	0.05	0	0.11
Total	49.95	50.31	52.63	56.81	48.81	48.86	53.67	54.08	54.41	59.86

Notes: Dol = dolomite; magnes = magnesite

Table 1d. Chemical analyses and formulae of chlorite group minerals (on the basis of 18 [O+(OH)] per formula unit)

Comment	DB402-C1-9 rim	DB402-C1-10 core	DB402-C2-8 rim	DB402-C2-9 core	DB402-C4-8 rim	DB402-C4-9 core	DB402-C5-6 rim	DB402-C5-5 core	DB321-C1-9 rim	DB321-C1-10 core	DB321-C2-1 alt.^ bel	DB321-C4-11 alt. bel	DB321-C1-1 alt. bel	DB402-C1-6 alt. bel
SiO_2	26.10	26.95	23.81	26.67	22.49	27.22	25.63	27.35	23.70	26.39	23.31	24.91	23.26	23.06
Al_2O_3	25.71	25.70	29.71	25.95	31.98	24.86	27.14	24.42	29.46	26.18	26.76	25.50	27.98	29.32
TiO_2	0.01	0.02	0.03	0	0	0	0.00	0.01	0.05	0.01	0.06	0	0.30	0.01
Cr_2O_3	0.35	0.20	0.19	0.24	0	0.22	0.09	0.11	0.02	0.28	1.04	0.40	1.33	0.42
FeO	8.33	6.31	9.42	6.25	10.68	6.47	8.50	6.05	11.56	6.54	17.83	17.59	16.69	14.01
MnO	0.02	0.08	0.05	0.03	0.06	0.07	0.08	0.07	0.05	0.06	0.11	0.15	0.11	0.05
V_2O_3	0.03	0.05	0.06	0.04	0.11	0	0.05	0.06	0.10	0.07	0.06	0.06	0.02	0.02
NiO	0	0.05	0.11	0.01	0.08	0.13	0.07	0.04	0.04	0.04	0.10	0	0.02	0.00
ZnO	0	0.06	0	0	0.12	0	0	0.06	0.13	0	0	0	0.03	0
MgO	26.36	27.88	24.25	27.94	22.78	28.42	25.79	28.24	23.06	27.58	19.01	20.10	19.34	21.04
H_2O*	12.36	12.55	12.38	12.54	12.39	12.55	12.42	12.45	12.32	12.51	11.88	12.00	12.06	12.13
Total	99.27	99.85	100.00	99.67	100.68	99.94	99.77	98.86	100.48	99.67	100.16	100.71	101.14	100.06
Si	2.53	2.57	2.30	2.55	2.17	2.6	2.47	2.63	2.30	2.53	2.35	2.49	2.31	2.28
^{T}Al	1.47	1.43	1.70	1.45	1.83	1.40	1.53	1.37	1.70	1.47	1.65	1.51	1.69	1.72
Ti	0	0	0	0	0	0	0	0	0	0	0	0	0.02	0.0
^{M}Al	1.47	1.46	1.69	1.47	1.82	1.39	1.56	1.40	1.68	1.48	1.53	1.49	1.59	1.69
Fe^{2+}	0.68	0.50	0.76	0.50	0.86	0.52	0.69	0.49	0.94	0.52	1.50	1.47	1.39	1.16
V^{3+}	0	0	0	0	0.01	0	0	0	0.01	0.01	0.01	0.01	0	0
Mn^{2+}	0	0.01	0	0	0	0.01	0.01	0.01	0	0.01	0.01	0.01	0.01	0
Mg	3.81	3.97	3.50	3.98	3.28	4.04	3.71	4.05	3.34	3.94	2.86	2.99	2.86	3.09
Cr	0.03	0.01	0.01	0.02	0	0.02	0.01	0.01	0	0.02	0.08	0.03	0.1	0.03
Ni^{2+}	0	0	0.01	0	0.01	0.01	0.01	0	0	0	0.01	0	0	0
Zn^{2+}	0	0	0	0	0.01	0	0	0	0.01	0	0	0	0	0
Σ cat	9.98	9.97	9.99	9.98	9.99	9.99	9.97	9.97	9.99	9.98	10.01	10.00	9.98	9.98
OH	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00

Notes: * Calculated; ^ alt. = alteration

Table 1e. Chemical profile of one magnesiobeltrandoite-2*N*3*S* grain. Formula on the basis of 40 O+(OH) per formula unit (Sn, Ca, Na, K and F within detection limits)

	DB321-C7-6	DB321-C7-7	DB321-C7-8	DB321-C7-9	DB321-C7-10
Comment	rim		core		rim
SiO_2	0.03	0.02	0.05	0	0
Al_2O_3	60.54	60.47	60.40	60.32	61.49
TiO_2	2.58	3.65	3.50	3.27	2.40
Cr_2O_3	2.02	1.63	1.98	2.04	1.98
FeO	12.36	11.52	11.502	10.86	11.70
Fe_2O_3	10.36	10.06	10.044	11.14	11.08
MnO	0.28	0.23	0.27	0.29	0.20
V_2O_3	0.15	0.16	0.21	0.16	0.14
NiO	0.05	0.01	0.06	0.11	0.09
ZnO	0.39	0.36	0.25	0.37	0.38
MgO	9.83	11.08	10.90	10.94	10.14
H_2O*	1.16	1.18	1.17	1.18	1.18
TOTAL	99.75	100.37	100.34	100.68	100.78
FeO_{tot}	21.68	20.57	20.54	20.89	21.67
Fe^{3+}/Fe_{tot}*	0.43	0.44	0.44	0.48	0.46
No. Oxy	40	40	40	40	40
Si	0.01	0	0.01	0	0
Ti	0.50	0.70	0.67	0.63	0.46
Al	18.45	18.21	18.22	18.15	18.50
Fe^{3+}	2.02	1.93	1.93	2.14	2.13
Cr	0.41	0.33	0.40	0.41	0.40
V^{3+}	0.03	0.03	0.04	0.03	0.03
Mn^{2+}	0.06	0.05	0.06	0.06	0.04
Fe^{2+}	2.67	2.46	2.46	2.32	2.50
Mg	3.79	4.22	4.16	4.16	3.86
Ni^{2+}	0.01	0	0.01	0.02	0.02
Zn^{2+}	0.07	0.07	0.05	0.07	0.07
Σ cat	28.02	28.02	28.02	27.99	28.01
R^{2+}	6.61	6.8	6.74	6.63	6.49
R^{3+}	21.38	21.18	21.22	21.33	21.49
OH	2.00	2.01	2.00	2.01	2.01

Notes: * Calculated;

Table 2. Analytical data (wt.%) for magnesiobeltrandoite-2*N*3*S* (average of 55 spot analyses).

	Mean	Range	SD	Standard (line)
MgO	10.43	9.33-11.11	0.45	olivine (*Kα*)
ZnO	0.34	0.14-0.52	0.07	rhodonite (*Kα*)
NiO	0.09	0-0.16	0.04	NiAs (*Kα*)
MnO	0.23	0.15-0.32	0.03	rhodonite (*Kα*)
FeO	11.80	10.83-14.18	0.69	fayalite (*Kα*)
Fe_2O_3**	10.83	9.66-12.13	0.57	
Al_2O_3	61.10	59.41-63.50	0.81	almandine (*Kα*)
Cr_2O_3	1.98	1.23-3.19	0.32	Cr (*Kα*)
V_2O_3	0.15	0.09-0.25	0.03	V (*Kα*)
TiO_2	2.91	1.14-4.49	0.26	ilmenite (*Kα*)
H_2O*	1.18	1.16-1.19	0.01	
Total	100.90			

Notes: *by stoichiometry assuming 2 (OH) pfu; ** by charge balance and 28 cations pfu

Table 3. Hyperfine parameters derived from the SMS spectrum of magnesiobeltrandoite-2*N*3*S*

	Component/ Colour in Fig. 3	**Coordination/ Rel. Distribution (%)**	**CS[a] mm/s**	**QS[b] mm/s**	**Area %**	**FWHM[c] mm/s**
Fe^{2+}/Fe_{tot} = 54 %	Fe^{2+} (red)	T sites[d] / 14(5) %	0.81(2)	0.98(5)	8(1)	0.12(5)
	Fe^{2+} (orange)	M sites[e] / 86(3) %	1.10(5)	1.02(8)	46(2)	0.50(4)
Fe^{3+}/Fe_{tot} = 46 %	Fe^{3+} (blue)	T sites / 83(4) %	0.29(2)	0.58(4)	38(1)	0.25(2)
	Fe^{3+} (cyan)	M sites / 17(5) %	0.49(2)	0.54(4)	8(1)	0.10(5)

Notes: [a] CS: centre shift relative to α-Fe; [b] QS: quadrupole splitting; [c] FWHM: full width at half maximum including the source linewidth; [d] T site: tetrahedral site; [e] octahedral site

Table 4. X-ray powder diffraction data for magnesiobeltrandoite-2*N*3*S**. The eight strongest reflections are reported in bold.

h	*k*	*l*	d_{obs}(Å)	d_{calc} (Å)	Int. (obs)	Int. (calc)
0	0	5	4.594	4.605	9.4	6.6
0	1	2	4.546	4.552	11.7	10.3
1	0	3	4.157	4.163	5.4	7.3
0	1	5	3.367	3.373	8.6	8.0
1	0	6	3.028	3.034	10.8	12.9
1	**1**	**0**	**2.858**	**2.861**	**42.2**	**43.8**
1	**0**	**7**	**2.735**	**2.740**	**51.2**	**45.6**
0	**1**	**8**	**2.484**	**2.489**	**45.9**	**38.9**
1	0	8	2.484	2.489	23.0	9.1
0	2	1	2.461	2.464	12.3	12.0
1	**1**	**5**	**2.427**	**2.430**	**100.0**	**100.0**
0	2	2	2.420	2.423	27.8	26.7
0	2	4	2.273	2.276	7.7	6.3
0	2	6	2.079	2.082	20.2	15.4
2	0	6	2.079	2.082	22.0	15.3
0	2	7	1.976	1.979	12.3	9.8
2	0	7	1.976	1.979	16.2	14.5
0	1	13	1.664	1.668	5.3	4.6
3	0	0	1.650	1.652	6.0	6.3
2	1	7	1.625	1.628	21.1	17.2
0	2	11	1.596	1.599	5.5	5.4
1	**2**	**8**	**1.568**	**1.570**	**29.0**	**21.7**
2	1	8	1.568	1.570	11.1	8.2
0	3	5	1.553	1.555	12.8	12.3
3	0	5	1.553	1.555	15.4	10.3
0	**2**	**12**	**1.514**	**1.517**	**29.6**	**21.9**
0	2	13	1.438	1.441	11.1	11.4
2	**0**	**13**	**1.438**	**1.441**	**42.2**	**30.9**
2	**2**	**0**	**1.429**	**1.431**	**71.8**	**61.2**
2	0	14	1.368	1.370	13.9	7.1
3	1	8	1.239	1.240	9.1	6.4
4	1	5	1.052	1.053	6.8	5.7
1	4	5	1.052	1.053	7.7	5.0
4	0	12	1.039	1.041	5.7	4.9
0	4	13	1.014	1.015	17.0	8.1

Notes: Reflections with $I_{rel} > 5\sigma(I_{rel})$ are listed

Table 5. Parameters for X-ray data collection and crystal-structure refinement of magnesiobeltrandoite-2*N*3*S* crystal.

Diffractometer	Xcalibur Rubi Gemini Ultra
X-ray radiation	Mo *K*α (0.71073 Å)
Temperature	293(2) K
Crystal size	0.08 x 0.05 x 0.02 mm^3
Space group	$P\bar{3}m1$
Unit cell dimensions (Å)	
	a = 5.7226(3)
	c = 23.0231(9)
Cell volume ($Å^3$)	652.95(5)
Refined formula	$Mg_{5.13}Fe_{4.83}Al_{18}O_{38}(OH)_2$
Z	1
Completeness	98.5 %
Average redundancy	8.2
Reflections collected	11966
θ-range for data collection (°)	3.54 to 40.91
Index ranges	$-10 \leq h \leq 10$,
	$-10 \leq k \leq 10$,
	$-41 \leq l \leq 36$
Unique reflections	1721
Reflections > 2σ(*I*)	1626
R_{int}	0.0340
R_σ	0.0195
Number of least-squares parameters	94
Goodness-of-fit on F^2	1.111
*R*1, *I*>2σ(*I*)	0.0219
*R*1, all data	0.0242
w*R*2 (on all F^2)	0.0603
Extinction coefficient	0.0019(7)
Largest diff. peak and hole	0.513 and -0.555 e.$Å^{-3}$
$\Delta\rho_{min}$ ($-e \cdot Å^{-3}$)	0.55 [0.93 A from O3]
$\Delta\rho_{max}$ ($e \cdot Å^{-3}$)	0.51 [0.77 Å from M6]

Table 6. Atoms, site occupancies, fractional atom coordinates (Å), and equivalent isotropic displacement parameters (Å^2) for the studied magnesiobeltrandoite-2*N*3*S* crystal.

Site	Refined occ.	*x*/*a*	*y*/*b*	*z*/*c*	*U_{eq}
M1	Al 1.037(7)	0	0	0	0.004(1)
T2	Fe^{2+} 0.480(5)/ Mg^{2+} 0.520(5)	1/3	-1/3	-0.0257(1)	0.007(1)
M3	Al 1.019(4)	0.3380(1)	0.1690(1)	-0.1016(1)	0.005(1)
T4	Fe^{2+} 0.211(5)/ Mg^{2+} 0.789(5)	1/3	-1/3	-0.1736(1)	0.004(1)
M5	Fe^{2+} 0.875(6)/ Mg^{2+} 0.125(6)	-1/3	-2/3	-0.2162(1)	0.004(1)
M6	Al 1.110(4)	0.1641(1)	0.3282(1)	-0.2962(1)	0.005(1)
T7	Fe^{2+} 0.469(5)/ Mg^{2+} 0.531(5)	1/3	2/3	0.3699(1)	0.006(1)
M8	Al 1.028(5)	-1/3	-2/3	0.3995(1)	0.005(1)
T9	Fe^{2+} 0.386(5)/ Mg^{2+} 0.614(5)	0	0	0.4241(1)	0.006(1)
M10	Al 1.044(4)	0	1/2	1/2	0.005(1)
O1		-0.2962(2)	-0.1481(1)	-0.0535(1)	0.008(1)
O2		-1/3	-2/3	-0.0590(1)	0.008(1)
O3		0.5098(1)	-0.5098(1)	-0.1491(1)	0.009(1)
O4		0	0	0.1450(1)	0.008(1)
O5		-0.1638(1)	0.1638(1)	-0.2545(1)	0.007(1)
O6		1/3	-1/3	-0.2535(1)	0.007(1)
O7		0.4808(1)	-0.4808(1)	-0.3473(1)	0.009(1)
O8		0	0	-0.3396(1)	0.006(1)
O9		-0.1856(1)	0.1856(1)	0.4532(1)	0.005(1)
O10		1/3	-1/3	0.4554(1)	0.006(1)
H		0	0	0.1912	0.009

Notes: *The temperature factor has the form exp(−T) where $T = 8\pi^2 U(\sin(\theta)/\lambda)^2$ for isotropic atoms

Table 7. Anisotropic displacement parameters* for magnesiobeltrandoite-2*N*3*S* (Å).

site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{13}
M1	0.0047(3)	0.0047(3)	0.0038(5)	0.000	0.000	0.00235(16)
T2	0.00721(19)	0.00721(19)	0.0061(2)	0.000	0.000	0.00361(10)
M3	0.0048(2)	0.00555(17)	0.00464(18)	0.00015(9)	0.00030(17)	0.00239(10)
T4	0.0045(2)	0.0045(2)	0.0032(2)	0.000	0.000	0.00224(11)
M5	0.00455(11)	0.00455(11)	0.00269(13)	0.000	0.000	0.00228(6)
M6	0.00460(14)	0.00446(16)	0.00446(15)	-0.00069(13)	-0.00035(6)	0.00223(8)
T7	0.00580(17)	0.00580(17)	0.0069(2)	0.000	0.000	0.00290(9)
M8	0.0054(2)	0.0054(2)	0.0043(3)	0.000	0.000	0.00271(12)
T9	0.00620(19)	0.00620(19)	0.0054(3)	0.000	0.000	0.00310(10)
M10	0.0044(2)	0.0046(2)	0.0044(2)	-0.00024(11)	-0.0005(2)	0.00218(12)
O1	0.0076(5)	0.0084(3)	0.0072(4)	-0.00029(16)	-0.0006(3)	0.0038(2)
O2	0.0081(5)	0.0081(5)	0.0074(6)	0.000	0.000	0.0040(2)
O3	0.0095(3)	0.0095(3)	0.0073(4)	0.00027(19)	-0.00027(19)	0.0035(4)
O4	0.0096(5)	0.0096(5)	0.0037(6)	0.000	0.000	0.0048(2)
O5	0.0072(3)	0.0072(3)	0.0063(4)	-0.00095(19)	0.00095(19)	0.0037(4)
O6	0.0071(5)	0.0071(5)	0.0064(6)	0.000	0.000	0.0035(2)
O7	0.0084(3)	0.0084(3)	0.0074(4)	0.00112(17)	-0.00112(17)	0.0032(4)
O8	0.0062(4)	0.0062(4)	0.0049(6)	0.000	0.000	0.0031(2)
O9	0.0056(3)	0.0056(3)	0.0051(4)	-0.00016(15)	0.00016(15)	0.0026(3)
O10	0.0056(4)	0.0056(4)	0.0060(6)	0.000	0.000	0.0028(2)

Notes: *The temperature factor has the form exp(−T) where T = $-2\pi^2$ [$h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + ... + 2hka^*b^*U_{12}$].

Table 8. Main interatomic distances (Å) and geometrical parameters for magnesiobeltrandoite-2*N*3*S*.

T2–O1 (×3)	1.9443(12)	M1–O1 (×6)	1.9164(11)
–O2	1.950(2)	<M1–O>	1.9164
<T2–O>	1.946	V(Å^3)	9.20
V(Å^3)	3.78	σ^2*	51.72
σ^2*	0.08	λ*	1.0136
λ*	1.000		
		M5–O3 (×3)	2.1917(12)
T4–O3 (×3)	1.8377(13)	M5–O5 (×3)	1.8972(12)
–O6	1.8381(18)	<M5–O>	2.0444
<T4–O>	1.8378	V(Å^3)	10.99
V(Å^3)	3.18	σ^2*	83.32
σ^2*	2.94	λ*	1.0295
λ*	1.0008		
		M6–O5 (×2)	1.8875(8)
T7–O7 (×3)	1.9146(12)	M6–O6	1.9439(9)
–O10	1.9688(18)	M6–O7 (×2)	1.9712(8)
<T7–O>	1.9281	M6–O8	1.9097(10)
V(Å^3)	3.66	<M6–O>	1.9285
σ^2*	15.41	V(Å^3)	9.40
λ*	1.0038	σ^2*	40.77
		λ*	1.0118
T9–O9 (×3)	1.9572(11)		
–O8	1.9453(18)	M8–O7 (×3)	1.8922(11)
<T9–O>	1.9542	M8–O9 (×3)	1.9159(11)
V(Å^3)	3.83	<M8–O>	1.9040
σ^2*	0.34	V(Å^3)	9.04
λ*	1.0001	σ^2*	47.12
		λ*	1.0125
M3–O1 (×2)	1.9303(8)		
M3–O2	1.9009(11)	M10–O9 (×4)	1.9018(7)
M3–O3 (×2)	1.9331(8)	M10–O10 (×2)	1.9448(9)
M3–O4	1.9506(10)	<M10–O>	1.9161
<M3–O>	1.9297	V(Å^3)	9.22
V(Å^3)	9.44	σ^2*	44.39
σ^2*	36.76	λ*	1.0119
λ*	1.0098		
		O4–H	1.0645(17)
		O4–H…O5	2.1810(12)
		O4–H–O5	131.89(3)°

Notes: *Mean quadratic elongation (λ) and the angle variance (σ^2) were computed according to Robinson *et al*. (1971)

Table 9. Refined site-scattering and assigned site-populations for magnesiobeltrandoite-2*N*3*S*.

	Al	Mg	Fe^{2+}	Fe^{3+}	Ti^{4+}	V^{3+}	Cr^{3+}	Mn^{2+}	Zn	Σ cat	s.s. $_{cal.}$	s.s. $_{obs.}$	Δ	$<R\text{-O}>_{obs}$	$<R\text{-O}>_{calc}$	Δ
M1	0.91			0.02		0.03	0.04			1.00	13.94	13.48	-0.46	1.916	1.917	-0.001
T2	0.15	0.43	0.39						0.03	1.00	36.30	37.45	1.15	1.946	1.950	-0.004
M3	0.89	0.08		0.01			0.02			1.00	79.62	79.48	-0.14	1.930	1.925	0.005
T4	0.62	0.24	0.06	0.08						1.00	29.16	29.92	0.76	1.838	1.842	-0.004
M5		0.07	0.17	0.47	0.28			0.01		1.00	47.78	48.49	0.71	2.044	2.034	0.010
M6	0.88			0.11			0.01			1.00	87.24	86.61	-0.63	1.929	1.922	0.007
T7	0.20	0.38	0.36	0.06						1.00	36.16	37.13	0.97	1.928	1.934	-0.006
M8	0.97						0.03			1.00	26.66	26.73	0.07	1.904	1.911	-0.007
T9	0.04	0.62	0.28	0.06						1.00	33.60	34.81	1.21	1.954	1.962	-0.008
M10	0.96						0.04			1.00	40.32	40.71	0.39	1.916	1.911	0.005
Σ*	18.37	3.96	2.52	2.08	0.56	0.03	0.40	0.02	0.06	28.00	430.78	434.81				

Notes: * Sums taking into account site multiplicity; s.s. $_{cal.}$ = calculated site scattering (in electrons per formula unit, e.p.f.u); s.s. $_{obs.}$ = observed site scattering (in electrons per formula unit, e.p.f.u); Δ = difference; $<R\text{-O}>_{obs}$ = observed mean bond length (in Å); $<R\text{-O}>_{calc}$ = calculated mean bond length (in Å).

Table 10. Bond-valence values* for structural sites of magnesiobeltrandoite-2*N*3*S*.

	M1	T2	M3	T4	M5	M6	T7	M8	T9	M10	H	Σ
O1	$0.501_{\times 6\downarrow}$	$0.518_{\times 3\downarrow}$	$0.465_{\times 2\downarrow}{}^{\times 2\rightarrow}$									1.948
O2		$0.510^{\times 3\rightarrow}$	0.502									2.017
O3			$0.462_{\times 2\downarrow}{}^{\times 2\rightarrow}$	$0.635_{\times 3\downarrow}$	$0.319_{\times 3\downarrow}$							1.878
^{III}O4			$0.441^{\times 3\rightarrow}$								0.590	1.913
O5					$0.702_{\times 3\downarrow}$	$0.549_{\times 2\downarrow}{}^{\times 2\rightarrow}$					$0.133_{\times 3\downarrow}$	1.933
O6				0.635		$0.472^{\times 3\rightarrow}$						2.050
O7						$0.439_{\times 2\downarrow}{}^{\times 2\rightarrow}$	$0.563_{\times 3\downarrow}$	$0.524_{\times 3\downarrow}$				2.121
O8						$0.517^{\times 3\rightarrow}$			0.515			2.066
O9								$0.492_{\times 3\downarrow}$	$0.499_{\times 3\downarrow}$	$0.512_{\times 4\downarrow}{}^{\times 2\rightarrow}$		2.015
O10							0.516			$0.457_{\times 2\downarrow}{}^{\times 3\rightarrow}$		1.859
BVS	3.006	2.064	2.797	2.540	3.063	2.964	2.175	3.048	2.012	2.961	0.989	
f.c.	3.000	2.150	2.900	2.700	3.030	3.000	2.260	3.000	2.100	3.000	1.000	

Notes: *Bond-valence parameters from Brown (1981); BVS = bond valence sum; f.c. = formal charge; anion sites coordination reported only for coordination other than IV.

Table 11. The högbomite supergroup. (References are given in brackets).

Högbomite supergroup
(Mills *et al.*, 2009)

$N \times \mathbf{TM}_4O_7(OH) \cdot S \times \mathbf{T}_2\mathbf{M}_4O_8$ (theoretical composition)

Högbomite group	Nigerite group	Taaffeite group	"Beltrandoite group" (*)
Ferrohögbomite-2*N*2*S* (1)(2)(3)(4)(5)	Ferronigerite-2*N*1*S* (1)(4)(14)(15)(16)(17)(18)	Ferrotaaffeite-2*N*'2*S* (1)(4)(23)(24)(25(26)	Magnesiobeltrandoite-2*N*3*S* (32)
Magnesiohögbomite-2*N*2*S* (1)(2)(3)(4)(5)	Ferronigerite-6*N*6*S* (1)(4)(14)(15)(16)(19)(20)	Ferrotaaffeite-6*N*'3*S* (1)(4)(23)(27)(28)(29)	
Magnesiohögbomite-2*N*3*S* (1)(2)(4)(6)	Magnesionigerite-2*N*1*S* (1)(4)(14)(15)(16)(19)(21)(22)	Magnesiotaaffeite-2*N*'2*S* (1)(4)(23)(26)(27)(29)(30)(31)	
Magnesiohögbomite-2*N*4*S* (1)(7)	Magnesionigerite-6*N*6*S* (1)(4)(14)(15)(16)(19)(21)(22)	Magnesiotaaffeite-6*N*'3*S* (1)(4)(23)(25)(27)(29)(30)	
Magnesiohögbomite-6*N*6*S* (1)(2)(4)(6)(8)			
Zincohögbomite-2*N*2*S* (1)(2)(4)(6)(9)(10)			
Zincohögbomite-2*N*6*S* (1)(2)(4)(11)(12)(13)			

Refs.: (*) Because magnesiobeltrandoite-2*N*3*S* is the only mineral in the relevant group, it should be classified as **Unassigned member of the högbomite supergroup;** (1) Armbruster (2002); (2) McKie (1963); (3) Gatehouse and Grey (1982); (4) Hejny and Armbruster (2002); (5) Hejny *et al.* (2002); (6) Gavelin (1916); (7) Shimura *et al.* (2012); (8) Schmetzer and Berger (1990); (9) Armbruster (1998); (10) Ockenga *et al.* (1998); (11) Moleva and Miasnikov (1952); (12) Yalçin *et al.* (1993); (13) Armbruster *et al.* (1998); (14) Bannister *et al*. (1947); (15) Jacobson and Webb (1947); (16) Burke *et al*. (1977); (17) Arakcheeva *et al.* (1995); (18) Yang *et al.* (2013); (19) Peacor (1967); (20) Grey and Gatehouse (1979); (21) Chen *et al.* (1989a); (22) Chen *et al.* (1989b); (23) Anderson *et al.* (1951); (24) Peng and Wang (1963); (25) Nuber and Schmetzer (1983); (26) Yang *et al.* (2012); (27) Hudson *et al.* (1967); (28) Burke and Lustenhouwer (1981); (29) Schmetzer (1983); (30) Bernhard *et al.* (2008); (31) Moor *et al.* (1981); (32) this work.

```
#
# h,k,l, Fc-squared, Fo-squared, sigma(Fo-squared) and status flag
#
data_magnesiobeltrandoite-2N3S
_shelx_title ' magnesiobeltrandoite-2N3S'
_shelx_refln_list_code          4
_shelx_F_calc_maximum      360.64
_exptl_crystal_F_000       756.98
_reflns_d_resolution_high  0.5426

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-y, x-y, z'
 'y, x, -z'
 '-x+y, -x, z'
 '-x, -x+y, -z'
 'x-y, -y, -z'
 '-x, -y, -z'
 'y, -x+y, -z'
 '-y, -x, z'
 'x-y, x, -z'
 'x, x-y, z'
 '-x+y, y, z'

_cell_length_a     5.7226
_cell_length_b     5.7226
_cell_length_c    23.0231
_cell_angle_alpha  90.000
_cell_angle_beta   90.000
_cell_angle_gamma 120.000

_shelx_F_squared_multiplier     1.000

loop_
 _refln_index_h
 _refln_index_k
 _refln_index_l
 _refln_F_squared_calc
 _refln_F_squared_meas
 _refln_F_squared_sigma
 _refln_observed_status
   0   1   0      525.20      575.68     11.37 o
  -1   2   0    18050.05    18289.60    217.28 o
   0   2   0     1350.33     1498.83     14.43 o
  -1   3   0      378.92      362.20      6.11 o
   0   3   0     9456.60     9106.71     79.17 o
  -2   4   0   130060.30   124307.27   1260.85 o
  -1   4   0      174.59      166.36      4.18 o
   0   4   0     1053.99     1017.69     15.31 o
  -2   5   0      130.23      134.64      3.67 o
  -1   5   0     5529.66     5683.46     40.65 o
   0   5   0      162.11      164.52      7.44 o
  -3   6   0     5356.51     5430.85     64.33 o
  -2   6   0      670.09      680.12     11.62 o
  -1   6   0       80.57       92.40      4.39 o
   0   6   0    33705.67    34272.93    394.74 o
  -3   7   0       95.70       97.86      4.85 o
  -2   7   0     2012.19     2010.11     26.71 o
  -1   7   0       44.13       52.07      4.93 o
```

0	7	0	46.46	40.67	7.88	o
-4	8	0	21284.25	21587.94	241.97	o
-3	8	0	34.25	33.78	5.04	o
-2	8	0	302.44	315.15	10.85	o
-1	8	0	2340.08	2391.67	43.86	o
0	8	0	239.17	224.79	22.00	o
-4	9	0	34.28	33.67	4.88	o
-3	9	0	1400.33	1378.92	24.74	o
-2	9	0	55.43	47.67	8.42	o
-1	9	0	38.22	34.52	7.79	o
0	9	0	670.63	675.64	40.13	o
-5	10	0	2116.21	2107.04	50.21	o
-4	10	0	179.58	178.68	12.05	o
-3	10	0	23.62	24.52	12.23	o
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0	1	1	175.34	172.71	3.30	o
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-1	2	1	1.63	3.95	1.09	o
0	2	1	3758.10	3941.01	35.99	o
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-1	3	1	396.36	378.04	7.64	o
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-1	4	1	78.86	77.65	2.96	o
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-5	5	1	159.65	158.48	7.31	o
-4	5	1	22.69	27.05	2.75	o
-3	5	1	107.65	102.27	3.19	o
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-1	5	1	22.99	24.72	2.66	o
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-6	6	1	2.03	4.38	6.38	o
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-4	7	1	85.53	86.35	4.67	o
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-6	8	1	455.14	464.23	13.01	o
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-1	8	1	6.56	6.79	4.28	o
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-6	9	1	8.78	14.47	5.34	o
-5	9	1	40.60	43.17	5.76	o
-4	9	1	39.81	40.23	6.81	o
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-7	10	1	47.55	40.95	11.16	o
-6	10	1	170.18	186.38	11.54	o
-5	10	1	7.14	11.77	5.68	o
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-1	2	2	100.13	123.13	2.60	o
0	2	2	8473.33	8918.94	91.85	o
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-2	3	2	411.49	419.85	5.82	o
-1	3	2	419.22	396.85	6.67	o
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-1	8	2	25.84	27.77	5.88	o
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-7	9	2	186.80	186.89	15.82	o

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-7	9	3	29.02	20.52	7.30	o
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-1	3	4	316.87	327.73	6.46	o
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-1	9	5	78.21	77.11	8.36	o
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-5	10	5	1609.02	1592.32	30.58	o
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-2	6	6	1713.73	1716.62	20.94	o
-1	6	6	291.35	293.91	8.65	o
0	6	6	18.64	28.33	5.46	o
-7	7	6	257.49	252.16	21.24	o
-6	7	6	189.08	203.05	10.56	o
-5	7	6	159.82	160.63	6.91	o
-4	7	6	351.92	338.73	8.88	o
-3	7	6	359.39	373.21	11.32	o
-2	7	6	159.85	171.29	8.21	o
-1	7	6	185.16	186.98	9.53	o
0	7	6	262.50	264.48	17.69	o
-8	8	6	378.68	354.25	27.41	o
-7	8	6	13.88	14.68	6.70	o
-6	8	6	602.20	633.60	17.97	o
-5	8	6	106.89	114.23	7.27	o
-4	8	6	11.51	12.86	3.40	o
-3	8	6	104.83	106.73	7.35	o
-2	8	6	601.81	582.05	15.93	o
-1	8	6	13.61	13.03	5.39	o
0	8	6	379.92	399.06	22.81	o
-8	9	6	102.10	104.24	12.11	o
-7	9	6	207.02	210.94	12.32	o
-6	9	6	42.07	33.53	6.03	o
-5	9	6	166.64	177.83	10.50	o
-4	9	6	170.04	151.47	9.66	o
-3	9	6	41.90	45.24	6.21	o

-2	9	6	202.70	202.41	12.16	o
-1	9	6	104.10	116.05	9.86	o
-7	10	6	53.02	51.22	9.72	o
-6	10	6	261.28	273.91	13.83	o
-5	10	6	6.29	12.05	6.46	o
-4	10	6	262.42	259.71	12.95	o
-3	10	6	53.67	64.17	10.58	o
0	0	7	54.38	111.09	15.27	o
-1	1	7	9908.36	10226.88	178.53	o
0	1	7	10119.87	10416.16	80.50	o
-2	2	7	12234.06	12792.14	162.61	o
-1	2	7	94.73	90.12	2.14	o
0	2	7	12285.93	12477.11	104.64	o
-3	3	7	36.40	36.25	3.59	o
-2	3	7	6742.04	6650.53	46.44	o
-1	3	7	6881.21	6715.31	50.47	o
0	3	7	36.17	33.33	3.30	o
-4	4	7	3804.76	3622.80	53.45	o
-3	4	7	4041.63	3963.52	29.63	o
-2	4	7	85.29	93.76	4.28	o
-1	4	7	3957.91	3851.29	45.41	o
0	4	7	3789.39	3765.94	38.69	o
-5	5	7	2758.88	2781.30	38.94	o
-4	5	7	35.30	33.50	2.25	o
-3	5	7	3140.71	3121.23	34.34	o
-2	5	7	3207.70	3235.20	28.85	o
-1	5	7	35.34	35.50	2.81	o
0	5	7	2703.84	2710.17	56.04	o
-6	6	7	39.12	42.60	4.67	o
-5	6	7	1589.30	1668.42	33.60	o
-4	6	7	1805.15	1865.27	20.08	o
-3	6	7	52.62	55.50	3.77	o
-2	6	7	1812.05	1811.14	21.84	o
-1	6	7	1621.50	1673.07	25.37	o
0	6	7	39.09	45.32	6.44	o
-7	7	7	1055.46	1068.52	43.95	o
-6	7	7	1053.52	1094.05	21.90	o
-5	7	7	16.45	15.71	3.71	o
-4	7	7	1538.70	1557.45	25.22	o
-3	7	7	1569.86	1564.86	20.18	o
-2	7	7	16.45	22.93	5.23	o
-1	7	7	1031.69	1003.28	23.78	o
0	7	7	1077.81	1027.29	35.09	o
-8	8	7	370.29	346.95	27.42	o
-7	8	7	41.84	48.42	7.03	o
-6	8	7	684.29	703.49	23.22	o
-5	8	7	727.10	742.16	16.53	o
-4	8	7	25.03	31.37	5.70	o
-3	8	7	712.85	682.31	17.21	o
-2	8	7	678.68	678.48	17.30	o
-1	8	7	41.80	44.50	6.69	o
0	8	7	372.67	392.08	22.90	o
-8	9	7	452.39	450.66	31.93	o
-7	9	7	744.13	774.96	23.37	o
-6	9	7	24.22	35.68	5.13	o
-5	9	7	719.59	700.52	23.40	o
-4	9	7	734.94	753.54	20.81	o
-3	9	7	24.18	19.47	5.02	o
-2	9	7	729.35	731.75	22.79	o
-1	9	7	461.29	462.00	17.98	o

-7	10	7	298.60	301.91	21.55	o
-6	10	7	264.89	283.30	14.13	o
-5	10	7	49.08	62.75	8.24	o
-4	10	7	267.43	295.48	13.89	o
-3	10	7	304.02	292.81	21.24	o
0	0	8	55.50	79.94	6.97	o
-1	1	8	13110.01	13279.80	221.04	o
0	1	8	12937.21	13477.65	117.45	o
-2	2	8	2418.20	2405.90	24.57	o
-1	2	8	0.22	1.46	0.75	o
0	2	8	2376.75	2388.44	25.45	o
-3	3	8	22.50	21.70	2.42	o
-2	3	8	12859.49	12643.84	72.99	o
-1	3	8	12736.83	12545.17	88.66	o
0	3	8	22.04	29.15	3.32	o
-4	4	8	746.31	753.25	16.05	o
-3	4	8	6298.27	6166.85	38.22	o
-2	4	8	138.19	133.15	4.51	o
-1	4	8	6368.19	6187.17	52.54	o
0	4	8	757.77	716.27	18.66	o
-5	5	8	5812.87	5946.98	73.46	o
-4	5	8	2.59	2.25	1.59	o
-3	5	8	3449.17	3471.27	36.43	o
-2	5	8	3397.43	3374.73	36.93	o
-1	5	8	2.62	4.79	1.92	o
0	5	8	5862.55	5880.81	105.84	o
-6	6	8	100.82	95.47	7.67	o
-5	6	8	3525.21	3638.97	44.33	o
-4	6	8	342.22	344.24	7.39	o
-3	6	8	8.71	14.36	3.27	o
-2	6	8	337.82	341.28	9.76	o
-1	6	8	3498.21	3485.58	39.78	o
0	6	8	100.93	115.66	9.10	o
-7	7	8	901.23	901.50	40.05	o
-6	7	8	1453.93	1516.53	26.77	o
-5	7	8	10.36	8.90	3.94	o
-4	7	8	3477.61	3551.92	34.39	o
-3	7	8	3450.24	3497.74	46.00	o
-2	7	8	10.16	9.21	4.39	o
-1	7	8	1471.52	1542.26	25.44	o
0	7	8	885.47	844.49	54.11	o
-8	8	8	62.04	65.05	13.21	o
-7	8	8	12.88	11.15	4.47	o
-6	8	8	149.02	158.76	10.27	o
-5	8	8	1554.03	1566.88	31.40	o
-4	8	8	85.46	86.63	6.22	o
-3	8	8	1565.48	1543.05	26.75	o
-2	8	8	152.09	142.61	8.24	o
-1	8	8	12.80	14.03	5.26	o
0	8	8	61.09	61.18	10.77	o
-8	9	8	1163.98	1150.99	48.26	o
-7	9	8	1706.95	1629.02	38.97	o
-6	9	8	0.93	5.59	5.30	o
-5	9	8	697.34	722.39	27.32	o
-4	9	8	686.13	693.37	18.66	o
-3	9	8	0.91	9.64	4.31	o
-2	9	8	1720.91	1693.75	39.41	o
-1	9	8	1156.91	1109.64	28.78	o
-7	10	8	896.32	762.50	59.35	o
-6	10	8	55.05	56.73	7.21	o

-5	10	8	30.97	29.03	6.36	o
-4	10	8	53.97	63.54	8.12	o
-3	10	8	892.63	895.44	51.86	o
0	0	9	39.86	41.17	3.97	o
-1	1	9	979.13	998.40	16.40	o
0	1	9	974.66	1005.62	12.25	o
-2	2	9	864.54	894.52	13.10	o
-1	2	9	273.63	268.94	4.83	o
0	2	9	859.74	866.12	12.58	o
-3	3	9	182.93	178.86	4.91	o
-2	3	9	2301.97	2268.14	16.43	o
-1	3	9	2279.01	2253.22	20.40	o
0	3	9	179.80	184.03	7.91	o
-4	4	9	360.53	353.41	8.01	o
-3	4	9	660.10	634.66	7.45	o
-2	4	9	29.60	29.08	2.74	o
-1	4	9	666.16	641.79	11.42	o
0	4	9	359.91	354.54	12.25	o
-5	5	9	1396.01	1403.37	32.70	o
-4	5	9	115.34	112.53	3.78	o
-3	5	9	76.77	85.23	3.79	o
-2	5	9	76.82	75.50	4.97	o
-1	5	9	117.21	116.01	5.26	o
0	5	9	1411.70	1404.57	29.36	o
-6	6	9	11.38	17.14	4.71	o
-5	6	9	681.21	712.48	13.33	o
-4	6	9	248.47	240.48	6.28	o
-3	6	9	103.95	97.72	4.80	o
-2	6	9	250.49	240.73	10.89	o
-1	6	9	673.38	648.03	15.70	o
0	6	9	11.40	17.19	5.59	o
-7	7	9	6.35	3.47	8.20	o
-6	7	9	62.96	65.03	6.83	o
-5	7	9	88.66	87.14	7.32	o
-4	7	9	832.24	842.64	14.49	o
-3	7	9	822.89	816.98	15.95	o
-2	7	9	86.82	78.32	5.96	o
-1	7	9	63.47	62.09	5.73	o
0	7	9	6.26	3.96	5.84	o
-8	8	9	141.70	137.53	19.32	o
-7	8	9	69.08	58.64	7.74	o
-6	8	9	111.53	115.89	10.47	o
-5	8	9	202.39	200.79	11.05	o
-4	8	9	6.69	8.73	3.88	o
-3	8	9	204.86	199.94	9.33	o
-2	8	9	111.04	107.79	7.54	o
-1	8	9	69.91	76.56	7.77	o
0	8	9	143.85	149.06	14.74	o
-8	9	9	251.79	304.08	18.76	o
-7	9	9	448.57	416.86	15.96	o
-6	9	9	61.44	64.23	7.78	o
-5	9	9	1.84	10.16	5.32	o
-4	9	9	1.86	6.24	4.57	o
-3	9	9	62.69	65.10	6.69	o
-2	9	9	453.49	439.76	17.64	o
-1	9	9	248.85	241.98	13.59	o
-6	10	9	97.76	105.94	10.08	o
-5	10	9	65.25	74.04	8.63	o
-4	10	9	98.99	118.69	10.17	o
0	0	10	1827.69	1536.44	29.68	o

-1	1	10	74.10	73.98	4.28	o
0	1	10	74.09	69.31	2.68	o
-2	2	10	2099.29	2118.87	42.94	o
-1	2	10	79.65	92.58	4.09	o
0	2	10	2136.31	2139.01	25.89	o
-3	3	10	9.65	15.22	5.41	o
-2	3	10	65.21	51.84	1.75	o
-1	3	10	64.18	58.66	2.91	o
0	3	10	9.56	12.00	2.87	o
-4	4	10	857.16	882.86	13.92	o
-3	4	10	22.43	24.84	1.91	o
-2	4	10	1060.20	925.14	11.74	o
-1	4	10	22.63	21.28	2.86	o
0	4	10	842.77	820.36	16.91	o
-5	5	10	43.43	39.33	7.03	o
-4	5	10	76.36	87.94	3.46	o
-3	5	10	23.40	22.96	2.25	o
-2	5	10	23.21	27.13	3.70	o
-1	5	10	76.44	77.50	4.74	o
0	5	10	44.36	47.30	4.78	o
-6	6	10	972.74	970.81	23.27	o
-5	6	10	9.20	13.79	3.59	o
-4	6	10	431.17	430.64	8.72	o
-3	6	10	240.70	242.12	7.55	o
-2	6	10	438.40	427.82	10.97	o
-1	6	10	9.03	9.69	3.40	o
0	6	10	972.41	935.90	31.21	o
-7	7	10	8.28	11.40	8.39	o
-6	7	10	3.70	4.01	3.41	o
-5	7	10	0.20	4.88	3.62	o
-4	7	10	21.13	24.79	3.33	o
-3	7	10	20.69	20.28	3.67	o
-2	7	10	0.20	2.88	3.51	o
-1	7	10	3.76	4.17	3.70	o
0	7	10	8.14	-3.84	6.50	o
-8	8	10	94.34	121.39	16.96	o
-7	8	10	153.12	153.65	10.21	o
-6	8	10	158.34	157.24	10.09	o
-5	8	10	0.77	9.71	4.06	o
-4	8	10	710.26	715.78	16.55	o
-3	8	10	0.78	0.83	3.88	o
-2	8	10	156.19	147.09	8.51	o
-1	8	10	153.10	154.70	10.66	o
0	8	10	95.72	100.32	16.50	o
-8	9	10	3.31	0.85	7.69	o
-7	9	10	14.09	22.02	5.73	o
-6	9	10	16.66	27.29	6.44	o
-5	9	10	4.61	7.30	5.40	o
-4	9	10	4.52	11.67	4.67	o
-3	9	10	16.65	14.27	4.33	o
-2	9	10	14.35	22.25	5.88	o
-1	9	10	3.24	1.95	5.59	o
-6	10	10	66.07	85.41	11.40	o
-5	10	10	243.04	247.94	15.69	o
-4	10	10	66.87	77.57	10.19	o
0	0	11	62.08	60.58	5.08	o
-1	1	11	20.91	24.00	2.66	o
0	1	11	21.26	21.05	1.90	o
-2	2	11	4769.70	4755.96	50.90	o
-1	2	11	151.90	151.30	3.72	o

0	2	11	4685.47	4718.76	45.46	o
-3	3	11	111.77	112.66	5.11	o
-2	3	11	285.51	271.12	4.67	o
-1	3	11	287.67	251.76	5.32	o
0	3	11	112.49	104.83	4.82	o
-4	4	11	2158.55	2242.92	38.06	o
-3	4	11	9.85	13.16	1.37	o
-2	4	11	15.70	15.18	1.85	o
-1	4	11	9.97	17.16	2.52	o
0	4	11	2198.88	2185.34	31.40	o
-5	5	11	346.21	340.53	12.29	o
-4	5	11	48.59	49.35	3.00	o
-3	5	11	72.02	72.66	3.61	o
-2	5	11	73.55	80.65	4.56	o
-1	5	11	48.64	39.75	3.36	o
0	5	11	343.30	355.44	11.74	o
-6	6	11	2.75	3.68	3.80	o
-5	6	11	81.17	87.49	5.54	o
-4	6	11	1404.17	1450.72	19.62	o
-3	6	11	26.79	27.10	3.63	o
-2	6	11	1377.65	1351.57	21.09	o
-1	6	11	81.86	84.62	6.15	o
0	6	11	2.80	9.18	6.04	o
-7	7	11	95.65	96.19	11.49	o
-6	7	11	13.65	17.39	4.24	o
-5	7	11	34.69	32.28	5.76	o
-4	7	11	186.60	192.17	7.52	o
-3	7	11	188.04	196.61	9.42	o
-2	7	11	34.54	31.91	4.45	o
-1	7	11	13.37	13.22	3.95	o
0	7	11	97.62	87.85	11.48	o
-8	8	11	599.15	643.96	36.66	o
-7	8	11	10.12	16.86	5.41	o
-6	8	11	567.04	540.08	17.03	o
-5	8	11	4.83	11.93	4.23	o
-4	8	11	0.37	7.72	4.15	o
-3	8	11	4.83	2.56	4.20	o
-2	8	11	578.68	596.77	16.47	o
-1	8	11	10.25	11.53	4.62	o
0	8	11	587.15	519.15	27.10	o
-8	9	11	38.96	46.49	9.11	o
-7	9	11	134.77	143.66	13.82	o
-6	9	11	17.76	29.72	6.45	o
-5	9	11	56.17	64.91	7.50	o
-4	9	11	57.34	58.97	8.87	o
-3	9	11	18.03	14.25	4.87	o
-2	9	11	134.14	131.42	10.13	o
-1	9	11	39.11	46.43	7.14	o
-6	10	11	420.79	430.43	23.03	o
-5	10	11	2.59	5.98	5.39	o
-4	10	11	412.18	389.66	34.90	o
0	0	12	302.11	346.33	11.87	o
-1	1	12	1074.36	1088.77	12.85	o
0	1	12	1091.09	1029.01	15.58	o
-2	2	12	20810.26	20179.43	262.19	o
-1	2	12	2.12	3.47	1.25	o
0	2	12	20382.82	20038.64	151.91	o
-3	3	12	10.69	10.39	1.91	o
-2	3	12	645.01	652.68	7.72	o
-1	3	12	638.11	629.24	7.38	o

0	3	12	10.78	10.96	2.53	o
-4	4	12	9211.96	9488.87	174.77	o
-3	4	12	594.54	596.91	7.89	o
-2	4	12	135.37	124.88	3.94	o
-1	4	12	588.25	622.29	10.07	o
0	4	12	9405.72	9347.51	109.66	o
-5	5	12	323.78	303.29	11.84	o
-4	5	12	6.53	6.96	2.15	o
-3	5	12	473.78	495.19	10.14	o
-2	5	12	483.66	497.50	10.29	o
-1	5	12	6.63	11.85	2.62	o
0	5	12	330.41	335.78	11.44	o
-6	6	12	36.31	44.77	5.38	o
-5	6	12	334.78	343.57	11.20	o
-4	6	12	5435.64	5480.45	112.30	o
-3	6	12	12.31	10.19	2.62	o
-2	6	12	5322.96	5358.11	52.82	o
-1	6	12	333.78	333.62	11.32	o
0	6	12	36.34	43.92	10.69	o
-7	7	12	247.46	265.03	18.41	o
-6	7	12	271.20	282.98	10.57	o
-5	7	12	8.24	11.79	4.94	o
-4	7	12	228.56	235.63	8.70	o
-3	7	12	224.69	216.07	9.98	o
-2	7	12	8.24	17.03	4.67	o
-1	7	12	266.26	257.10	10.45	o
0	7	12	252.57	255.31	17.89	o
-8	8	12	1748.08	1781.69	63.02	o
-7	8	12	21.59	21.22	6.13	o
-6	8	12	2066.45	2081.33	45.22	o
-5	8	12	292.18	283.99	11.40	o
-4	8	12	20.87	20.47	4.66	o
-3	8	12	289.24	273.71	11.27	o
-2	8	12	2110.13	2156.19	33.18	o
-1	8	12	21.77	22.66	5.51	o
0	8	12	1711.54	1633.43	88.93	o
-8	9	12	140.97	140.38	13.46	o
-7	9	12	105.68	98.99	8.66	o
-6	9	12	9.10	10.43	6.53	o
-5	9	12	192.13	180.19	11.90	o
-4	9	12	196.21	197.23	11.40	o
-3	9	12	9.27	12.66	4.43	o
-2	9	12	107.82	101.62	9.21	o
-1	9	12	140.60	142.84	12.83	o
-6	10	12	1212.97	1202.37	53.60	o
-5	10	12	36.95	40.32	9.72	o
0	0	13	107.45	109.03	6.79	o
-1	1	13	4718.64	4560.36	46.06	o
0	1	13	4672.88	4497.79	43.84	o
-2	2	13	44440.45	44326.97	485.13	o
-1	2	13	54.66	61.01	2.35	o
0	2	13	44874.14	44227.78	331.10	o
-3	3	13	51.04	48.11	3.75	o
-2	3	13	2788.43	2720.05	19.94	o
-1	3	13	2772.97	2686.29	19.40	o
0	3	13	50.33	51.13	4.29	o
-4	4	13	21078.17	21623.49	315.93	o
-3	4	13	2509.32	2565.51	20.02	o
-2	4	13	46.62	49.24	2.74	o
-1	4	13	2533.39	2578.59	24.83	o

0	4	13	20876.87	21341.27	225.09	o
-5	5	13	965.40	970.83	22.08	o
-4	5	13	27.80	29.51	2.54	o
-3	5	13	1820.05	1839.46	21.07	o
-2	5	13	1800.96	1846.76	21.16	o
-1	5	13	28.15	35.44	3.44	o
0	5	13	966.57	1011.45	20.96	o
-6	6	13	9.69	12.94	6.21	o
-5	6	13	1234.87	1236.80	22.83	o
-4	6	13	12021.33	12414.33	154.52	o
-3	6	13	17.79	17.72	2.88	o
-2	6	13	12137.82	12322.91	110.44	o
-1	6	13	1224.48	1241.46	22.72	o
0	6	13	9.69	1.80	6.14	o
-7	7	13	684.89	640.19	23.61	o
-6	7	13	961.21	977.92	22.01	o
-5	7	13	19.81	19.48	4.77	o
-4	7	13	743.55	770.88	17.40	o
-3	7	13	740.74	740.76	16.72	o
-2	7	13	19.45	19.84	4.63	o
-1	7	13	971.97	997.99	22.28	o
0	7	13	676.78	670.69	28.90	o
-8	8	13	3791.10	3776.94	100.61	o
-7	8	13	8.77	4.00	4.75	o
-6	8	13	5209.02	5283.27	71.47	o
-5	8	13	966.40	1016.71	27.13	o
-4	8	13	4.99	3.80	3.92	o
-3	8	13	977.46	986.82	19.75	o
-2	8	13	5163.81	5088.00	62.74	o
-1	8	13	8.87	3.03	4.67	o
0	8	13	3828.19	3881.11	83.22	o
-8	9	13	467.96	429.33	21.97	o
-7	9	13	299.99	299.40	15.87	o
-6	9	13	9.87	13.23	5.28	o
-5	9	13	565.09	552.86	18.47	o
-4	9	13	558.50	562.89	18.59	o
-3	9	13	10.05	21.32	5.63	o
-2	9	13	300.26	294.92	13.63	o
-1	9	13	463.85	457.02	18.57	o
0	0	14	1272.90	1308.93	28.86	o
-1	1	14	309.95	281.01	6.73	o
0	1	14	307.88	282.68	6.16	o
-2	2	14	11317.53	11279.79	101.30	o
-1	2	14	255.59	264.06	4.57	o
0	2	14	11431.74	11440.68	92.20	o
-3	3	14	430.68	414.35	10.54	o
-2	3	14	87.40	85.30	3.10	o
-1	3	14	87.55	82.16	2.66	o
0	3	14	421.95	411.48	9.11	o
-4	4	14	5097.53	5193.42	59.98	o
-3	4	14	226.52	236.60	5.01	o
-2	4	14	612.91	595.35	8.32	o
-1	4	14	227.76	223.53	5.64	o
0	4	14	5041.01	5153.44	87.09	o
-5	5	14	3.39	4.22	4.78	o
-4	5	14	203.21	197.33	6.71	o
-3	5	14	225.89	227.79	6.48	o
-2	5	14	223.67	231.17	7.05	o
-1	5	14	207.48	216.41	7.74	o
0	5	14	3.33	8.77	4.41	o

-6	6	14	236.46	251.67	12.05	o
-5	6	14	70.19	66.46	5.64	o
-4	6	14	2858.55	2917.30	33.63	o
-3	6	14	113.17	121.08	5.48	o
-2	6	14	2892.82	2944.61	35.29	o
-1	6	14	70.12	77.43	6.00	o
0	6	14	238.06	229.94	16.00	o
-7	7	14	90.41	83.03	9.46	o
-6	7	14	116.74	117.87	7.31	o
-5	7	14	235.32	221.92	10.22	o
-4	7	14	5.21	17.97	4.05	o
-3	7	14	5.29	8.00	3.39	o
-2	7	14	231.00	222.52	10.18	o
-1	7	14	117.71	109.63	8.59	o
0	7	14	89.27	83.33	11.35	o
-8	8	14	856.36	909.39	81.09	o
-7	8	14	77.32	67.98	7.62	o
-6	8	14	1152.01	1159.92	22.25	o
-5	8	14	101.50	88.71	6.98	o
-4	8	14	162.63	160.64	9.01	o
-3	8	14	102.02	98.60	6.71	o
-2	8	14	1137.10	1108.21	23.36	o
-1	8	14	78.44	66.94	8.52	o
0	8	14	868.02	893.17	36.13	o
-8	9	14	11.89	21.91	14.20	o
-7	9	14	4.04	17.49	5.15	o
-6	9	14	95.97	100.82	8.72	o
-5	9	14	66.92	67.81	6.75	o
-4	9	14	66.13	72.43	7.65	o
-3	9	14	97.99	103.55	8.59	o
-2	9	14	4.11	0.90	5.33	o
-1	9	14	11.90	10.97	7.83	o
0	0	15	10917.28	10319.66	155.72	o
-1	1	15	234.39	219.33	5.88	o
0	1	15	229.60	221.06	5.29	o
-2	2	15	1246.64	1243.76	19.28	o
-1	2	15	91.39	87.82	3.07	o
0	2	15	1269.90	1273.95	16.41	o
-3	3	15	78.41	76.58	5.03	o
-2	3	15	172.33	169.62	4.28	o
-1	3	15	169.02	169.25	3.83	o
0	3	15	79.94	76.82	4.05	o
-4	4	15	840.08	827.06	21.18	o
-3	4	15	69.72	76.52	3.03	o
-2	4	15	7076.54	7052.40	42.53	o
-1	4	15	71.19	67.63	3.32	o
0	4	15	822.87	804.76	20.82	o
-5	5	15	117.11	126.50	10.33	o
-4	5	15	63.08	60.87	4.65	o
-3	5	15	85.92	88.80	4.01	o
-2	5	15	84.23	82.62	4.42	o
-1	5	15	62.12	61.79	4.08	o
0	5	15	119.00	116.32	13.36	o
-6	6	15	2853.25	2958.16	71.78	o
-5	6	15	26.75	24.92	4.27	o
-4	6	15	552.16	548.09	13.22	o
-3	6	15	70.05	62.34	4.44	o
-2	6	15	563.93	581.38	13.70	o
-1	6	15	26.26	26.51	4.46	o
0	6	15	2855.34	2812.25	61.61	o

-7	7	15	65.47	77.31	9.28	o
-6	7	15	25.98	37.05	5.11	o
-5	7	15	31.80	29.77	4.98	o
-4	7	15	56.02	51.56	5.27	o
-3	7	15	54.98	53.44	6.18	o
-2	7	15	32.38	40.81	7.64	o
-1	7	15	26.53	38.37	6.48	o
0	7	15	64.41	86.95	12.03	o
-8	8	15	251.26	253.48	23.96	o
-7	8	15	27.41	32.22	5.99	o
-6	8	15	353.02	362.90	12.39	o
-5	8	15	13.72	16.16	4.27	o
-4	8	15	1964.61	1995.72	32.28	o
-3	8	15	13.71	13.94	4.24	o
-2	8	15	345.88	324.82	12.61	o
-1	8	15	27.16	30.44	5.55	o
0	8	15	256.42	228.52	18.57	o
-7	9	15	52.33	38.05	6.14	o
-6	9	15	13.12	21.97	5.74	o
-5	9	15	47.83	44.37	6.11	o
-4	9	15	47.02	52.43	7.21	o
-3	9	15	12.87	17.03	6.94	o
-2	9	15	53.20	50.30	7.36	o
-1	9	15	10.54	-6.25	10.40	o
0	0	16	1369.47	1441.04	33.15	o
-1	1	16	419.70	421.25	7.58	o
0	1	16	419.40	407.57	7.62	o
-2	2	16	546.91	509.11	11.69	o
-1	2	16	257.29	236.01	4.95	o
0	2	16	536.56	516.54	9.49	o
-3	3	16	514.49	507.03	12.35	o
-2	3	16	135.06	139.02	3.81	o
-1	3	16	133.16	125.55	3.44	o
0	3	16	524.80	527.55	10.49	o
-4	4	16	449.51	425.75	11.52	o
-3	4	16	123.33	123.85	4.38	o
-2	4	16	643.12	625.99	8.16	o
-1	4	16	123.71	124.28	4.33	o
0	4	16	459.08	447.02	13.59	o
-5	5	16	61.65	56.89	6.77	o
-4	5	16	296.41	292.27	8.36	o
-3	5	16	279.47	287.82	6.81	o
-2	5	16	281.13	281.15	7.44	o
-1	5	16	290.26	282.03	7.85	o
0	5	16	62.94	66.13	7.08	o
-6	6	16	219.41	237.20	11.98	o
-5	6	16	19.99	24.83	4.38	o
-4	6	16	349.11	324.63	11.43	o
-3	6	16	144.24	139.92	5.84	o
-2	6	16	341.97	334.12	10.61	o
-1	6	16	19.58	25.77	4.33	o
0	6	16	218.30	215.23	15.80	o
-7	7	16	186.62	196.83	13.74	o
-6	7	16	60.85	57.06	6.25	o
-5	7	16	386.66	388.58	18.73	o
-4	7	16	33.31	35.28	4.89	o
-3	7	16	32.63	30.16	4.71	o
-2	7	16	392.81	384.46	13.48	o
-1	7	16	60.73	62.01	6.52	o
0	7	16	188.07	225.06	17.73	o

-8	8	16	168.45	180.65	31.51	o
-7	8	16	116.75	122.80	9.54	o
-6	8	16	170.59	164.62	8.72	o
-5	8	16	7.16	5.39	3.88	o
-4	8	16	141.36	144.79	8.18	o
-3	8	16	7.31	2.56	4.31	o
-2	8	16	174.01	171.36	9.92	o
-1	8	16	114.58	112.20	8.88	o
0	8	16	165.17	170.23	15.75	o
-7	9	16	25.32	20.94	5.36	o
-6	9	16	177.89	192.89	11.32	o
-5	9	16	112.69	127.33	12.58	o
-4	9	16	113.42	121.41	9.51	o
-3	9	16	174.48	161.36	9.79	o
-2	9	16	25.82	19.24	5.50	o
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-1	1	17	971.03	919.60	12.52	o
0	1	17	978.44	921.72	12.08	o
-2	2	17	819.46	807.23	15.39	o
-1	2	17	90.93	85.26	2.90	o
0	2	17	813.16	779.86	16.91	o
-3	3	17	89.85	88.48	5.58	o
-2	3	17	400.00	392.52	7.02	o
-1	3	17	406.77	397.08	6.04	o
0	3	17	90.92	85.49	4.31	o
-4	4	17	508.61	488.87	15.02	o
-3	4	17	598.70	588.69	9.98	o
-2	4	17	38.14	40.99	2.62	o
-1	4	17	591.38	586.82	9.95	o
0	4	17	515.26	508.13	13.61	o
-5	5	17	97.54	92.57	8.22	o
-4	5	17	35.16	41.35	5.30	o
-3	5	17	678.02	667.77	12.06	o
-2	5	17	680.52	681.00	11.12	o
-1	5	17	34.71	35.41	3.21	o
0	5	17	95.52	92.85	7.46	o
-6	6	17	1.74	5.77	5.48	o
-5	6	17	223.96	199.17	9.28	o
-4	6	17	313.10	331.03	10.72	o
-3	6	17	9.73	15.77	3.21	o
-2	6	17	308.31	288.71	8.92	o
-1	6	17	228.47	222.18	8.68	o
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-7	7	17	347.29	350.03	18.04	o
-6	7	17	309.41	316.88	12.52	o
-5	7	17	40.94	35.18	6.16	o
-4	7	17	84.65	70.08	6.20	o
-3	7	17	86.46	85.42	6.29	o
-2	7	17	41.57	44.82	5.38	o
-1	7	17	305.62	287.43	11.67	o
0	7	17	347.43	350.22	18.80	o
-8	8	17	88.13	101.90	16.49	o
-7	8	17	3.79	5.84	5.36	o
-6	8	17	148.17	148.40	8.39	o
-5	8	17	238.53	242.60	10.89	o
-4	8	17	0.53	8.97	4.41	o
-3	8	17	233.87	223.10	11.73	o
-2	8	17	149.84	159.13	9.24	o
-1	8	17	3.73	3.88	5.48	o
0	8	17	86.51	65.58	10.07	o

-7	9	17	20.74	26.84	6.15	o
-6	9	17	14.96	13.09	4.86	o
-5	9	17	241.47	254.70	14.01	o
-4	9	17	242.63	262.52	13.47	o
-3	9	17	14.73	19.33	6.62	o
-2	9	17	20.37	20.41	7.41	o
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-1	1	18	5622.96	5323.54	45.66	o
0	1	18	5583.10	5379.99	43.27	o
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-1	2	18	5.02	5.69	1.56	o
0	2	18	1013.13	974.87	13.77	o
-3	3	18	17.19	22.38	3.78	o
-2	3	18	2739.45	2638.90	23.17	o
-1	3	18	2715.69	2730.07	21.77	o
0	3	18	16.83	14.43	3.26	o
-4	4	18	551.05	540.98	16.94	o
-3	4	18	2962.56	2975.04	27.14	o
-2	4	18	301.27	309.87	6.44	o
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-5	5	18	891.04	879.28	24.82	o
-4	5	18	3.97	7.32	3.03	o
-3	5	18	3256.24	3256.78	31.65	o
-2	5	18	3234.88	3284.72	30.14	o
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0	5	18	898.81	921.30	22.60	o
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-4	7	18	638.51	651.80	17.96	o
-3	7	18	632.42	638.23	15.47	o
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-1	7	18	1305.88	1271.36	24.83	o
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-7	8	18	19.90	18.61	4.76	o
-6	8	18	137.05	148.96	9.74	o
-5	8	18	801.14	765.45	19.21	o
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-3	8	18	810.98	813.79	22.06	o
-2	8	18	135.81	134.01	8.73	o
-1	8	18	19.75	33.19	8.22	o
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-7	9	18	218.53	206.14	31.03	o
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-5	9	18	1089.45	1096.21	29.13	o
-4	9	18	1081.65	1100.13	27.34	o
-3	9	18	4.52	15.63	5.08	o
-2	9	18	220.25	222.27	23.33	o
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0	1	19	968.63	949.94	12.91	o

-2	2	19	272.19	247.91	8.93	o
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0	2	19	269.22	276.17	9.27	o
-3	3	19	476.79	474.63	12.83	o
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0	3	19	478.76	490.97	12.82	o
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-3	4	19	454.08	449.99	10.54	o
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-1	4	19	462.57	470.44	9.22	o
0	4	19	141.46	148.95	7.76	o
-5	5	19	131.11	141.83	10.09	o
-4	5	19	281.22	275.00	8.77	o
-3	5	19	599.42	594.44	11.68	o
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-1	5	19	280.21	280.79	8.99	o
0	5	19	133.87	147.62	9.21	o
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-5	6	19	126.89	129.19	7.86	o
-4	6	19	74.65	70.37	6.10	o
-3	6	19	193.75	190.94	7.61	o
-2	6	19	73.34	76.28	5.82	o
-1	6	19	124.36	126.36	7.90	o
0	6	19	97.80	82.77	9.11	o
-7	7	19	290.77	310.22	20.38	o
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-5	7	19	206.67	189.61	11.08	o
-4	7	19	85.76	86.66	7.18	o
-3	7	19	83.98	86.26	6.75	o
-2	7	19	208.06	212.51	10.29	o
-1	7	19	180.67	190.91	11.65	o
0	7	19	285.32	302.49	23.43	o
-8	8	19	29.49	23.74	16.02	o
-7	8	19	95.06	93.25	8.16	o
-6	8	19	50.67	44.08	5.39	o
-5	8	19	74.28	86.76	9.25	o
-4	8	19	86.81	80.89	8.21	o
-3	8	19	75.78	81.90	8.03	o
-2	8	19	51.58	60.50	8.93	o
-1	8	19	94.78	107.48	8.73	o
0	8	19	29.01	27.30	9.64	o
-6	9	19	116.86	128.96	11.46	o
-5	9	19	176.15	194.73	12.55	o
-4	9	19	172.78	197.98	12.75	o
-3	9	19	116.20	112.07	8.73	o
0	0	20	14997.17	14541.33	180.02	o
-1	1	20	1631.78	1571.03	19.45	o
0	1	20	1608.44	1609.22	19.13	o
-2	2	20	124.23	130.39	6.12	o
-1	2	20	6511.01	6549.99	41.51	o
0	2	20	125.39	124.49	5.38	o
-3	3	20	5291.07	5369.69	59.18	o
-2	3	20	1151.83	1101.91	13.67	o
-1	3	20	1135.14	1118.22	14.42	o
0	3	20	5299.21	5379.17	58.67	o
-4	4	20	57.13	66.17	5.76	o
-3	4	20	1011.31	1006.93	17.29	o
-2	4	20	7070.31	7162.85	50.56	o
-1	4	20	1026.29	1014.28	17.10	o

0	4	20	56.72	73.38	5.95	o
-5	5	20	524.78	506.77	19.09	o
-4	5	20	2822.01	2821.14	34.24	o
-3	5	20	787.84	776.17	13.65	o
-2	5	20	776.57	787.31	13.02	o
-1	5	20	2817.88	2883.87	31.38	o
0	5	20	532.36	522.44	17.16	o
-6	6	20	2267.67	2167.26	63.72	o
-5	6	20	592.92	569.32	15.88	o
-4	6	20	40.23	40.35	5.08	o
-3	6	20	1772.38	1808.71	24.57	o
-2	6	20	40.44	38.60	4.22	o
-1	6	20	584.42	576.39	14.25	o
0	6	20	2268.51	2252.48	69.98	o
-7	7	20	329.93	311.54	30.72	o
-6	7	20	434.25	415.22	16.18	o
-5	7	20	1997.53	1991.61	48.15	o
-4	7	20	422.87	443.29	16.51	o
-3	7	20	417.00	406.14	13.76	o
-2	7	20	2002.70	2078.38	33.17	o
-1	7	20	440.64	441.56	15.80	o
0	7	20	325.28	340.74	28.94	o
-7	8	20	660.18	647.34	19.91	o
-6	8	20	19.19	12.58	4.63	o
-5	8	20	433.49	437.10	19.42	o
-4	8	20	1387.65	1413.90	32.25	o
-3	8	20	439.83	454.59	16.72	o
-2	8	20	19.03	25.93	5.22	o
-1	8	20	659.31	657.66	20.39	o
0	8	20	22.62	28.96	19.57	o
-6	9	20	908.77	759.59	59.78	o
-5	9	20	264.97	270.34	14.56	o
-4	9	20	261.17	276.81	15.02	o
-3	9	20	906.74	883.99	37.77	o
0	0	21	684.43	838.84	21.50	o
-1	1	21	4457.26	4497.10	41.01	o
0	1	21	4500.30	4463.47	40.93	o
-2	2	21	976.29	955.52	17.06	o
-1	2	21	1059.95	1046.48	12.88	o
0	2	21	968.20	1006.15	16.38	o
-3	3	21	885.74	860.55	20.04	o
-2	3	21	2610.15	2641.55	25.63	o
-1	3	21	2639.03	2623.66	25.57	o
0	3	21	875.23	859.94	20.58	o
-4	4	21	549.20	572.19	15.38	o
-3	4	21	2603.78	2570.50	23.58	o
-2	4	21	408.32	413.04	8.54	o
-1	4	21	2580.31	2583.85	33.30	o
0	4	21	554.50	542.33	15.07	o
-5	5	21	1050.50	1058.13	33.93	o
-4	5	21	573.35	583.92	13.40	o
-3	5	21	2494.87	2500.52	28.81	o
-2	5	21	2516.60	2531.48	29.26	o
-1	5	21	579.35	589.05	12.68	o
0	5	21	1036.31	1078.40	36.15	o
-6	6	21	217.37	185.32	18.18	o
-5	6	21	1157.37	1172.39	22.33	o
-4	6	21	429.67	430.39	13.93	o
-3	6	21	476.32	462.79	12.66	o
-2	6	21	424.91	424.98	11.68	o

-1	6	21	1168.94	1148.56	27.69	o
0	6	21	218.13	216.47	18.63	o
-7	7	21	1203.75	1131.11	39.60	o
-6	7	21	1170.96	1147.58	27.46	o
-5	7	21	389.26	391.20	15.62	o
-4	7	21	769.38	752.61	25.24	o
-3	7	21	779.52	795.75	20.77	o
-2	7	21	382.74	364.73	13.41	o
-1	7	21	1162.25	1154.15	26.16	o
0	7	21	1213.61	1209.70	45.21	o
-7	8	21	251.77	234.92	13.38	o
-6	8	21	215.00	219.73	10.82	o
-5	8	21	878.50	891.08	27.94	o
-4	8	21	173.13	179.18	12.31	o
-3	8	21	872.03	888.78	23.86	o
-2	8	21	217.78	204.73	10.85	o
-1	8	21	253.42	247.70	12.84	o
-5	9	21	877.29	918.38	56.89	o
-4	9	21	883.95	892.12	38.32	o
0	0	22	336.34	355.93	20.17	o
-1	1	22	1142.66	1179.83	16.14	o
0	1	22	1160.96	1162.38	16.24	o
-2	2	22	192.74	193.98	7.54	o
-1	2	22	37.78	47.27	2.92	o
0	2	22	194.45	197.20	9.60	o
-3	3	22	27.30	23.95	3.85	o
-2	3	22	347.71	364.48	8.32	o
-1	3	22	353.14	351.23	8.04	o
0	3	22	27.58	27.47	4.43	o
-4	4	22	164.08	150.60	8.76	o
-3	4	22	749.02	737.26	11.99	o
-2	4	22	209.67	195.08	6.01	o
-1	4	22	735.68	736.81	13.55	o
0	4	22	163.74	164.79	8.67	o
-5	5	22	22.55	24.47	5.51	o
-4	5	22	22.54	21.24	3.58	o
-3	5	22	913.63	935.27	16.34	o
-2	5	22	929.18	954.10	16.77	o
-1	5	22	22.34	21.52	3.77	o
0	5	22	22.47	20.20	5.52	o
-6	6	22	112.43	112.47	12.20	o
-5	6	22	213.94	209.18	9.53	o
-4	6	22	122.54	124.64	8.11	o
-3	6	22	25.48	25.73	4.20	o
-2	6	22	122.96	119.97	6.61	o
-1	6	22	218.25	217.95	9.91	o
0	6	22	112.41	111.67	13.64	o
-7	7	22	488.78	469.47	38.67	o
-6	7	22	457.63	433.45	16.67	o
-5	7	22	8.68	9.29	4.88	o
-4	7	22	25.61	26.60	8.58	o
-3	7	22	26.00	21.80	5.08	o
-2	7	22	8.84	13.07	4.58	o
-1	7	22	448.83	440.45	16.15	o
0	7	22	497.38	469.38	26.28	o
-7	8	22	15.47	16.46	5.91	o
-6	8	22	95.43	101.29	9.70	o
-5	8	22	312.59	304.97	16.43	o
-4	8	22	90.21	107.33	14.47	o
-3	8	22	306.13	323.20	15.69	o

-2	8	22	95.97	110.29	8.14	o
-1	8	22	15.37	18.17	4.91	o
0	0	23	108.58	113.01	8.00	o
-1	1	23	206.39	194.30	7.33	o
0	1	23	202.27	194.79	6.20	o
-2	2	23	739.20	695.70	14.76	o
-1	2	23	274.98	266.81	6.17	o
0	2	23	749.93	731.42	21.88	o
-3	3	23	224.61	233.32	8.95	o
-2	3	23	59.98	51.43	3.31	o
-1	3	23	59.25	58.94	3.72	o
0	3	23	225.10	229.10	10.14	o
-4	4	23	556.11	513.61	17.28	o
-3	4	23	172.53	173.88	6.59	o
-2	4	23	52.40	48.29	3.90	o
-1	4	23	176.08	159.51	6.55	o
0	4	23	547.30	509.10	17.07	o
-5	5	23	14.87	15.50	8.76	o
-4	5	23	149.04	145.39	7.51	o
-3	5	23	181.65	184.11	8.32	o
-2	5	23	177.86	181.23	7.20	o
-1	5	23	148.72	147.73	7.82	o
0	5	23	14.59	17.82	5.11	o
-6	6	23	13.18	3.24	6.01	o
-5	6	23	69.87	70.92	6.06	o
-4	6	23	376.70	399.28	18.16	o
-3	6	23	119.58	124.34	7.13	o
-2	6	23	383.12	370.41	11.86	o
-1	6	23	68.69	82.68	6.44	o
0	6	23	13.17	23.13	8.47	o
-7	7	23	90.22	94.43	13.13	o
-6	7	23	120.17	118.71	9.34	o
-5	7	23	98.26	112.73	10.26	o
-4	7	23	11.33	17.68	5.70	o
-3	7	23	11.54	15.17	5.45	o
-2	7	23	98.64	95.78	9.68	o
-1	7	23	122.72	128.90	8.67	o
0	7	23	88.36	92.59	13.31	o
-7	8	23	55.98	52.08	10.14	o
-6	8	23	255.11	294.46	14.73	o
-5	8	23	117.84	108.26	11.21	o
-4	8	23	6.12	12.17	6.07	o
-3	8	23	120.27	124.23	10.33	o
-2	8	23	250.20	257.29	12.27	o
-1	8	23	55.85	56.80	11.29	o
0	0	24	868.79	1008.98	25.46	o
-1	1	24	127.79	115.10	5.84	o
0	1	24	125.18	130.44	5.23	o
-2	2	24	179.86	182.88	10.47	o
-1	2	24	134.40	124.91	4.55	o
0	2	24	179.55	163.67	7.79	o
-3	3	24	293.25	284.40	10.00	o
-2	3	24	117.74	114.39	4.69	o
-1	3	24	115.38	117.85	5.44	o
0	3	24	299.30	291.34	11.45	o
-4	4	24	115.09	103.73	7.39	o
-3	4	24	71.83	73.29	4.58	o
-2	4	24	588.62	578.40	11.90	o
-1	4	24	73.14	76.15	4.88	o
0	4	24	114.81	109.55	9.10	o

-5	5	24	81.39	98.29	9.33	o
-4	5	24	178.79	181.48	8.23	o
-3	5	24	64.17	65.22	5.27	o
-2	5	24	62.87	66.02	4.86	o
-1	5	24	175.09	168.21	7.93	o
0	5	24	83.08	93.74	9.47	o
-6	6	24	340.11	309.65	19.15	o
-5	6	24	44.10	34.49	4.75	o
-4	6	24	71.35	71.29	7.40	o
-3	6	24	67.27	56.09	5.84	o
-2	6	24	71.44	77.75	8.24	o
-1	6	24	43.62	44.07	5.10	o
0	6	24	338.57	333.72	21.72	o
-7	7	24	37.26	54.26	10.37	o
-6	7	24	34.01	46.42	6.65	o
-5	7	24	278.81	280.22	15.34	o
-4	7	24	50.03	50.63	8.58	o
-3	7	24	49.11	43.40	6.59	o
-2	7	24	283.64	286.42	13.18	o
-1	7	24	34.51	29.82	6.89	o
0	7	24	36.50	50.15	9.69	o
-6	8	24	42.77	45.11	7.01	o
-5	8	24	29.27	30.43	6.75	o
-4	8	24	270.97	226.26	14.88	o
-3	8	24	29.26	38.61	7.03	o
-2	8	24	42.43	64.66	8.53	o
0	0	25	17728.69	17321.45	279.07	o
-1	1	25	149.03	151.73	6.89	o
0	1	25	150.24	148.60	7.14	o
-2	2	25	2568.75	2496.86	32.71	o
-1	2	25	84.26	88.00	4.07	o
0	2	25	2602.77	2479.63	39.79	o
-3	3	25	59.24	61.90	5.45	o
-2	3	25	95.12	96.66	4.49	o
-1	3	25	95.86	94.35	5.14	o
0	3	25	59.78	67.33	6.30	o
-4	4	25	1539.26	1484.93	25.77	o
-3	4	25	142.27	146.09	6.01	o
-2	4	25	10633.98	10515.61	82.66	o
-1	4	25	141.41	140.00	6.53	o
0	4	25	1518.10	1515.26	40.18	o
-5	5	25	32.34	32.89	6.26	o
-4	5	25	83.25	76.35	6.12	o
-3	5	25	97.99	91.56	6.05	o
-2	5	25	98.55	106.20	6.28	o
-1	5	25	82.82	83.38	5.86	o
0	5	25	32.13	22.63	6.48	o
-6	6	25	4872.20	4713.31	77.79	o
-5	6	25	110.35	112.01	7.41	o
-4	6	25	989.77	949.00	26.16	o
-3	6	25	130.92	133.34	8.21	o
-2	6	25	1004.04	1022.15	20.48	o
-1	6	25	110.76	124.02	8.36	o
0	6	25	4870.19	4786.16	113.14	o
-7	7	25	41.93	32.31	8.92	o
-6	7	25	92.86	93.62	9.69	o
-5	7	25	50.29	42.81	7.17	o
-4	7	25	44.87	43.22	7.39	o
-3	7	25	45.04	55.47	8.39	o
-2	7	25	50.82	48.56	6.75	o

-1	7	25	92.64	104.83	8.77	o
0	7	25	42.04	38.61	14.52	o
-6	8	25	456.81	481.30	18.76	o
-5	8	25	130.75	138.00	12.09	o
-4	8	25	3551.64	3657.40	64.45	o
-3	8	25	130.50	156.53	11.51	o
-2	8	25	449.72	458.18	21.22	o
0	0	26	1653.54	1889.06	55.14	o
-1	1	26	772.59	772.97	15.73	o
0	1	26	786.10	753.82	19.10	o
-2	2	26	7967.40	7904.84	96.39	o
-1	2	26	729.01	744.99	12.30	o
0	2	26	7904.50	7742.97	90.35	o
-3	3	26	662.84	650.05	15.81	o
-2	3	26	837.06	833.56	14.44	o
-1	3	26	850.45	833.90	14.49	o
0	3	26	656.32	671.12	24.13	o
-4	4	26	4932.90	4921.14	83.03	o
-3	4	26	631.10	614.36	12.64	o
-2	4	26	1126.00	1120.39	18.10	o
-1	4	26	620.39	618.44	12.76	o
0	4	26	4973.46	4932.18	62.82	o
-5	5	26	550.75	532.74	20.84	o
-4	5	26	428.32	417.22	14.45	o
-3	5	26	317.14	317.24	10.89	o
-2	5	26	323.30	291.78	10.67	o
-1	5	26	432.26	413.54	11.93	o
0	5	26	542.53	564.43	20.51	o
-6	6	26	633.27	606.56	24.06	o
-5	6	26	549.49	539.50	20.17	o
-4	6	26	3265.18	3231.20	49.99	o
-3	6	26	310.70	298.86	11.67	o
-2	6	26	3238.59	3229.59	52.29	o
-1	6	26	558.22	547.04	16.48	o
0	6	26	634.53	660.95	36.25	o
-7	7	26	111.99	103.33	16.25	o
-6	7	26	282.32	249.03	16.46	o
-5	7	26	359.97	349.93	17.28	o
-4	7	26	447.06	446.18	19.79	o
-3	7	26	453.79	460.65	20.19	o
-2	7	26	354.60	297.63	13.82	o
-1	7	26	277.08	266.44	13.56	o
0	7	26	114.34	118.71	27.09	o
-5	8	26	411.20	380.58	18.82	o
-4	8	26	503.50	510.15	22.17	o
-3	8	26	404.28	422.21	23.65	o
0	0	27	727.07	796.75	34.74	o
-1	1	27	1.44	16.24	3.68	o
0	1	27	1.43	9.27	4.51	o
-2	2	27	3451.65	3381.59	85.63	o
-1	2	27	36.18	48.41	4.87	o
0	2	27	3388.57	3462.54	50.57	o
-3	3	27	41.75	31.96	4.37	o
-2	3	27	21.34	30.30	3.49	o
-1	3	27	21.14	25.35	3.70	o
0	3	27	41.36	42.30	6.23	o
-4	4	27	2127.68	2164.59	48.63	o
-3	4	27	2.55	11.00	3.18	o
-2	4	27	541.83	523.31	12.21	o
-1	4	27	2.53	4.53	3.20	o

0	4	27	2167.77	2084.80	36.87	o
-5	5	27	24.88	27.12	5.79	o
-4	5	27	20.89	20.19	4.29	o
-3	5	27	22.22	23.96	5.35	o
-2	5	27	21.84	23.23	5.10	o
-1	5	27	21.13	30.01	4.30	o
0	5	27	25.17	40.21	6.90	o
-6	6	27	346.99	363.76	18.83	o
-5	6	27	17.39	10.03	4.84	o
-4	6	27	1408.95	1371.33	30.54	o
-3	6	27	6.78	16.49	4.46	o
-2	6	27	1381.93	1399.24	26.53	o
-1	6	27	17.37	17.69	4.66	o
0	6	27	346.98	327.48	19.60	o
-7	7	27	41.87	38.25	14.96	o
-6	7	27	3.31	8.51	5.52	o
-5	7	27	29.93	37.08	10.49	o
-4	7	27	17.46	5.55	5.39	o
-3	7	27	17.33	23.62	6.65	o
-2	7	27	29.48	32.22	5.97	o
-1	7	27	3.37	13.62	8.01	o
-5	8	27	9.51	30.04	19.57	o
-4	8	27	289.63	295.72	39.68	o
0	0	28	2032.48	1943.02	55.17	o
-1	1	28	88.44	88.51	5.76	o
0	1	28	89.48	90.48	7.17	o
-2	2	28	1817.14	1876.82	28.28	o
-1	2	28	483.13	485.73	10.14	o
0	2	28	1845.05	1809.23	34.41	o
-3	3	28	446.91	443.38	13.43	o
-2	3	28	2.92	8.13	2.99	o
-1	3	28	2.94	2.97	3.19	o
0	3	28	445.68	417.68	16.21	o
-4	4	28	1196.35	1242.45	26.43	o
-3	4	28	48.15	59.80	4.56	o
-2	4	28	1479.01	1453.89	21.25	o
-1	4	28	47.61	52.79	4.68	o
0	4	28	1178.88	1214.97	34.86	o
-5	5	28	10.89	12.28	6.79	o
-4	5	28	270.40	265.76	12.59	o
-3	5	28	190.38	181.57	8.35	o
-2	5	28	192.61	176.06	8.31	o
-1	5	28	271.06	272.73	9.67	o
0	5	28	10.91	26.58	7.76	o
-6	6	28	909.35	849.37	33.92	o
-5	6	28	1.97	5.28	4.33	o
-4	6	28	875.76	833.73	30.52	o
-3	6	28	169.93	194.41	9.88	o
-2	6	28	887.55	861.63	22.48	o
-1	6	28	1.98	13.42	4.45	o
0	6	28	909.62	915.81	32.61	o
-6	7	28	75.26	81.24	9.07	o
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'Roberto Compagnoni'
'Dip. di Scienze della Terra - Via Valperga Caluso, 35 - 10125 Torino'

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;
CrysAlisPro, Agilent Technologies,
Version 1.171.37.31 (release 14-01-2014 CrysAlis171 .NET)
(compiled Jan 14 2014,18:38:05)
;
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR
and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors
based
 on F^2^ are statistically about twice as large as those based on F, and
R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
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```
 'calc w=1/[\s^2^(Fo^2^)+(0.0327P)^2^+0.0089P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     constr
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0019(3)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          1721
_refine_ls_number_parameters      94
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0242
_refine_ls_R_factor_gt            0.0219
_refine_ls_wR_factor_ref          0.0603
_refine_ls_wR_factor_gt           0.0593
_refine_ls_goodness_of_fit_ref    1.111
_refine_ls_restrained_S_all       1.111
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T2A Fe 0.3333 -0.3333 -0.02571(2) 0.00686(15) Uani 0.480(5) 6 d SP . .
T2B Mg 0.3333 -0.3333 -0.02571(2) 0.00686(15) Uani 0.520(5) 6 d SP . .
M3 Al 0.33800(9) 0.16900(5) -0.101571(16) 0.00508(12) Uani 1.019(4) 2 d
SP . .
T4A Fe 0.3333 -0.3333 -0.17363(3) 0.00405(18) Uani 0.211(5) 6 d SP . .
T4B Mg 0.3333 -0.3333 -0.17363(3) 0.00405(18) Uani 0.789(5) 6 d SP . .
M5A Fe -0.3333 -0.6667 -0.216201(15) 0.00393(9) Uani 0.875(6) 6 d SP . .
M5B Mg -0.3333 -0.6667 -0.216201(15) 0.00393(9) Uani 0.125(6) 6 d SP . .
M6 Al 0.16412(4) 0.32823(9) -0.296154(16) 0.00452(10) Uani 1.110(4) 2 d
SP . .
T7A Fe 0.3333 0.6667 0.36991(2) 0.00619(14) Uani 0.469(5) 6 d SP . .
T7B Mg 0.3333 0.6667 0.36991(2) 0.00619(14) Uani 0.531(5) 6 d SP . .
M8 Al -0.3333 -0.6667 0.39954(3) 0.00504(19) Uani 1.028(5) 6 d SP . .
T9A Fe 0.0000 0.0000 0.42410(2) 0.00594(17) Uani 0.386(5) 6 d SP . .
T9B Mg 0.0000 0.0000 0.42410(2) 0.00594(17) Uani 0.614(5) 6 d SP . .
M10 Al 0.0000 0.5000 0.5000 0.00452(15) Uani 1.044(4) 4 d SP . .
O1 O -0.2962(2) -0.14811(12) -0.05351(5) 0.0078(2) Uani 1 2 d S . .
O2 O -0.3333 -0.6667 -0.05901(8) 0.0079(3) Uani 1 6 d S . .
O3 O 0.50978(13) -0.50978(13) -0.14912(5) 0.0093(2) Uani 1 2 d S . .
O4 O 0.0000 0.0000 0.14498(8) 0.0077(3) Uani 1 6 d S . .
H H 0.0000 0.0000 0.1912 0.009 Uiso 1 6 d S . .
O5 O -0.16381(13) 0.16381(13) -0.25446(4) 0.00683(17) Uani 1 2 d S . .
O6 O 0.3333 -0.3333 -0.25347(7) 0.0069(3) Uani 1 6 d S . .
O7 O 0.48076(11) -0.48076(11) -0.34733(5) 0.0085(2) Uani 1 2 d S . .
O8 O 0.0000 0.0000 -0.33961(7) 0.0057(3) Uani 1 6 d S . .
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O9 O -0.18555(10) 0.18555(10) 0.45318(4) 0.00547(18) Uani 1 2 d S . .
O10 O 0.3333 -0.3333 0.45542(7) 0.0058(3) Uani 1 6 d S . .

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T2B 0.00721(19) 0.00721(19) 0.0061(2) 0.000 0.000 0.00361(10)
M3 0.0048(2) 0.00555(17) 0.00464(18) 0.00015(9) 0.00030(17) 0.00239(10)
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T4B 0.0045(2) 0.0045(2) 0.0032(2) 0.000 0.000 0.00224(11)
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M5B 0.00455(11) 0.00455(11) 0.00269(13) 0.000 0.000 0.00228(6)
M6 0.00460(14) 0.00446(16) 0.00446(15) -0.00069(13) -0.00035(6)
0.00223(8)
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M8 0.0054(2) 0.0054(2) 0.0043(3) 0.000 0.000 0.00271(12)
T9A 0.00620(19) 0.00620(19) 0.0054(3) 0.000 0.000 0.00310(10)
T9B 0.00620(19) 0.00620(19) 0.0054(3) 0.000 0.000 0.00310(10)
M10 0.0044(2) 0.0046(2) 0.0044(2) -0.00024(11) -0.0005(2) 0.00218(12)
O1 0.0076(5) 0.0084(3) 0.0072(4) -0.00029(16) -0.0006(3) 0.0038(2)
O2 0.0081(5) 0.0081(5) 0.0074(6) 0.000 0.000 0.0040(2)
O3 0.0095(3) 0.0095(3) 0.0073(4) 0.00027(19) -0.00027(19) 0.0035(4)
O4 0.0096(5) 0.0096(5) 0.0037(6) 0.000 0.000 0.0048(2)
O5 0.0072(3) 0.0072(3) 0.0063(4) -0.00095(19) 0.00095(19) 0.0037(4)
O6 0.0071(5) 0.0071(5) 0.0064(6) 0.000 0.000 0.0035(2)
O7 0.0084(3) 0.0084(3) 0.0074(4) 0.00112(17) -0.00112(17) 0.0032(4)
O8 0.0062(4) 0.0062(4) 0.0049(6) 0.000 0.000 0.0031(2)
O9 0.0056(3) 0.0056(3) 0.0051(4) -0.00016(15) 0.00016(15) 0.0026(3)
O10 0.0056(4) 0.0056(4) 0.0060(6) 0.000 0.000 0.0028(2)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are
taken
 into account individually in the estimation of s.u.'s in distances,
angles
 and torsion angles; correlations between s.u.'s in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

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M1 O1 1.9164(11) 9 ?
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M1 M3 2.8765(4) 9 ?
M1 M3 2.8765(4) 7 ?
M1 M3 2.8765(4) . ?
M1 M3 2.8765(4) 2 ?
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T2A O1 1.9443(12) 9_545 ?
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T2A O2 1.950(2) 7_545 ?
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T2A M3 3.3527(6) 7_655 ?
M3 O2 1.9009(11) 1_665 ?
M3 O1 1.9304(8) 9 ?
M3 O1 1.9304(8) 2 ?
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M5A M6 3.4024(3) 1_545 ?
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M6 O5 1.8875(8) 4 ?
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M6 M8 2.9119(7) 7 ?
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T7A O7 1.9146(12) 10_455 ?
T7A O7 1.9146(12) 8_675 ?
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O1 T2A M3 79.75(2) 1_655 . ?
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M3 T2A M3 49.770(16) 2_655 . ?
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M3 T2A M3 51.282(16) 9 . ?
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O1 T2A M3 79.75(2) 9_545 9_655 ?
O1 T2A M3 29.977(19) 1_655 9_655 ?
O2 T2A M3 121.400(9) 7_545 9_655 ?
M3 T2A M3 51.282(16) 2_655 9_655 ?
M3 T2A M3 95.327(13) 2_545 9_655 ?
M3 T2A M3 117.195(19) 9 9_655 ?
M3 T2A M3 49.770(16) 1_545 9_655 ?
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M3 T2A M3 95.620(12) . 8 ?
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 _geom_hbond_atom_site_label_A
 _geom_hbond_distance_DH
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 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
O4 H O5  1.0645(17) 2.1810(12) 2.9983(19) 131.89(3) 5

_diffrn_measured_fraction_theta_max    0.985
_diffrn_reflns_theta_full              40.91
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_refine_diff_density_max    0.513
_refine_diff_density_min   -0.555
_refine_diff_density_rms    0.122

# start Validation Reply Form
_vrf_PLAT075_magnesiobeltrandoite-2N3S
;
PROBLEM: Occupancy      1.037 greater than 1.0 for ......         M1
RESPONSE: this site host other species with higher scattering than Al,
but refining a mixed occupancy model in this site by imposing full
occupancy through restrains would not allow to reach convergence easily
and produce non reliable errrs in site occupancy.
;
_vrf_PLAT077_magnesiobeltrandoite-2N3S
;
PROBLEM: Unitcell contains non-integer number of atoms ..     Please
Check
RESPONSE: this is linked to the previous problem.
;
_vrf_PLAT355_magnesiobeltrandoite-2N3S
;
PROBLEM: Long    O-H (X0.82,N0.98A)  O4     -   H      ..       1.06 Ang.
RESPONSE: the position of hydrogen atom was located in the Fourier
difference
map and was added to the model fixing coordinates and restaining thermal
motion
to 1.2 imes the isotropic displacement of the oxygen to wich is bound (as
usual)
;
_vrf_PLAT701_magnesiobeltrandoite-2N3S
;
PROBLEM: Bond    Calc   3.3733(2), Rep   3.3737(2), Dev..       2.00
Sigma
RESPONSE: it must be related to the restrains applied to the H atom
;
_vrf_PLAT702_magnesiobeltrandoite-2N3S
```

;
PROBLEM: Angle   Calc   121.41(1), Rep   121.40(1), Dev..   1.10
Sigma
RESPONSE: it must be related to the restrains applied to the H atom
;
_vrf_PLAT751_magnesiobeltrandoite-2N3S
;
PROBLEM: Bond   Calc   1.06000, Rep 1.0645(17) ...... Senseless s.u.
RESPONSE: it must be related to the restrains applied to the H atom
;
_vrf_PLAT755_magnesiobeltrandoite-2N3S
;
PROBLEM: D-H   Calc   1.06000, Rep 1.0645(17) ...... Senseless s.u.
RESPONSE: it must be related to the restrains applied to the H atom
;
_vrf_PLAT756_magnesiobeltrandoite-2N3S
;
PROBLEM: H...A   Calc   2.18000, Rep 2.1810(12) ...... Senseless s.u.
RESPONSE: it must be related to the restrains applied to the H atom
;
_vrf_PLAT790_magnesiobeltrandoite-2N3S
;
PROBLEM: Centre of Gravity not Within Unit Cell: Resd. #   1 Note
RESPONSE: We have refined the structure starting form the atom
coordinates
of a previously publisehd model of an isostruttural mineral. It does not
seem
us a sufficient reason to change the model and create confussion in
litterature.
;
end Validation Reply Form