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Metavivianite, $Fe^{2+}Fe_2^{3+}(PO_4)_2(OH)_2{\cdot}6H_2O$: new data and formula revision

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ABSTRACT

The composition, structure, X-ray powder diffraction pattern, optical properties, density, infrared, Raman and Mössbauer spectra, and thermal properties of a homogeneous sample of metavivianite from the Boa Vista pegmatite, near Galiléia, Minas Gerais, Brazil are reported for the first time. Metavivianite is biaxial (+) with α = 1.600(3), β = 1.640(3), γ = 1.685(3) and $2V_{meas}$ = 85(5)º. The measured and calculated densities are D_{meas} = 2.56(2) and D_{calc} = 2.579 g cm^{-3}. The chemical composition, based on electron-microprobe analyses, Mössbauer spectroscopy (to determine the Fe^{2+}:Fe^{3+} ratio) and gas chromatography (to determine H_2O) is MgO 0.70, MnO 0.92, FeO 17.98, Fe_2O_3 26.60, P_2O_5 28.62, H_2O 26.5; total 101.32 wt.%. The empirical formula is $(Fe^{3+}_{1.64}Fe^{2+}_{1.23}Mg_{0.085}Mn_{0.06})_{\Sigma 3.015}(PO_4)_{1.98}(OH)_{1.72}{\cdot}6.36H_2O$. Metavivianite is triclinic, $P\bar{1}$, a = 7.989(1), b = 9.321(2), c = 4.629(1) Å, α = 97.34(1), β = 95.96(1), γ = 108.59(2)º, V = 320.18(11) Å^3 and Z = 1. The crystal structure was solved using a single-crystal techniques to an agreement index R = 6.0%. The dominant cations in the independent sites are Fe^{2+} and Fe^{3+}, with multiplicities of 1 and 2, respectively. The simplified crystal-chemical formula for metavivianite is $Fe^{2+}(Fe^{3+},Fe^{2+})_2(PO_4)_2(OH,H_2O)_2{\cdot}6H_2O$; the endmember formula is $Fe^{2+}Fe_2^{3+}(PO_4)_2(OH)_2{\cdot}6H_2O$, which is dimorphous with ferrostrunzite.

Keywords: metavivianite, formula revision, crystal chemistry, Minas Gerais, Brazil.

Introduction

Metavivianite has a complex history. It was discovered at the Big Chief mine, near Glendale, South Dakota, USA and was originally thought to be dimorphous with vivianite, $Fe_3(PO_4)_2{\cdot}8H_2O$, and isostructural with symplesite, $Fe_3(AsO_4)_2{\cdot}8H_2O$ (Ritz *et al*., 1974). The original description was based on a heterogeneous sample and is incomplete. The density was not measured due to the presence of impurities and the hardness was not determined. Although most of the crystals in the sample were described as either opaque or translucent, the optical properties of rare pale grains were reported, resulting in incorrect values for the refractive indices. The original infrared (IR) data is now known to include contributions

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from disordered phases such as X-ray amorphous santabarbaraite, $Fe^{3+}_3(PO_4)_2(OH)_3{\cdot}5H_2O$, and does not correspond to pure vivianite and metavivianite. No separate analyses for Fe^{2+} and Fe^{3+} and no determination of H_2O was made. The crystal structure was considered to be similar to symplesite on the basis of similarities in the X-ray powder-diffraction patterns, but no single-crystal studies were attempted.

Subsequent investigations have shown that metavivianite contains Fe^{3+} and that it is not dimorphous with vivianite (Dormann and Poullen, 1980; Dormann *et al*., 1982; Rodgers and Johnston, 1985; Rodgers, 1986). On the basis of Fe^{2+}:Fe^{3+} ratios obtained from Mössbauer spectroscopy, Rodgers (1986) suggested the formula $Fe^{2+}_{3-x}Fe^{3+}_x(PO_4)_2(OH)_x{\cdot}(8-x)H_2O$ with x >1.4. This formula is in much better agreement with the general composition of metavivianite, but it is written without regard to the two independent sites for iron in the structure (Dormann *et al*., 1982). Within the compositional limits (with x ranging from 1.4 to almost 3), this formula includes two possible endmember compositions, which are either Fe^{2+}- or Fe^{3+}-dominant, and it therefore represents two mineral species.

In this work, a pure monomineralic metavivianite sample from the Boa Vista pegmatite, near Galiléia, Minas Gerais, Brazil was investigated. We report detailed chemical data; a crystal structure analysis, with bond valence calculations for all sites; determinations of the optical characteristics and density; infrared, Raman and Mössbauer spectra; thermal analyses including thermogravimetry (TG), differential thermogravimetry (DTG) and differential thermal analysis (DTA); and a complete X-ray powder diffraction pattern.

Geological setting, occurrence and general appearance

The Boa Vista mine is located in the municipality of Galiléia and is well known to mineralogists as a source of pegmatite phosphates (Cassedanne and Cassedanne, 1979). The mine is located in the Conselheiro Pena pegmatite district, a subdivision of the Eastern Brazilian Pegmatite province (EBP) which encompasses an area of about 150,000 km^2, extending from Bahia to Rio de Janeiro states (Pedrosa Soares *et al.*, 2011). About 90% of the province is situated in the eastern part of Minas Gerais. The Conselheiro Pena pegmatite district covers an area of about 5000 km^2 in the municipalities of Conselheiro Pena and Galiléia, in the Doce river basin, about 360 km northeast of Belo Horizonte.

The pegmatite district is a part of the central domain of the Araçuaí mobile belt (Almeida, 1977), which was formed during the Brasiliano orogeny (630–490 Ma) by accretion to the eastern margin of the São Francisco craton. In this area, several suites of granitic rocks (e.g. Urucum and Palmital of Eocambrian to Palaeozoic age, and Galiléia of Neoproterozoic age), intrude schistose rocks of the Neoproterozoic São Tomé Formation (Chaves *et al*., 2005).

The São Tomé Formation and associated granites crop out along a north–south trending synclinorium with metasedimentary rocks dominating in the synclines and granitic intrusions in the adjacent anticlines. The granites, which are typically S-type and peraluminous, were generated during the syn-collisional stage of the Araçuaí orogen. Pegmatites (with ages of ~580 Ma; Nalini, 1997) are related to the G2 granite super-suite (Pedrosa-Soares *et al*., 2001) and are common in the metasedimentary rocks.

The Boa Vista pegmatite is worked for industrial feldspar; gemstones and mineral specimens are a minor by-product. The pegmatite is heterogeneous with well developed mineralogical and textural zonation. It has an asymmetric lens shape with the long axis trending northwest–southeast and dips at about 65º to the northeast. The strike extension is up to about 80 m and the body is ~10 m thick. The pegmatite is hosted by quartz-mica schist of the São Tomé Formation which is tourmalinized at the contact. Hydrothermal and metasomatic processes have produced extensive albitization (Cassedanne and Cassedanne, 1978).

The primary assemblage includes quartz, muscovite, microcline, schorl, dravite, beryl, graftonite and triphylite. The secondary assemblage includes albite, Li-rich micas, Sn, Nb, W and Ta oxides, sulfides, siderite and a complex phosphate assemblage formed by the alteration of primary triphylite (Cassedanne and Cassedanne, 1978, 1982; Chaves *et al.*, 2005).

Secondary phosphates including heterosite, wolfeite, arrojadite, beryllonite, alluaudite, amblygonite, hydroxylherderite, vivianite, ludlamite, rockbridgeite, phosphosiderite and tavorite are common in miarolitic cavities and in metre-scale blocks that are formed by the alteration of primary triphylite (Cassedanne and Cassedanne, 1979).

Bladed metavivianite crystals up to 3.0 cm along the *c* axis occur with siderite, ludlamite, albite and muscovite (Fig. 1). Fragments of a crystal of metavivianite ~2.0 cm in length were selected for this study. The crystal was extracted from a massive block where it was associated with siderite and ludlamite.

Physical properties

Metavivianite is translucent and very dark blue-green, with a vitreous lustre. The streak is blue. It is brittle and the Mohs' hardness measured using calcite and gypsum as standards is 2½. The cleavage is perfect on $(1\bar{1}0)$ and distinct in two directions across $(1\bar{1}0)$. The density measured by flotation in heavy liquids is 2.56(2) g cm^{-3}; the calculated density is 2.579 g cm^{-3}.

Optically, metavivianite is biaxial (+), with α = 1.600(3), β = 1.640(3), γ = 1.685(3), $2V_{meas}$ = 85(5)º and $2V_{calc}$ = 89º. The dispersion is very strong, $r < v$. The optical orientation is $X \perp (1\bar{1}0)$; $Z \wedge a$ = 33º. Pleochroism is very strong, with *X* (dark indigo blue) >> *Y* (light khaki green) ⩾ *Z* (yellowish green). It seems probable that the refractive indices reported in the original description of metavivianite using atypical pale grains [α = 1.579(6), β = 1.603(2), γ = 1.629(2); Ritz *et al*., 1974] refer in fact to admixed vivianite. If they are attributed to metavivianite, these parameters, produce a very poor Gladstone–Dale compatibility index (Mandarino, 1981) of about 0.14.

Vibrational (infrared and Raman) spectroscopy

Our initial infrared absorption spectra were recorded using powdered samples, which were mixed with anhydrous KBr, pelletized and analysed using a Specord 75 IR spectrometer. The IR spectrum of a pure KBr disk was subtracted from the overall spectrum. The accuracy of the spectra in the ranges 3000−4000 and 1500−1800 cm^{-1} was proved in a separate experiment using dry mineral oil as an immersion medium. Polystyrene and gaseous NH_3 were used as frequency standards. The precision of measurement is ±1 cm^{-1} and the mean resolution for the region 400−1600 cm^{-1} is 0.8 cm^{-1}.

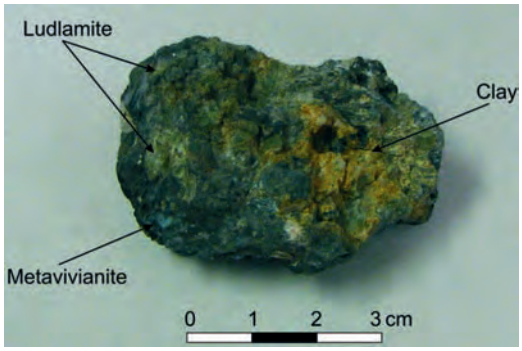

FIG. 1. A fragment of pegmatite with metavivianite from Boa Vista.

Absorption bands in the IR spectrum of metavivianite (Fig. 2), abbreviated as strong (s) and shoulder (sh), and their assignments, are as follows: 3350(s), 3240(s), 3145(s), 2850(sh), O−H stretching vibrations of H_2O molecules and OH groups; 2370, PO−H stretching; 1670, 1625, 1580(sh), bending vibrations of H_2O molecules; 1060(sh), 1024(s), 967(s), 945(sh), asymmetric stretching vibrations of PO_4^{3-} ions; 865(sh), 777, Fe···O−H bending and H_2O libration; 670(sh), 582(s), 560(sh), bending vibrations of PO_4^{3-} ions; and 475(sh) cm^{-1} Fe−O stretching vibrations.

The IR spectra of vivianite and santabarbaraite are included in Fig. 2 for comparative purposes. The splitting of the asymmetric P−O stretching vibrations indicates a relatively strong distortion of the PO_4 tetrahedra. The presence of a shoulder at 2370 cm^{-1}, indicates the presence of trace amounts of HPO_4^{2-} ions in metavivianite as a result of the substitution $PO_4^{3-} + H_2O \leftrightarrow HPO_4^{2-} + OH^-$. This is commonly observed in hydrous phosphates and arsenates (Pekov *et al*., 2001). Analogous bands are present in the IR spectra of vivianite and santabarbaraite.

The Raman spectrum of metavivianite from the Boa Vista pegmatite was recorded at room temperature using a triple monochromator spectrometer (JY T64000) in backscatter configuration. Excitation was by an argon ion laser operating at a wavelength of 514.5 nm and a power of 10 mW. The spectrum (Fig. 3) is similar to the vivianite spectrum reported by Frost *et al*. (2004), but not to their metavivianite spectrum. The positions and intensities of the Raman bands, abbreviated as strong (s), medium (m) and weak (w), are as follows: 8 lines in region A at 143(m), 166(m), 197(m), 236(m), 256(m), 289(m), 322(m) and 374(w) cm^{-1}; 3 lines in region B at 461(m), 506(s) and 579(m) cm^{-1}; 3 lines in region C at 970(s), 1022(m) and 1089(w) cm^{-1}; 5 lines in region D at 3194(s), 3257(s), 3299(s), 3378(s) and 3431(s) cm^{-1}.

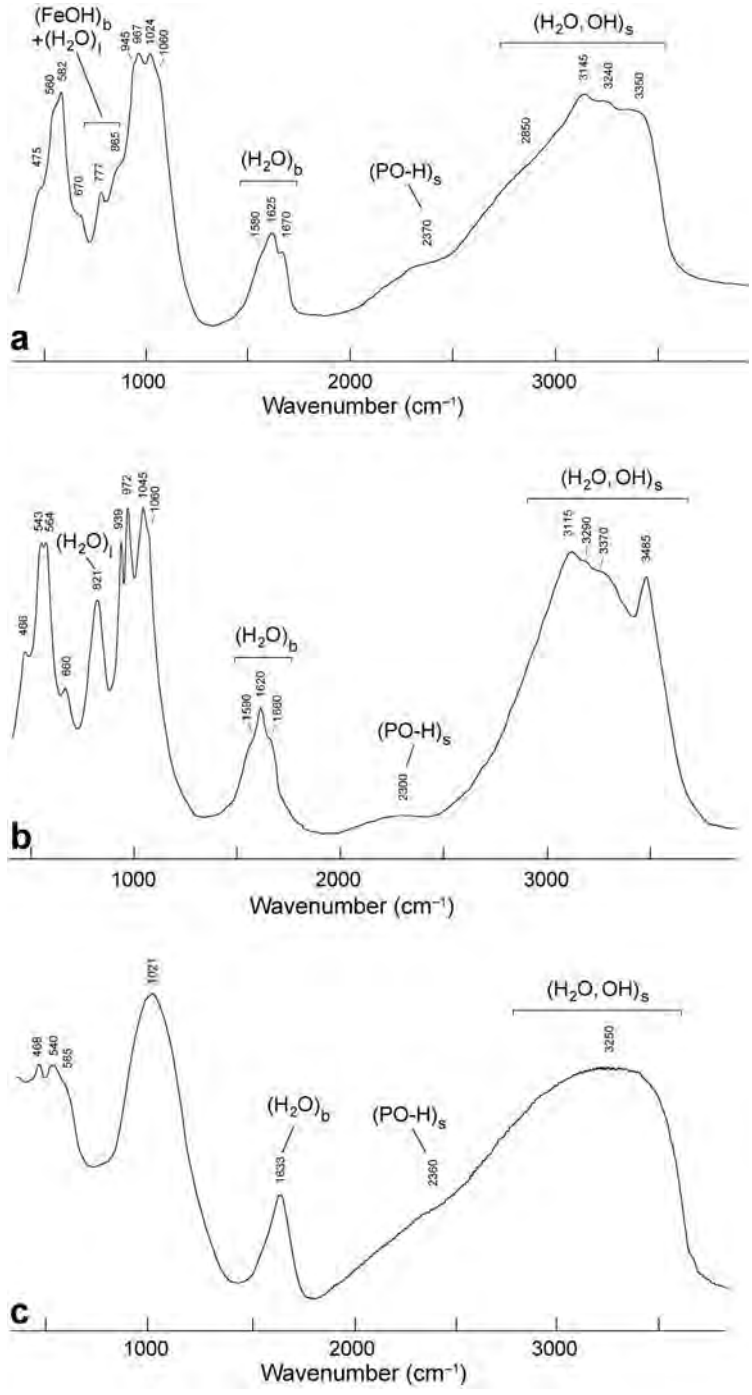

FIG. 2. Infrared spectra of metavivianite and related minerals. (*a*) Infrared spectrum of metavivianite from Boa Vista. (*b*) Infrared spectrum of vivianite from the Kamysh-Burun deposit, Kerch peninsula, Crimea, Ukraine. (*c*) Infrared spectrum of santabarbaraite from the Kamysh-Burun deposit, Kerch peninsula, Crimea, Ukraine. Ranges for different H-bearing groups are indicated.

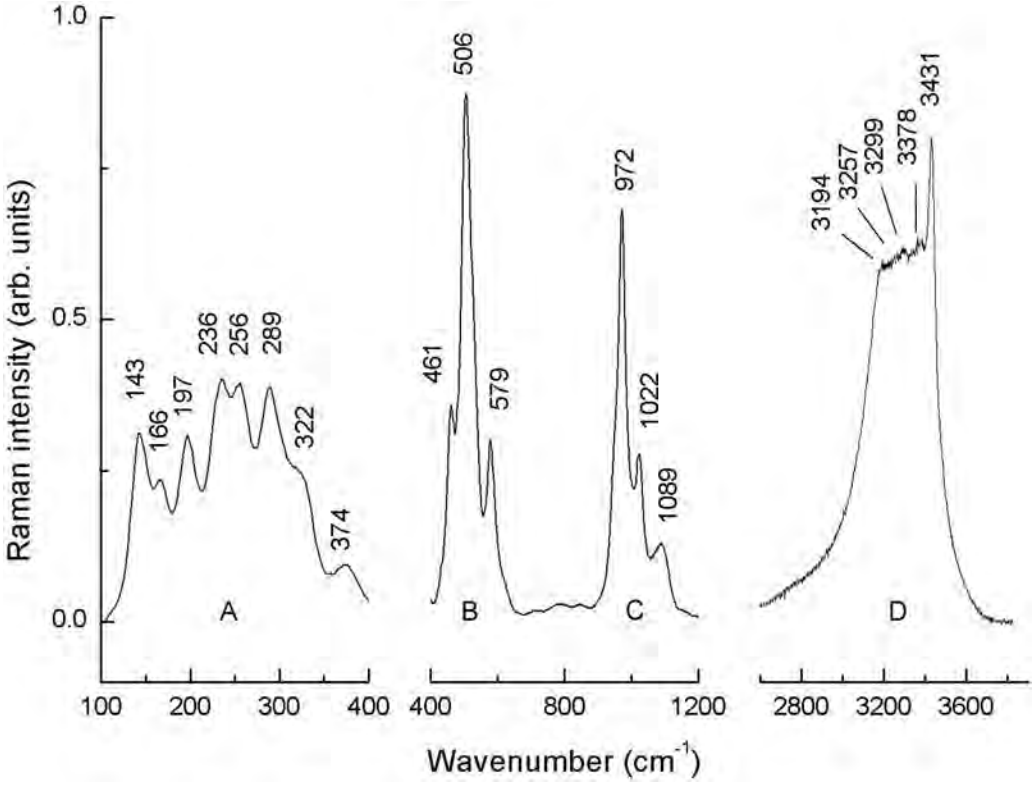

FIG. 3. The Raman spectrum of metavivianite from Boa Vista showing the four principal regions (A–D) of interest.

By analogy with vivianite, the strong band at 970 cm^{-1} corresponds to the symmetric stretching mode of PO_4^{3-} ions, and the bands about 1022 and 1089 cm^{-1} correspond to asymmetric P–O stretching vibrations. Numerous bands at wavenumbers lower than 580 cm^{-1} correspond to bending vibrations of PO_4^{3-} ions combined with Fe–O stretching and H_2O libration; unambiguous assignments could not be made based on the available data. The Raman spectrum of metavivianite from the Boa Vista pegmatite has O–H stretching bands at 3194, 3257, 3299, 3378 and 3431 cm^{-1}, the latter being the most intense. All the bands observed in this region correspond to hydroxyl groups and water molecules forming hydrogen bonds.

The Raman spectrum of metavivianite reported by Frost *et al*. (2004) contains broad poorly resolved bands of low intensity, which are characteristic of amorphous substances. In this context it is worthwhile noting that metavivianite is commonly admixed with an amorphous secondary Fe^{3+} phosphate (see below).

Mössbauer spectroscopy

The Mössbauer spectrum was recorded at room temperature in the Physics Department of the Federal University of Minas Gerais, using a spectrometer with a $^{57}Co/Rh$ (50 mCi) source and a drive operating at constant acceleration. A thin metallic iron foil (α-Fe) was used as a calibration. The *NORMOS* program (Brand, 1987) was used to fit the spectrum.

The Mössbauer spectrum of metavivianite from the Boa Vista pegmatite (Fig. 4) contains two doublets, which correspond to octahedrally coordinated Fe^{2+} and Fe^{3+}, in the ratio 43:57. Due to the absorber thickness effect, which reduces the accuracy of the relative ferrous and ferric fractions obtained from the Mössbauer spectrum, the uncertainty is estimated to be ~2%. Hyperfine parameters and the sub-spectral areas are listed in Table 1. Additional doublets have been reported in Mössbauer spectra of metavivianite (Dormann and Poullen, 1980; Rodgers and Johnston, 1985, Rodgers, 1986) and partially oxidized vivianite (Marincea *et al*.,

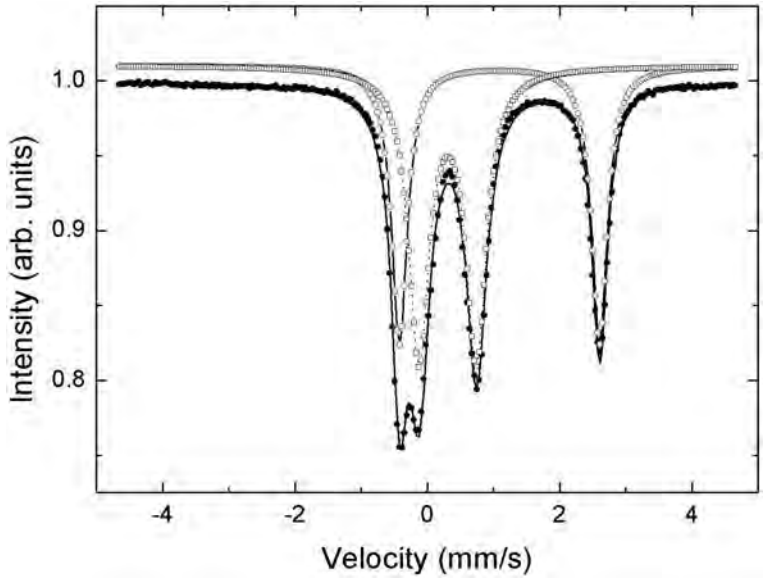

FIG. 4. Mössbauer spectrum of metavivianite from Boa Vista. Filled circles are experimental data; open circles are the fitted Fe^{2+} subspectrum; open squares are the fitted Fe^{3+} subspectrum.

1997), but these were not detected in the Mössbauer spectrum of the sample from Boa Vista.

Thermal data and chemical composition

Thermal data for metavivianite were obtained using a Shimadzu analyser in a nitrogen atmosphere at a gas flow rate of 50 cm^3 min^{-1}. Differential thermal analysis (DTA) and thermogravimetric (TG) and differential thermogravimetric (DTG) analyses were carried out simultaneously; 10 mg of sample was heated in an open platinum crucible at a rate of 10.0ºC min^{-1} up to a temperature of 950ºC.

The TG curve (Fig. 5) of metavivianite shows a total mass loss of about 21% on heating to 950ºC. The DTG curve has two main maxima, one centred at about 152.5ºC and the other at 185.6ºC, these are probably due to loss of loosely bound water molecules. The total mass loss of 21% corresponds to about 6 water molecules p.f.u. The discrepancy between the total mass loss of 21% by TG and the H_2O content determined by gas chromatography at 1200ºC (26.5 wt.%, see below) can be explained by the loss of hydroxyl groups above 950ºC. The IR spectrum of vivianite heated to 800ºC contains a strong band corresponding to O–H-stretching vibrations, whereas the H–O–H bending vibrations have a very low intensity (Pei-lin Tien and Waugh, 1969). The oxidation of iron in a reaction with H_2O or OH^- (self-oxidation after Frost *et al.*, 2004), can be represented by the following simplified schemes:

$$2Fe^{2+} + H_2O \rightarrow 2Fe^{3+} + (O^{2-})_{solid} + H_2\uparrow$$
$$2Fe^{2+} + 2OH^- \rightarrow 2Fe^{3+} + 2(O^{2-})_{solid} + H_2\uparrow$$

TABLE 1. Characteristics of the Mössbauer spectrum of iron in metavivianite from Boa Vista.

Doublet	Isomer shift δ (mm s^{-1})	Quadrupole splitting Δ (mm s^{-1})	Area (%)	Valency
1	1.20	3.025	43	Fe^{2+}
2	0.42	0.865	57	Fe^{3+}

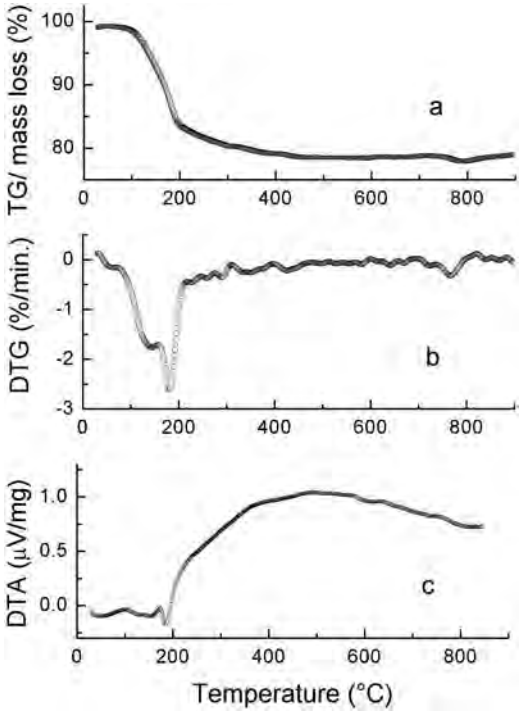

FIG. 5. The TG, DTG and DTA curves of metavivianite from room temperature to 950ºC.

In the course of gas chromatography, the evolved hydrogen would be oxidized by atmospheric oxygen and determined as H_2O. The second scheme (with OH^-) is more probable taking into account the low weight loss and the presence of a broad maximum on the DTA curve (that may indicate the self-oxidation process) in the temperature range 300 to 800ºC. Manganese can oxidize (to Mn^{3+} or, more probably, to Mn^{4+}) in a similar way.

Electron-microprobe analyses were carried out using a VEGA TS 5130MM SEM equipped with an EDX analyser (INCA Si(Li) detector) at an accelerating voltage of 15.7 kV and a beam current of 0.5 nA. The electron beam was rastered over an area of 16×16 μm. This type of analysis was chosen due to the instability of metavivianite under the electron beam. Attempts to analyse metavivianite using wavelength-dispersive spectrometry were unsuccessful due to its instability at even the smallest probe current (10 nA). Water was determined by gas chromatography of the products of annealing at 1200ºC; CO_2 was not analysed by this method as bands corresponding to vibrations of C−O bonds are absent in the IR spectrum. Iron was apportioned between FeO and Fe_2O_3 on the basis of the Mössbauer data. Other elements including F, Na, Al, Si, S, Cl, Ca, Ti, Cr, Co and Ni were sought, but were below detection limits. Analytical results are given in Table 2. The charge-balanced empirical formula of metavivianite (calculated on the basis of 16 oxygen atoms) is $(Fe^{3+}_{1.64}Fe^{2+}_{1.23}Mg_{0.085}Mn_{0.06})_{\Sigma 3.015}(PO_4)_{1.98}(OH)_{1.72}\cdot 6.36H_2O$. The simplified formula, taking into account structural data (see below), can be written $Fe^{2+}(Fe^{3+},Fe^{2+})_2(PO_4)_2(OH,H_2O)_2\cdot 6H_2O$. The Gladstone−Dale compatibility index, $1 - (K_P/K_c)$, (Mandarino, 1981) calculated from the empirical formula is 0.043 (good) using D_{calc} and 0.035 (excellent) using D_{meas}.

TABLE 2. Composition of metavivianite from Boa Vista based on five electron-microprobe analyses.

Constituent	Content (wt.%)	Range	Analytical standard
MgO	0.70	0.59−0.88	Diopside
MnO	0.92	0.77−1.04	Mn metal
FeO*	17.98	41.96−42.86**	Natural Fe_2O_3
Fe_2O_3*	26.60		
P_2O_5	28.62	28.37−28.82	Synthetic $LaPO_4$
H_2O***	26.5(5)		
Total	101.32		

* Total iron content analysed as FeO is 42.33 wt.% and is divided between FeO and Fe_2O_3 based on the Mössbauer data.
** For total iron measured as FeO.
*** H_2O determined by gas chromatography.

X-ray diffraction study and crystal structure determination

The X-ray powder diffraction data for metavivianite (Table 3) were collected on a STOE IPDS II single-crystal diffractometer equipped with an image plate detector (Mo$K\alpha$ radiation) using the Gandolfi method. These data were indexed on the triclinic unit cell found by single-crystal studies. The unit-cell parameters refined from the powder

TABLE 3. X-ray powder diffraction data for metavivianite from Boa Vista.

I_{obs}†	d_{obs}	I_{calc}*	d_{calc}**	*h k l*
40	8.72	37	8.705	010
9	7.53	9	7.482	100
100	6.95	100	6.947	$1\bar{1}0$
32	4.926	24	4.915	110
19	4.351	3, 8	4.352, 4.338	020, $0\bar{1}1$
12	4.206	5	4.174	$\bar{1}01$
8	3.983	6	3.954	$2\bar{1}0$
34	3.804	11, 9, 11	3.810, 3.787, 3.768	$\bar{1}11$, $1\bar{1}1$, 011
11	3.658	7	3.639	101
2	3.453	1	3.449	$0\bar{2}1$
2	3.319	1, 1	3.327, 3.309	$1\bar{2}1$, 120
23	3.060	2, 14	3.077, 3.047	$1\bar{3}0$, 111
24	2.974	22	2.967	$\bar{1}\bar{2}1$
24	2.776	12, 8	2.767, 2.749	$\bar{2}21$, $2\bar{2}1$
12	2.679	4, 2, 6	2.698, 2.690, 2.659	$1\bar{3}1$, 201, $0\bar{3}1$
3	2.589	2	2.569	$3\bar{2}0$
14	2.454	10, 5	2.452, 2.433	121, $2\bar{3}1$
9	2.346	4, 1, 3	2.353, 2.343, 2.328	211, $\bar{3}01$, $\bar{2}31$
8	2.315	5	2.308	$1\bar{4}0$
8	2.184	3, 1, 5	2.182, 2.182, 2.178	$3\bar{2}1$, $3\bar{1}1$, $1\bar{4}1$
5	2.156	2, 1	2.160, 2.152	$\bar{1}12$, $1\bar{1}2$
3	2.109	2	2.107	$0\bar{4}1$
6	2.070	4, 2	2.068, 2.057	$\bar{3}31$, $3\bar{3}1$
4	2.004	2, 1	2.002, 1.995	221, 131
3	1.954	1, 1	1.958, 1.956	$\bar{1}22$, $0\bar{3}2$
6	1.919	5	1.920	112
5	1.898	3, 1	1.899, 1.894	$2\bar{1}2$, $\bar{4}11$
5	1.857	3, 2	1.860, 1.851	$\bar{2}22$, $\bar{1}\bar{3}2$
6	1.833	3	1.831	$\bar{4}01$
6	1.822	5	1.823	$\bar{3}02$
8	1.740	3, 5, 4	1.741, 1.738, 1.737	050, $1\bar{4}2$, $4\bar{4}0$
5	1.714	4, 3	1.720, 1.714	$\bar{2}32$, 410
6	1.650	1, 2, 3, 3	1.655, 1.655, 1.654, 1.643	032, 240, $3\bar{2}2$, 401
4	1.630	2, 2	1.638, 1.625	330, $\bar{1}51$
2	1.591	3	1.588	$\bar{4}12$
3	1.547	2, 1	1.550, 1.549	$\bar{4}\bar{2}1$, $\bar{5}21$
5	1.528	2, 2	1.524, 1.521	222, 132
3	1.486	2, 3	1.491, 1.484	$\bar{1}\bar{2}3$, $\bar{2}\bar{4}2$
3	1.478	2	1.473	$\bar{3}\bar{3}2$
2	1.457	1, 1	1.456, 1.453	$0\bar{6}1$, $3\bar{6}1$
1	1.446	1	1.449	013
4	1.388	1, 4, 1, 1	1.390, 1.389, 1.383, 1.383	$\bar{2}23$, $5\bar{5}0$, $\bar{4}42$, $2\bar{2}3$

† The seven strongest lines are indicated in bold face.
* In the calculated X-ray pattern, only reflections with intensities $\geqslant 1$ are given.
** For the unit-cell parameters calculated from single-crystal data.

data (using the *KRIST* program, least-squares method) are a = 8.00(1), b = 9.35(7), c = 4.62(4) Å, α = 97.3(2), β = 96.0 (2), γ = 108.5(2)º and V = 321(2) Å^3.

Our X-ray powder diffraction pattern is a significant improvement on the data reported by Ritz *et al*. (1974) and Sameshima *et al*. (1985). It has more reflections and the d spacings and intensities are in good agreement with the calculated structural data.

The crystal structure of an Fe^{3+}-rich mineral related to metavivianite was solved by Dormann *et al*. (1982), but with a high R factor of 13.3%. The Fe^{2+}:Fe^{3+} ratio of 0.176 in this sample, which was described using the name metavivianite, is much lower than that in metavivianite from the type locality (0.613; Rodgers and Johnston, 1985). The crystal structure of metavivianite was investigated in the present work for these reasons.

Single-crystal X-ray studies of metavivianite from Boa Vista were carried out using an Xcalibur S diffractometer with a CCD detector. Details of data collection and structure refinement are given in Table 4. The crystal structure of metavivianite (Figs 6–8) was solved by the 'charge flipping' method using *Jana2006* (Petricek *et al*., 2006) and refined in space group $P\bar{1}$ to an R value of 6.0% for 1350 independent reflections with $|F_{obs}| > 3\sigma(F)$. Final atom parameters for metavivianite are given in Table 5, and interatomic distances in Table 6. The relatively high R value is due to the poor quality of the crystals. A crystallographic information file has been deposited with the Principal Editor of *Mineralogical Magazine* and is available at www.minersoc.org/pages/e_journals/dep_mat.html.

The metavivianite structure consists of heteropolyhedral layers which are coplanar with (1$\bar{1}$0). Each layer contains double Fe^{3+}-centred octahedral groups [$Fe_2^{3+}O_6(H_2O,OH)_4$] and isolated Fe^{2+}-centred octahedra [$Fe^{2+}O_2(H_2O)_4$] connected via [PO_4] tetrahedra. The layers are linked by hydrogen bonds between H_2O molecules and hydroxyl groups.

The hydrogen atoms were not located in the structural analysis, but the distances between some of the O atoms suggest the existence of strong hydrogen bonds formed by H_2O and OH^- with each other and with PO_4^{3-} groups. According to Brown (1976), the bond-valence contributions of hydrogen bonds are dependent on the O–O distances and they are as follows: 0.2 for $W1$–$W4$ (2.74 Å), 0.18 for $W1$–O2 (2.8 Å), 0.22 for $W4$–O3 (2.72 Å), 0.18 for $W2$–$W3$ (2.79 Å), 0.20 for $W2$–O1 (2.74 Å) and 0.22 for $W3$–O1 (2.70 Å). These values are listed in Table 7. On the basis of the values we assume that the $W1$ and $W3$ sites contain OH groups as well as water molecules.

TABLE 4. Crystal structure, data collection and refinement details for metavivianite from Boa Vista.

Chemical formula	$Fe^{2+}Fe_2^{3+}(PO_4)_2(OH)_2{\cdot}6H_2O$
a, b, c (Å)	7.989(1), 9.321(2), 4.629(1)
α, β, γ (º)	97.34(1), 95.96(1), 108.59(2)
V (Å^3)	320.2(1)
Space group	$P\bar{1}$
Z	1
μ (mm^{-1})	3.689
F(000)	236
D_{calc} (g cm^{-3})	2.5048
Crystal dimensions (mm)	0.23 × 0.23 × 0.17
Radiation	Mo$K\alpha$
θ_{max}	55.95
R_{int}	0.096
Reflection collected $\|F_{all}\|$	7242
Unique reflection $\|F_{obs}\| > 3\sigma\|F\|$	1350
GooF	1.04
Final R value (%)*	6.0
wR (%)*	6.5

* Refinement was by a full-matrix least squares fit on F^2 using the weighting scheme $w = 1/(\sigma^2(F) + 0.0016810001F^2)$.

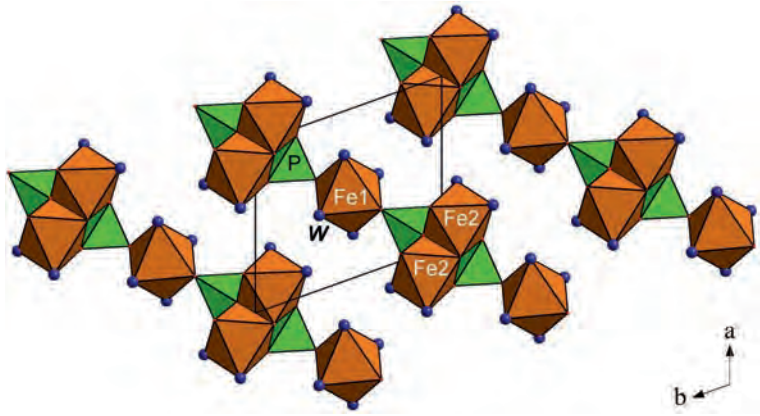

FIG. 6. The crystal structure of metavivianite from Boa Vista, (001) projection.

The O–O distances listed above are in good agreement with those estimated from the correlation between O–H stretching frequencies and O–H···O hydrogen bond lengths (Libowitzky, 1999) from 2.62 to 2.77 (based on IR absorption data) and from 2.70 to 2.82 Å (based on Raman shifts). The latter values are more precise because the widths of the bands in the Raman spectrum are lower than that in the IR spectrum.

The refined crystal-chemical formula of metavivianite (Z = 1) is $[(Fe^{2+}_{0.94}Mn_{0.06})(H_2O)_4][(Fe^{3+}_{0.82}Fe^{2+}_{0.14}Mg_{0.04})_2(H_2O,OH)_4][PO_4]_2$. The distribution of cations between different octahedral sites was calculated on the basis of the Fe^{2+}:Fe^{3+} ratio of 43:57, obtained from the Mössbauer spectrum, interatomic distances (Table 6) and the results of bond-valence calculations (Table 7).

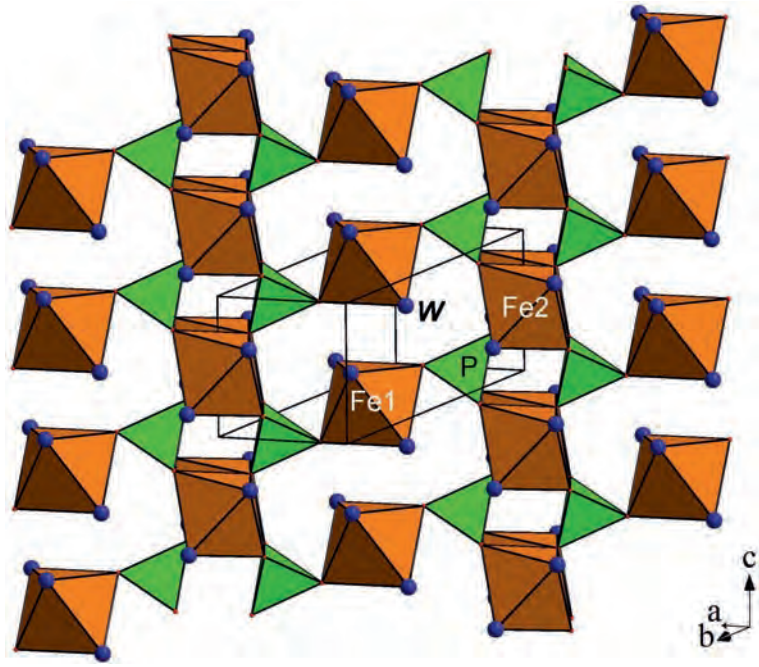

FIG. 7. Mixed octahedral-tetrahedral layer in the crystal structure of metavivianite from Boa Vista.

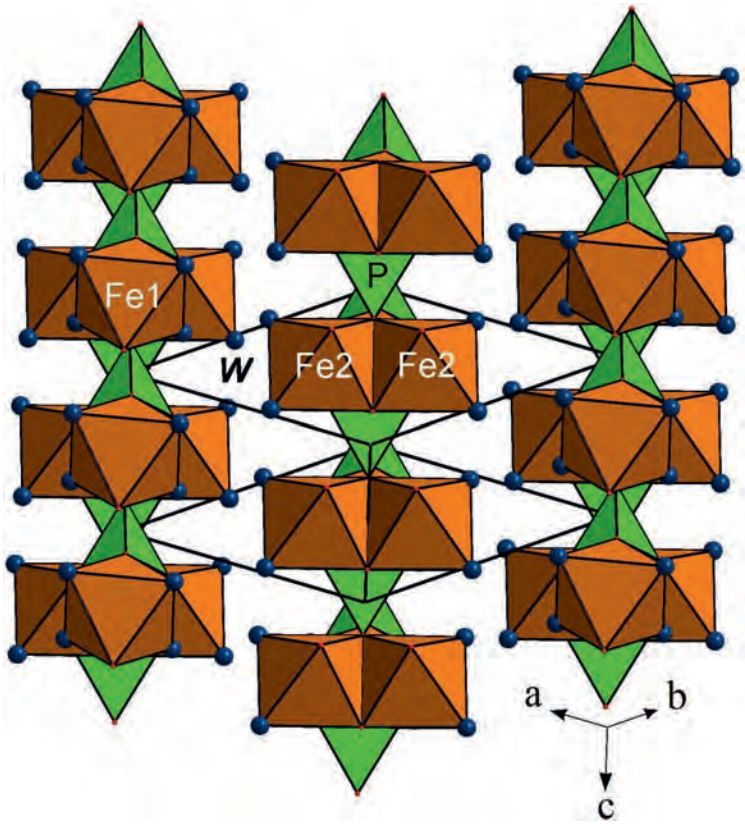

FIG. 8. The crystal structure of metavivianite from Boa Vista, (111) projection.

Discussion

On the basis of available data, Rodgers (1986) cast doubt on the homogeneity of some of the investigated metavivianite samples, including the type material (Ritz *et al*., 1974) from the Big Chief pegmatite, South Dakota. The existence of an

TABLE 5. Fractional coordinates, site multiplicities (Wyckoff) and equivalent displacement parameters U_{eq} (Å^2) for metavivianite from Boa Vista.

Site	*x*/*a*	*y*/*b*	*z*/*c*	Wyckoff	U_{eq}
Fe1	0.5	0.5	0	1g	0.0112(4)
Fe2	0.1305(1)	−0.0845(1)	−0.5020(2)	2i	0.0117(3)
P	0.1888(2)	0.1768(2)	0.0579(3)	2i	0.0098(4)
O1	0.045(1)	0.219(1)	−0.129(1)	2i	0.013(1)
O2	0.257(1)	0.064(1)	−0.129(1)	2i	0.013(1)
O3	0.343(1)	0.324(1)	0.189(1)	2i	0.015(1)
O4	0.105(1)	0.101(1)	0.312(1)	2i	0.013(1)
O*W*1	0.351(1)	−0.080(1)	−0.678(1)	2i	0.024(2)
O*W*2	0.259(1)	0.477(1)	0.697(1)	2i	0.020(2)
O*W*3	0.137(1)	−0.275(1)	−0.310(1)	2i	0.028(2)
O*W*4	0.560(1)	0.342(1)	0.696(1)	2i	0.020(2)

TABLE 6. Bond lengths (Å) for metavivianite.

—— This work ——		Calculated from the data of Dormann *et al.* (1982)	
Fe1–O3	2.075(4) ×2	Fe1–O3	1.977(22) ×2
–O*W*4	2.111(5) ×2	–O4	1.991(18) ×2
–O*W*2	2.196(5) ×2	–O6	2.012(18) ×2
Mean	**2.127**	**Mean**	**1.994**
Fe2–O*W*1	2.010(6)	Fe2–O1	2.016(16)
–O2	2.015(4)	–O8	2.021(23)
–O1	2.072(4)	–O2	2.063(15)
–O4	2.084(5)	–O5	2.080(22)
–O*W*3	2.093(6)	–O7	2.123(18)
–O4	2.127(5)	–O7	2.149(18)
Mean	**2.067**	**Mean**	**2.075**
P–O3	1.525(4)	P–O1	1.517(22)
–O2	1.541(5)	–O2	1.520(20)
–O1	1.546(5)	–O3	1.531(16)
–O4	1.551(5)	–O7	1.532(17)
Mean	**1.541**	**Mean**	**1.525**

oxidation series vivianite → metavivianite → santabarbaraite was subsequently established by Pratesi *et al*. (2003). Naturally oxidized vivianite samples are often heterogeneous and they commonly contain two or even all three of these minerals. This may account for the inconsistencies in earlier publications. In particular, the optical data reported by Ritz *et al*. (1974) on the palest grains (extracted from a heterogeneous sample) are identical to those of non-oxidized vivianite; and the second Fe^{3+} doublet in the Mössbauer spectra (reported by Dormann and Poullen, 1980; Marincea *et al*., 1997) is probably produced by admixed santabarbaraite, $Fe^{3+}_3(PO_4)_2(OH)_3{\cdot}5H_2O$. Note that the homogeneity of metavivianite before its structural investigation by Dormann and Poullen (1982) was checked by X-ray diffraction, but this technique would not reveal admixtures of amorphous santabarbaraite. The existence of homogeneous metavivianite with Fe^{3+}:Fe^{2+} = 2.9:0.1 (Dormann and Poullen, 1980; Rodgers and Johnston, 1985) is even more questionable.

Santabarbaraite is an amorphous phase produced by the transformation (oxidation) process described by Pratesi *et al*. (2003), it is trimorphous with ferristrunzite and allanpringite (crystalline Fe^{3+} phosphates that are isostructural with strunzite and wavellite, respectively).

TABLE 7. Bond-valence calculations for metavivianite from Boa Vista.

Site	O1	O2	O3	O4	O*W*1	O*W*2	O*W*3	O*W*4	ΣV_i
Fe1			0.40 (×2)→ 0.40↓			0.29 (×2)→ 0.29↓		0.36 (×2)→ 0.36↓	2.1
Fe2	0.43	0.50		(0.41 + 0.37)↓→	0.51		0.41		2.63
P	1.21	1.23	1.28	1.19					4.91
ΣV_i*	1.64 (0.42)	1.73 (0.18)	1.68 (0.22)	1.97	0.51 (0.2)	0.29 (0.18)	0.41 (0.18)	0.36 (0.2)	

* Bond valences for anions are supplemented by contributions (in brackets) due to hydrogen bonding from the hydrogen atoms of H_2O molecules.

Investigations using a polarizing microscope showed that our sample from the Boa Vista pegmatite does not contain any admixed amorphous phase and the Mössbauer spectrum of this sample contains only one doublet for Fe^{3+}.

Bond-valence calculations for our metavivianite sample (Table 7) show that Fe^{2+} and Fe^{3+} are the dominant components in the Fe1 and Fe2 sites, respectively. Therefore, the idealized (endmember) formula is $Fe^{2+}Fe^{3+}_2(PO_4)_2(OH)_2{\cdot}6H_2O$ and not $Fe_3(PO_4)_2{\cdot}8H_2O$ or $(Fe^{2+},Fe^{3+})_3(PO_4)_2{\cdot}8H_2O$, as reported previously (Ritz *et al*., 1974; Back and Mandarino, 2008). The formula $Fe^{2+}_{3-x}Fe^{3+}{}_x(PO_4)_2(OH)_x{\cdot}(8-x)H_2O$, $x > 1.4$ (Rodgers, 1986) is misleading because it represent two possible endmember compositions (Fe^{2+}- and Fe^{3+}-dominant) and does not reflect the presence of two independent sites with different occupancies in the crystal structure. The formula $(Fe^{2+},Fe^{3+})_3(PO_4)_2(OH)_2{\cdot}8H_2O$ is also given in the IMA list of mineral species and should be amended. On the basis of our data, endmember metavivianite is dimorphous with ferrostrunzite.

The crystal structure of strunzite, $Mn^{2+}Fe^{3+}_2(PO_4)_2(OH)_2{\cdot}6H_2O$, (Fig. 9) was investigated by Fanfani *et al*. (1978). Ferrostrunzite, $Fe^{2+}Fe^{3+}_2(PO_4)_2(OH)_2{\cdot}6H_2O$, is considered to be the Fe^{2+}-analogue of strunzite (Peacor *et al*., 1983; Hawthorne, 1998; Frost *et al*., 2002). The atomic arrangement of strunzite-group minerals (strunzite, ferrostrunzite and ferristrunzite) consists of chains of Fe coordination octahedra sharing vertices; PO_4 tetrahedra link together adjacent octahedra. Parallel chains are connected by PO_4 groups to form thick slabs. Parallel slabs are connected by isolated Mn^{2+}-, Fe^{2+}- or Fe^{3+}-centred coordination octahedra, to form a heteropolyhedral framework (Fig. 10).

Unlike ferrostrunzite, metavivianite is a 'transformational' mineral species which is formed as a result of the natural oxidation of vivianite. Rodgers (1986) showed that the transition to the triclinic structure takes place when the Fe^{3+} content exceeds 1.4 p.f.u. The crystal structure of vivianite (Fig. 11) is related to that of metavivianite but differs in the shifting of heteropolyhedral layers.

Metavivianite from the type locality has an Fe^{2+}:Fe^{3+} ratio of 0.615 (Rodgers and Johnston, 1985). If the Fe^{3+} is concentrated in the Fe1 site and minor Mn is present in the Fe2 site, this sample has the same general formula, $(Fe^{2+},Mn^{2+})(Fe^{3+},Fe^{2+})_2(PO_4)_2(OH,H_2O)_2{\cdot}6H_2O$, as our sample from Boa Vista.

Dormann *et al*. (1982) investigated a triclinic mineral which is isostructural with metavivianite from the Kamysh-Burun deposit, Kerch iron-ore basin, Crimea, Ukraine, described as α-kerchenite. The Mössbauer spectrum of this mineral indicates an Fe^{2+}:Fe^{3+} ratio of 15:85, which would mean that Fe^{3+} is the dominant component in both the Fe1 and Fe2 sites, a conclusion which is supported by the shorter Fe1–O distances in comparison to our sample from Boa Vista (Table 6). The dominance of Fe^{3+} in both the Fe1 and Fe2 sites in the sample investigated by

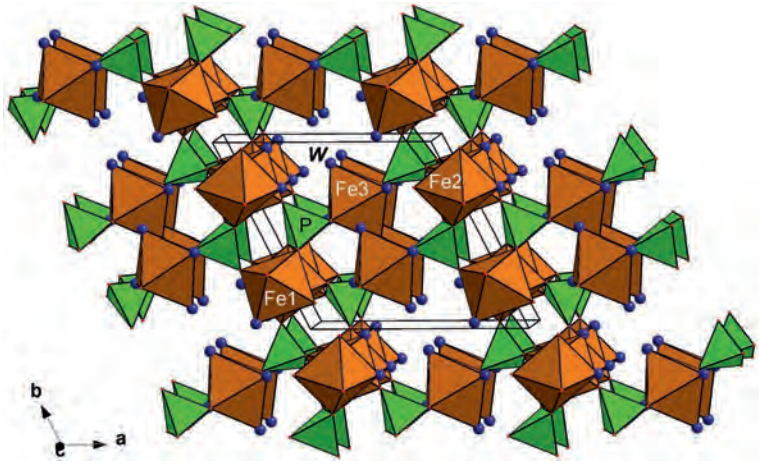

FIG. 9. The crystal structure of strunzite-type minerals, (001) projection. In ferrostrunzite, the Fe3-octahedron is occupied predominantly by Fe^{2+}.

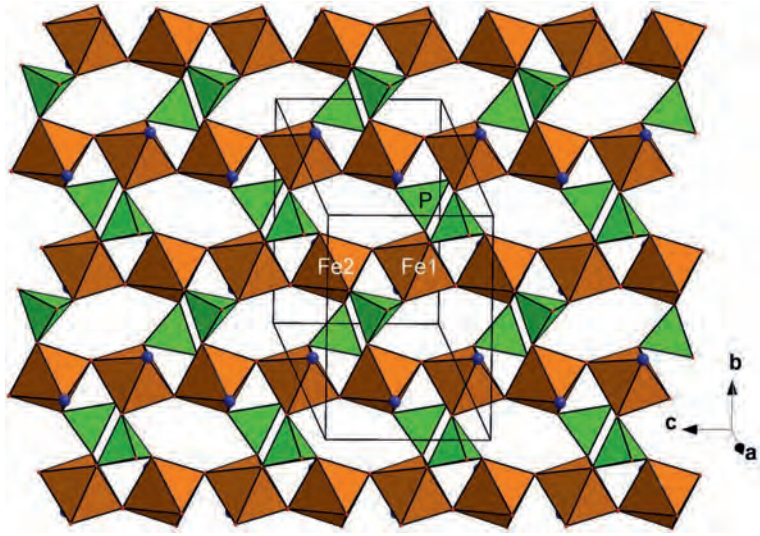

FIG. 10. Heteropolyhedral layer in the structures of strunzite and ferrostrunzite.

Dormann *et al*. (1982) is in agreement with bond-valence calculations (Table 8). Therefore, α-kerchenite is probably a distinct mineral species and not metavivianite, although its homogeneity and the absence of admixed amorphous phases such as santabarbaraite would need to be confirmed. A hypothetical mineral species with the endmember formula $Fe_3^{3+}(PO_4)_2(OH)_3{\cdot}5H_2O$ would be isostructural with metavivianite and (in its idealized

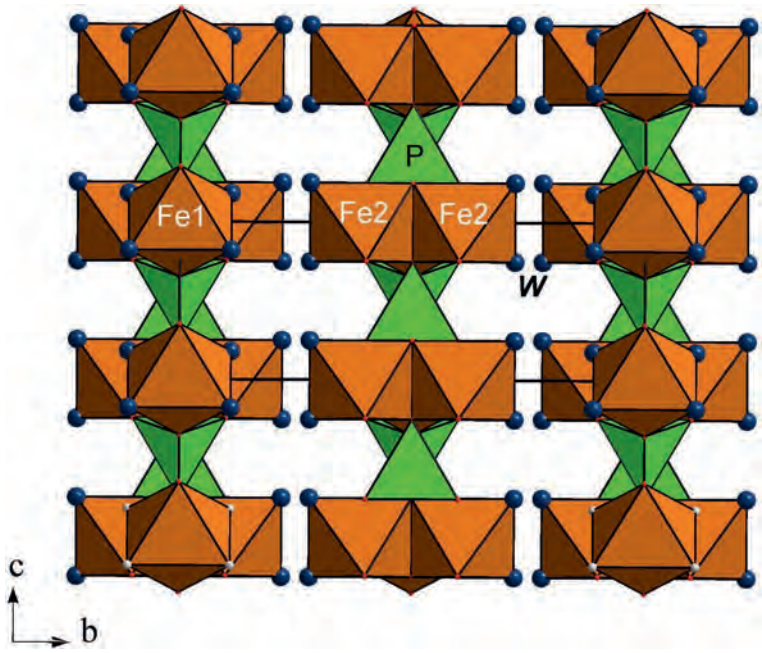

FIG. 11. The crystal structure of vivianite based on the data of Mori and Ito (1950), (100) projection.

TABLE 8. Bond-valence calculations for α-kerchenite from Kamysh-Burun, Kerch, Crimea, Ukraine.

Site	O1	O2	O3	O7	O8	O6	O5	O4	ΣV_i
Fe1			0.55 (×2)→ 0.55↓			0.50 (×2)→ 0.50↓		0.53 (×2)→ 0.53 ↓	3.16
Fe2	0.50	0.44		(0.37 + 0.35)↓→	0.49		0.42		2.57
P	1.31	1.30	1.26	1.26					5.13
ΣV_i	1.81	1.74	1.81	1.98	0.49	0.50	0.42	0.53	

Calculated from the data of Dormann *et al*. (1982).

TABLE 9. Comparative data for metavivianite, vivianite and ferrostrunzite.

Mineral Idealized formula Space group	Metavivianite $Fe^{2+}Fe_2^{3+}(PO_4)_2(OH)_2\cdot 6H_2O$ $P\bar{1}$	Vivianite $Fe_3^{2+}(PO_4)_2\cdot 8H_2O$ $C2/m$	Ferrostrunzite $Fe^{2+}Fe_2^{3+}(PO_4)_2(OH)_2\cdot 6H_2O$ $P\bar{1}$ or $P1$
a (Å)	7.989(1)	4.69–4.71	10.17–10.23
b (Å)	9.321(2)	13.43–13.44	9.77–9.78
c (Å)	4.629(1)	10.03–10.09	7.37–7.40
α (°)	97.34(1)	90	88.63–89.65
β (°)	95.96(1)	102.7–104.3	97.60–98.28
γ (°)	108.59(2)	90	117.26–117.60
Z	1	2	2
Strongest lines in the X-ray powder-diffraction pattern *d* (Å) *I* (%)	8.72 (40) 6.95 (100) 4.926 (32) 3.804 (34) 3.060 (23) 2.974 (24) 2.776 (24)	7.93 (13) 6.73 (100) 4.90 (12) 4.081 (12) 3.210 (16) 2.985 (10) 2.728 (9)	8.94 (80) 5.29 (100) 4.47 (30) 4.33 (20) 3.452 (30) 3.277 (40) 3.213 (30)
Strongest bands of the IR spectrum (cm^{-1})*	3350, 3240, 3145, 1625, 1024, 967, 777, 582	3485, 3115, 1620, 1045, 972, 939, 821, 564, 543, 466	3470, 3360, 3090, 1630, 1103, 1006, 584, 518
Optical data:			
α	1.600	1.579**	1.628
β	1.640	1.602**	1.682
γ	1.685	1.629**	1.724
Optical sign, 2V (°)	+85	+87 (calculated)	−80
Measured and calculated density, (g cm^{-3})	2.56 2.579	2.68 2.69	2.50 2.57
References	This work	Fejdi *et al*. (1980); Feklichev (1989); Rodgers *et al*. (1993).	Peacor *et al*. (1983); Coveney *et al*. (1984); van Tassel and de Grave (1992); our data on the IR spectrum.

* Shoulders are omitted.

** Lowest values for non-oxidized vivianite.

endmember formula presentation) polymorphous with santabarbaraite, ferristrunzite and allanpringite. Comparative data for metavivianite, vivianite and ferrostrunzite are given in Table 9.

Frost *et al*. (2004) proposed that the oxidation of vivianite may result in the formation of ferrostrunzite or ferristrunzite. However, this study and the available published data indicate that natural low-temperature oxidation of vivianite results in the transformation series vivianite → partly oxidized vivianite → metavivianite → Fe^{3+}-analogue of metavivianite → santabarbaraite. The members of this series, except for X-ray amorphous santabarbaraite, have similar crystal structures which make the transformations easy.

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References

Almeida, F.F.M. (1977) O Craton do São Francisco. *Revista Brasileira de Geociências*, **7**, 349–364.

Back, M.E. and Mandarino, J.A. (2008) *Fleischer's Glossary of Mineral Species*. The Mineralogical Record, Tucson, Arizona, USA, 344 pp.

Brand, R.A. (1987) Improving the validity of hyperfine field distributions from magnetic alloys. *Nuclear Instruments and Methods*, **B28**, 398–416.

Brown I.D. (1976) On the geometry of O–H...O hydrogen bonds. *Acta Crystallographica*, **A32**, 24–31.

Cassedanne, J.P. and Cassedanne, J.O. (1978) Présence de wolframite dans une pegmatite près de Galiléia, (MG). *Anais da Academia Brasileira de Ciências*, **50**, 89–93.

Cassedanne, J.P. and Cassedanne, J.O. (1979) Les minéraux de la pegmatite de Boa Vista (MG) et leur gangue. *Anais da Academia Brasileira de Ciências*, **51**, 311–326.

Cassedanne, J.P. and Cassedanne, J.O. (1982) Présence de legrandite dans une pegmatite de Minas Gerais, Brésil. *The Canadian Mineralogist*, **20**, 87–89.

Chaves, M.L.S.C., Scholz, R., Atencio, D. and Karfunkel, J. (2005) Assembléias e paragêneses minerais singulares nos pegmatitos da região de Galiléia (Minas Gerais). *Geociências*, **24**, 143–161.

Coveney R.M. Jr, Allen, A.V., Blankenship, J.C. and Simmons W.B. (1984) Hawleyite and phosphate minerals from Bethel Church, Indiana, including a second occurrence for ferrostrunzite. *Mineralogical Record*, **15**, 351–357.

Dormann, J. and Poullen, J.-F. (1980) Étude par spectroscopie Mössbauer de vivianites oxydées naturelles. *Bulletin de Minéralogie*, **103**, 633–639.

Dormann, J., Gaspérin, M. and Poullen, J.-F. (1982) Étude structurale de la séquence d'oxydation de la vivianite $Fe_3(PO_4)_2{\cdot}8(H_2O)$. *Bulletin de Minéralogie*, **105**, 147–160.

Fanfani, L., Tomassini, M., Zanazzi, P.F. and Zanzari. A.R. (1978) The crystal structure of strunzite, a contribution to the crystal chemistry of basic ferric-manganous hydrated phosphates. *Mineralogy and Petrology*, **25**, 77–87.

Fejdi, P., Poullen, J.-F. and Gasperin, M. (1980) Affinement de la structure de la vivianite $Fe_3(PO_4)_2{\cdot}8(H_2O)$. *Bulletin de Minéralogie*, **103**, 135–138.

Feklichev, V.G. (1989) *Diagnostic Constants of Minerals*. Nedra, Moscow, 480 pp., [in Russian].

Frost, R.L., Kloprogge, T., Martens, W.N. and Williams, P. (2002) Vibrational spectroscopy of the basic manganese, ferric and ferrous phosphate minerals: strunzite, ferristrunzite and ferrostrunzite. *Neues Jahrbuch für Mineralogie, Monatschefte*, **2002**, 481–496.

Frost, R.L., Weier, M.L. and Lyon, W. (2004) Metavivianite, an intermediate mineral phase between vivianite, and ferro/ferristrunzite – a Raman spectroscopic study. *Neues Jahrbuch für Mineralogie, Monatshefte*, **2004**, 228–240.

Hawthorne, F.C. (1998) Structure and chemistry of phosphate minerals. *Mineralogical Magazine*, **62**, 141–164.

Libowitzky, E. (1999) Correlation of O–H stretching frequencies and O–H···O hydrogen bond lengths in minerals. *Monatshefte für Chemie*, **130**, 1047–1059.

Mandarino, J.A. (1981) The Gladstone–Dale relationship: part IV. The compatibility concept and its application. *The Canadian Mineralogist*, **19**, 441–450.

Marincea, S., Constantinescu, E. and Ladriere, J. (1997) Relatively unoxidized vivianite in limnic coal from Capeni, Baraolt Basin, Romania. *The Canadian Mineralogist*, **35**, 713–722.

Mori, H. and Ito, T. (1950) The structure of vivianite and symplesite. *Acta Crystallographica*, **3**, 1–6.

Nalini H.A. Jr (1997) Caractérisation des suites magmatiques néoprotérozoïques de la region de Conselheiro Pena et Galiléia (Minas Gerais,

Brésil). Unpublished PhD thesis, Ecole Nationale Superieure des Mines de Saint Étienne, Saint Étienne, France, 237 pp.

Peacor, D.R., Dunn, P.J. and Simmons, W.B. (1983) Ferrostrunzite, the ferrous iron analogue of strunzite from Mullica Hill, New Jersey. *Neues Jahrbuch für Mineralogie, Monatshefte*, **1983**, 524–528.

Pedrosa-Soares, A.C., Noce, C.M., Wiedemann, C.M. and Pinto, C.P. (2001) The Araçuaí-West Congo orogen in Brazil: an overview of a confined orogen formed during Gondwanaland assembly. *Precambrian Research*, **110**, 307–323.

Pedrosa-Soares, A.C., Campos, C.M. De, Noce, C.M., Silva, L.C. da, Novo, T.A., Roncato, J., Medeiros, S.M., Castañeda, C., Queiroga, G.N., Dantas, E., Dussin, I.A. and Alkmim, F. (2011) Late Neoproterozoic–Cambrian granitic magmatism in Araçuaí orogen (Brazil), the Eastern Brazilian Pegmatite Province and related mineral resources. *Geological Society Special Publication*, **350**, 25–51.

Pekov, I.V., Vinogradova, R.A., Chukanov, N.V. and Kulikova, I.M. (2001) On magnesium and cobalt arsenates of the fairfieldite and roselite groups. *Zapiski Vserossiiskogo Mineralogicheskogo Obshchestva*, **130**, 10–23, [in Russian].

Pen-li Tien and Waugh, T.C. (1969) Thermal and X-ray studies on earthy vivianite in Graneros Shale (Upper Cretaceous), Kansas. *American Mineralogist*, **54**, 1355–1362.

Petricek, V., Dusek, M. and Palatinus, L. (2006) *Jana2006. Structure Determination Software Programs*. Institute of Physics, Praha, Czech Republic.

Pratesi, G., Cipriani, C., Giuli, G. and Birch W.D. (2003) Santabarbaraite: a new amorphous phosphate mineral. *European Journal of Mineralogy*, **15**, 185–192.

Ritz, C., Essene, E.J. and Peacor, D.R. (1974) Metavivianite, $Fe_3(PO_4)_2{\cdot}8H_2O$, a new mineral. *The American Mineralogist*, **59**, 896–899.

Rodgers, K.A. (1986) Metavivianite and kerchenite: a review. *Mineralogical Magazine*, **50**, 687–691.

Rodgers, K.A., Kobe, H.W. and Childs, C.W. (1993) Characterization of vivianite from Catavi, Llallagua, Bolivia. *Mineralogy and Petrology*, **47**, 193–208.

Rodgers, K.A. and Johnston, J.H. (1985) Type metavivianite: Mössbauer evidence for a revised composition. *Neues Jahrbuch für Mineralogie, Monatshefte*, **1985**, 539–542.

Sameshima, T., Henderson, G.S., Black, P.M. and Rodgers, K.A. (1985) X-ray diffraction studies of vivianite, metavivianite, and baricite. *Mineralogical Magazine*, **49**, 81–85.

Van Tassel, R. and de Grave, E. (1992) Ferrostrunzite from Arnsberg, Sauerland, Germany. *Neues Jahrbuch für Mineralogie, Monatshefte*, **1992**, 207–212.

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;
_journal_techeditor_code                ?
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_journal_volume                         ?
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# 2. SUBMISSION DETAILS

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Petricek, V., Dusek, M. & Palatinus L. (2006). Jana2006.
Structure Determination Software Programs.
Institute of Physics, Praha, Czech Republic.

Palatinus L. & Chapuis G. (2007). J. Appl. Cryst. 40, 786-790.

# enable this reference if Diamond ver. 2 was used for visualization
#Brandenburg, K. (1999). DIAMOND. Version. 2.1c.
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#Crystal Impact GbR, Bonn, Germany.

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#Brandenburg, K. & Putz, H. (2005). DIAMOND Version 3.
#Crystal Impact GbR, Postfach 1251, D-53002 Bonn, Germany.

# enable this reference if SIR97 was used for solving of the structure
#Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C.,
#Guagliardi, A., Moliterni, A. G. G., Polidori, G., Spagna, R. (1997).
#SIR97. A Package for Crystal Structure Solution by Direct Methods
#and Refinement, Bari, Rome, Italy.

# use this reference if SIR2002 was used for solving of the structure
#Burla, M.C., Camalli, M., Carrozzini, B., Cascarano, G., Giacovazzo, C.,
#Polidori, G., Spagna, R.
#SIR2002: the program, J. Appl. Cryst, (2003). 36, 1103

# enable this reference if bond valences were calculated
#Brown, I. D. (1996). J. Appl. Cryst. 29, 479-480.

# enable this reference if Xshape wase used for crystal shape refinement
#Stoe & Cie (1998). X-SHAPE. Stoe & Cie, Darmstadt, Germany.


# enable this reference if Flack coefficient was refined
#Flack, H. D. (1983). Acta Cryst. A39, 876-881.
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_cell_length_c                           9.3358(7)
_cell_angle_alpha                        108.649(8)
_cell_angle_beta                         97.387(7)
_cell_angle_gamma                        95.834(7)
_cell_volume                             321.74(5)

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_diffrn_reflns_limit_l_min              -19
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# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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  Fe2 Fe -0.50203(19) 0.13050(11) -0.08450(10) Uani 0.0117(3) 2 1 d . . .
  P1 P 0.0579(3) 0.18877(19) 0.17684(17) Uani 0.0098(4) 2 1 d . . .
  O1 O -0.6777(11) 0.3514(7) -0.0802(6) Uani 0.0238(18) 2 1 d . . .
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  O2 O 0.6971(11) 0.2587(6) 0.4767(6) Uani 0.0200(15) 2 1 d . . .
  O3 O -0.1286(9) 0.0448(5) 0.2191(5) Uani 0.0129(13) 2 1 d . . .
  O4 O -0.3100(12) 0.1365(8) -0.2746(6) Uani 0.028(2) 2 1 d . . .
  O5 O -0.1288(9) 0.2569(5) 0.0642(5) Uani 0.0130(12) 2 1 d . . .
  O6 O 0.1888(9) 0.3428(6) 0.3243(5) Uani 0.0153(13) 2 1 d . . .
  O7 O 0.6956(10) 0.5601(7) 0.3416(6) Uani 0.0197(16) 2 1 d . . .
  O8 O 0.3123(9) 0.1050(5) 0.1012(5) Uani 0.0126(12) 2 1 d . . .

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 Fe2 Fe 0.0078(4) 0.0126(4) 0.0105(4) 0.0011(3) -0.0007(3) -0.0008(3)
 P1 P 0.0065(6) 0.0103(6) 0.0078(6) 0.0010(4) 0.0000(5) -0.0030(4)
 O1 O 0.018(2) 0.025(2) 0.030(3) -0.0004(19) -0.004(2) 0.015(2)
 O2 O 0.019(2) 0.020(2) 0.019(2) 0.0003(17) 0.0024(18) 0.0048(17)
 O3 O 0.015(2) 0.0140(17) 0.010(2) 0.0018(14) 0.0064(16) 0.0037(14)
 O4 O 0.028(3) 0.037(3) 0.028(3) 0.017(2) 0.014(2) 0.017(2)
 O5 O 0.0091(18) 0.0103(16) 0.015(2) -0.0006(13) -0.0001(15) -0.0007(14)
 O6 O 0.0093(18) 0.0162(18) 0.012(2) 0.0009(14) 0.0011(15) -0.0056(14)
 O7 O 0.014(2) 0.029(2) 0.016(2) 0.0080(18) -0.0010(18) 0.0074(18)
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  O7 Fe1 O7 1_455 . 2_666 180.0(5) ?
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  O8 Fe2 O8 1_455 . 2_555 89.66(18) ?
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  O3 P1 O6 . . . 108.4(3) ?
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  Fe2 O5 P1 . . . 128.2(3) ?
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  -4   1   0    99.30   119.44  20.82 o
   1   1   0  2686.82  2584.21  22.56 o
   2   1   0   206.66   222.53  13.89 o
   3   1   0  1764.52  1802.00  28.39 o
   4   1   0    66.53    78.58  20.10 o
   5   1   0  1310.08  1422.20  38.35 o
   7   1   0   487.44   407.49  57.46 o
  -6   2   0   168.93   255.98  78.88 o
  -5   2   0   567.40   604.61  43.25 o
  -4   2   0   287.02   274.22  24.95 o
  -3   2   0   792.48   755.69  15.82 o
  -6   3   0   453.76   393.11  41.47 o
  -4   3   0   925.36   884.64  32.55 o
  -3   3   0   491.16   592.08  19.05 o
  -2   3   0  7692.99  7429.57  44.05 o
   0   3   0  4093.59  3997.81  26.08 o
   1   3   0   394.02   478.17  15.09 o
   2   3   0  1607.04  1568.51  27.37 o
   4   3   0  1105.62  1159.45  44.95 o
   5   3   0   227.61   217.97  29.25 o
  -7   4   0   304.23   347.13  49.34 o
  -6   4   0   181.49   132.12  40.89 o
  -5   4   0   223.37   246.45  33.78 o
  -4   4   0   829.24   920.71  36.23 o
  -3   4   0   117.18   135.62  15.14 o
  -2   4   0   411.00   413.42  17.24 o
  -1   4   0  3854.26  4289.23  29.59 o
   2   4   0    69.62   102.90  15.86 o
   3   4   0  1708.77  2086.93  41.23 o
   5   4   0   776.12   921.65  42.67 o
   7   4   0   283.22   366.52  50.62 o
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   3   5   0   114.28   156.82  28.44 o
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3	-5	3	49.75	63.06	18.00	o
4	-5	3	1775.66	1468.80	38.72	o
-6	-4	3	128.67	142.20	34.31	o
-5	-4	3	223.41	211.48	30.59	o
-4	-4	3	117.64	92.65	20.76	o
-3	-4	3	655.84	624.60	27.50	o
-2	-4	3	519.83	458.27	22.50	o
-1	-4	3	759.63	736.98	23.37	o
0	-4	3	837.07	952.43	23.12	o
1	-4	3	200.75	249.09	15.43	o
2	-4	3	641.38	754.26	21.37	o
-8	-2	3	375.74	396.82	50.06	o
-6	-2	3	298.15	337.42	40.46	o

-4	-2	3	92.46	85.60	27.19	o
-3	-2	3	3147.76	3078.73	32.67	o
-2	-2	3	3285.50	2955.93	28.06	o
-1	-2	3	3491.03	3368.59	27.87	o
2	-2	3	8041.60	7582.43	44.02	o
3	-2	3	1417.80	1350.08	25.90	o
4	-2	3	1687.26	1570.46	35.06	o
-7	-1	3	364.89	313.38	40.44	o
-5	-1	3	593.83	507.48	29.86	o
-4	-1	3	78.32	70.63	19.08	o
-3	-1	3	3042.63	2802.34	32.09	o
-1	-1	3	2672.32	2529.59	20.59	o
0	-1	3	966.27	1035.00	16.37	o
1	-1	3	998.01	963.65	31.79	o
2	-1	3	514.20	541.66	12.27	o
3	-1	3	220.90	209.52	14.75	o
4	-1	3	469.17	495.18	29.47	o
5	-1	3	264.50	247.21	62.41	o
-4	0	3	294.58	274.06	17.61	o
-3	0	3	630.79	610.75	19.44	o
-2	0	3	1219.74	1294.72	20.68	o
-1	0	3	4475.30	4437.24	27.61	o
0	0	3	1080.77	1029.59	18.98	o
1	0	3	311.67	312.09	16.65	o
2	0	3	1727.96	1824.20	19.47	o
3	0	3	438.89	468.91	18.00	o
-5	1	3	126.92	131.90	22.19	o
-4	1	3	444.50	556.52	26.15	o
0	1	3	74.79	72.46	9.62	o
3	1	3	102.75	91.77	13.11	o
-7	2	3	801.42	985.87	57.88	o
-6	2	3	109.42	131.85	31.96	o
-4	2	3	66.81	108.76	26.01	o
0	2	3	211.88	234.13	12.71	o
3	2	3	1162.89	1327.42	29.10	o
4	2	3	334.55	362.06	33.46	o
5	2	3	245.59	261.97	56.93	o
-6	3	3	160.99	216.77	34.88	o
-4	3	3	491.24	546.21	25.19	o
-2	3	3	4810.60	5065.42	49.81	o
-1	3	3	603.68	692.76	18.29	o
0	3	3	4378.58	4752.75	42.13	o
2	3	3	495.19	545.45	18.14	o
3	3	3	409.65	369.11	22.21	o
4	3	3	240.50	194.42	32.20	o
-4	4	3	128.89	130.95	23.71	o
0	4	3	655.99	619.16	19.33	o
2	4	3	519.30	472.88	21.26	o
3	4	3	444.74	414.65	30.84	o
4	4	3	270.50	221.67	58.54	o
5	4	3	179.14	207.30	64.30	o
6	4	3	221.55	192.12	48.28	o
-7	5	3	349.04	340.72	50.94	o
-5	5	3	420.34	412.86	35.17	o
-3	5	3	794.72	772.02	27.72	o
-2	5	3	415.56	415.53	19.33	o
-1	5	3	451.02	464.63	18.75	o
0	5	3	506.45	502.19	19.54	o
1	5	3	151.45	177.46	18.97	o
3	5	3	303.64	384.41	28.31	o
5	5	3	215.79	269.61	72.85	o

-8	6	3	187.34	203.80	60.06	o
-6	6	3	229.12	306.73	46.71	o
-4	6	3	1603.21	1858.33	39.59	o
1	6	3	48.85	56.58	17.43	o
3	6	3	92.20	87.35	27.19	o
-4	7	3	176.51	206.96	28.11	o
-3	7	3	263.64	240.49	22.25	o
0	7	3	303.20	286.69	19.41	o
1	7	3	616.32	660.86	32.17	o
3	7	3	581.43	603.71	38.29	o
-3	8	3	102.48	97.45	22.53	o
3	8	3	74.89	118.18	32.92	o
-6	9	3	289.33	202.90	57.24	o
-4	9	3	602.10	582.71	36.48	o
-2	9	3	387.92	334.01	27.02	o
0	9	3	492.88	507.59	32.18	o
-3	10	3	316.39	272.05	30.17	o
-1	10	3	207.56	203.21	33.17	o
1	10	3	652.93	752.24	46.27	o
-3	13	3	153.36	156.38	51.35	o
3	-13	4	149.85	201.89	51.89	o
-1	-11	4	314.36	275.07	34.78	o
0	-11	4	116.49	125.89	31.56	o
-1	-10	4	215.88	193.66	31.12	o
1	-10	4	211.59	221.06	35.43	o
3	-10	4	299.76	297.18	33.30	o
5	-10	4	374.72	333.79	43.37	o
-4	-9	4	186.19	168.85	34.48	o
-1	-9	4	448.27	444.08	27.58	o
0	-9	4	451.00	523.17	31.11	o
1	-9	4	213.98	234.08	27.54	o
6	-9	4	377.54	450.13	72.67	o
-1	-8	4	463.71	478.87	28.45	o
1	-8	4	273.65	317.76	22.71	o
3	-8	4	458.30	493.03	29.87	o
4	-8	4	135.08	174.25	38.77	o
-2	-7	4	135.35	125.06	25.06	o
-1	-7	4	510.66	506.78	41.50	o
0	-7	4	484.75	421.78	23.76	o
1	-7	4	470.72	395.12	20.27	o
2	-7	4	532.07	472.96	21.60	o
3	-7	4	255.19	183.34	31.09	o
-6	-6	4	165.74	155.10	43.10	o
-2	-6	4	842.35	835.55	46.02	o
-1	-6	4	515.65	491.28	25.29	o
0	-6	4	203.88	176.91	20.99	o
1	-6	4	224.23	218.02	16.97	o
4	-6	4	1356.27	1136.79	42.44	o
6	-6	4	293.42	254.11	55.99	o
-7	-5	4	309.38	235.89	58.95	o
-5	-5	4	862.75	736.83	38.42	o
-3	-5	4	969.73	858.10	37.21	o
-2	-5	4	196.40	154.11	22.10	o
-1	-5	4	2449.95	2134.97	37.65	o
0	-5	4	182.56	153.22	20.09	o
1	-5	4	1033.47	1004.16	25.96	o
2	-5	4	282.13	297.79	20.63	o
3	-5	4	478.92	407.23	20.92	o
4	-5	4	310.67	332.48	39.29	o
5	-5	4	272.03	240.57	45.37	o
6	-5	4	170.23	188.23	54.31	o

-6	-4	4	79.37	111.60	34.63	o
1	-4	4	112.33	106.85	13.52	o
3	-4	4	59.58	73.99	14.04	o
4	-4	4	709.34	816.83	44.74	o
-3	-3	4	74.16	67.36	15.97	o
-2	-3	4	101.92	106.38	13.64	o
-1	-3	4	124.07	98.95	15.99	o
0	-3	4	706.18	693.29	20.59	o
1	-3	4	594.72	683.26	17.15	o
2	-3	4	661.36	664.73	16.83	o
3	-3	4	168.83	171.21	16.07	o
-7	-2	4	283.85	258.95	39.83	o
-5	-2	4	567.16	512.43	30.43	o
-3	-2	4	3337.87	2961.67	31.76	o
-2	-2	4	106.92	126.93	12.65	o
-1	-2	4	2917.18	2470.09	25.32	o
0	-2	4	762.15	712.80	18.55	o
1	-2	4	615.81	583.86	22.43	o
2	-2	4	882.16	774.55	12.69	o
3	-2	4	185.17	208.39	19.89	o
4	-2	4	378.22	331.20	33.40	o
5	-2	4	227.43	294.50	65.78	o
7	-2	4	239.10	355.34	91.66	o
-7	-1	4	236.98	170.62	39.02	o
-6	-1	4	559.05	528.31	37.60	o
-4	-1	4	484.18	406.47	28.21	o
-3	-1	4	320.66	330.54	16.95	o
-1	-1	4	4884.00	4738.73	29.87	o
0	-1	4	4966.72	4771.76	36.56	o
1	-1	4	566.79	641.91	33.39	o
2	-1	4	1806.29	1772.66	30.60	o
4	-1	4	2689.65	2818.38	64.44	o
5	-1	4	322.65	341.81	68.93	o
-4	0	4	298.05	354.06	27.89	o
-2	0	4	79.21	73.30	11.06	o
-1	0	4	1684.45	1849.90	19.28	o
2	0	4	32.40	40.54	12.38	o
3	0	4	1315.04	1579.88	28.27	o
5	0	4	674.74	848.27	51.83	o
7	0	4	208.36	334.29	94.93	o
-7	1	4	290.29	385.10	49.82	o
-5	1	4	838.03	955.95	29.48	o
-2	1	4	75.25	98.11	13.52	o
-1	1	4	1268.45	1368.11	21.98	o
0	1	4	322.34	359.23	13.60	o
1	1	4	120.65	149.40	9.91	o
-7	2	4	174.79	136.81	38.71	o
-6	2	4	282.63	288.93	35.11	o
-4	2	4	641.43	674.70	30.42	o
-3	2	4	125.68	118.31	17.07	o
-2	2	4	8611.00	7573.50	54.40	o
0	2	4	3582.85	4317.50	38.90	o
2	2	4	1435.36	1400.37	23.09	o
3	2	4	986.10	832.19	31.43	o
4	2	4	367.50	353.73	53.78	o
-6	3	4	312.97	253.24	31.01	o
-5	3	4	216.15	184.59	25.68	o
-3	3	4	791.11	789.42	25.28	o
-2	3	4	1099.94	945.45	24.46	o
-1	3	4	1530.39	1635.95	26.82	o
1	3	4	1207.85	1240.04	25.15	o

3	3	4	1962.55	1684.85	56.50	o
5	3	4	1107.82	883.03	82.47	o
-6	4	4	330.15	268.00	38.81	o
-4	4	4	281.81	269.89	26.29	o
-1	4	4	313.09	392.91	22.00	o
2	4	4	250.61	230.60	21.43	o
-6	5	4	69.04	110.62	35.56	o
-4	5	4	779.41	894.15	36.45	o
-3	5	4	177.89	252.54	27.02	o
-1	5	4	356.94	452.79	24.49	o
-7	6	4	167.21	188.46	50.41	o
-6	6	4	160.62	174.18	38.20	o
-4	6	4	267.05	362.83	32.92	o
-3	6	4	305.12	336.86	24.45	o
-2	6	4	58.92	76.47	17.73	o
-1	6	4	1466.80	1640.60	33.36	o
1	6	4	959.49	1035.80	28.75	o
3	6	4	940.59	998.61	41.13	o
-6	7	4	256.49	243.90	48.08	o
-4	7	4	149.19	140.39	32.35	o
-2	7	4	622.61	610.36	22.44	o
-1	7	4	284.97	255.55	21.32	o
0	7	4	45.68	58.18	19.24	o
1	7	4	259.60	278.60	29.52	o
4	7	4	572.60	501.80	82.25	o
-5	8	4	215.05	148.36	38.28	o
-4	8	4	285.08	237.01	35.63	o
-3	8	4	187.68	152.89	27.73	o
-1	8	4	283.13	261.77	24.51	o
0	8	4	92.24	95.33	22.59	o
-3	9	4	92.53	132.37	26.05	o
-1	9	4	428.11	398.25	28.13	o
0	9	4	140.94	140.02	34.47	o
-4	10	4	145.92	146.21	38.66	o
-3	10	4	121.61	145.96	28.53	o
-1	10	4	132.91	145.86	32.66	o
2	10	4	234.94	246.26	42.34	o
-3	11	4	503.91	449.96	42.69	o
-1	11	4	131.31	143.67	37.52	o
-3	-12	5	146.42	145.87	37.00	o
-1	-12	5	287.49	270.47	37.45	o
1	-12	5	271.79	231.51	42.07	o
2	-11	5	299.01	268.51	41.30	o
4	-11	5	248.60	207.34	59.61	o
-3	-9	5	363.98	385.95	27.39	o
-1	-9	5	676.36	681.29	29.14	o
1	-9	5	388.64	348.92	29.05	o
-5	-8	5	183.16	181.63	36.03	o
-4	-8	5	233.51	256.84	31.28	o
-2	-8	5	212.66	211.05	21.79	o
0	-8	5	1127.35	1154.59	33.53	o
1	-8	5	142.91	123.75	24.41	o
2	-8	5	1297.99	1270.03	35.20	o
4	-8	5	320.04	372.49	54.71	o
6	-8	5	356.03	338.26	89.48	o
-1	-7	5	312.56	305.46	33.41	o
0	-7	5	188.44	179.06	26.89	o
3	-7	5	331.14	318.34	43.77	o
5	-7	5	452.99	382.81	80.71	o
-5	-6	5	460.75	447.11	43.49	o
-4	-6	5	113.64	104.59	24.90	o

-3	-6	5	273.57	261.88	27.53	o
-1	-6	5	176.85	195.55	22.90	o
1	-6	5	294.60	271.31	21.83	o
-5	-5	5	300.67	327.24	40.52	o
1	-5	5	45.38	53.87	16.26	o
4	-5	5	544.07	591.67	66.67	o
6	-5	5	445.17	459.59	86.85	o
-7	-4	5	94.06	167.01	43.49	o
-6	-4	5	110.19	139.23	34.18	o
-5	-4	5	298.12	338.48	32.27	o
-4	-4	5	91.28	130.15	23.95	o
-3	-4	5	353.05	322.81	23.44	o
-2	-4	5	518.74	456.88	20.87	o
-1	-4	5	505.92	493.54	21.93	o
0	-4	5	955.31	907.42	27.43	o
1	-4	5	1411.34	1373.25	25.88	o
2	-4	5	105.07	101.83	12.37	o
3	-4	5	1085.27	889.72	38.60	o
5	-4	5	816.78	640.37	81.42	o
7	-4	5	534.87	290.80	93.20	o
-6	-3	5	128.49	102.98	29.88	o
-4	-3	5	763.93	689.69	29.71	o
-3	-3	5	213.03	203.35	16.49	o
-2	-3	5	1036.90	922.80	20.73	o
1	-3	5	82.55	89.45	11.88	o
2	-3	5	195.92	227.44	19.36	o
3	-3	5	87.31	64.80	15.58	o
-6	-2	5	121.11	135.52	32.70	o
-4	-2	5	441.54	389.97	21.59	o
-3	-2	5	313.29	278.68	16.63	o
-2	-2	5	1693.80	1531.51	21.88	o
0	-2	5	1002.33	944.45	21.05	o
1	-2	5	282.29	328.33	17.11	o
2	-2	5	1497.17	1391.13	48.81	o
4	-2	5	691.15	551.82	40.56	o
-7	-1	5	378.67	381.24	41.72	o
-5	-1	5	128.35	157.65	27.47	o
-4	-1	5	980.88	944.95	42.21	o
-3	-1	5	99.24	86.51	18.13	o
-2	-1	5	687.49	610.67	17.36	o
-1	-1	5	3071.21	3310.61	30.02	o
3	-1	5	1417.66	1730.82	49.20	o
7	-1	5	347.17	558.63	96.93	o
-3	0	5	173.97	199.87	18.27	o
-2	0	5	1224.65	1487.04	23.39	o
3	0	5	204.72	184.50	18.49	o
4	0	5	481.79	547.49	49.77	o
5	0	5	115.26	160.94	41.37	o
6	0	5	492.29	706.32	91.57	o
-5	1	5	431.79	470.33	24.29	o
-4	1	5	143.75	161.60	25.36	o
-3	1	5	465.78	534.75	22.47	o
-2	1	5	379.13	355.94	17.10	o
-1	1	5	1549.78	1722.14	28.84	o
0	1	5	581.49	624.16	15.73	o
2	1	5	103.35	103.90	12.19	o
3	1	5	158.72	127.78	39.96	o
-5	2	5	224.66	218.13	25.72	o
-4	2	5	137.44	126.04	22.84	o
-3	2	5	209.06	214.32	20.23	o
0	2	5	124.43	148.80	12.38	o

1	2	5	2321.85	2201.96	28.61	o
2	2	5	133.75	129.09	14.48	o
3	2	5	646.18	701.33	58.14	o
5	2	5	533.78	521.65	72.32	o
-8	3	5	318.68	279.18	61.32	o
-6	3	5	1040.60	1047.97	39.73	o
-4	3	5	395.87	316.29	26.83	o
-2	3	5	817.88	848.58	25.17	o
-1	3	5	2509.31	2572.64	39.63	o
0	3	5	886.70	1064.78	26.65	o
2	3	5	432.93	475.24	23.28	o
3	3	5	325.18	436.13	54.98	o
4	3	5	427.72	456.54	64.05	o
-7	4	5	157.24	200.21	49.07	o
-5	4	5	402.04	435.70	35.87	o
-1	4	5	3777.69	4227.49	51.25	o
0	4	5	64.83	74.20	21.43	o
4	4	5	182.24	205.71	61.61	o
-2	5	5	150.80	176.99	24.29	o
-1	5	5	153.29	162.86	31.59	o
2	5	5	626.72	643.66	41.01	o
3	5	5	364.09	396.82	33.31	o
4	5	5	321.22	333.85	71.84	o
-6	6	5	298.11	254.33	40.53	o
-4	6	5	121.18	99.79	31.03	o
-3	6	5	174.80	132.94	23.38	o
-2	6	5	243.49	236.75	20.78	o
1	6	5	134.63	114.10	31.91	o
2	6	5	128.71	102.92	28.59	o
-7	7	5	277.02	207.64	60.52	o
-5	7	5	723.30	597.33	43.29	o
-3	7	5	561.32	493.91	30.70	o
-1	7	5	999.02	883.15	29.66	o
1	7	5	452.45	468.38	35.04	o
3	7	5	171.72	193.95	34.00	o
-2	8	5	259.45	246.37	30.62	o
0	8	5	1062.74	1123.71	37.58	o
1	8	5	66.96	115.20	32.30	o
2	8	5	269.01	321.02	36.65	o
-5	10	5	214.16	179.62	55.55	o
-3	10	5	308.77	290.48	35.81	o
-1	10	5	157.22	215.29	34.53	o
-2	11	5	360.04	277.39	50.19	o
0	11	5	264.03	168.40	47.87	o
2	11	5	259.05	173.18	51.49	o
0	-12	6	111.38	134.79	40.37	o
2	-12	6	350.96	310.16	45.65	o
-2	-11	6	83.88	94.57	30.28	o
0	-11	6	93.43	99.27	27.37	o
1	-11	6	146.74	177.33	39.53	o
3	-11	6	93.19	175.67	41.66	o
-3	-10	6	79.27	82.25	26.78	o
-2	-10	6	385.26	384.70	28.14	o
0	-10	6	178.57	177.87	30.45	o
-2	-9	6	103.06	110.27	23.48	o
0	-9	6	156.63	132.43	27.05	o
2	-9	6	359.91	355.24	36.87	o
3	-9	6	195.04	162.55	37.68	o
-5	-8	6	192.76	165.50	44.07	o
-4	-8	6	148.70	142.60	30.93	o
-2	-8	6	104.21	116.15	21.57	o

-1	-8	6	137.60	128.49	22.07	o
0	-8	6	227.02	258.94	26.20	o
1	-8	6	423.62	428.91	30.98	o
2	-8	6	155.65	163.37	29.89	o
3	-8	6	234.82	204.74	42.79	o
5	-8	6	287.97	209.40	58.24	o
-4	-7	6	633.59	632.78	33.16	o
-2	-7	6	703.95	670.44	27.09	o
0	-7	6	344.91	359.14	24.79	o
1	-7	6	128.87	154.84	26.84	o
2	-7	6	669.31	673.44	26.83	o
3	-7	6	287.85	276.55	32.85	o
2	-6	6	311.12	319.23	27.27	o
3	-6	6	114.88	147.54	48.45	o
-3	-5	6	336.72	294.13	26.80	o
-2	-5	6	140.63	134.76	23.91	o
0	-5	6	287.27	278.55	27.91	o
1	-5	6	109.07	93.75	18.86	o
3	-5	6	497.98	471.04	52.64	o
5	-5	6	517.43	396.61	76.53	o
-8	-4	6	136.32	151.47	48.11	o
-6	-4	6	406.10	370.16	37.21	o
-4	-4	6	2018.64	1895.18	41.81	o
-2	-4	6	133.98	127.40	22.20	o
0	-4	6	1955.34	1733.68	33.29	o
1	-4	6	1627.84	1427.94	25.86	o
2	-4	6	1571.21	1496.02	36.85	o
5	-4	6	353.51	342.70	68.92	o
-5	-3	6	151.02	129.84	28.97	o
-4	-3	6	79.31	134.79	25.12	o
-3	-3	6	1202.89	1118.61	26.22	o
-2	-3	6	126.93	128.90	15.57	o
-1	-3	6	2758.01	2346.79	42.09	o
1	-3	6	2143.01	2295.27	45.06	o
3	-3	6	1411.56	1410.76	69.20	o
-4	-2	6	89.36	81.49	22.17	o
0	-2	6	511.21	574.94	21.46	o
1	-2	6	171.92	215.24	13.86	o
4	-2	6	519.05	533.09	38.64	o
-4	-1	6	853.43	954.67	26.62	o
-3	-1	6	121.33	114.43	17.24	o
0	-1	6	1622.32	1770.79	26.94	o
4	-1	6	331.24	316.31	41.27	o
6	-1	6	246.75	316.69	85.45	o
-5	0	6	1262.46	1284.47	30.82	o
-3	0	6	1474.16	1352.67	31.60	o
-2	0	6	53.44	48.69	12.97	o
-1	0	6	1968.44	1642.96	26.28	o
1	0	6	4862.55	4525.05	46.95	o
3	0	6	979.77	850.44	52.91	o
6	0	6	215.87	251.52	82.51	o
-5	1	6	281.21	259.77	23.36	o
-4	1	6	242.30	200.38	23.35	o
-3	1	6	332.46	333.79	20.29	o
-2	1	6	53.69	55.79	15.05	o
0	1	6	2231.03	2219.63	28.88	o
2	1	6	1899.46	1768.12	35.90	o
4	1	6	395.14	263.96	52.88	o
6	1	6	509.20	538.41	94.14	o
-6	2	6	203.20	278.82	32.75	o
-5	2	6	126.94	112.25	25.55	o

-4	2	6	142.70	160.02	26.32	o
-3	2	6	203.38	193.68	24.02	o
-2	2	6	120.82	156.86	17.59	o
-1	2	6	73.58	76.29	19.71	o
-7	3	6	110.20	175.86	39.44	o
-3	3	6	2176.01	2383.02	42.18	o
3	3	6	278.31	381.72	55.18	o
-5	4	6	357.75	466.15	36.90	o
-4	4	6	318.69	401.96	31.23	o
-2	4	6	440.91	518.32	27.93	o
-1	4	6	271.90	293.92	25.76	o
0	4	6	1400.47	1673.03	37.84	o
1	4	6	111.02	133.35	35.19	o
2	4	6	1002.50	1098.07	46.45	o
3	4	6	201.01	269.13	59.97	o
4	4	6	1159.66	973.35	90.97	o
-7	5	6	180.28	172.53	47.23	o
-5	5	6	490.30	457.52	38.21	o
-4	5	6	140.04	116.41	31.24	o
-1	5	6	166.83	151.26	33.45	o
0	5	6	164.43	153.98	26.22	o
1	5	6	329.67	365.65	28.12	o
2	5	6	57.30	123.92	34.64	o
-5	6	6	298.53	297.87	38.38	o
-3	6	6	289.84	246.81	26.34	o
-2	6	6	340.08	325.27	27.43	o
-1	6	6	450.86	446.23	28.97	o
0	6	6	80.03	85.54	23.21	o
1	6	6	148.49	131.20	34.80	o
-4	7	6	119.62	147.14	34.12	o
-2	7	6	373.37	422.71	27.27	o
1	7	6	82.91	138.85	31.05	o
-5	8	6	273.38	314.68	40.83	o
-2	8	6	133.61	153.31	29.68	o
-1	8	6	95.59	115.33	28.11	o
0	8	6	384.09	494.08	38.13	o
1	8	6	109.79	126.28	33.44	o
3	8	6	227.09	288.23	48.72	o
-6	9	6	169.03	179.63	58.31	o
-4	9	6	287.55	251.44	44.21	o
-2	9	6	93.39	129.43	36.03	o
-2	10	6	291.31	237.15	43.67	o
1	-13	7	92.33	145.38	36.81	o
-4	-11	7	109.82	177.69	40.09	o
0	-11	7	99.89	113.47	28.07	o
2	-11	7	201.60	195.47	42.47	o
-3	-10	7	113.79	157.65	27.54	o
-1	-10	7	119.94	133.21	27.62	o
1	-10	7	313.47	352.60	39.35	o
3	-10	7	372.05	421.25	43.98	o
-4	-8	7	340.56	364.83	37.87	o
-2	-8	7	495.31	518.91	24.93	o
-1	-8	7	137.22	157.89	22.83	o
0	-8	7	273.74	327.42	32.00	o
2	-8	7	136.38	129.98	32.38	o
3	-8	7	174.50	200.50	45.18	o
-5	-7	7	125.24	205.13	43.91	o
1	-7	7	1418.69	1572.11	46.05	o
5	-7	7	292.18	337.93	79.07	o
-3	-6	7	68.97	86.95	23.29	o
-2	-6	7	274.25	243.50	27.36	o

-1	-6	7	354.81	333.04	26.17	o
2	-6	7	452.70	432.46	29.62	o
4	-6	7	485.24	531.19	67.05	o
-6	-5	7	135.96	141.95	43.42	o
-5	-5	7	172.14	193.58	39.24	o
-4	-5	7	261.08	269.76	30.39	o
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-2	-5	7	128.04	143.00	24.07	o
1	-5	7	118.91	80.50	24.03	o
2	-5	7	116.19	115.11	32.13	o
-3	-4	7	648.03	613.82	25.16	o
-2	-4	7	105.59	108.48	22.21	o
-1	-4	7	2983.59	2754.11	46.25	o
0	-4	7	105.10	76.62	19.02	o
1	-4	7	1292.39	1219.89	32.70	o
3	-4	7	599.66	644.03	54.53	o
-8	-3	7	155.78	172.19	47.57	o
-4	-3	7	560.94	546.97	28.14	o
-3	-3	7	1062.94	1116.02	34.57	o
-2	-3	7	614.14	596.14	25.09	o
0	-3	7	72.75	113.68	23.09	o
1	-3	7	1018.43	971.83	27.48	o
2	-3	7	2555.53	3160.58	91.53	o
4	-3	7	777.37	941.40	76.62	o
6	-3	7	517.57	503.30	92.36	o
-7	-2	7	223.50	320.85	45.57	o
-3	-2	7	582.16	642.74	24.90	o
-1	-2	7	725.32	883.13	26.16	o
1	-2	7	172.40	141.20	14.59	o
2	-2	7	316.23	356.95	37.48	o
5	-2	7	151.86	209.66	66.79	o
-5	-1	7	155.86	133.29	23.16	o
-4	-1	7	221.54	190.22	21.11	o
-3	-1	7	700.66	664.57	24.49	o
-1	-1	7	551.14	479.93	19.11	o
0	-1	7	1221.90	1229.87	26.25	o
1	-1	7	652.96	625.21	48.69	o
2	-1	7	166.42	177.81	39.20	o
-5	0	7	395.14	356.57	24.22	o
-4	0	7	307.47	310.33	20.11	o
-3	0	7	548.29	474.76	35.30	o
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1	0	7	39.11	36.38	11.66	o
4	0	7	274.18	203.17	45.48	o
6	0	7	721.13	821.30	106.51	o
-7	1	7	179.67	191.32	39.28	o
-5	1	7	575.39	566.21	26.51	o
-3	1	7	2105.34	1944.86	42.52	o
-1	1	7	193.88	201.71	18.22	o
0	1	7	799.21	762.90	22.19	o
1	1	7	340.69	334.64	24.24	o
2	1	7	786.52	856.70	37.69	o
3	1	7	390.13	354.33	33.73	o
-6	2	7	107.90	161.05	30.22	o
-5	3	7	112.19	122.72	33.56	o
-2	3	7	191.85	191.37	24.23	o
0	3	7	516.00	521.59	27.15	o
2	3	7	326.17	347.71	37.13	o
3	3	7	301.10	389.38	61.75	o
4	3	7	525.46	484.69	74.55	o
-7	4	7	376.93	411.63	54.47	o

-5	4	7	414.89	450.65	39.15	o
-4	4	7	184.56	160.98	30.63	o
-3	4	7	199.80	206.59	27.50	o
-2	4	7	312.61	263.84	29.00	o
-1	4	7	305.36	294.08	28.08	o
0	4	7	105.19	99.15	32.75	o
1	4	7	322.19	285.81	35.61	o
2	4	7	262.96	249.84	57.41	o
-6	5	7	158.75	133.67	38.77	o
-4	5	7	1049.03	916.54	41.77	o
-2	5	7	1014.59	868.03	38.89	o
-1	5	7	132.69	157.78	28.98	o
0	5	7	986.11	1020.74	40.38	o
1	5	7	159.70	167.86	27.19	o
2	5	7	211.87	203.62	59.43	o
3	5	7	187.65	221.28	65.73	o
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1	6	7	719.32	810.06	47.42	o
2	6	7	96.02	180.99	41.13	o
3	6	7	312.52	421.28	46.81	o
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-3	7	7	60.32	97.72	28.95	o
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-2	8	7	411.69	341.23	33.72	o
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2	8	7	146.14	150.33	38.43	o
-1	9	7	511.46	424.58	50.43	o
1	9	7	364.26	363.70	42.54	o
3	9	7	158.95	190.98	59.68	o
-1	12	7	234.54	360.51	88.99	o
-1	-11	8	156.49	186.06	29.88	o
3	-11	8	293.41	285.20	45.38	o
-2	-10	8	103.89	117.26	25.86	o
-1	-10	8	228.81	267.32	29.49	o
0	-10	8	130.45	141.79	36.81	o
4	-10	8	310.67	367.16	65.38	o
-3	-9	8	269.20	278.23	31.31	o
-1	-9	8	268.38	290.58	27.72	o
2	-9	8	155.69	175.32	36.80	o
1	-8	8	261.21	273.89	33.09	o
2	-8	8	206.84	191.65	35.31	o
3	-8	8	239.37	232.23	47.89	o
-3	-7	8	302.75	304.19	28.47	o
-1	-7	8	194.89	231.54	28.98	o
2	-7	8	560.22	513.42	45.45	o
-5	-6	8	253.25	280.29	43.94	o
-3	-6	8	897.10	870.67	30.85	o
-1	-6	8	546.91	558.35	30.46	o
0	-6	8	117.98	115.48	31.48	o
1	-6	8	292.12	321.49	37.45	o
3	-6	8	213.10	292.95	70.95	o
4	-6	8	199.94	234.94	63.43	o
-2	-5	8	701.69	604.44	27.30	o
-1	-5	8	189.17	174.24	28.18	o
0	-5	8	1008.36	850.54	36.57	o
2	-5	8	484.05	500.71	67.36	o
4	-5	8	257.09	186.38	57.84	o
-2	-4	8	109.87	93.16	22.41	o
2	-4	8	245.48	298.91	30.25	o
3	-4	8	123.97	180.38	44.68	o

5	-4	8	219.48	200.69	66.86	o
-5	-3	8	741.12	913.34	52.58	o
-1	-3	8	775.54	742.34	27.57	o
1	-3	8	641.47	566.19	38.25	o
2	-3	8	213.51	156.42	49.25	o
3	-3	8	202.99	223.17	50.77	o
-7	-2	8	148.62	133.99	42.96	o
-4	-2	8	415.11	394.83	25.42	o
-2	-2	8	2947.56	2684.24	44.49	o
0	-2	8	1300.73	1150.47	28.72	o
1	-2	8	162.92	137.23	29.96	o
2	-2	8	1209.96	1061.18	60.52	o
4	-2	8	400.94	408.91	40.45	o
-2	-1	8	148.60	129.87	22.06	o
-1	-1	8	130.67	104.83	17.42	o
1	-1	8	514.30	454.40	32.86	o
-7	0	8	185.64	180.88	40.94	o
-5	0	8	200.39	209.55	23.75	o
-4	0	8	193.40	169.05	20.02	o
-3	0	8	637.75	611.16	26.95	o
-1	0	8	355.72	326.22	24.74	o
0	0	8	228.80	200.91	17.35	o
-8	1	8	126.80	182.36	56.13	o
-3	1	8	59.15	72.33	19.12	o
-7	2	8	141.36	169.01	40.93	o
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-3	2	8	373.81	422.72	23.61	o
-2	2	8	127.38	139.46	25.44	o
-1	2	8	984.85	1072.96	31.21	o
1	2	8	768.13	817.67	56.86	o
3	2	8	1041.73	981.04	78.04	o
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-6	4	8	162.40	124.70	39.12	o
-4	4	8	664.56	724.96	40.34	o
-2	4	8	530.18	528.55	36.79	o
-1	4	8	109.94	142.44	28.58	o
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-5	5	8	170.31	234.52	37.72	o
-3	5	8	423.62	495.40	37.99	o
-2	5	8	154.66	201.20	32.91	o
-1	5	8	263.84	338.46	33.00	o
-8	6	8	257.25	293.61	61.84	o
-3	6	8	176.56	186.74	36.89	o
-2	6	8	97.55	122.99	33.12	o
-1	6	8	122.36	155.88	27.53	o
2	6	8	276.86	364.11	73.97	o
-3	7	8	490.49	461.08	35.13	o
-2	7	8	203.56	147.73	30.20	o
-1	7	8	70.43	113.08	31.37	o
-3	8	8	186.20	171.15	33.24	o
-1	8	8	304.40	218.27	36.67	o
1	8	8	273.07	226.78	52.85	o
3	8	8	274.83	312.08	61.89	o
-5	10	8	208.96	199.36	55.60	o
-1	-13	9	70.99	116.93	37.97	o
2	-12	9	105.97	165.23	43.99	o
-3	-10	9	153.81	192.85	31.52	o
-1	-10	9	326.84	334.77	33.94	o
1	-10	9	110.54	159.77	38.51	o
2	-9	9	282.37	322.95	40.18	o

4	-9	9	286.83	311.67	99.79	o
1	-8	9	85.69	106.06	32.69	o
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-2	-7	9	137.87	117.46	27.31	o
-1	-7	9	233.61	265.10	26.87	o
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-1	-6	9	175.64	172.92	29.02	o
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1	-6	9	142.96	193.79	62.94	o
2	-6	9	445.89	489.28	73.76	o
4	-6	9	883.44	940.06	103.34	o
-3	-5	9	65.02	81.36	26.01	o
-2	-5	9	158.60	164.10	24.70	o
-1	-5	9	323.13	368.03	32.54	o
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1	-5	9	283.47	313.50	64.15	o
3	-5	9	437.86	631.27	82.27	o
-6	-4	9	183.79	290.85	54.66	o
-5	-4	9	169.96	195.12	47.13	o
-4	-4	9	182.18	219.32	28.34	o
-2	-4	9	55.27	90.95	22.28	o
-4	-3	9	147.83	132.50	23.31	o
-2	-3	9	1364.56	1298.02	35.15	o
0	-3	9	974.33	949.65	65.05	o
1	-3	9	169.23	121.20	37.91	o
2	-3	9	455.20	433.55	56.26	o
-5	-2	9	163.69	154.17	33.51	o
-3	-2	9	333.25	309.53	23.58	o
-2	-2	9	512.35	431.71	24.13	o
-1	-2	9	269.09	244.05	20.05	o
0	-2	9	326.27	319.37	49.23	o
5	-2	9	646.78	591.14	84.11	o
-6	-1	9	376.60	367.45	33.60	o
-4	-1	9	241.87	216.35	23.31	o
-2	-1	9	589.81	534.60	28.38	o
-1	-1	9	395.53	337.30	20.42	o
0	-1	9	239.33	204.82	30.92	o
4	-1	9	170.27	176.19	53.48	o
-1	0	9	578.48	556.09	31.81	o
0	0	9	153.31	197.67	45.41	o
2	0	9	236.32	256.03	45.05	o
-7	1	9	108.17	142.89	40.41	o
-6	1	9	99.27	111.34	28.77	o
-4	1	9	238.65	255.74	25.40	o
-1	1	9	1160.41	976.05	36.02	o
1	1	9	523.98	472.23	56.30	o
3	1	9	454.76	377.07	65.18	o
-8	2	9	177.96	231.79	59.91	o
-6	2	9	346.44	393.25	40.11	o
-4	2	9	390.44	362.09	27.18	o
-3	2	9	113.09	102.26	22.26	o
-2	2	9	798.45	697.77	34.42	o
-1	2	9	289.37	261.80	35.17	o
1	2	9	345.70	339.25	51.71	o
3	2	9	243.77	280.11	60.48	o
4	2	9	474.58	344.06	68.92	o
-5	3	9	298.42	247.97	36.06	o
-4	3	9	147.68	166.82	31.90	o
-3	3	9	463.12	415.94	35.55	o
-1	3	9	874.31	760.56	36.52	o
0	3	9	98.62	91.70	27.50	o

1	3	9	378.77	424.34	56.33	o
-1	4	9	137.96	167.19	31.03	o
0	4	9	244.52	205.88	39.64	o
2	4	9	229.47	323.93	63.77	o
-8	5	9	238.45	285.13	63.34	o
-4	5	9	177.97	189.49	35.28	o
-3	5	9	102.88	171.50	36.04	o
-2	5	9	77.07	125.39	33.46	o
-1	5	9	116.13	154.21	33.15	o
2	5	9	238.74	305.82	74.37	o
-7	6	9	175.34	223.32	60.46	o
-5	6	9	157.02	150.79	42.05	o
-3	6	9	1091.59	1036.32	50.85	o
-1	6	9	480.60	426.83	41.88	o
3	6	9	190.15	230.50	56.79	o
-2	7	9	213.88	151.52	32.79	o
0	7	9	244.82	204.34	47.78	o
2	7	9	284.16	282.98	60.95	o
-5	9	9	246.53	297.45	59.14	o
-3	9	9	220.71	270.40	39.75	o
-2	10	9	275.03	224.06	53.81	o
2	10	9	186.56	235.61	75.76	o
0	-13	10	144.02	193.50	40.33	o
0	-9	10	143.51	229.75	49.23	o
1	-9	10	135.97	160.18	38.85	o
-4	-8	10	277.34	259.87	44.95	o
-2	-8	10	267.08	234.69	31.66	o
0	-8	10	161.22	165.96	44.60	o
1	-8	10	147.56	175.79	46.37	o
-1	-7	10	74.69	88.25	26.72	o
2	-7	10	199.77	307.51	79.16	o
3	-7	10	285.32	262.07	80.98	o
-4	-6	10	160.29	195.49	39.97	o
-2	-6	10	82.83	99.25	26.75	o
-1	-6	10	153.17	189.80	33.32	o
1	-6	10	231.68	374.14	74.67	o
3	-6	10	195.40	323.49	79.26	o
-4	-5	10	401.81	499.57	40.92	o
-2	-5	10	275.03	264.38	27.43	o
0	-5	10	922.25	958.66	50.07	o
1	-5	10	229.35	314.30	71.58	o
-3	-4	10	261.44	237.79	27.63	o
-1	-4	10	760.24	650.18	34.17	o
1	-4	10	899.93	748.16	74.01	o
1	-3	10	221.76	215.79	52.81	o
4	-3	10	229.83	254.51	67.80	o
-8	-2	10	157.75	180.79	53.29	o
-6	-2	10	466.71	484.41	41.95	o
-4	-2	10	149.90	176.47	27.98	o
-2	-2	10	389.64	373.89	24.98	o
-1	-2	10	339.26	345.52	30.61	o
0	-2	10	257.84	262.35	36.60	o
-7	-1	10	87.97	173.10	40.85	o
-6	-1	10	110.65	125.93	32.30	o
-2	-1	10	110.13	135.99	33.48	o
-1	-1	10	1938.90	2090.24	56.38	o
3	-1	10	285.35	348.04	52.40	o
-6	0	10	53.23	96.35	31.45	o
-5	0	10	61.45	116.19	30.75	o
-2	0	10	108.35	124.69	26.81	o
0	0	10	383.86	419.20	59.09	o

2	0	10	471.19	383.98	54.69	o
4	0	10	432.09	327.88	66.97	o
-6	1	10	131.73	132.03	36.23	o
-4	1	10	108.16	99.97	25.06	o
-2	1	10	104.65	106.47	28.07	o
-7	2	10	125.57	181.41	56.61	o
-5	2	10	645.06	595.51	33.82	o
-3	2	10	379.74	319.78	35.54	o
-1	2	10	738.09	617.25	35.98	o
1	2	10	828.03	744.39	67.57	o
-5	3	10	181.96	213.80	36.89	o
-4	3	10	43.58	98.40	32.22	o
-2	3	10	433.15	411.10	35.19	o
0	3	10	963.14	1031.55	50.45	o
-5	4	10	122.30	121.11	38.43	o
-5	5	10	136.68	154.05	42.74	o
-3	5	10	305.60	351.67	44.12	o
-2	5	10	105.02	113.71	36.27	o
-1	5	10	312.58	319.88	37.61	o
-2	6	10	359.10	260.07	34.75	o
0	6	10	354.95	258.78	76.50	o
-2	7	10	149.92	138.12	34.87	o
-1	7	10	226.96	160.20	39.35	o
-3	8	10	93.70	118.85	38.44	o
-2	8	10	96.50	153.14	48.33	o
-4	-12	11	108.73	182.14	56.42	o
2	-12	11	160.33	179.25	49.28	o
-1	-11	11	138.38	221.72	43.91	o
1	-11	11	138.26	222.93	56.38	o
-4	-9	11	176.09	227.49	48.05	o
-1	-8	11	273.65	324.17	39.46	o
1	-8	11	383.45	549.76	88.68	o
3	-8	11	343.06	489.33	96.99	o
-4	-6	11	192.07	228.01	40.62	o
-2	-6	11	134.02	135.80	29.26	o
-3	-5	11	249.88	236.45	31.57	o
-1	-5	11	396.85	359.92	34.21	o
1	-5	11	780.80	800.24	82.46	o
-5	-4	11	167.75	173.63	39.14	o
-4	-4	11	200.84	173.96	27.48	o
0	-4	11	476.97	443.17	68.03	o
1	-4	11	136.94	204.20	63.41	o
2	-4	11	531.96	443.90	75.88	o
-5	-3	11	158.49	131.04	37.24	o
-3	-2	11	601.31	683.59	37.07	o
-2	-2	11	378.31	415.97	32.28	o
1	-2	11	295.33	283.01	55.31	o
-6	-1	11	165.69	148.71	38.00	o
-5	-1	11	121.41	187.71	32.77	o
-4	-1	11	111.80	135.87	35.19	o
-1	-1	11	230.44	209.97	57.16	o
0	-1	11	577.93	571.12	66.05	o
2	-1	11	377.25	279.91	60.12	o
-5	0	11	447.97	381.77	35.08	o
-1	0	11	258.28	164.29	36.10	o
0	0	11	160.94	191.95	57.23	o
1	0	11	309.79	281.94	57.86	o
-5	1	11	83.28	99.40	32.44	o
-4	1	11	250.97	236.21	31.46	o
-2	1	11	328.72	333.74	33.38	o
-1	1	11	115.84	119.89	36.56	o

0	1	11	276.11	266.37	59.18	o
-2	2	11	179.50	217.53	34.58	o
1	2	11	134.18	180.56	55.55	o
2	2	11	301.52	456.38	70.20	o
-5	3	11	311.91	396.77	44.98	o
-3	3	11	281.42	337.36	38.20	o
-2	3	11	77.30	135.62	33.71	o
0	3	11	445.55	522.03	46.34	o
-6	4	11	248.23	226.11	58.50	o
-4	4	11	328.33	406.14	44.83	o
-2	4	11	329.91	373.14	40.16	o
0	4	11	402.76	340.53	66.91	o
2	4	11	238.60	232.55	75.07	o
-2	5	11	141.21	115.85	38.05	o
-1	5	11	231.10	170.90	37.29	o
-6	7	11	205.12	189.27	59.75	o
-4	7	11	346.55	416.13	57.98	o
-2	7	11	277.28	265.96	51.16	o
0	7	11	220.76	280.46	73.93	o
-1	8	11	193.98	219.37	68.06	o
1	8	11	309.67	324.31	78.16	o
-1	-9	12	182.29	207.58	55.77	o
-3	-8	12	152.48	161.12	42.68	o
2	-8	12	285.96	470.77	93.51	o
-3	-7	12	254.93	297.11	41.07	o
-1	-7	12	184.19	209.60	38.06	o
0	-6	12	257.69	251.61	45.47	o
-5	-4	12	238.88	203.88	40.79	o
-3	-4	12	480.27	465.18	39.27	o
-1	-4	12	133.75	145.69	28.19	o
0	-4	12	177.80	213.61	45.72	o
-1	-3	12	93.62	147.08	30.48	o
0	-3	12	418.15	428.74	67.23	o
-7	-1	12	186.10	159.63	51.06	o
-5	-1	12	132.97	136.01	41.53	o
-3	-1	12	99.02	112.72	34.78	o
-4	0	12	694.07	586.36	43.34	o
-2	0	12	531.57	464.53	72.36	o
0	0	12	756.04	668.51	75.61	o
-3	1	12	126.36	139.10	36.07	o
1	1	12	696.37	683.05	77.77	o
3	1	12	375.12	356.35	79.87	o
-6	3	12	209.75	213.32	57.54	o
-4	3	12	247.34	351.06	43.16	o
-2	3	12	344.20	286.98	38.33	o
0	3	12	321.50	257.53	45.13	o
-4	4	12	160.75	135.84	43.51	o
1	4	12	390.78	328.68	78.67	o
-1	7	12	180.33	224.07	69.58	o
1	7	12	339.99	396.01	79.47	o
-2	-10	13	135.25	180.28	46.12	o
-2	-7	13	356.72	351.12	36.99	o
2	-7	13	389.61	443.51	90.47	o
-4	-3	13	135.78	168.04	33.73	o
3	-3	13	389.89	264.63	84.13	o
-4	-2	13	110.89	156.14	39.34	o
-4	-1	13	179.77	170.54	40.83	o
-3	-1	13	137.55	144.26	38.39	o
-3	0	13	110.52	174.03	50.84	o
1	0	13	372.29	413.66	73.38	o
3	0	13	461.11	420.68	93.58	o

-4	1	13	141.28	181.50	41.66	o
-3	1	13	86.32	129.26	37.55	o
-2	1	13	164.12	183.97	35.85	o
-3	2	13	487.92	500.73	44.28	o
-1	2	13	167.24	168.86	47.13	o
-5	5	13	251.14	316.98	57.45	o
-3	5	13	204.09	187.17	52.07	o
-3	8	13	210.06	188.13	55.06	o
-2	-6	14	288.56	246.77	40.35	o
-1	-5	14	190.13	169.50	48.04	o
-6	-3	14	131.01	137.22	42.61	o
-4	-3	14	182.38	191.28	45.12	o
-2	-3	14	193.18	195.47	48.12	o
-3	-2	14	250.34	203.48	41.61	o
-1	-2	14	449.66	329.12	78.36	o
-3	1	14	519.19	479.69	59.71	o
-1	1	14	395.24	306.92	53.63	o
-2	2	14	158.29	125.12	40.74	o
-5	4	14	146.29	196.42	55.69	o
-3	4	14	131.76	150.91	49.95	o
-3	-6	15	139.17	222.93	48.99	o
-1	-6	15	224.14	296.83	54.91	o
0	-2	15	183.52	256.36	83.79	o
-5	-5	16	100.68	144.05	44.08	o
-2	2	16	178.82	251.77	79.91	o
-1	3	16	151.07	228.53	70.38	o