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Ferrotitanowodginite, $Fe^{2+}TiTa_2O_8$, a new mineral of the wodginite group from the San Elías pegmatite, San Luis, Argentina

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ABSTRACT

Ferrotitanowodginite is a new mineral of the wodginite group, which is found in and defined from two closely adjacent pegmatites in the San Luis province, Argentina, but previously encountered in the Tanco (Manitoba) and Marko's (Ontario) pegmatites. In the San Elías pegmatite, ferrotitanowodginite occurs aggregated with ferrowodginite and associated with microlite, ferrotapiolite, cleavelandite, and quartz. In La Viquita pegmatite, ferrotitanowodginite occurs in a replacement unit associated with wodginite, ferrowodginite, titanowodginite and ferrotapiolite in yellow muscovite and quartz. Ferrotitanowodginite is very dark brown to black, with a dark brown streak and submetallic luster. Mohs hardness is $5^1/_2$ and D_{calc} = 7.368 g/cm^3. In reflected light, it is creamy white and gray in air and oil, respectively; anisotropy is distinct, bireflectance and pleochroism moderate. Ferrotitanowodginite is monoclinic, space group *C2/c*, Z = 4. Unit-cell dimensions for San Elías'material are a = 9.403(4) Å, b = 11.384(3) Å, c = 5.075(1) Å, β = 90.55° (2), V = 543.24(22) Å^3. The strongest lines in the X-ray powder diffraction are d = 2.963 Å, I = 100%, (hkl = $22\bar{1}$); d = 2.939 Å, I = 90% (hkl = 221); d = 3.626 Å, I = 70% (hkl = 220); and d = 1.715 Å, I = 50% (hkl = 402). Eighteen analyses by electron microprobe gave the following mean composition: WO_3 0.02, Nb_2O_5 6.52, Ta_2O_5 70.68, TiO_2 7.10, SnO_2 1.25, ThO_2 0.01, UO_2 0.02, As_2O_3 0.03, Sb_2O_3 0.02, Bi_2O_3 0.03, Fe_2O_3 2.18, MgO 0.01, CaO 0.01, MnO 1.05, FeO 10.27, PbO 0.05, total 99.25 wt%. The La Viquita sample is much richer in Mn and Sn. The simplified formula for ferrotitanowodginite is: $(Fe^{2+},Mn^{2+})(Ti,Sn^{4+},Ta,Fe^{3+})(Ta,Nb)_2O_8$, ideally $Fe^{2+}TiTa_2O_8$.

INTRODUCTION

Wodginite was described as a new mineral species by Nickel et al. (1963) from granitic pegmatites at Wodgina, western Australia and Tanco, Canada. The structure of wodginite was initially refined by Grice (1973) and Graham and Thornber (1974). Ferguson et al. (1976) improved on the earlier results and established the general formula ABC_2O_8 with Z of 4 and space group *C*2/*c*, and all three cation sites in octahedral coordination. The A site is usually dominated by Mn, B by Sn, and C by Ta, but diadochy of Fe^{2+} in A, Ti, Ta, or Fe^{3+} in B, and Nb or W in C are widespread.

Extensive substitutions of Fe for Mn and Ti for Sn were recognized soon after the discovery of wodginite (Vorma and Siivola 1967; Grice et al. 1972). New minerals based on these substitutions were described by Ercit et al. (1992a, 1992b, 1992c). Extension of the wodginite group was anticipated by Ercit et al. (1992c), who obtained (Fe^{2+},Ti)-dominant compositions on two samples from the Tanco pegmatite in Manitoba, but lack of material prevented complete description of yet another member of the group. Tindle et al. (1998) also reported such compositions from Marko's pegmatite in Ontario.

During a systematic study of Nb,Ta-oxide minerals from rare-element pegmatites of the Pampean pegmatite province carried out at the University of Manitoba, some samples yielded chemical compositions and X-ray powder diffraction data corresponding to wodginite minerals in general, and to (Fe^{2+},Ti)-dominant wodginite in particular. This paper describes a new member of the group that was named ferrotitanowodginite, following the classification scheme and rules of nomenclature approved by the Commission on New Minerals and Mineral Names of the I.M.A. (Table 1, modified from Ercit et al. 1992c). Type material is preserved in polished sections at the Museum Prof. Manuel Tellechea, Centro Regional de Investigaciones Científicas y Técnicas of CONICET, Mendoza, Argentina (catalog no. 8554).

This study is dedicated to the memory of our colleague and friend, Gene Foord, who contributed to our understanding of the wodginite-ionolite mineral family.

PARENT PEGMATITES AND PARAGENESIS

Ferrotitanowodginite occurs in San Elías and in La Viquita pegmatites, located in the Sierra de la Estanzuela, departamento Chacabuco, San Luis province, República Argentina, approximately at 32°51' latitude S and 65°06' longitude W, and separated from each other by 300 m. The pegmatites are emplaced

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TABLE 1. Classification of the wodginite group

Restricitions for			
A site	B site	Name	End-member formula
≤50% Li, ≤50% Fe^{2+}	≤50% Ti, ≤25% Fe^{3+}	Wodginite	$MnSnTa_2O_8$
≤50% Li, ≤50% Fe^{2+}	>50% Ti	Titanowodginite	$MnTiTa_2O_8$
≤50% Li, ≤50% Fe^{2+}	>25% Fe^{3+}, >25% Ta	(unnamed)	$Mn(Fe^{3+}_{0.5}Ta_{0.5})Ta_2O_8$
>50% Fe^{2+}	≤50% Ti, ≤25% Fe^{3+}	Ferrowodginite	$Fe^{2+}SnTa_2O_8$
>50% Fe^{2+}	>50% Ti	Ferrotitanowodginite	$Fe^{2+}TiTa_2O_8$
>50% Fe^{2+}	>25% Fe^{3+}, >25% Ta	(unnamed)	$Fe^{2+}(Fe^{3+}_{0.5}Ta_{0.5})Ta_2O_8$
>50% Li	>50% Ta	Lithiowodginite	$LiTaTa_2O_8$

in a locally tourmalinized quartz-mica schist of medium metamorphic grade, probably of Lower Paleozoic age.

The San Elías pegmatite was opened in 1957 as a potential source of beryl and lepidolite, but after extensive excavation the activity ceased and the mine is at present inactive. It is accessible in several quarries opened along its strike. Internal structure and mineralogy of the complex-type, rare-element-class San Elías pegmatite were initially described by Angelelli and Rinaldi (1963) and Herrera (1963). The pegmatite is a N-S striking, steeply east-dipping, 140 m long tabular body. It is only partially exposed because the eastern side is covered by Quaternary loess; consequently, the width in outcrop varies between 15 and 27 m. The pegmatite is zoned with border, wall and intermediate zones, and a core. The border and wall zones are fine- and medium-grained, respectively, principally composed of plagioclase (An ~15), quartz, and muscovite, and are only exposed in the western part of the pegmatite. The intermediate zone has a medium- to coarse-grained association of potassium feldspar, quartz, and cleavelandite as main minerals. In the southern part of the pegmatite, a poorly defined subzone consist of cleavelandite and small crystals and nodules of amblygonite-montebrasite, with blue, green, colorless, and pink tourmaline as principal accessory minerals. Nb-Ta minerals and yellow beryl are scarce in this zone, as are some relics of Mn-Fe-Li phosphates and nodules of an unknown phase completely replaced by a white clay material. At the inner side, this subzone contains widespread gray, pink or purple, fine-grained, massive lepidolite. The core is irregular and is composed of quartz with a few euhedral megacrystals of potassium feldspar. Abundant vugs in cleavelandite, with late-stage quartz, cookeite, herderite, and apatite decorate the core margin. The pegmatite is geochemically considerably evolved, with an abundance of Na, Li, Be, Ta>Nb, B, and F bearing minerals, suggestive of high chemical potentials of PFO_2 and LiF+KF at relatively low acidity during advanced stages of consolidation (cf. London 1982). It can be provisionally classified as a lepidolite-subtype pegmatite.

The sample of San Elías ferrotitanowodginite was found in broken rubble of a small dump, located inside the southern quarry. Ferrotitanowodginite forms submillimetric domains intergrown with Ti-rich ferrowodginite. Both minerals form a composite aggregate 0.7 cm long and 0.5 cm wide, enclosed in cleavelandite and quartz together with a few small grains of microlite and ferrotapiolite. The composite aggregate is diamond-shaped in cross-section, resembling a section across the characteristic flat "bipyramidal" morphology of wodginite described by Ercit (1992b), which results from the widespread penetration twinning, with (001) or (100) as composition planes of individuals defined mainly by {111} faces.

La Viquita is a spodumene-subtype, complex type, rare-element pegmatite, which was exploited for spodumene and tantalite, and contains a fair abundance of several Nb-Ta-Sn-Ti oxide minerals. The geology of this pegmatite was described by Angelelli and Rinaldi (1963) and Herrera (1963) with slight differences. According to the former authors, the pegmatite is 150 m long, 60 m wide, and strikes NNE-SSW. The pegmatite is zoned with border, wall, and three intermediate zones, and an irregular quartz core. The mineralogy of the intermediate zones is dominated by spodumene, albite, potassium feldspar, quartz, and muscovite, with beryl and amblygonite-montebrasite as main accessory minerals. Ferrotitanowodginite occurs associated with wodginite, ferrowodginite, titanowodginite, ferrotapiolite, and cassiterite, as dark millimeter-sized intergrowths contained in a mass of yellow fine-grained muscovite, quartz, and minor cleavelandite. The studied material was sampled from dumps in 1989. During later visits to the mine, a similar assemblage was observed in situ in an oval-shaped replacement unit ~0.8 m in diameter, located in the inner intermediate zone close to the core. Ferrotitanowodginite from La Viquita pegmatite forms millimetric domains that pass in optical continuity to wodginite.

PHYSICAL AND OPTICAL PROPERTIES

The San Elías aggregate of ferrotitanowodginite and ferrowodginite is very dark brown to black, with a dark brown streak. The luster is submetallic and the Mohs hardness 5 $^1/_2$. Cleavage was not observed; the aggregate is brittle and the fracture is irregular. The density of ferrotitanowodginite could not be measured because of the very small size of the domains of this composition. The density calculated on the basis of the empirical formula and unit-cell dimensions is 7.368 g/cm^3. Microscopically, in reflected light, ferrotitanowodginite is creamy white in air, and gray in oil. It shows very abundant yellow, orange, and purplish-orange internal reflections in air, and green, yellow, orange, and purplish-brown in oil. Anisotropy is distinct, from light greenish-gray to gray in air, and from light greenish gray to olive-greenish gray in oil. Bireflectance is moderate in both air and oil. Pleochroism is moderate, from creamy white to creamy gray in air, and from light greenish gray to gray in oil. The reflectance values (Table 2) were obtained using a silicon sample (Pauly 1986) as a standard because of instrumental limitations, the data collected at 420, 640, and 660 nm are inaccurate and consequently not reported.

The physical and optical properties of the La Viquita ferrotitanowodginite are similar. In reflected light, ferrotitanowodginite is slightly darker than wodginite.

CHEMICAL COMPOSITION

Electron-microprobe analyses of ferrotitanowodginite were carried out in the wavelength-dispersion mode on a Cameca

TABLE 2. Reflectance values in air for ferrotitanowodginite

λ(nm)	R_{max} (%)	R_{min} (%)
400	22.2 (1)	22.2 (1)
440	19.5 (2)	18.6 (1)
460	19.1 (1)	18.1 (1)
470 (COM)	18.7 (2)	18.2 (3)
480	18.4 (3)	17.5 (2)
500	18.6 (1)	17.2
520	18.4 (1)	17.0
540	18.8	17.7
546 (COM)	19.1 (1)	18.1 (1)
560	18.5	17.0 (1)
580	17.9 (1)	16.6 (1)
589 (COM)	17.9	16.9
600	18.1	16.8 (1)
620	16.4 (1)	14.6 (1)
650 (COM)	16.4 (2)	15.6 (1)
680	15.9 (3)	15.2 (3)
700	12.9	11.5 (1)

Notes: McCrone Microscope-Photometer Type MPA 1 continuous monochromator, band width of 4.5 nm.COM = wavelengths required by the IMA Commision on Ore Minerals.

SX50 equipment, with a beam diameter of 1–2 μm and an acceleration potential of 15 kV. A sample current of 20 nA measured on Faraday cup and a counting time of 20 s were used for Fe, Mn, Sn, Ti, Nb, and Ta. For Mg, Ca, Sb, As, Bi, Sc, Zr, and U, 40 nA and 50 s were used. The standards used were: manganotantalite (Ta*M*α), $FeNb_2O_6$ (Fe*K*α), $MnNb_2O_6$ (Nb*L*α, Mn*K*α), SnO_2 (Sn*L*α), rutile (Ti*K*α), ZrO_2 (Zr*L*α), $NaScSi_2O_6$ (Sc*K*α), YAG (Y*L*α), gahnite (Zn*K*α), $MgNb_2O_6$ (Mg*K*α), $BiTaO_4$ (Bi*M*α), $CaWO_4$ (W*M*β), mimetite (As*L*α Pb *M*α), $CaNb_2O_6$ (Ca*K*α), stibiotantalite (Sb*L*α), ThO_2 glass (Th*M*α), and UO_2 (U*M*α). Data were reduced using the PAP routine of Pouchou and Pichoir (1985).

Chemical compositions are represented in Table 3. The complete results can be obtained on request from the authors. The cation contents were calculated for 32 O atoms and 16 cations per unit cell (to quantify minor cations which would be sup-

TABLE 3. Representative chemical compositions of ferrotitanowodginite

	ELI2AA	ELI2AE	ELI2AG	ELI2J	ELI2K	ELI2Q	ELI2V	MEAN	1σ	RANGE	VI3AB	VI3BA
						Oxides (wt%)						
WO_3	0.00	0.00	0.00	0.03	0.15	0.02	0.00	0.02	0.04	0.15–0.00	0.05	0.00
Nb_2O_5	5.87	6.37	5.93	10.66	11.38	5.93	5.40	6.52	1.67	11.38–5.40	6.99	7.36
Ta_2O_5	71.65	70.99	71.60	62.91	62.51	71.68	72.14	70.68	2.93	72.32–62.51	64.42	63.80
TiO_2	7.07	7.43	6.66	8.40	7.83	7.18	6.92	7.10	0.47	8.40–6.52	7.40	6.90
ZrO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00–0.00	0.43	0.42
SnO_2	1.35	1.20	1.12	2.84	3.33	1.02	1.17	1.25	0.69	3.33–0.74	7.26	8.06
ThO_2	0.00	0.04	0.00	0.00	0.00	0.00	0.04	0.01	0.04	0.16–0.00	0.00	0.00
UO_2	0.00	0.03	0.05	0.00	0.02	0.00	0.17	0.02	0.04	0.17–0.00	0.01	0.00
Fe_2O_3	2.33	1.92	2.55	1.56	1.84	2.10	2.26	2.19	0.26	2.57–1.56	0.54	0.70
Sc_2O_3	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.03–0.00	0.00	0.00
As_2O_3	0.03	0.03	0.03	0.03	0.05	0.04	0.01	0.03	0.02	0.06–0.00	0.03	0.02
Y_2O_3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00–0.00	0.00	0.00
Sb_2O_3	0.00	0.00	0.07	0.00	0.09	0.00	0.00	0.02	0.04	0.11–0.00	0.03	0.00
Bi_2O_3	0.00	0.08	0.00	0.04	0.04	0.16	0.00	0.03	0.05	0.16–0.00	0.00	0.08
MgO	0.00	0.01	0.00	0.00	0.02	0.01	0.00	0.01	0.01	0.02–0.00	0.10	0.07
CaO	0.04	0.01	0.00	0.00	0.00	0.00	0.02	0.01	0.01	0.04–0.00	0.02	0.03
MnO	0.54	0.46	0.47	5.30	5.49	0.60	0.34	1.05	1.58	5.49–0.34	3.79	5.37
FeO	10.96	10.75	10.85	6.59	6.44	10.60	10.80	10.26	1.37	10.96–6.44	7.53	6.12
ZnO	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.01	0.05–0.00	0.03	0.00
PbO	0.00	0.00	0.00	0.02	0.04	0.00	0.00	0.05	0.06	0.18–0.00	0.02	0.00
Total	99.85	99.33	99.38	98.38	99.23	99.34	99.27	99.25	0.50		98.65	98.93
						cations (pfu)						
W	0.000	0.000	0.000	0.003	0.015	0.002	0.000	0.001	0.004	0.015–0.001	0.005	0.000
Nb	1.069	1.163	1.089	1.891	2.003	1.087	0.995	1.188	0.283	2.003–0.995	1.273	1.339
Ta	6.931	6.837	6.911	6.106	5.982	6.911	7.005	6.810	0.285	7.005–5.982	6.722	6.661
∑(C site)	8.000	8.000	8.000	8.000	8.000	8.000	8.000				8.000	8.000
Ti	2.143	2.256	2.035	2.479	2.293	2.190	2.122	2.158	0.116	2.479–2.008	2.242	2.088
Zr	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000–0.000	0.084	0.082
Sn	0.217	0.193	0.181	0.444	0.517	0.165	0.190	0.201	0.106	0.517–0.119	1.166	1.293
Ta	0.923	0.958	0.999	0.608	0.638	0.996	0.994	0.970	0.130	1.146–0.608	0.335	0.321
Sc	0.004	0.004	0.000	0.000	0.000	0.000	0.000	0.001	0.003	0.011–0.000	0.000	0.000
As	0.007	0.007	0.007	0.007	0.012	0.010	0.003	0.007	0.004	0.015–0.000	0.007	0.005
Fe^{3+}	0.706	0.583	0.778	0.460	0.539	0.640	0.693	0.665	0.083	0.783–0.460	0.164	0.212
∑(B site)	4.000	4.001	4.000	3.998	3.999	4.001	4.002				3.998	4.001
Th	0.000	0.004	0.000	0.000	0.000	0.000	0.004	0.001	0.004	0.015–0.000	0.000	0.000
U	0.000	0.003	0.005	0.000	0.002	0.000	0.015	0.002	0.004	0.015–0.000	0.001	0.000
Y	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000–0.000	0.000	0.000
Sb	0.000	0.000	0.012	0.000	0.014	0.000	0.000	0.004	0.006	0.018–0.000	0.005	0.000
Bi	0.000	0.006	0.000	0.003	0.003	0.011	0.000	0.002	0.004	0.011–0.000	0.011	0.002
Mg	0.000	0.006	0.000	0.000	0.012	0.006	0.000	0.003	0.005	0.012–0.000	0.060	0.042
Ca	0.017	0.004	0.000	0.000	0.000	0.000	0.009	0.003	0.005	0.017–0.000	0.009	0.013
Mn	0.184	0.157	0.162	1.761	1.811	0.206	0.117	0.352	0.523	1.811–0.117	1.293	1.830
Fe^{2+}	3.694	3.630	3.686	2.162	2.097	3.595	3.682	3.475	0.492	3.694–2.097	2.536	2.059
Zn	0.000	0.000	0.015	0.000	0.000	0.000	0.000	0.000	0.001	0.015–0.000	0.009	0.000
Pb	0.000	0.000	0.000	0.002	0.004	0.000	0.000	0.000	0.006	0.019–0.000	0.002	0.000
∑(A site)	3.895	3.810	3.880	3.928	3.943	3.818	3.827				3.926	3.946
Total	15.895	15.811	15.880	15.926	15.942	15.819	15.829				15.924	15.947

Notes: ELI = San Elías; MEAN = average of all 18 compositions obtained on San Elías material. VI = La Viquita. See text for method of calculating unit-cell contents. Sums refer to the preceding lists of cations.

pressed in a formula unit), following the criteria established by Ercit et al. (1992b), and adjusted for additional cations: (1) all Nb and W were assigned to the C site, which was then complemented to 8 by Ta; (2) all the Ti, Sn, Zr, Sc, As, and remaining Ta were assigned to the *B* site, and complemented to 4 by Fe^{3+} calculated to eliminate apparent surplus of cations over 16; (3) all Fe^{2+} and Mn^{2+} was assumed to be in A site; the traces of Mg, Th, U^{4+}, Y, Sb^{3+}, Bi, Ca, Zn, and Pb^{2+} were assigned to this structural position on the basis of their ionic radius (Shannon 1976). The slight shortage in the A site was considered a vacancy, but may be occupied, at least in part, by Li that could not be analyzed (cf. Ercit et al. 1992b).

The empirical unit formula of San Elías ferrotitanowodginite is $(Fe^{2+}_{0.869}Mn^{2+}_{0.088}\square_{0.039}Mg_{0.001}Ca_{0.001}Sb^{3+}_{0.001}Pb^{2+}_{0.001})_{\Sigma 1.000}(Ti^{4+}_{0.540}Ta_{0.244}Fe^{3+}_{0.166}Sn^{4+}_{0.050})_{\Sigma 1.000}(Ta_{1.702}Nb_{0.297})_{\Sigma 1.999}O_8$. The La Viquita ferrotitanowodginite gives $(Fe^{2+}_{0.574}Mn^{2+}_{0.390}\square_{0.017}Mg_{0.013}Ca_{0.003}Bi_{0.002}Zn_{0.001}Sb_{0.001})_{S1.000}(Ti^{4+}_{0.541}Sn^{4+}_{0.307}Ta_{0.082}Fe^{3+}_{0.047}Zr^{5+}_{0.021}As_{0.001})_{\Sigma 0.999}(Ta_{1.672}Nb_{0.327})_{\Sigma 1.999}O_8$. The simplified unit formula for the mineral is $(Fe^{2+},Mn^{2+})(Ti,Sn^{4+},Ta,Fe^{3+})(Ta,Nb)_2O_8$, ideally $Fe^{2+}TiTa_2O_8$.

X-RAY CRYSTALLOGRAPHY

The material available was not suitable for extraction of single-crystal fragments. X-ray powder diffraction data were obtained by means of a Philips 1710 automated powder diffractometer using monochromatic Cu$K\alpha_1$ radiation. The data were collected from 10° to 70° 2θ at a speed of 0.6° per minute. CaF_2 (a = 5.45935 Å) was used as an internal standard, and the intensities were observed at peak maxima. For the San Elías ferrotitanowodginite, the X-rayed material was separated from the counterpart of the analyzed polished section, but minor contamination by the associated Ti-rich ferrowodginite could not be avoided. The La Viquita ferrotitanowodginite was extracted from the analyzed polished section. Both diffractograms match the X-ray powder diffraction patterns of wodginite, ferrowodginite, and titanowodginite (Nickel et al. 1963, Ercit et al. 1992c) and confirm monoclinic 2/*m* symmetry and space-group *C*2/*c* for ferrotitanowodginite. Measured and calculated interplanar spacing for the San Elías ferrotitanowodginite are given in Table 4. Least-squares unit-cell refinement with the program CELREF (Appleman and Evans 1973) gave a = 9.403(4) Å, b = 11.384(3) Å, c = 5.075(1) Å, β = 90.55°(2) V = 543.24(22) Å^3, and axial ratios 0.826:1:0.446. The a and b cell parameters are in full agreement with those anticipated for Fe,Ti-rich wodginite by Ercit et al. (1992b, Fig. 12), and the low value of β indicates a high degree of cation disorder (Ercit et al. 1992b, Table 12). However, the I(021)/I(220) ratio, which is also indicative of cation disorder (Ercit et al. 1992b, Fig. 6), is quite anomalous at 0.28, off-scale beyond the ordered extreme of the range. The high Ti content, not encountered in any of the Ercit et al. samples, might be responsible. The unit-cell dimensions of La Viquita ferrotitanowodginite are a = 9.505(2) Å, b = 11.445(3) Å, c = 5.141(1) Å, β = 90.50°(1) and V = 559.26(16) Å^3. The difference relative to the San Elías data is undoubtedly caused by the much higher Mn and Sn contents, and possibly by contamination of the X-rayed sample by wodginite proper, into which this ferrotitanowodginite is transitional.

TABLE 4. X-ray powder diffraction pattern of the San Elías ferrotitanowodginite

d_{obs} (Å)	d_{calc} (Å)	*hkl*	*I* (%)
7.230	7.250	110	10
5.692	5.692	020	10
4.693	4.701	200	20
4.163	4.172	$\bar{1}11$	15
3.790	3.788	021	20
3.626	3.625	220	70
3.521	3.519	130	15
2.963	2.960	$\bar{2}21$	100
2.939	2.939	221	90
2.849	2.846	040	25
2.539	2.538	002	30
2.484	2.482	041	45
2.350	2.352	400	15
2.242	2.242	$\bar{2}02$	10
2.191	2.190	241	10
2.086	2.087	$\bar{2}22$	15
2.072	2.071	222	10
1.980	1.990	421	10
1.893	1.894	042	20
1.812	1.812	440	15
1.759	1.759	260	45
1.737	1.735	$\bar{3}51$	25
1.715	1.716	402	50
1.711	1.711	$\bar{4}41$	45
1.704	1.703	441	30
1.537	1.537	$\bar{2}23$	15
1.528	1.528	223	18
1.447	1.448	$\bar{2}62$	40
1.444	1.443	262	30
1.361	1.362	280	30

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