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HAINITE FROM POÇOS DE CALDAS, MINAS GERAIS, BRAZIL

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ABSTRACT

Hainite occurs in evolved alkaline rocks (nepheline syenites and tinguaites) of the Poços de Caldas massif, Minas Gerais, Brazil. It forms pale brownish yellow anhedral, elongate or tabular crystals. The crystals display a perfect {100} cleavage, indistinct and irregular {010} and {001} cleavages, and twinning on {100} that may be either simple or lamellar. Its streak is pale yellow. Hainite is generally poikilitic (except inside the vugs), enclosing alkali feldspar, nepheline and other minerals. Optically, the mineral is biaxial (+), with α 1.662(1), β 1.663(1), γ 1.675(1), $2V_z$ (obs.) 30 to 45°, $2V_z$ (calc.) 32.4°. Dispersion $r < v$ crossed, very strong. Its pleochroic scheme is: X colorless, Y colorless to pale yellow, and Z golden yellow. The mineral is triclinic, space group $P1$, a 9.584(2), b 7.267(2), c 5.708(1) Å, α 89.85(2), β 101.22(2), γ 101.03(1)°, V 382.50 Å^3, $Z = 1$. The calculated density is 3.170 g/cm^3. The strongest seven lines of the observed X-ray powder-diffraction pattern [d in Å(I)(hkl)] are 3.081(100)(300), 2.970(43)(021), 2.635(11)(20$\bar{2}$), 1.904(10)(4$\bar{2}$1), 2.312(9)(30$\bar{2}$), 2.496(8)(301) and 3.966(7)(20$\bar{1}$). The empirical formulae, derived from results of electron-microprobe analyses, are in good agreement with the structural formula $\{Na_2Ca[Ti(OH)_2(Si_2O_7)_2]\}\{Ca_3(Ca_{0.7}Mn_{0.1}Fe_{0.1}Ce_{0.1})\}F_2$. The simplified formula is $Na_2Ca_5Ti(Si_2O_7)_2(OH)_2F_2$.

Keywords: hainite, silicate, crystal structure, optical properties, chemical composition, Poços de Caldas, Minas Gerais, Brazil.

SOMMAIRE

On trouve la haïnite dans les roches alcalines évoluées, par exemple, syénites néphéliniques et tinguaïtes, du complexe alcalin de Poços de Caldas, Minas Gerais, Brésil. Elle se présente en cristaux xénomorphes jaune brunâtre pâle, allongés ou tabulaires. Ils font preuve d'un clivage {100} parfait, de clivages {010} et {001} indistincts et irréguliers, et de macles sur {100}, soit simples ou lamellaires. La rayure est jaune pâle. La haïnite est poecilitique, en général (sauf où elle se trouve dans des cavités), renfermant le feldspath alcalin, la néphéline, et autres minéraux. Il s'agit d'un minéral biaxe (+), avec α 1.662(1), β 1.663(1), γ 1.675(1), $2V_z$ (obs.) 30 à 45°, $2V_z$ (calc.) 32.4°. La dispersion $r < v$ est croisée, et intense. Elle est pléochroïque: X incolore, Y incolore à jaune pâle, et Z jaune doré. La haïnite est triclinique, groupe spatial $P1$, a 9.584(2), b 7.267(2), c 5.708(1) Å, α 89.85(2), β 101.22(2), γ 101.03(1)°, V 382.50 Å^3, $Z = 1$. La densité calculée est 3.170 g/cm^3. Les sept raies les plus intenses du spectre de diffraction (méthode des poudres) [d en Å(I)(hkl)] sont: 3.081(100)(300), 2.970(43)(021), 2.635(11)(20$\bar{2}$), 1.904(10)(4$\bar{2}$1), 2.312(9)(30$\bar{2}$), 2.496(8)(301) et 3.966(7)(20$\bar{1}$). La formule empirique, dérivée des résultats d'analyses à la microsonde électronique, concorde bien avec la formule $\{Na_2Ca[Ti(OH)_2(Si_2O_7)_2]\}\{Ca_3(Ca_{0.7}Mn_{0.1}Fe_{0.1}Ce_{0.1})\}F_2$. La formule simplifiée serait $Na_2Ca_5Ti(Si_2O_7)_2(OH)_2F_2$.

(Traduit par la Rédaction)

Mots-clés: haïnite, silicate, structure cristalline, propriétés optiques, composition chimique, Poços de Caldas, Minas Gerais, Brésil.

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INTRODUCTION

Hainite was originally described by Blumrich (1893); it was discovered in cavities and groundmass of phonolites and tinguaites from Hradište (formerly "Hoher Hain"), near Frýdlant (Friedland), northern Bohemia, Czech Republic, and was named on the basis of incomplete optical and qualitative chemical data. Complete chemical analysis and X-ray powder-diffraction data were only recently published by Johan & Čech (1989). A second occurrence of hainite has now been established in the alkaline massif of Poços de Caldas, Minas Gerais and São Paulo states, Brazil. In terms of chemical composition and X-ray-diffraction data, the hainite from Poços de Caldas is very similar to that from the Czech Republic. Morphological and optical data for hainite from Poços de Caldas also are presented. These data agree very well with those obtained by Guimarães (1948) for "giannettite" from Poços de Caldas. Apparently, Guimarães did not have access to the paper by Blumrich (1893). The original description of "giannettite" is so poor that the species and name have not been considered valid. In addition, as hainite has historical priority (Blumrich 1893) over "giannettite" (Guimarães 1948), the mineral is more properly to be called hainite. Unfortunately, the name "giannettite" has appeared in the literature since then, as in the structure description by Rastsvetaeva *et al.* (1995). Although a formal discreditation of "giannettite" is not possible because the type specimen of "giannettite" cannot be located, the authors are convinced that "giannettite" is equal to hainite.

OCCURRENCE

Hainite occurs in evolved alkaline rocks, in particular nepheline syenites and tinguaites, of the Poços de Caldas massif (Fig. 1). The following listing of accessory, vug- and fracture-filling minerals, mostly identified by optical means, has been cited as occurring in the Poços de Caldas massif: eudialyte, catapleiite, lamprophyllite, rinkite, neptunite, manganoan pectolite, kupletskite, låvenite, normandite, rosenbuschite, narsarsukite, tainiolite, the problematic "mosandrite", "giannettite", "rinkolite" and "pennaite" (not yet fully described in the literature), wadeite, aenigmatite, astrophyllite, fersmanite, elpidite, gaidonnayite, hilairite, burbankite, calcite, fluorite, natrolite, analcime, pyrite, galena, manganoan ilmenite, strontianite, ankerite, kutnohorite, ancylite-(Ce), chamosite, berthierine-1*M* and lorenzenite. Complete mineralogical data are lacking for these minerals. For background information on the geology and mineralogy of the Poços de Caldas area, see Schorscher & Shea (1992) and Ulbrich & Ulbrich (1992).

The hainite crystals described here were collected from vugs in the subvolcanic phonolite (tinguaite) mined at Bortolan quarry (sample 5), and also from the matrix of the tinguaite at Pedreira da Prefeitura ("City Hall Quarry") (sample 6).

The abundance of hainite in the rocks ranges from 0 to 5%. As the crystals are generally poikilitic, their shapes adapt to the available spaces. The dimensions of the crystals reach a maximum of 0.5 mm in the fine-grained rocks and 2.5 mm in the coarse-grained rocks. Inside the vugs, extremely rare tabular crystals of hainite reach up to 2 mm in length and 0.3 mm in width. Hainite also occurs intimately associated with manganoan pectolite in elongate (up to 3 cm in length and 1 mm in width) crystals in vugs (Fig. 2).

Hainite is late magmatic where it poikilitically encloses alkali feldspar, nepheline and other minerals, and clearly postmagmatic in cases where it occurs in vugs.

The vug-filling crystals of hainite are associated with unidentified minerals. Mineral UPC1 (= unidentified from Poços de Caldas #1), displaying rectangular con-

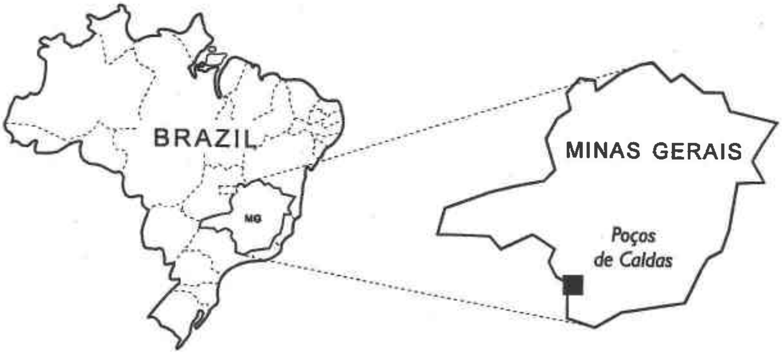


FIG. 1. Location map of Poços de Caldas, Minas Gerais, Brazil.

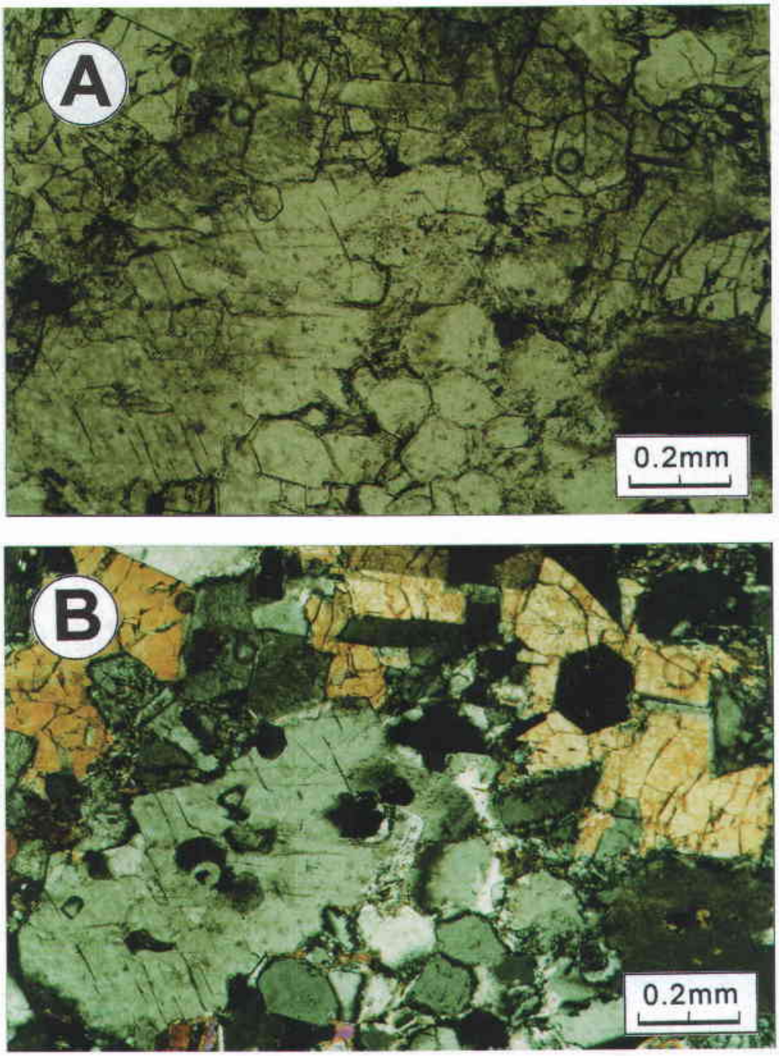
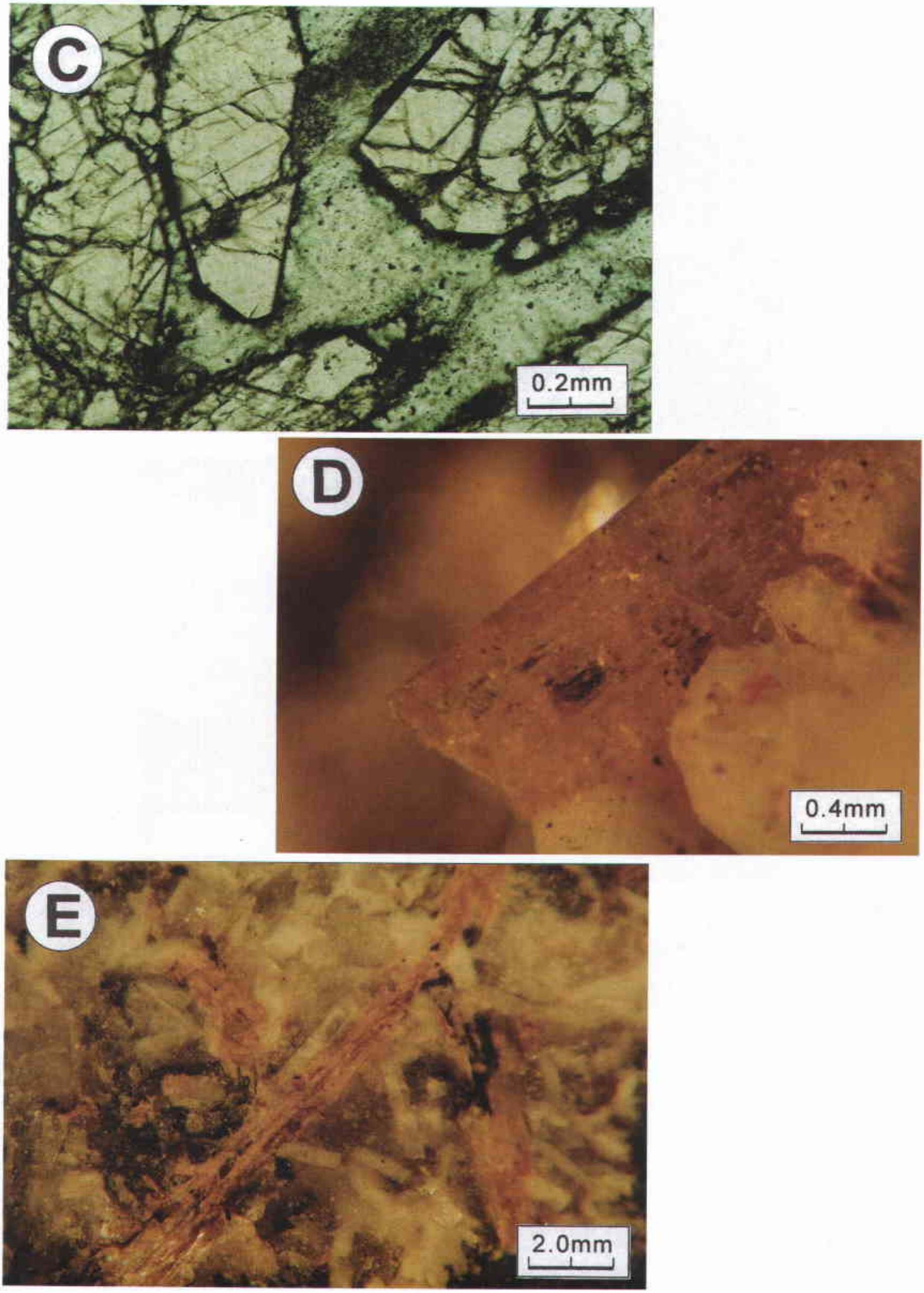


FIG. 2. A and B. Poikilitic hainite, associated with nepheline, alkali feldspar and aegirine in tinguaite from Pedreira da Prefeitura, Poços de Caldas. A. Plane-polarized light. B. The same view under cross-polarized light. Hainite shows a yellow interference-color. In the top center, a twinned crystal can be seen. C. Sections of larger euhedral tabular crystals of hainite near a vug in tinguaite from Pedreira Bortolan, Poços de Caldas; plane-polarized light. D. Euhedral tabular crystal of hainite (yellow) inside the vug of C, associated with natrolite, analcime, and alkali feldspar. E. Elongate crystals of hainite (yellow) intimately associated with manganoan pectolite, inside a vug in tinguaite from Pedreira Bortolan, Poços de Caldas, with natrolite, alkali feldspar, aegirine, and nepheline. F. Detail of Figure 2E.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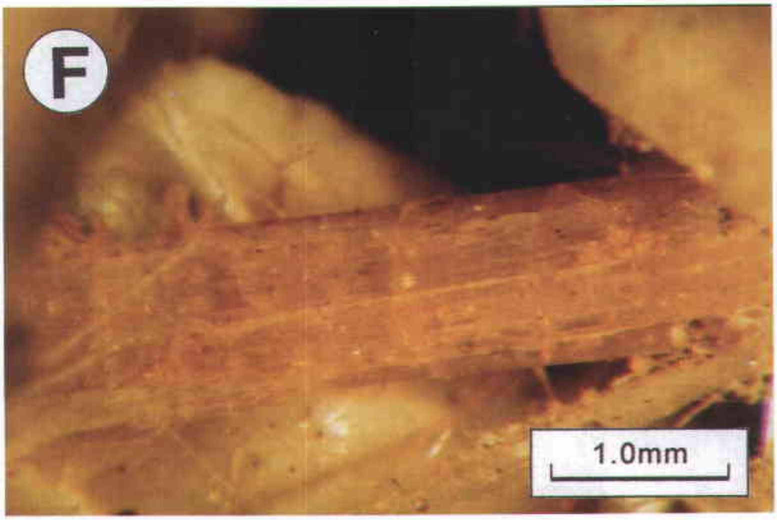

tours and maximum dimensions of 8 × 0.2 µm, develops along fracture surfaces of hainite crystals. Energy-dispersion analyses indicate a Sr, Ce, Ca, La and Na silicate-phosphate, with F and Cl. A second unidentified mineral (UPC2) grew around the same grain of hainite. It is anhedral, about 10 × 10 µm in area, and is a Ba, Na, Nb, Ti and Ca silicate. In another sample, hainite is associated with manganoan pectolite, a mineral similar to tuperssuatsiaite and a third unidentified mineral (UPC3). The latter is a Ti, Na, Mn, Fe, Ca, K and Al silicate with rectangular contours and maximum dimensions of 120 × 15 µm. It is difficult to evaluate the extent of interference by the matrix hainite in the resulting chemical data.

HABIT AND PHYSICAL PROPERTIES

Hainite occurs as pale brownish yellow anhedral, elongate or tabular crystals. Its streak is pale yellow. The {010}, {012}, {250}, {111}, {320} and {120} forms were identified by Guimarães (1948), who also quoted a perfect {100} cleavage, indistinct and irregular {010} and {001} cleavages, and twinning on {100}, which may be either simple or lamellar. Hainite from the rock matrix is generally poikilitic. Hainite from vugs, here described for the first time, is inclusion-free, but may show an intimate association with unidentified minerals UPC1, UPC2 and UPC3, and with manganoan pectolite, or else it may appear idiomorphic and isolated in the cavity. Microcline, aegirine and natrolite also are present inside the vugs.

The calculated density is 3.170 g/cm^3 (vug crystals, sample 5), close to 3.148 g/cm^3 given by Blumrich (1893) for hainite.

Crystal forms, optical orientation, $2V$ and dispersion of the optic axes were determined in thin sections with the help of a universal stage. Indices of refraction were measured by immersion of grains in liquids calibrated with the Abbé refractometer. Table 1 compares the results obtained by Guimarães (1948) with those found in the present work. Note that the data in columns 1 and 2 of Table 1 are almost identical. The so-called "giannettite" of Guimarães (1948) is certainly the same mineral described here. The optical properties are clearly different from those attributed to hainite in the standard texts (Winchell 1964, Tröger 1969).

Figure 3 illustrates the optical orientation and the three-dimensional shapes of crystals as deduced from a combination of different sections seen under the microscope. Extinction angles measured on the universal stage

TABLE 1. OPTICAL PROPERTIES FOR HAINITE FROM POÇOS DE CALDAS, MINAS GERAIS, BRAZIL

	1	2		1	2
α	1.663(2)	1.662(1)	$2V_z$ obs. (°)	30	30 to 45
β	1.664(2)	1.663(1)	$2V_z$ calc. (°)	33.7	32.4
γ	1.675(2)	1.675(1)	$c \wedge Y$ (°)	23	20
birefringence	0.012	0.013			
dispersion	not cited	$r < v$ very strong, crossed			
pleochroism	colorless to pale yellow	X = colorless Y = colorless to pale yellow Z = golden yellow			

1. Guimarães (1948), XY plane is nearly perpendicular to (010), and X is at about 16° to the normal to the (010) face.
2. This paper (three crystals from vugs, sample 5). Average values for indices of refraction, $2V$ and $c \wedge Y$. Other average values: on (100): $c \wedge Y' = ca.$ 18°; on (010): $c \wedge Y' = ca.$ 2°; on section ⊥ c: trace of (100) $\wedge X'$ = 14°.

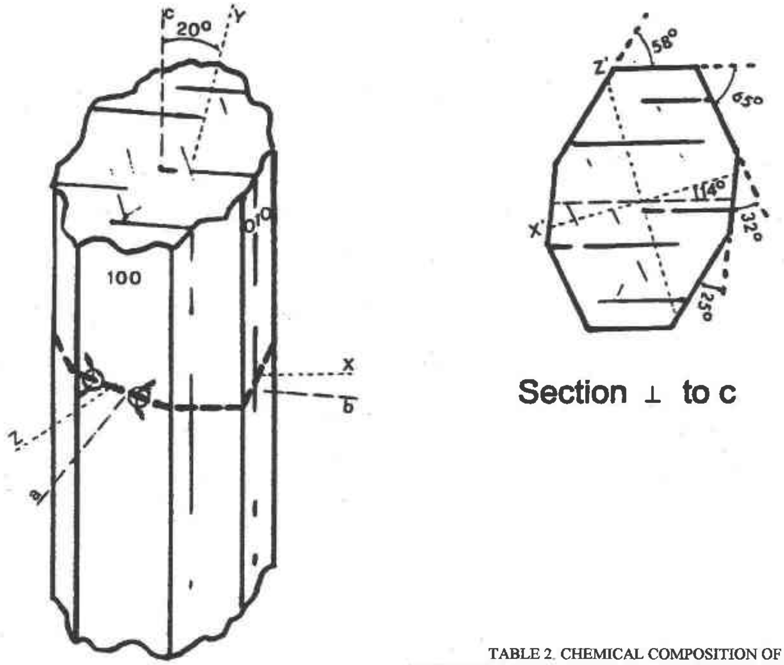

FIG. 3. Optical orientation for hainite.

TABLE 2. CHEMICAL COMPOSITION OF HAINITE
ELECTRON-MICROPROBE DATA (WAVELENGTH-DISPERSION MODE)

	1	2	3	4	5	ave.	6	ave.
SiO_2	32.07	30.30	30.09	29.96	31.44	30.37-32.14	31.70	31.33-32.03
TiO_2	8.06	9.23	8.92	9.12	9.83	9.71-9.99	9.39	9.18-9.47
ZrO_2	6.58	4.91	3.43	3.45	2.33	2.13-2.65	2.84	2.22-3.81
HfO_2	n.a.	n.a.	0.06	0.08	n.a.		n.a.	
Al_2O_3	0.03	0.02	n.d.	n.d.	0.04	0.04-0.04	0.05	0.04-0.06
Fe_2O_3	1.25	n.a.	n.a.	n.a.	n.a.		n.a.	
Nb_2O_5	1.38	1.21	1.01	0.76	0.82	0.78-0.84	1.06	0.97-1.13
Ta_2O_5	0.22	n.a.	n.a.	n.a.	n.a.		n.a.	
MnO	2.06	1.49	0.75	1.65	0.92	0.82-1.04	0.68	0.54-0.92
MgO	n.a.	0.02	n.d.	n.d.	0.03	0.03-0.04	0.04	0.03-0.05
FeO	n.a.	0.64	0.79	0.36	0.75	0.74-0.77	0.81	0.60-0.99
CaO	32.05	32.36	34.21	32.98	36.03	35.94-36.09	34.77	33.90-35.10
SrO	n.a.	0.75	0.44	2.02	0.79	0.69-0.92	0.60	0.41-0.88
La_2O_3	0.60	n.a.	1.38	0.94	1.17	1.00-1.31	1.20	0.73-1.44
Ce_2O_3	1.01	1.64	2.50	1.62	1.96	1.61-2.21	2.86	2.13-3.39
Pr_2O_3	n.a.	n.a.	n.a.	n.a.	0.18	0.15-0.20	0.27	0.23-0.36
Nd_2O_3	n.a.	n.a.	n.a.	n.a.	0.39	0.34-0.43	0.81	0.68-0.92
Y_2O_3	n.a.	0.16	0.94	0.49	0.11	0.06-0.16	0.49	0.43-0.57
ThO_2	n.a.	n.a.	n.a.	n.a.	0.11	0.11-0.12	0.08	0.04-0.11
Na_2O	7.46	7.44	6.30	6.60	6.17	5.48-6.54	6.74	6.36-7.26
K_2O	n.a.	0.03	n.d.	n.d.	n.d.		n.d.	
H_2O	n.a.	n.a.	n.a.	n.a.	2.43		2.46	
F	12.09	7.73	9.22	10.38	5.13	4.53-5.82	5.19	4.81-5.48
Cl	n.a.	0.01	n.d.	n.d.	<0.02		<0.02	
	104.86	97.94	100.03	100.40	100.63	99.28-101.63	102.04	100.97-102.61
–O-F	5.09	3.26	3.87	4.36	2.16	1.90-2.44	2.18	2.02-2.30
Total	99.77	94.68	96.16	96.04	98.47	96.85-99.52	99.86	98.85-101.42

Compositions are quoted in wt.% oxides. 1. Hradište, Bohemia, Czech Republic (Johan & Čech 1989). 2. Morro do Cristo, Poços de Caldas, Minas Gerais, Brazil (Soubiès *et al.* 1991, average of eight analyses). 3. Pedreira da Prefeitura, Poços de Caldas, Minas Gerais, Brazil (Schorscher *et al.* 1992). 4. Pedreira Bortolan, Poços de Caldas, Minas Gerais, Brazil (Schorscher *et al.* 1992). 5. Pedreira Bortolan, Poços de Caldas, Minas Gerais, Brazil; vug sample, this paper [average of three analyses; H_2O content calculated on the basis of 2(OH) per formula unit]. 6. Pedreira da Prefeitura, Poços de Caldas, Minas Gerais, Brazil; rock matrix sample, this paper [average of six analyses; H_2O content calculated on the basis of 2(OH) per formula unit). n.a.: not analyzed, n.d.: not detected.

are imprecise owing to strong dispersion, and only average numbers are given.

Owing to the poor quality and paucity of the crystals, no observations could be made about terminal faces, twin laws, the indexing of faces and cleavage planes, and about hardness and density.

CHEMICAL DATA

The chemical data obtained by Guimarães (1948) are considered inaccurate. He made a spectrographic study of a few grains and showed the presence of Si, Ti, Zr, Mn, Fe, Ca, and Na, with traces of Ta and absence of rare-earth elements. Since the mineral could not be separated, chemical analyses were performed on material dissolved from two rock samples.

Electron-microprobe data for hainite (wavelength-dispersion mode) are presented in Table 2. The chemical analyses were done at Instituto de Geociências of the Universidade de São Paulo using a JEOL JXA–8600 electron-microprobe and a Noran system for automation and data reduction. Careful wavelength scans were conducted under a variety of beam conditions to determine the trace elements present and background positioning. Quantitative point analyses were made with a defocused (20 μm) beam. The crystals were first analyzed for F, Na, Si, Ti, and Ca under an excitation voltage of 15 kV and a beam current of 20 nA in order to reduce the effects of Na and F loss. A second run for Si, Ti, Ca and the remaining elements was performed at 20 kV and 50 nA. Peaks were counted for 10 s for F, Na, Si, Ti and Ca, and 100 s for the remaining elements or a maximum 2σ counts of 1% and 5%, respectively. Matrix corrections were made with the PROZA program, as provided by Tracor. Standards and elements lines were as follows: synthetic diopside (Si$K\alpha$, Ca$K\alpha$ and Mg$K\alpha$), rutile (Ti$K\alpha$), Amelia albite (Na$K\alpha$), magnesian manganoan fayalite (Fe$K\alpha$, Mn$K\alpha$), synthetic anorthite (Al$K\alpha$), fluorite (F$K\alpha$), synthetic strontian anorthite (Sr$L\alpha$), synthetic oxides for Zr$L\alpha$ and Th$M\alpha$, metallic Nb for Nb$L\alpha$, and the standard *REE* glasses of Drake & Weill (1972) for La$L\alpha$, Ce$L\alpha$, Pr$L\beta$, Nd$L\beta$ and Y$L\alpha$. The H_2O content could not be determined owing to insufficient amount of pure material. It was therefore calculated on the basis of 2(OH) per formula unit, from the results of the crystal-structure analysis.

The empirical formulae derived from columns 5 and 6 in Table 2 [based on 18 (O + OH + F)] are, respectively,

$$\{(Na_{1.48}Ca_{0.20})_{\Sigma 1.68}\ Ca[(Ti_{0.79}Zr_{0.14}Nb_{0.05}Al_{0.01})_{\Sigma 0.99}(OH)_2\ (Si_{1.94}Ti_{0.06}O_7)_2]\}\ \{Ca_3(Ca_{0.57}Mn_{0.10}Ce_{0.09}Fe_{0.08}Sr_{0.06}La_{0.05}Nd_{0.02}Y_{0.01}Pr_{0.01}Mg_{0.01})_{\Sigma 1.00}\}\ F_2$$

and

$$\{(Na_{1.60}Ca_{0.03})_{\Sigma 1.63}\ Ca[(Ti_{0.77}Zr_{0.17}Nb_{0.06}Al_{0.01})_{\Sigma 1.01}(OH)_2\ (Si_{1.95}Ti_{0.05}O_7)_2]\}\ \{Ca_3(Ca_{0.54}Ce_{0.13}Fe_{0.08}Mn_{0.07}La_{0.05}Sr_{0.04}Nd_{0.04}Y_{0.03}Pr_{0.01}Mg_{0.01})_{\Sigma 1.00}\}\ F_2,$$

in good agreement with the structural formula (Rastsvetaeva *et al.* 1995), $\{Na_2Ca[Ti(O,OH)_2(Si_2O_7)_2]\}\{Ca_3(Ca_{0.7}Mn_{0.1}Fe_{0.1}Ce_{0.1})\}F_2$. In the given formula, the $(O,OH)_2$ must have a charge of 2– to achieve neutrality. Therefore, it is more likely to be $(OH)_2$. The simplified formula is $Na_2Ca_5Ti(Si_2O_7)_2(OH)_2F_2$.

The compositions shown in columns 1 to 4, quoted from the literature, are also in agreement with the structural formula, except for the higher F content, possibly due to analytical problems or marked chemical differences in the mineral specimens studied.

CRYSTALLOGRAPHY AND CRYSTAL STRUCTURE

The mineral is triclinic, space group *P*1. X-ray powder-diffraction data for hainite from Poços de Caldas (sample 5) were obtained by means of graphite-monochromatized Cu$K\alpha$ radiation and a Siemens D5000 diffractometer. The results are compared with the calculated pattern and with the observed data for hainite from Czech Republic in Table 3.

The parameters of the triclinic unit-cell were refined on an Enraf–Nonius CAD–4F diffractometer (monochromatized Mo$K\alpha$, $\lambda = 0.71073$ Å) (Table 4). The *a:b:c* relation for the unit-cell parameters is 1.3188:1:0.7855.

TABLE 3. X-RAY POWDER-DIFFRACTION DATA FOR HAINITE

1		2				
$d_{obs.}$	$I_{obs.}$	$d_{obs.}$	$I_{obs.}$	$d_{calc.}$*	$I_{calc.}$*	*h k l*
4.295	10			4.269	6	$2\bar{1}0$
3.961	50	3.966	7	3.964	41	$20\bar{1}$
3.557	10	3.578	2	3.568	7	210
				3.563	5	111
3.340	10			3.273	8	$21\bar{1}$
3.259	10			3.256	5	201
3.073	90	3.081	100	3.074	90	300
2.961	100	2.970	43	2.958	100	021
2.824	30	2.842	3	2.838	18	$10\bar{2}$
2.628	50	2.635	11	2.634	36	$20\bar{2}$
2.493	50	2.496	8	2.494	11	301
2.309	10	2.312	9	2.309	8	$30\bar{2}$
2.244	20	2.250	3	2.246	14	$1\bar{2}\bar{2}$
				2.240	16	$02\bar{2}$
2.200	30	2.204	4	2.201	14	$2\bar{2}\bar{2}$
2.043	20	2.049	2	2.050	6	$3\bar{2}\bar{2}$
				2.044	4	$22\bar{2}$
1.984	20	1.986	2	1.982	9	$40\bar{2}$
1.896	70	1.904	10	1.895	30	$4\bar{2}1$
				1.894	32	321
1.865	30	1.868	4	1.865	13	$50\bar{1}$, 003
1.822	50	1.825	6	1.817	41	$1\bar{4}0$
1.787	10	1.789	2	1.782	5	222, 040
1.680	40	1.683	5	1.681	11	$1\bar{2}\bar{3}$, 041
1.633	20			1.636	6	$42\bar{2}$
1.571	20	1.567	3	1.565	8	440
1.532	20	1.542	3	1.532	4	$4\bar{2}\bar{3}$, $2\bar{4}\bar{2}$

* Calculated with the program LAZY PULVERIX.
1. Hradište, Bohemia, Czech Republic (Johan & Čech 1989).
2. Pedreira Bortolan, Poços de Caldas, Minas Gerais, Brazil (corresponds to #5 in Table 2; observed values: this paper; calculated values: Rastsvetaeva *et al.* 1995).

Calculations using the Gladstone–Dale relationship were performed using the chemical data, the calculated density and the recorded indices of refraction of the vug crystals (sample 5). From these calculations, the compatibility index is 0.037, indicating, according to Mandarino (1979), excellent compatibility.

The atomic arrangement in hainite (Rastsvetaeva *et al.* 1995) corresponds basically to the structure models of götzenite (Cannillo *et al.* 1972), rosenbuschite (Shibayeva & Belov 1962), rinkite (Rastsvetaeva *et al.* 1991) and seidozerite (Simonov & Belov 1960). The main specific feature of all these structures is the (100) "walls" of polyhedra linked by the "ribbons" of octahedra parallel to [010], and by $[Si_2O_7]$ groups. Figure 4 is a schematic attempt to discriminate between these struc-

TABLE 4. UNIT-CELL PARAMETERS FOR HAINITE

	a (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	*V* (Å³)
1	9.586(3)	7.259(3)	5.676(2)	90.27(4)	101.14(4)	101.08(4)	379.94
2	9.584(2)	7.267(2)	5.708(1)	89.85(2)	101.22(2)	101.03(1)	382.50

1. Hradište, Bohemia, Czech Republic (Johan & Čech 1989); the *a* and *c* axes were interchanged.
2. Pedreira Bortolan, Poços de Caldas, Minas Gerais, Brazil. Corresponds to #5 in Table 2; derived from single-crystal studies: Rastsvetaeva *et al.* (1995).

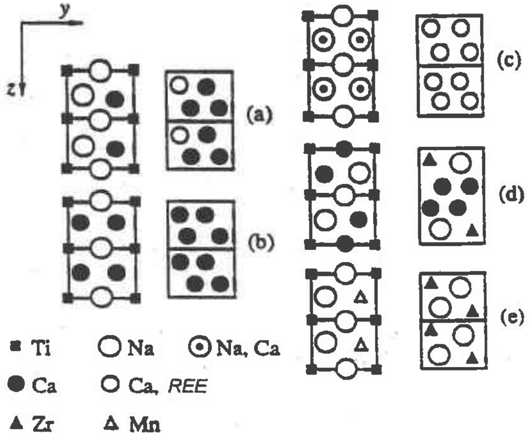

FIG. 4. Schematic view of the arrangement of cations in the "walls" (left) and in the "ribbons" (right) of: a) hainite, b) götzenite, c) rinkite, d) rosenbuschite, and e) seidozerite (Rastsvetaeva *et al.* 1995, modified from Cannillo *et al.* 1972).

tures primarily on the basis of different types of cation ordering. Thus, the "walls" of hainite contain completely ordered Ca- and Na-atoms in two crystallographically independent octahedra (space group $P1$), whereas in götzenite, $Na(Ca_{1.2}Na_{0.8})\ Ca_4Ti(Si_2O_7)_2(F,OH,O)_4$, according to Cannillo *et al.* (1972), they are randomly distributed in two symmetrically related octahedra (space group $P\bar{1}$).

In summary, götzenite is characterized by one atom of Na, and hainite, by two atoms of Na for 18 (O,OH,F), which leads to ordering and, consequently, to the structure transformation from centrosymmetric space-group $P\bar{1}$ (götzenite) to acentric $P1$ (hainite).

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REFERENCES

BLUMRICH, J. (1893): Die Phonolithe des Friedländer Bezirkes in Nordböhmen. *Tschermaks Mineral. Petrogr. Mitt.* **13**, 465-495.

CANNILLO, E., MAZZI, F. & ROSSI, G. (1972): Crystal structure of götzenite. *Sov. Phys. Crystallogr.* **16**, 1026-1030.

DRAKE, M.J. & WEILL, D.F. (1972): New rare earth element standards for electron microprobe analysis. *Chem. Geol.* **10**, 179-181.

GUIMARÃES, D. (1948): The zirconium ore deposits of the Poços de Caldas plateau, Brazil, and zirconium geochemistry. *Instituto de Tecnologia Industrial, Boletim* **6**.

JOHAN, Z. & ČECH, F. (1989): Nouvelles données sur la haïnite, $[Na_2Ca_4(Ti,Zr,Mn,Fe,Nb,Ta)_{1,50}\square_{0,50}](Si_2O_7)_2F_4$ et ses relations cristallochimiques avec la götzenite, $Na_2Ca_5Ti(Si_2O_7)_2F_4$. *C.R. Acad. Sci. Paris* **308**, *Sér.* **II**, 1237-1242.

MANDARINO, J.A. (1979): The Gladstone–Dale relationship. III. Some general applications. *Can. Mineral.* **17**, 71-76.

RASTSVETAEVA, R.K., BORUTZKII, B.E. & SHLIUKOVA, Z.V. (1991): Crystal structure of Khibinian rinkite. *Sov. Phys. Crystallogr.* **36**, 349-351.

________, PUSHCHAROVSKY, D.YU. & ATENCIO, D. (1995): Crystal structure of giannettite. *Crystallogr. Rep.* **40**, 574-578.

SCHORSCHER, H.D., MONTEIRO, M.M.G., PÉREZ AGUILAR, A., GARDA, G.M., BOHLAND, F., NETO & SCHULZ-DOBRICK, B. (1992): Contribuição ao conhecimento da giannettita do complexo alcalino de Poços de Caldas, MG. *Boletim IG-USP, Publicação Especial* II (*Jornadas Científicas*) **12**, 105-107.

________ & SHEA, M.E. (1992): The regional geology of the Poços de Caldas alkaline complex: mineralogy and geochemistry of selected nepheline syenites and phonolites. *J. Geochem. Explor.* **45**, 25-51.

SHIBAYEVA, R.P. & BELOV, N.V. (1962): Crystal structure of rosenbuschite, $(Ca,Na)_3(Zr,Ti)[Si_2O_7](O,F)_2$. *Dokl. Acad. Sci. USSR, Earth Sci. Sect.* **143**, 113-116.

SIMONOV, V.I. & BELOV, N.V. (1960): The determination of the crystal structure of seidozerite. *Sov. Phys. Crystallogr.* **4**, 146-157.

SOUBIÈS, F., MELFI, A.J., DELVIGNE, J. & SARDELA, I.A. (1991): Mobilidade do zircônio na bauxitização de rochas alcalinas do maciço de Poços de Caldas, Minas Gerais. *Revista Brasileira de Geociências* **21**(1), 17-22.

TRÖGER, W.E. (1969): *Optische Bestimmung der gesteinsbildenden Minerale.* 2. *Textband.* Schweizerbart, Stuttgart, Germany.

ULBRICH, H.H.G.J. & ULBRICH, M.N.C. (1992): O maciço alcalino de Poços de Caldas, MG-SP: características petrográficas e estruturais. *Roteiro das Excursões do 37º Congresso Brasileiro de Geologia* (*São Paulo*) **5**.

WINCHELL, A.N. (1964): *Elements of Optical Mineralogy.* II. *Description of Minerals* (fourth ed.). John Wiley & Sons, New York, N.Y.

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