

Bahianite, $\text{Sb}_3\text{Al}_5\text{O}_{14}(\text{OH})_2$, a new species

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SUMMARY. Bahianite, $\text{Sb}_3\text{Al}_5\text{O}_{14}(\text{OH})_2$ - $\text{Sb}_3\text{Al}_5(\text{Al}, \text{Be}, \text{Si})_2\text{O}_{16}$, monoclinic, a 9.406(6), b 11.541(8), c 4.410(3) Å, β 90.94(3)°, $Z = 2$, space group $C2/m$, is a new species from the Paramirim region, south central Bahia state, Brazil. It occurs as water-worn pebbles ('favas') with quartz, andalusite, kyanite, diaspore, eskolaite, cassiterite, etc. Colour tan to cream, crystals in vugs colourless, tan or pale violet. Specific gravity ranges from 4.89 to 5.46 (5.26 g cm^{-3} for $\text{Sb}_3\text{Al}_5\text{O}_{14}(\text{OH})_2$); hardness 9, cleavage {100} perfect, lustre adamantine, biaxial (-), $2V$ large, $\alpha = 1.81$, $\beta = 1.87$, $\gamma = 1.92$, dispersion $r > v$.

The crystal structure represents a new type and is based on hexagonal close-packed oxygens. It is related to the structure of simpsonite $\text{Ta}_3\text{Al}_4\text{O}_{13}(\text{OH})$.

BAHIANITE, a new species whose detailed crystal structure was recently reported (Moore and Araki, 1976), has been found only in stream gravel concentrates and not in place in rock. Samples were submitted to the Government Analytical Laboratory in Rio de Janeiro where it was first recognized as a new species by Carlos Barbosa, who first investigated its composition and properties.

It was first observed in cassiterite concentrates by *garimpeiros* (= prospectors) mining tin ores in the Paramirim region, south central Bahia state, Brazil, near the village of Paramirim das Crioulas, Municipio de (County of) Agua Quente. Subsequently it has been found elsewhere in the region, roughly within a 25-km radius of the Pico das Almas in the Serra das Almas, usually in cassiterite concentrates.

The Serra das Almas is a NW.-SE. trending range lying about 25 km east of the city of Paramirim in the County of Paramirim. The highest points in the range attain an altitude of about 2000 m, and most of it is accessible only on foot or on horseback. Bahianite has been observed

in the counties of Agua Quente, Rio das Contas, Livramento do Brumado, and Paramirim, all of which are traversed by the Serra das Almas with the Pico das Almas at the juncture of three of them. Approximate geographic coordinates of the Pico das Almas are 13° 33' S. 41° 57' W.

The geology of the region has not been studied in detail, but is believed to be complex, comprised mainly of pre-Cambrian metamorphic units, and sandstones, serpentine, quartzites, and rhyolite or rhyodacite. Gold and cassiterite are recovered from the placers, and there are known to be prospects for copper, zinc, and other metals. It is not possible to assess any genetic connection between cassiterite and bahianite, which quite likely are of different origins. The cassiterite is definitely associated with the extrusive units, and is of the wood-tin variety, which occurs in shallow, high-temperature environments.

Minerals found in the placers with the bahianite include quartz, andalusite of the bright green gem variety (viridine), kyanite, diaspore, zircon staurolite, cassiterite, gold, and eskolaite in small sharp crystals. The bahianite itself is found as abraded and water-worn pebbles, more or less bean-shaped, whence the local term 'favas'. The largest piece seen was 17 grams, but a *garimpeiro* in the region reported having seen pieces well over 100 grams in weight. The larger pieces are seldom pure, but commonly contain inclusions of quartz. They are polycrystalline and often show radial-fibrous structure. The pebbles are often vuggy, the vugs being lined with crystals of bahianite which, although lustrous, present curved facets unsuitable for goniometric measurement.

Owing to the lack of material found *in situ*, it is

TABLE I. *Bahianite*. X-ray powder data*

I_{obs}	I_{calc}	d_{obs}	d_{calc}	hkl	I_{obs}	I_{calc}	d_{obs}	d_{calc}	hkl
—	29	—	7.291	110	—	5	—	1.396	203
—	15	—	5.771	020	20	3	1.392	1.396	442
70	90	4.712	4.702	200	70	29	1.373	1.377	640
40	46	4.425	4.409	001	20	5	1.353	1.356	133
20	23	3.794	3.794	$\bar{1}11$	10	1	1.328	1.332	532
20	19	3.765	3.752	111	—	8	—	1.318	281
10	8	3.648	3.645	220	30b	8	1.313	1.314	281
30	32	3.564	3.561	130	—	15	—	1.309	043
30	23	3.508	3.504	021	50b	5	1.305	1.306	172
100	100	3.241	3.243	$\bar{2}01$	10	3	1.285	1.287	602
100	100	3.194	3.191	201	—	4	—	1.268	730
—	2	—	3.025	310	20b	3	1.264	1.268	602
30	24	2.885	2.885	040	30	7	1.253	1.257	243
20	15	2.825	2.827	$\bar{2}21$	10	4	1.238	1.240	570
—	13	—	2.792	221	10	5	1.226	1.230	480
50b	35	2.772	2.779	$\bar{1}31$	10	4	1.219	1.221	372
—	30	—	2.762	131	10	4	1.212	1.213	372
20	10	2.509	2.513	311	10	3	1.206	1.207	082
—	7	—	2.476	311	10	4	1.194	1.197	571
70	53	2.457	2.459	240	10	5	1.187	1.190	571
—	16	—	2.430	330	10	4	1.179	1.182	481
70	58	2.411	2.414	041	—	5	—	1.176	642
40	21	2.349	2.351	400	40	5	1.173	1.175	800
20	10	2.206	2.205	002	10	3	1.165	1.167	282
80	55	2.156	2.156	241	20	5	1.158	1.161	642
—	17	—	2.140	$\bar{3}31$	40	7	1.149	1.151	443
10	10	2.121	2.117	331	40	7	1.135	1.137	443
50	24	2.060	2.061	401	20	3	1.115	1.117	533
10	6	2.008	2.009	$\bar{2}02$	40	11	1.100	1.102	004
30	14	1.982	1.984	202	20	6	1.090	1.091	173
20	7	1.877	1.880	$\bar{1}32$	20	5	1.087	1.088	173
30	13	1.823	1.823	440	20	6	1.084	1.086	572
30	10	1.754	1.752	042	10	7	1.079	1.081	603
50	24	1.693	1.692	441	—	14	—	1.078	482
50	24	1.677	1.677	441	—	4	—	1.077	204
70	35	1.648	1.649	242	40	7	1.076	1.076	572
70	38	1.635	1.635	242	30	12	1.069	1.070	482
—	11	—	1.642	170	20	8	1.062	1.063	603
70	23	1.624	1.622	402	40	10	1.060	1.061	841
30	18	1.589	1.595	402	20	10	1.052	1.053	841
10	8	1.580	1.586	531	30	8	1.043	1.044	802
—	8	—	1.570	531	20	6	1.041	1.043	1.11.0
20	5	1.563	1.567	600	20	8	1.038	1.039	373
—	10	—	1.525	$\bar{1}71$	10	7	1.033	1.035	681
30b	10	1.518	1.522	171	—	8	—	1.032	373
20	7	1.479	1.485	601	—	9	—	1.030	802
20	6	1.464	1.469	601	—	2	—	1.029	083
10	5	1.457	1.459	370	50b	6	1.028	1.029	681
30	13	1.436	1.442	080	—	11	—	1.016	771
—	7	—	1.414	442	30	13	1.013	1.015	1.11.1
30b	7	1.407	1.409	203	50	15	1.008	1.009	244

* 114.6 mm camera diameter, Fe- K_{α} radiation. The sample was a spherical powdered aggregate, and the film was corrected for shrinkage. The observed spacings were corrected for absorption effects and are here reported after the correction was made. The calculated data obtain from the structure study of Moore and Araki (1976).

not possible to ascertain the paragenetic setting for bahianite. We speculate that it is a metamorphic product, formed at moderate temperatures, of pre-existing weathered and oxidized antimony ores that are recrystallized in a locally peraluminous environment. The chemical content of bahianite pebbles is quite variable and they commonly contain subsidiary amounts of W, Ti, Fe, Be, and Si, again suggesting the existence of local concentrations of pre-existing weathered and subsequently agglomerated ores and siliceous matter.

Physical properties. Bahianite is most commonly tan to cream in colour. Crystals in vugs may be colourless, tan, or pale violet. Other colours noted in the pebbles are orange-brown to brown. The colour variation seems to be associated with variation in composition, with the orange varieties corresponding to a content of several per cent Ti. Specific gravities, based on pure grains from selected pebbles, are: 4.89, 4.98, 5.05, 5.16, 5.23, 5.29 (Berman torsion balance); and 5.08, 5.17 (pycnometer). The clear crystal, a portion of which was used towards the structure analysis, gave 5.46 (Berman microbalance). The computed density for $\text{Sb}_3\text{Al}_5\text{O}_{14}(\text{OH})_2$ is 5.26 g cm^{-3} but we provide evidence further on that the structure tolerates additional and variable amounts of other cations.

Crystals, although too rough for goniometric measurements, are commonly striated; cleavage

{100} perfect; lustre adamantine; hardness 9. The mineral is highly resistant to attack by acids or bases and wet chemical analysis required fusion in Na_2CO_3 .

X-ray crystallography. Bahianite is monoclinic, pseudo-orthorhombic, space group $C2/m$, $a = 9.406(6) \text{ \AA}$, $b = 11.541(8) \text{ \AA}$, $c = 4.410(3) \text{ \AA}$, $\beta = 90.94(3)^\circ$, $Z = 2$ for $\text{Sb}_3\text{Al}_5\text{O}_{14}(\text{OH})_2$. Crystal cell parameters were obtained by least-squares refinement of the powder data in Table I. The crystal structure, known in detail ($R = 0.046$ for 1044 independent F_0), is allied to simpsonite $\text{Ta}_3\text{Al}_4\text{O}_{13}(\text{OH})$ in that both compounds are based on hexagonal close-packed oxygens parallel to {001}. In bahianite the structure is based on layers of $[\text{Al}_5\text{O}_{14}(\text{OH})_2]$ edge-sharing sheets corner-linked at adjacent layers to linear $[\text{Sb}_3\text{O}_{14}]^{13-}$ trimers, representing a unique structure type (Moore and Araki, 1976). Since the b -axis is parallel to the chain component in the edge-sharing sheets, $\sqrt{3}b/2 \sim a$.

Optical properties. Biaxial (-), $2V_x$ large, $\alpha = 1.81$; $\beta = 1.87$, $\gamma = 1.92$ all ± 0.01 ; dispersion $r > v$. Utilizing the ideal formula and the Gladstone-Dale relationship, $\langle n \rangle = 1.90$.

Chemical composition. Like simpsonite, bahianite is variable in composition and this results from both substitution over the four non-equivalent octahedral (M) sites in the structure and the

TABLE II. Bahianite analyses*

	1	2	3	4	5	6	7
Sb_2O_5	(55.35)	56.70	57.86	n.d.	(63.6)	57.28	5.61
Al_2O_3	(41.10)	35.23	35.51	(33.3)	(38.9)	35.37	10.98
Fe_2O_3	(0.94)	1.24	0.90	1.0	(< 0.1)	1.04	0.21
WO_3	n.d.	1.34	1.05	n.d.	(< 0.1)	1.20	0.08
BeO	(1.08)	n.d.	0.55	0.95	n.d.	0.75	0.47
SiO_2	1.03	n.d.	n.d.	n.d.	(< 0.1)	1.03	0.27
CaO	(1.00)	n.d.	n.d.	n.d.	(< 0.1)	—	—
H_2O^+	n.d.	n.d.	n.d.	2.77	n.d.	2.77	(4.87)
Total	(100.5)	94.51	95.87	(38.02)	(102.6)	99.44	17.62

* Results in parentheses are semi-quantitative and were not used in the final average. Water was determined by the Penfield tube technique, the sample fused in anhydrous Na_2CO_3 .

n.d. = not determined.

1. Barbosa, by wet chemical means.

2. A. M. Clark, British Museum (Natural History), electron probe analysis.

3. N. Schuhwerk, Kawecki Berylco Industries.

4. J. Ito, by wet-chemical techniques. Pale-yellow grains.

5. A. J. Irving, by electron microprobe, using Sb metal and corundum standards. The analysis is semi-quantitative.

6. Average of 1-4, with the exception of results in parentheses.

7. Cations per cell based on (6), specific gravity = 5.46 and $V = 487.66 \text{ \AA}^3$. H was not included in the sum.

possibility of partial tetrahedral (*T*) occupancy. Moore and Araki (1976) have demonstrated that in both simpsonite and bahianite, tetrahedrally coordinated cations can exist without violating electrostatic principles and that the upper compositional limit for bahianite is $2M_8T_2O_{16}$, where all electrostatically favoured tetrahedral sites are occupied. It was further proposed that Si and Be, and excess Al reported in some of the analyses, may indeed partially occupy these available sites.

Partial chemical analyses are presented in Table II and the averaged results were used to calculate cell contents. Neglecting the presence of water the cation cell contents nearly balance the anhydrous oxide fraction, that is, $Al_{10.98}Sb_{5.61}Fe_{0.21}^{3+}W_{0.08}Be_{0.47}Si_{0.27}O_{32.06}$, or partitioning over octahedral and tetrahedral sites, $\Sigma M = Al_{10.10}Sb_{5.61}Fe_{0.21}^{3+}W_{0.08}$ ($= 16.00$) and $\Sigma T = Al_{0.88}Be_{0.47}Si_{0.27}$ ($= 1.62$). This yields a calculated density of 5.31 g cm^{-3} and an average of 3.1 electrons per tetrahedral site.

Thus, bahianite's formula can be written as a series $Sb_3Al_5O_{14}(OH)_2-Sb_3Al_5(Al, Be, Si)_{<2}O_{16}$. The crystal structure analysis, indeed, supports the presence of disordered hydroxyl groups, although

electron density was not definitely established over the tetrahedral sites, doubtless owing to a low residual density over these sites distributed in a matrix of rather high mean atomic number.

Name and disposition of the type specimen. The name bahianite refers to the State of Bahia from within which state the specimens were found. The sample that formed the basis of the structure analysis, the powder pattern, and the semi-quantitative electron probe analysis is designated as the type and is deposited in the U.S. National Museum of Natural History (Smithsonian Institution), Washington, D.C., U.S.A.

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REFERENCE

- Moore (P. B.) and Araki (T.), 1976. *Neues Jb. Mineral., Abh.* **126**, 113.

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