**THE CRYSTAL STRUCTURE OF NATURAL LIPSCOMBITE**

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The mineral name "lipscombite" was first given by Gheith (1) for a synthetic iron phosphate forming black tetragonal bipyramidal crystals, stable above 290°C. This compound is the high-temperature polymorph of another synthetic phase called by Gheith the "ferrous ferric lazulite", of monoclinic symmetry (1), later defined as barbosalite (2). Natural lipscombite was described by Lindberg (3) in the Sapucaia pegmatite, Brazil, where it shows a chemical composition significantly enriched in manganese.

The crystal structure of lipscombite is known from synthetic material (4-6), but was never determined on a natural sample. During a mineralogical investigation of the Eduardo pegmatite, Minas Gerais, Brazil, black pseudo-cubic crystals were found, associated with hureaulite and jahnsite-group minerals. A single-crystal X-ray investigation (Rigaku Xcalibur, EOS detector, MoKα radiation) showed them to be tetragonal, space group *P*41212, *a* = 7.4195(17) and *c* = 13.023(5) Å. This mineral therefore corresponds to lipscombite, and its empirical formula was determined by electron microprobe (WDS, 15 kV, 5 nA, 5 µm beam diameter, average of 11 point analyses): [Fe(II)0.93Mn(II)0.14]Fe(III)2.00(PO4)2(OH)2·0.23H2O.

The structure of lipscombite from the Edurado pegmatite was refined satisfactorily to *R*1 = 0.0996. All atoms were refined anisotropically, except O1, O3 and O6. Fe occurs in two weakly-distorted Fe1O6 and Fe2O6 octahedra, and P occurs in the P1O4 tetrahedron; the average Fe1-O, Fe2-O, and P1-O bond distances are 2.077, 2.053, and 1.539 Å, respectively. The structure is characterized by trimers of face-sharing FeO6 octahedra, which are connected to similar trimers by corner-sharing to form infinite octahedral chains runing along the [110] direction. The chains are located in planes, perpendicular to the *c* axis, and these planes are connected together by PO4 tetrahedra or by sharing octahedral corners. Bond-valence sums were calculated on all sites, showing the presence of 0.57 Fe(II) + 0.43 Fe(III) on the Fe1 site, and of 0.29 Fe(II) + 0.71 Fe(III) on the Fe2 site. O1 to O4 correspond to O atoms, O4 to an OH group, and O6 to an H2O molecule. The resulting crystal-chemical formula of lipscombite is revised as: Fe(II)Fe(III)2(PO4)2(OH)2·H2O.

1. Gheith, M.A. (1953). *American Mineralogist*, 38, 612-628.
2. Lindberg, M.L. & Pecora, W.T. (1955). *American Mineralogist*, 40, 952-966.
3. Lindberg, M.L. (1962). *American Mineralogist*, 47, 353-359.
4. Katz, L. & Lipscomb, W.N. (1951). *Acta Crystallographica*, 4, 345-348.
5. Matvienko, E.N., Yakubovich, O.V., Simonov, M.A. & Belov, N.V. (1981). *Zhurnal Strukturnoi Khimii*, 22, 121-125.
6. Vencato, I., Mattievich, E. & Mascarenhas, Y.P. (1989). *American Mineralogist*, 74, 456-460.