# The Crystal Structure of Natural Lipscombite

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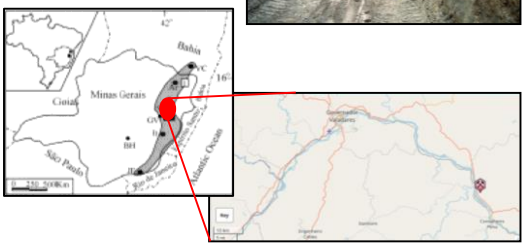
## Introduction

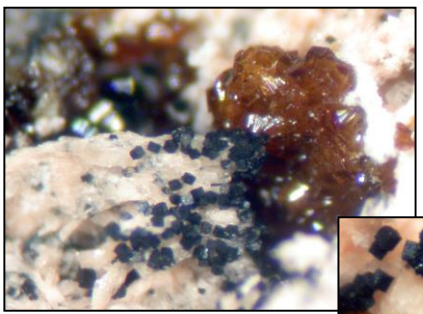
- The name “lipscombite” was first given for a synthetic tetragonal iron phosphate of composition $Fe^{2+}Fe^{3+}_2(PO_4)_2(OH)_2$, stable above 290°C.
- Its low-temperature monoclinic polymorph is known as barbosalite.
- Natural lipscombite has been described in the Sapucaia pegmatite, Brazil, but the crystal structure of this mineral was never determined on a natural sample.
- We report here the first structure refinement of a natural lipscombite sample, which was collected in the Eduardo pegmatite, Minas Gerais, Brazil.

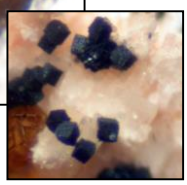
## Occurrence

- Eduardo claim (or « Boa Vista »)
- LCT-type pegmatite
- Conseilhero Pena
- Minas Gerais, Brazil




## Mineralogical characterization



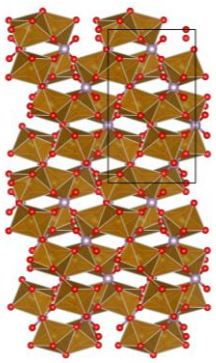


- Black pseudo-cubic crystals
- Associated with hureaulite and jahnsite
- Chemical composition (EMPA): $(Fe^{2+}_{0.93}Mn_{0.14})Fe^{3+}_2(PO_4)_2(OH)_2 \cdot 0.23H_2O$

## Bond-valence table

| | Fe1 | Fe2 | P | Sum | Attribution |
|---|---|---|---|---|---|
| O1 | 0.392 (x2↓) | 0.510 | 1.086 | 1.99 | $O^{2-}$ |
| O2 | - | 0.625 | 1.189 | 1.81 | $O^{2-}$ |
| O3 | - | 0.461 | 1.482 | 1.95 | $O^{2-}$ |
| O4 | 0.391 (x2↓) | 0.787 | - | 1.18 | $OH^-$ |
| O5 | 0.433 (x2↓) | 0.332 | 1.222 | 1.99 | $O^{2-}$ |
| O6 | - | - | - | 0.00 | $H_2O$ |
| **Sum** | **2.43** | **2.72** | **4.98** | **-** | **-** |
| % $Fe^{2+}$ | 57 | 28.5 | - | - | - |
| % $Fe^{3+}$ | 43 | 71.5 | - | - | - |

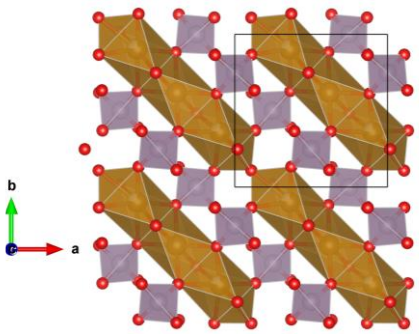
## Crystal structure description




$a$ = 7.4195(17) Å
$c$ = 13.023(5) Å
SG: $P4_12_12$
$R_1$ = 0.0996

- Fe1 [6], Fe2 [6], P [4]
- <Fe1-O> = 2.077 Å
- <Fe2-O> = 2.053 Å
- <P-O> = 1.539 Å

- Trimers of face-sharing octahedra, connected to similar trimers by corners
- Octahedral chains aligned along the [110] and [1-10] directions
- Octahedral planes perpendicular to the $c$ axis
- Chains connected by corner-sharing $PO_4$ tetrahedra




## Conclusions

- The crystal structure of natural lipscombite has been determined for the first time.
- A bond-valence analysis shows that $Fe^{2+}$ and $Fe^{3+}$ are disordered over the Fe1 and Fe2 positions. However, $Fe^{2+}$ shows a significant preference for the Fe1 site, and $Fe^{3+}$ for the Fe2 site.
- The position O6 corresponds to a water molecule, which was not observed previously in synthetic equivalents.
- The ideal formula of lipscombite should consequently be revised as: $Fe^{2+}Fe^{3+}_2(PO_4)_2(OH)_2 \cdot H_2O$

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