

Supplementary Information

Iron Ore Tailings: Characterization and Applications

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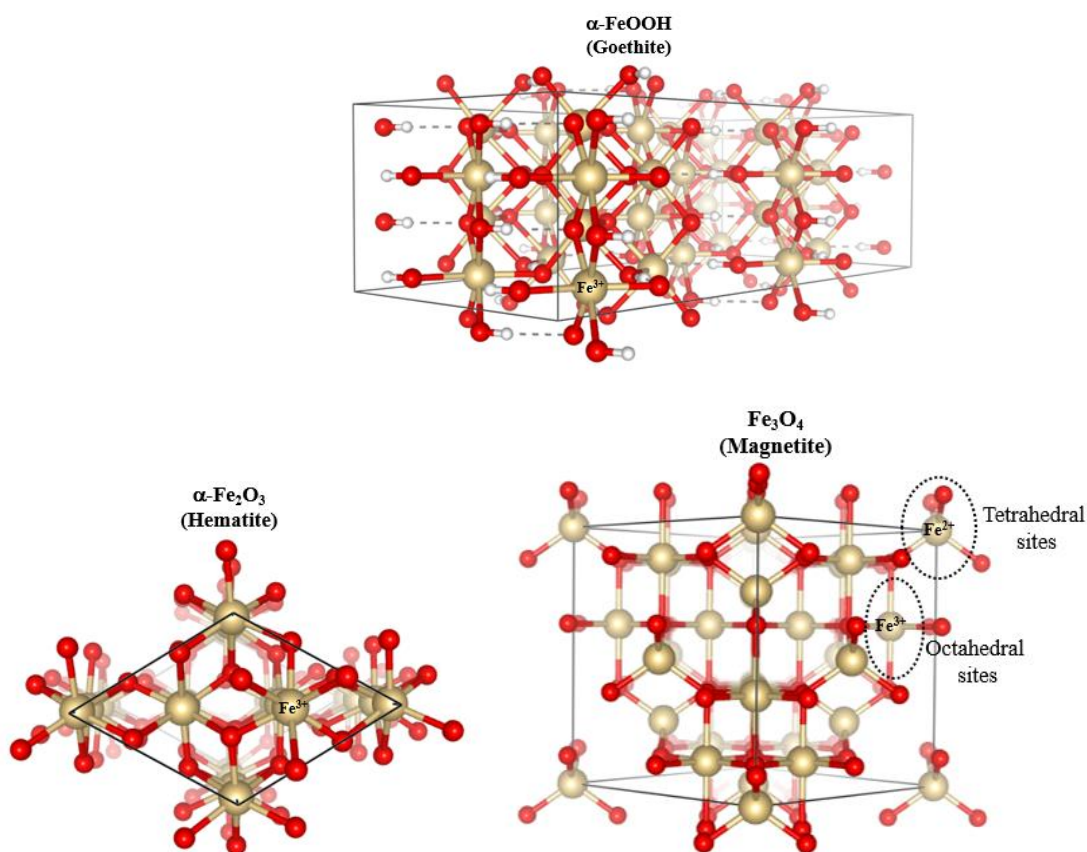


Figure S1. Three-dimensional structures of the main phases of iron oxides found in IOT. All structures were generated from the crystallographic information file (CIF)¹ taken from the database, Crystallography Open Database and generated from Vesta Visualization software for Electronic and Structure Analysis.²

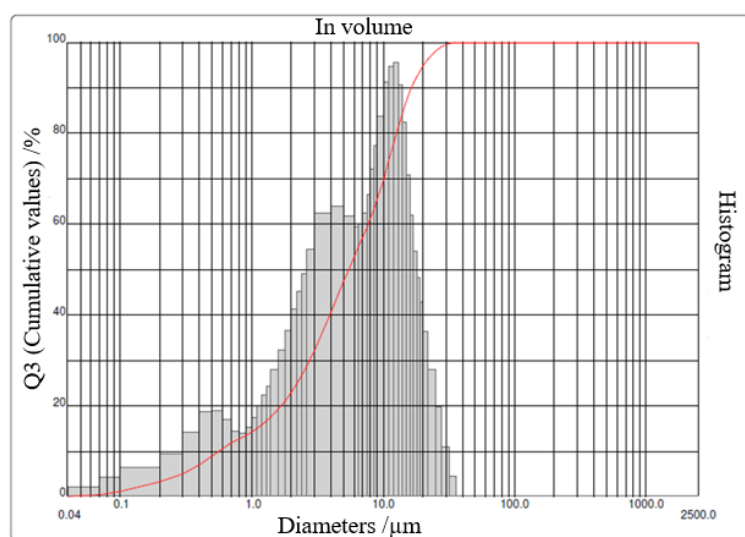


Figure S2. The granulometric distribution curve of fine tailings from iron mining from the Quadrilátero Ferrífero region (Brazil-MG).

Table S1. Main characteristics of the iron phases found in iron mining tailings: color, morphology, magnetism, and type of structure

Phase and color	Morphology and type of magnetism	Structure
α -FeOOH (goethite) Oxyhydroxid Yellow/brown	crystals acicular and elongated antiferromagnetic	orthorhombic: the structures consist of an array of anions (O^{2-} and OH^-) stacked along the direction with Fe^{3+} ions occupying half the octahedral interstices within the layer; at the crystal surfaces, the empty sites appear as grooves
α -Fe ₂ O ₃ (hematite) Oxide Red	plates and discs, rods, spheres, ellipsoids, rhombohedra, stars, and cubes; antiferromagnetic	rhombohedral/hexagonal: the structures can be described as consisting of arrays of oxygen ions stacked along the [001] direction; two-thirds of the sites are filled with Fe^{3+} ions which are arranged regularly with two filled sites being followed by one vacant site; the arrangement of cations produces pairs of $Fe(O)_6$ octahedral; each octahedron shares edges with three neighboring octahedron in the same plane and one face with an octahedron in an adjacent plane
Fe ₃ O ₄ (magnetite) Oxide Black	particles spheroidal ferrimagnetic	cubic structure of spinel: the structure is that of an inverse spinel; it has a face-centered cubic unit cell based on 32 O^{2-} ions which are regularly cubic close-packed along the plane [111]; features tetrahedral sites occupied by Fe^{3+} ions, and octahedral sites occupied by Fe^{2+} and Fe^{3+} ions

Table S2. Hyperfine parameters for iron ore tailings (adapted from Silva *et al.*³⁾)

	Phase/oxidation state	$\delta \pm 0.05$ / (mm s ⁻¹)	$\Delta/\epsilon \pm 0.05$ / (mm s ⁻¹)	$B_{HF} \pm 0.5$ / T	Relative area ± 1 / %
IOT	α -Fe ₂ O ₃	0.36	-0.18	51.8	51
	α -FeOOH	0.36	-0.24	37.8	43

IOT: iron ore tailings; δ : isomeric shift; Δ : quadrupole splitting; B_{HF} : hyperfine field.

References

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2. Momma, K.; Izumi, F.; *J. Appl. Crystallogr.* **2011**, *44*, 1272.
3. Silva, R. C. F.; Ardisson, J. D.; Cotta, A. A. C.; Araujo, M. H.; Teixeira, A. P. C.; *Environ. Pollut.* **2020**, *260*, 114099.

