

The crystal chemistry of julgoldite-Fe³⁺ from Bombay, India, studied using synchrotron X-ray powder diffraction and ⁵⁷Fe Mössbauer spectroscopy

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ABSTRACT

The crystal structure of julgoldite-Fe³⁺ from Bombay, India, was investigated by ⁵⁷Fe Mössbauer spectroscopy and synchrotron X-ray powder diffraction. Only ferric iron was detected in the Mössbauer measurements and it occurs at two different octahedral sites in the atomic ratio 20:80. Based on Rietveld refinements, the Fe³⁺ cations are located at the X- and Y-octahedral sites with atomic percentages of about 25% and 75%, respectively. The resulting chemical formula of the Bombay julgoldite sample is Ca₈(Fe_{2.7}³⁺Al_{1.1}Mg_{0.2})(Fe_{8.0}³⁺)Si₁₂O₄₂(OH)₁₄. The oxidation state of Fe is not the same as that arrived at through simple crystal-chemical considerations. Such analysis cannot give quantitative results for the valence state of mixed-valence cations in pumpellyite-type minerals and their intracrystalline partitioning behavior. Assignments of the Mössbauer absorption doublets and an analysis of Fe-intracrystalline partitioning behavior are discussed with reference to previous works on different pumpellyite-type minerals.