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## Low-symmetry spin Hamiltonian and crystal field tensors analysis: Fe<sup>3+</sup> in natrolite

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### Abstract

Electron paramagnetic resonance study of a natural single crystal of natrolite was carried out at the frequency  $\nu = 36.772$  GHz at room temperature. The angular dependence of the four symmetry-related spectra of Fe<sup>3+</sup> in the three crystallographic planes was fitted to a spin Hamiltonian ( $S = 5/2$ ) of symmetry  $C_i$ . The rank 4 crystal field tensors at tetrahedral sites were calculated using the point-charge model to determine the principal axes orientations of their cubic and trigonal components. The analysis of zero-field splitting tensors and comparison with crystal field ones suggests that Fe<sup>3+</sup> substitutes for Al<sup>3+</sup> with no significant distortion of the coordination tetrahedron in natrolite. Comparison of data for several natural and synthetic crystals reveals that the 4-rank zero-field splitting tensor invariants for Fe<sup>3+</sup> at the tetrahedral oxygen-coordinated sites are distinguishably smaller than those for Fe<sup>3+</sup> at octahedral sites. Such comparative analysis may help to determine the substitutional sites in other crystals. © 2002 Elsevier Science (USA).

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### Keywords

Crystal field, Low symmetry effect, Natrolite, Spin Hamiltonian, Tensor invariants