

# Hyperfine field and electronic structure of magnetite

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Recently, Senn et al. [1] determined precise structure of low temperature  $Cc$  phase of magnetite and introduced a trimeron model for the ordering of the octahedrally coordinated iron cations. The present work studies the electronic ordering and hyperfine field (HF) at the iron sites in order to verify the model. A reanalysis of published dependences of the  $^{57}\text{Fe}$  nuclear magnetic resonance frequencies [2] on external magnetic field direction was performed to investigate HF anisotropy in  $Cc$  phase of magnetite. Isotropic parts and anisotropy tensors of the hyperfine interaction were extracted. Next, ab initio calculations of HF in dependence on magnetization direction yielded analogical data. Comparison of the two data sets revealed matching groups of the octahedral iron sites. Further, iron valences, minority spin valence electron density maps and populations were calculated. The results support the trimeron model.

## References:

- [1] M. S. Senn, J. P. Wright and J. P. Attfield, *Nature* **481**, 173-176 (2012).
- [2] M. Mizoguchi, *J. Phys. Soc. Jap.* **70**, 2333 (2001).