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## Mössbauer Spectroscopy of the New Iron Oxide $\text{Fe}_3\text{B}_7\text{O}_{13}(\text{OH})$

text, two Figs, refs.

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### Summary

Boracite  $\text{Fe}_3\text{B}_7\text{O}_{13}(\text{OH})$  is a new iron oxide synthesized by hydrothermal method [1]. The crystal structure is trigonal ( $R\bar{3}c$ ) with the lattice constants of  $a=8.590\text{\AA}$  and  $c=21.107\text{\AA}$  (hexagonal notation) at room temperature. Iron ion,  $\text{Fe}^{2+}$ , occupies a pentahedral site. Three pentahedrons share the upper corner, which is probably occupied by  $\text{OH}^-$  ion [2,3], and thus three  $\text{Fe}^{2+}$  ions form a triangular cluster in the  $c$ -plane. The material is an antiferromagnet with  $T_N=4.9\text{K}$ . Ising-like behavior is observed [1]. In order to investigate the local structure and the magnetic structure, we have applied  $^{57}\text{Fe}$  Mössbauer spectroscopy. The spectra were measured in conventional transmission geometry by using  $^{57}\text{Co}$ -in-Rh as the  $\gamma$ -ray source. The powdered specimen was used as an absorber.

The paramagnetic spectrum at  $293\text{K}$  is shown in Fig.1. The spectrum is composed of a paramagnetic doublet with sharp line widths ( $0.24\text{mm/s}$ ), indicating that there is only one crystallographic Fe site. The room-temperature value of isomer shift (IS) is  $1.16\text{mm/s}$ , which indicates that the Fe ions are in high spin  $\text{Fe}^{2+}$  state. The quadrupole splitting (QS) is very large ( $3.21\text{mm/s}$ ) due to the valence electron contribution. The spectrum at  $4.2\text{K}$ , just below  $T_N$ , is shown in Fig.2. The spectrum is a well-resolved hyperfine sextet with sharp line widths ( $0.30\text{mm/s}$ ), indicating that the hyperfine field ( $H_{\text{hf}}$ ) grows rather rapidly below  $T_N$ . We can obtain the best fit curve with the parameters;  $\text{IS}=1.29\text{mm/s}$ ,  $\text{QS}=3.52\text{ mm/s}$ ,  $H_{\text{hf}}=3.6\text{T}$ , asymmetry parameter  $\eta=0.5$ , and Euler angles  $\theta=20^\circ$  and  $\varphi=0^\circ$ . By evaluating the principal axis of electric field gradient (EFG) from the lattice contribution, we can deduce that each three  $\text{Fe}^{2+}$  magnetic moment is directed from  $\text{Fe}^{2+}$  ion to  $\text{OH}^-$  ion. Taking into account that the system is antiferromagnetic as a whole, a probable magnetic structure is 6-sublattice model, which is consistent with that derived from the static magnetic properties [1].

### References

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- [2] D. Andreica, et al., *Ferroelectrics*, 204 (1997) 73.
- [3] U. Werthmann, et al., *Z.Kristallogr.*215 (2000) 393.

**Primary author:** Prof. NAKAMURA, Shin (Teikyo University)

**Co-authors:** Prof. SATO, Hirohiko (Chuo University); Mr NOMOTO, Ippei (Chuo University); Prof. TSUNODA, Yorihiro (Waseda University)

**Presenter:** Prof. NAKAMURA, Shin (Teikyo University)

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