

Review of:

Polyakov V.B., Clayton R.N., Horita J. and Mineev S.D. (2007) Equilibrium iron isotope fractionation factors of minerals: Reevaluation from the data of nuclear inelastic resonant X-ray scattering and Mössbauer spectroscopy. *Geochim. Cosmochim. Acta* 71, 3833-3846.

Major points:

- Builds on earlier work by Polyakov and others to **calculate iron isotopic β -factors** from measured Mössbauer second-order Doppler shift (SOD) and adds new calculations based on the phonon density of state determined by inelastic nuclear resonance x-ray scattering (INXRS)
- Does this for several crystalline solids, including metallic iron, iron oxides, and iron sulfides with an emphasis on examining the widest possible range of oxidation states
- Finds good agreement between methods as well as with established sulfur isotope geothermometers among sulfides, calls into question the Mössbauer SOD for magnetite as reported by De Grave et al (1993) and Persoons et al. (1993) and adjusts these calculations
- Demonstrates correlation between β -factors and iron oxidation state; β -factors are larger for higher oxidation states.

Methods:

This paper uses the **primary equation**,

$$\ln\beta = \frac{\Delta m}{m^*} \left(\frac{KE}{RT} - \frac{3}{2} \right)$$

where KE is the kinetic energy per mole of iron. This quantity is determined by one of two methods:

Mössbauer spectroscopy, using the equation,

$$S = \frac{-KE}{mc}$$

where S is the Mössbauer second-order Doppler shift.

Inelastic Nuclear Resonant X-ray Scattering measures the PDOS $g(e)$ directly,

$$KE = \frac{3}{2} \int_0^{e_{max}} E (e/kT) g(e) de$$

$$\frac{E(e/kT)}{kT} \equiv \frac{e/kT}{\exp(e/kT)-1} + 0.5 e/kT \quad (\text{This is a Bose-Einstein distribution})$$

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