Supporting Information

for

Magnetic ground state of nanosized β-Fe_2O_3 and its remarkable electronic features

Ondřej Malina,[1] Jiří Tuček,[1,] Petr Jakubec,[1] Josef Kašlík,[1] Ivo Medřík,[1] Hiroko Tokoro,[2] Marie Yoshikiyo,[2] Asuka Namai,[2] Sin-ichi Ohkoshi,[2] and R. Zbořil,[1,*]*

[1] Regional Centre of Advanced Technologies and Materials, Departments of Physical Chemistry and Experimental Physics, Faculty of Science, Palacky University, Slechtitelu 11, 783 71 Olomouc, Czech Republic

[2] Department of Chemistry, School of Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

* Corresponding authors: Phone: +420 585634337, Fax: +420 585634761, E-mail address: radek.zboril@upol.cz (Radek Zbořil); Phone: +420 585634950, Fax: +420 585634958, E-mail address: jiri.tucek@upol.cz (Jiří Tuček).

Number of pages: 5
Number of figures: 1
Number of tables: 2

Supporting Figures

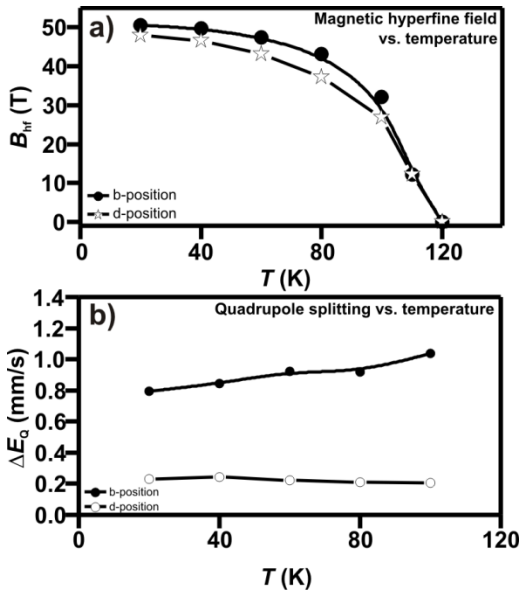

Figure S1. a) Temperature behavior of the hyperfine magnetic field (B_{hf}) for both sites and b) temperature evolution of the quadrupole splitting (ΔE_Q) for both sites below the Néel temperature.

Supporting Tables

Table S1. Values of the Mössbauer hyperfine parameters derived from the zero-field and in-field Mössbauer spectra of the prepared β-Fe_2O_3 phase recorded at various temperatures where T is the temperature of the measurement, B_{ext} is the external magnetic field, δ is the isomer shift, ΔE_Q is the quadrupole splitting, B_{hf} is hyperfine magnetic field, B_{eff} is the effective hyperfine magnetic field (i.e., B_{eff} is vector sum of the external magnetic field B_{ext} and the hyperfine field B_{hf}), and RA is relative spectra area of each component.

T (K)	B_{ext} (T)	Component	δ ± 0.01 (mm/s)	ΔE_Q ± 0.01 (mm/s)	B_{hf} ± 0.3 (T)	B_{eff} ± 0.3 (T)	RA ± 1 (%)	Assignment
20	0	Sextet 1	0.50	0.23	47.9	-	75	d-sites
		Sextet 2	0.49	0.80	50.6	-	25	b-sites
40	0	Sextet 1	0.50	0.24	46.6	-	75	d-sites
		Sextet 2	0.50	0.85	49.8	-	25	b-sites
60	0	Sextet 1	0.50	0.22	43.1	-	75	d-sites
		Sextet 2	0.51	0.92	47.4	-	25	b-sites
80	0	Sextet 1	0.48	0.21	37.3	-	45	d-sites
		Sextet 2	0.47	0.92	43.1	-	15	b-sites
		Singlet	0.48	-	-	-	40	relaxation c.
100	0	Sextet 1	0.49	0.21	26.8	-	21	d-sites
		Sextet 2	0.48	1.04	32.1	-	7	b-sites
		Singlet	0.48	-	-	-	72	relaxation c.
110	0	Doublet	0.47	0.75	-	-	17	
		Sextet	0.52	0.11	12.1	-	83	
120	0	Doublet 1	0.47	0.68	-	-	75	d-sites
		Doublet 2	0.47	1.05	-	-	25	b-sites
140	0	Doublet 1	0.47	0.68	-	-	75	d-sites
		Doublet 2	0.46	1.07	-	-	25	b-sites

160	0	Doublet 1	0.46	0.68	-	-	75	d-sites
		Doublet 2	0.45	1.05	-	-	25	b-sites
180	0	Doublet 1	0.45	0.69	-	-	75	d-sites
		Doublet 2	0.44	1.07	-	-	25	b-sites
200	0	Doublet 1	0.45	0.73	-	-	75	d-sites
		Doublet 2	0.43	0.92	-	-	25	b-sites
220	0	Doublet 1	0.42	0.70	-	-	75	d-sites
		Doublet 2	0.41	1.13	-	-	25	b-sites
240	0	Doublet 1	0.41	0.68	-	-	75	d-sites
		Doublet 2	0.40	1.06	-	-	25	b-sites
260	0	Doublet 1	0.39	0.73	-	-	75	d-sites
		Doublet 2	0.40	0.94	-	-	25	b-sites
280	0	Doublet 1	0.39	0.69	-	-	75	d-sites
		Doublet 2	0.39	1.02	-	-	25	b-sites
300	0	Doublet 1	0.37	0.68	-	-	75	d-sites
		Doublet 2	0.37	1.07	-	-	25	b-sites
5	0	Sextet 1	0.50	0.25	48.7	-	75	d-sites
		Sextet 2	0.47	0.84	50.9	-	25	b-sites
	1	Sextet 1	0.52	0.25	-	48.7	75	d-sites
		Sextet 2	0.46	0.84	-	50.9	25	b-sites
	2	Sextet 1	0.52	0.24	-	48.1	75	d-sites
		Sextet 2	0.44	0.77	-	50.5	25	b-sites
	3.5	Sextet 1	0.48	0.29	-	50.0	48	A-sublattice
		Sextet 2	0.51	0.25	-	46.4	52	B-subblatice
	5	Sextet 1	0.47	0.32	-	59.2	50	A-sublattice
		Sextet 2	0.48	0.20	-	44.8	50	B-subblatice
	8	Sextet 1	0.47	0.27	-	49.4	45	A-sublattice
		Sextet 2	0.49	0.25	-	44.9	27	B-sublattice
		Sextet 3	0.48	0.13	-	41.1	28	B-sublattice

Table S2. Values of the physical parameters derived from the Mössbauer spectra of the prepared β-Fe_2O_3 sample above the Néel temperature, where δ corresponds to the isomer shift, $A(T)$ is the resonant area under the Mössbauer spectrum at a temperature T, M_{eff} refers to an effective mass of the Mössbauer probed atom, and Θ_D is the Debye temperature of the solid.

	obtained parameters for the d-position	**obtained parameters for the b-position**
$d\delta/dT$ (mm/s K^{-1})	-5.75×10^{-4}	5.27×10^{-4}
M_{eff} (amu)	72	79
$d\ln[A(T)/A(120\ K)]/dT$ (K^{-1})	-3.50×10^{-3}	-3.52×10^{-3}
Θ_D (K)	175	167