

EDTA-Na₃ Functionalized Fe₃O₄

Nanoparticles: Grafting Density Control for MRSA Eradication

Palash Kumar Manna,^{*,†} Rachel Nickel,[†] Jie Li,[‡] Yaroslav Wroczynskyj,[†] Song Liu,[‡] and Johan van Lierop^{*,†,¶}

[†]*Department of Physics and Astronomy, University of Manitoba, Winnipeg, MB, R3T 2N2,
Canada*

[‡]*Department of Biosystems Engineering, Faculty of Agricultural and Food Sciences,
University of Manitoba, Winnipeg R3T 2N2, Canada*

[¶]*Manitoba Institute for Materials, University of Manitoba, Winnipeg, MB R3T 2N2
Canada*

E-mail: Palash.Manna@umanitoba.ca; Johan.van.Lierop@umanitoba.ca

Supporting Information Available

Fit results of Mössbauer spectra

A) The detailed fit results of the Mössbauer spectra (velocity scale: ~ 2.8 mm/s) of the Fe_3O_4 -EDTA- Na_3 nanoparticles are tabulated below.

Table 1: The isomer shift (δ), quadrupole shift (Δ), lorentzian linewidth (Γ , FWHM) and relative spectral area of the EDTA- Na_3 coated and as-synthesized nanoparticles obtained from the fits of the Mössbauer spectra.

Sample	δ (mm/s)	Δ (mm/s)	Γ (mm/s)	Area (%)	Phases
without EDTA- Na_3	0.42 \pm 0.01	2.72 \pm 0.01	0.19 \pm 0.01	100	Fe_3O_4 core
	0.50 \pm 0.01	2.04 \pm 0.01	0.19 \pm 0.01		
4 hr	0.42 \pm 0.01	2.72 \pm 0.01	0.19 \pm 0.01	56	Fe_3O_4 core
	0.50 \pm 0.01	2.04 \pm 0.01	0.19 \pm 0.01		
	0.36 \pm 0.01	0.73 \pm 0.01	0.40 \pm 0.14	37	Fe-EDTA monomer
	0.31 \pm 0.02	2.29 \pm 0.05	0.35 \pm 0.09	7	Fe-EDTA dimer
3 hr	0.42 \pm 0.01	2.72 \pm 0.01	0.19 \pm 0.01	37	Fe_3O_4 core
	0.50 \pm 0.01	2.04 \pm 0.01	0.19 \pm 0.01		
	0.36 \pm 0.01	0.70 \pm 0.01	0.38 \pm 0.12	57	Fe-EDTA monomer
	0.26 \pm 0.04	2.08 \pm 0.05	0.35 \pm 0.09	6	Fe-EDTA dimer
2 hr	0.42 \pm 0.01	2.72 \pm 0.01	0.19 \pm 0.01	40	Fe_3O_4 core
	0.50 \pm 0.01	2.04 \pm 0.01	0.19 \pm 0.01		
	0.36 \pm 0.01	0.72 \pm 0.01	0.42 \pm 0.16	54	Fe-EDTA monomer
	0.26 \pm 0.05	2.06 \pm 0.03	0.32 \pm 0.07	6	Fe-EDTA dimer
1 hr	0.42 \pm 0.01	2.72 \pm 0.01	0.19 \pm 0.01	6	Fe_3O_4 core
	0.50 \pm 0.01	2.04 \pm 0.01	0.19 \pm 0.01		
	0.37 \pm 0.01	0.71 \pm 0.01	0.39 \pm 0.13	71	Fe-EDTA monomer
	0.35 \pm 0.02	1.83 \pm 0.06	0.54 \pm 0.28	23	Fe-EDTA dimer
25 min	0.42 \pm 0.01	2.72 \pm 0.01	0.19 \pm 0.01	1	Fe_3O_4 core
	0.50 \pm 0.01	2.04 \pm 0.01	0.19 \pm 0.01		
	0.37 \pm 0.01	0.69 \pm 0.01	0.37 \pm 0.11	85	Fe-EDTA monomer
	0.42 \pm 0.03	1.68 \pm 0.10	0.45 \pm 0.19	14	Fe-EDTA dimer

B) The hyperfine parameters of the as synthesized Fe₃O₄ nanoparticle (velocity scale: \sim 11 mm/s) are given below:

Table 2: Hyperfine field (B_{hf}), isomer shift (δ), lorenzian linewidth (Γ), and area ratio of the A and B site components of the as synthesized Fe₃O₄ nanoparticles.

	B _{hf} (T)	δ (mm s ⁻¹)	Γ (mm s ⁻¹)	Area (%)
A	48.9 \pm 0.3	0.32 \pm 0.01	0.24 \pm 0.01	57.0 \pm 4.2
B	45.2 \pm 0.6	0.60 \pm 0.01	0.34 \pm 0.01	43.0 \pm 3.6