

Article

Supplementary Materials: First-Row-Transition Ion Metals(II)-EDTA Functionalized Magnetic Nanoparticles as Catalysts for Solvent-Free Microwave-Induced Oxidation of Alcohols

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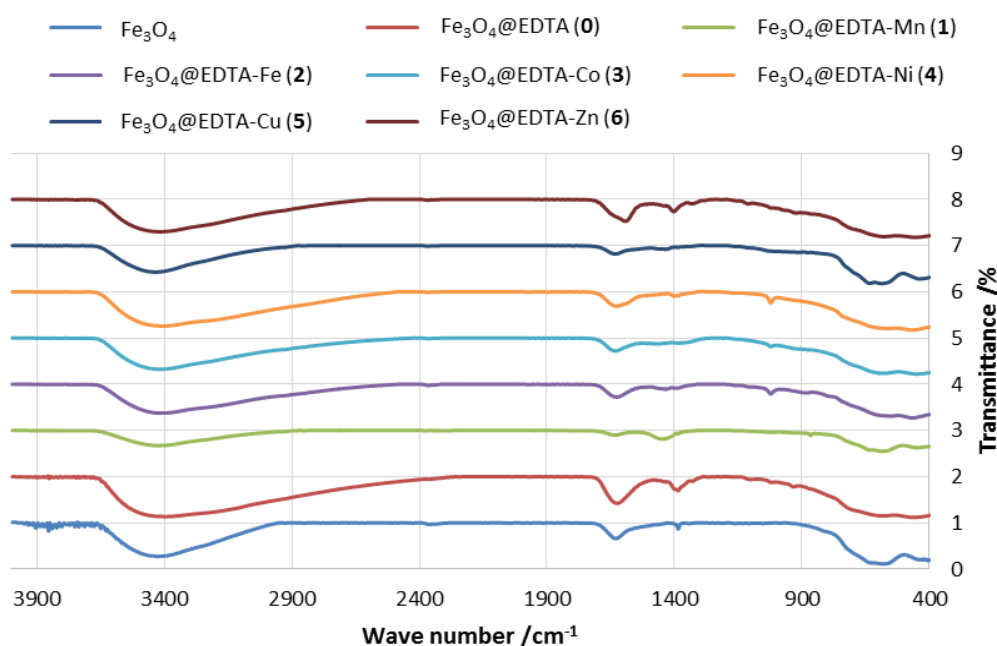


Figure S1. FT-IR spectrum of Fe_3O_4 and 0–6 MNPs in the range of 4000–400 cm^{-1} .

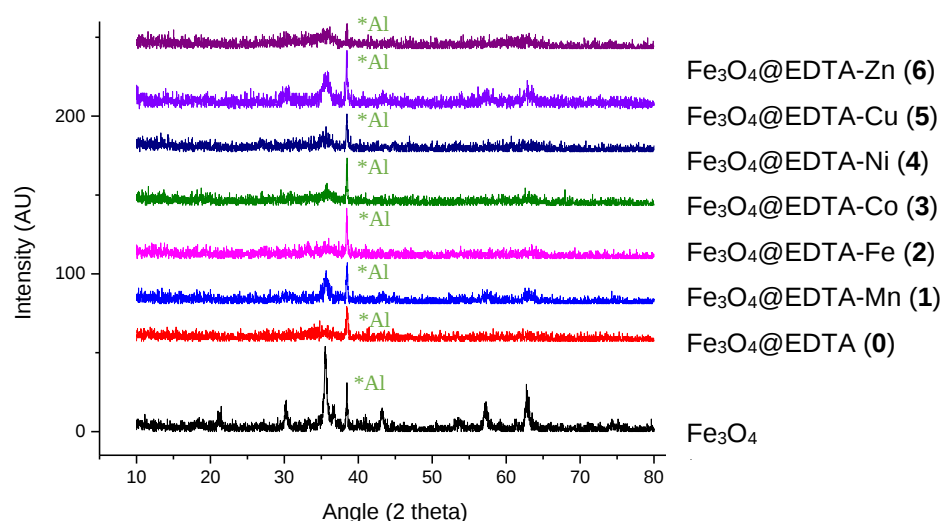


Figure S2. X-ray diffraction patterns of Fe_3O_4 and 0–6 MNPs (aluminum sample holder XRD peak marked *).

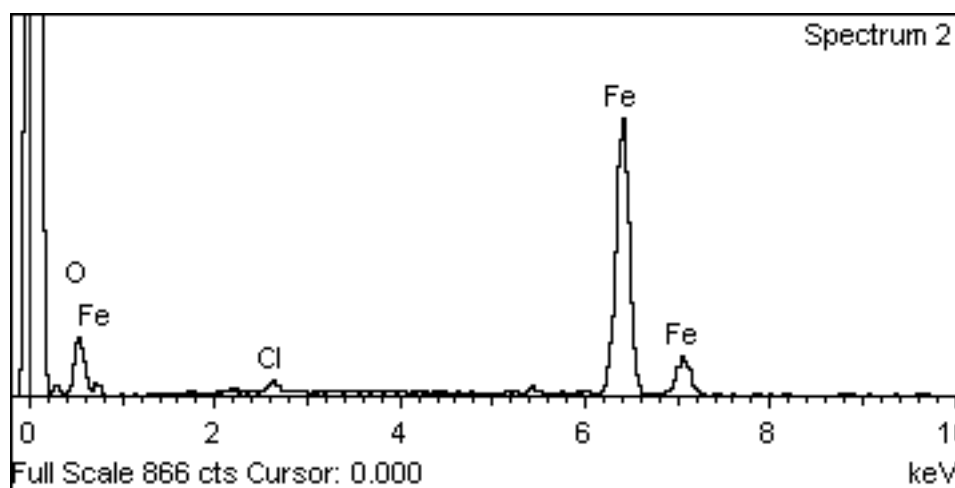


Figure S3. EDS spectrum of Fe₃O₄@EDTA (0) MNPs.

Table S1. Obtained EDS data related to Fe₃O₄@EDTA (0) MNPs.

Element	App	Intensity	Weight %	Weight %	Atomic %
	Conc.	Corrn.		Sigma	
O K	1792.93	1.3105	19.56	0.94	45.69
Cl K	62.61	0.7319	1.22	0.25	1.29
Fe K	5316.38	0.9594	79.22	0.95	53.02
Totals			100.00		

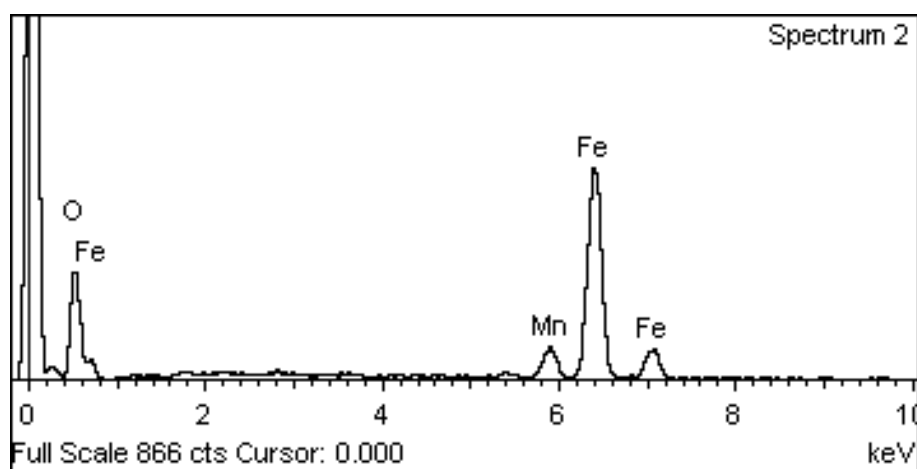


Figure S4. EDS spectrum of Fe₃O₄@EDTA-Mn²⁺ (1) MNPs.

Table S2. Obtained EDS data related to Fe₃O₄@EDTA-Mn²⁺ (1) MNPs.

Element	App	Intensity	Weight %	Weight %	Atomic %
	Conc.	Corrn.		Sigma	
O K	3992.34	1.4973	32.34	0.90	62.49
Mn K	559.39	0.9184	7.39	0.43	4.16
Fe K	4666.28	0.9392	60.27	0.88	33.36
Totals			100.00		

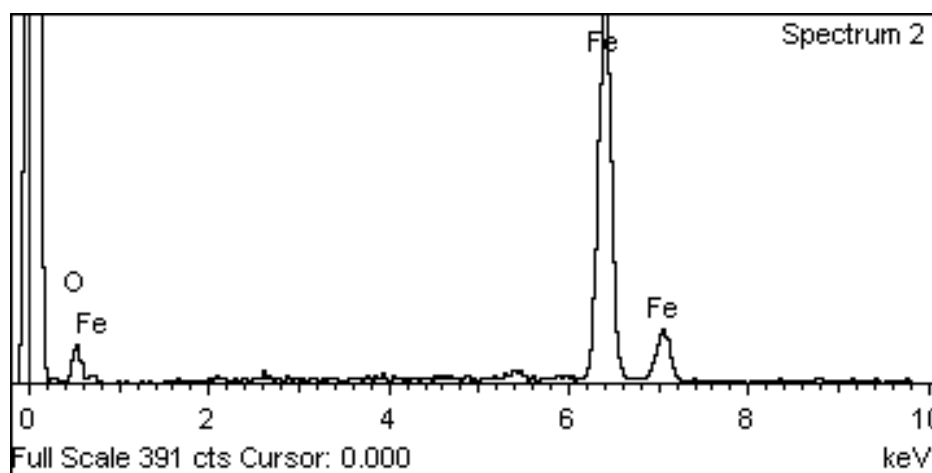


Figure S5. EDS spectrum of Fe₃O₄@EDTA-Fe²⁺ (2) MNPs.

Table S3. Obtained EDS data related to Fe₃O₄@EDTA-Fe²⁺ (2) MNPs.

Element	App	Intensity	Weight %	Weight %	Atomic %
	Conc.	Corrn.		Sigma	
O K	590.64	1.2964	11.15	0.98	30.45
Fe K	3551.20	0.9777	88.85	0.98	69.55
Totals			100.00		

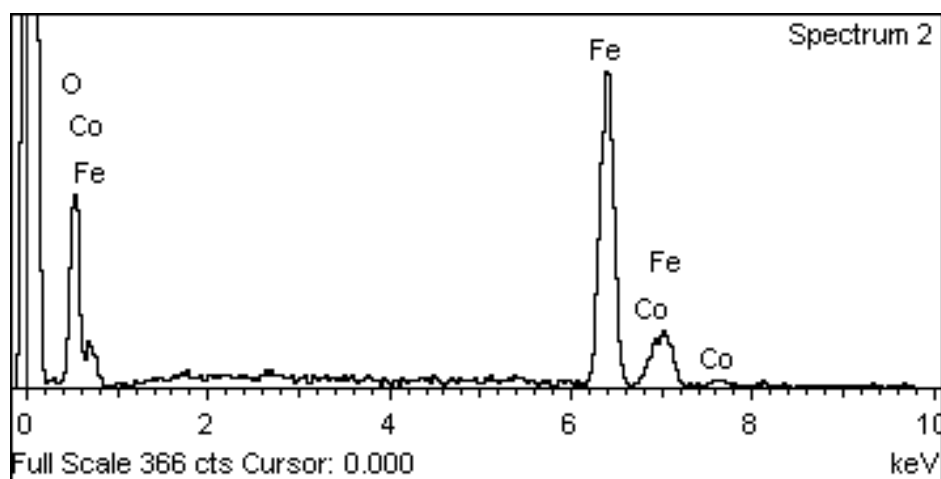


Figure S6. EDS spectrum of Fe₃O₄@EDTA-Co²⁺ (3) MNPs.

Table S4. Obtained EDS data related to Fe₃O₄@EDTA-Co²⁺ (2) MNPs.

Element	App	Intensity	Weight %	Weight %	Atomic %
	Conc.	Corrn.		Sigma	
O K	2761.02	1.5035	35.77	1.15	66.15
Fe K	2771.54	0.9321	57.92	1.16	30.68
Co K	296.01	0.9151	6.30	0.73	3.16
Totals			100.00		

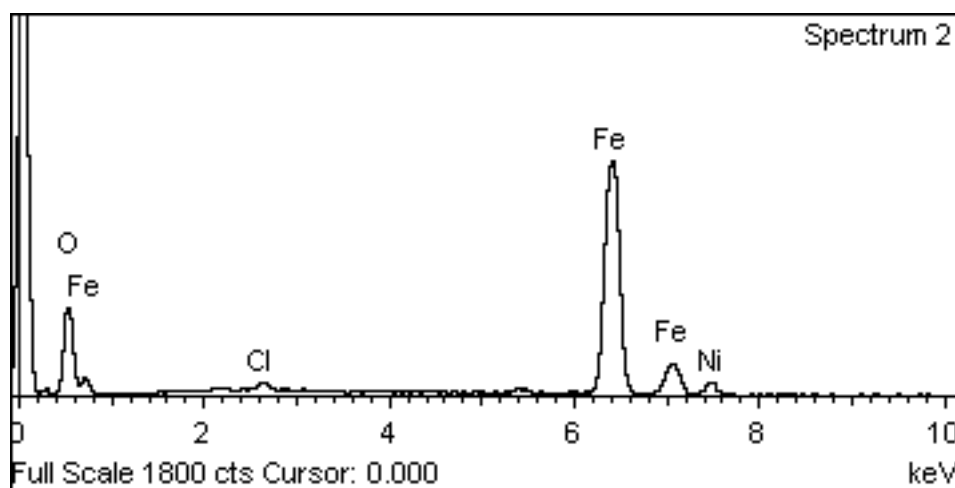


Figure S7. EDS spectrum of $\text{Fe}_3\text{O}_4\text{@EDTA-Ni}^{2+}$ (4) MNPs.

Table S5. Obtained EDS data related to $\text{Fe}_3\text{O}_4\text{@EDTA-Ni}^{2+}$ (4) MNPs.

Element	App	Intensity	Weight %	Weight %	Atomic %
	Conc.	Corrn.		Sigma	
O K	6561.07	1.3710	28.85	0.62	58.47
Cl K	131.65	0.7321	1.08	0.16	0.99
Fe K	10262.76	0.9489	65.21	0.64	37.86
Ni K	667.27	0.8289	4.85	0.32	2.68
Totals			100.00		

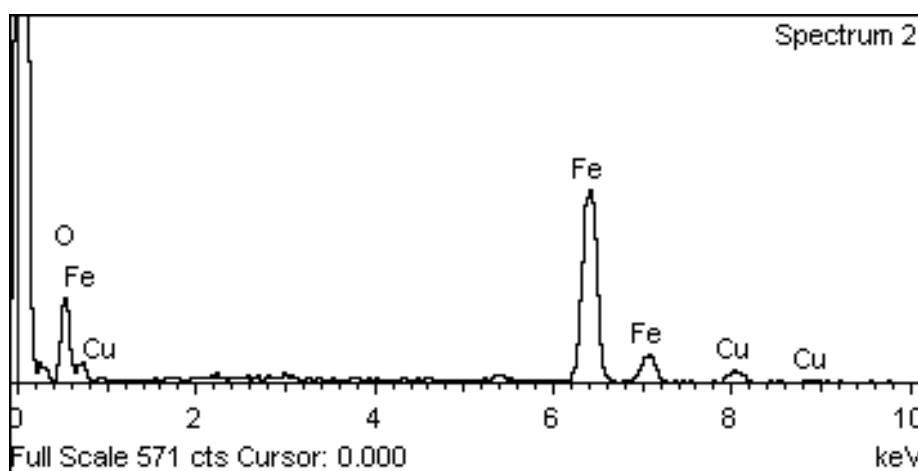


Figure S8. EDS spectrum of $\text{Fe}_3\text{O}_4\text{@EDTA-Cu}^{2+}$ (5) MNPs.

Table S6. Obtained EDS data related to $\text{Fe}_3\text{O}_4\text{@EDTA-Cu}^{2+}$ (5) MNPs.

Element	App	Intensity	Weight %	Weight %	Atomic %
	Conc.	Corrn.		Sigma	
O K	2142.26	1.4284	31.55	1.16	61.95
Fe K	2790.08	0.9484	61.90	1.18	34.81
Cu K	253.17	0.8134	6.55	0.70	3.24
Totals			100.00		

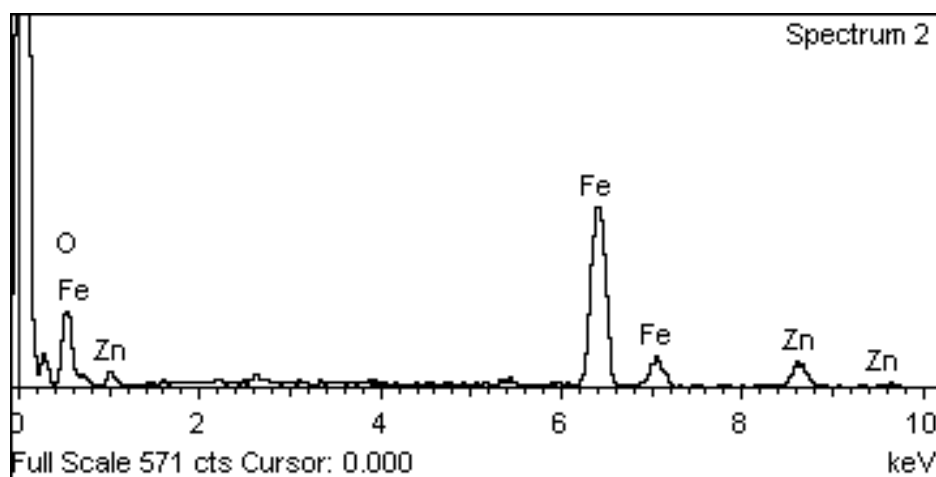


Figure S9. EDS spectrum of $\text{Fe}_3\text{O}_4\text{@EDTA-Zn}^{2+}$ (6) MNPs.

Table S7. Obtained EDS data related to $\text{Fe}_3\text{O}_4\text{@EDTA-Zn}^{2+}$ (6) MNPs.

Element	App	Intensity	Weight %	Weight %	Atomic %
	Conc.	Corrn.		Sigma	
O K	1940.30	1.3164	30.10	1.25	60.80
Fe K	2583.99	0.9588	55.03	1.23	31.85
Zn K	613.87	0.8426	14.88	0.97	7.35
Totals			100.00		

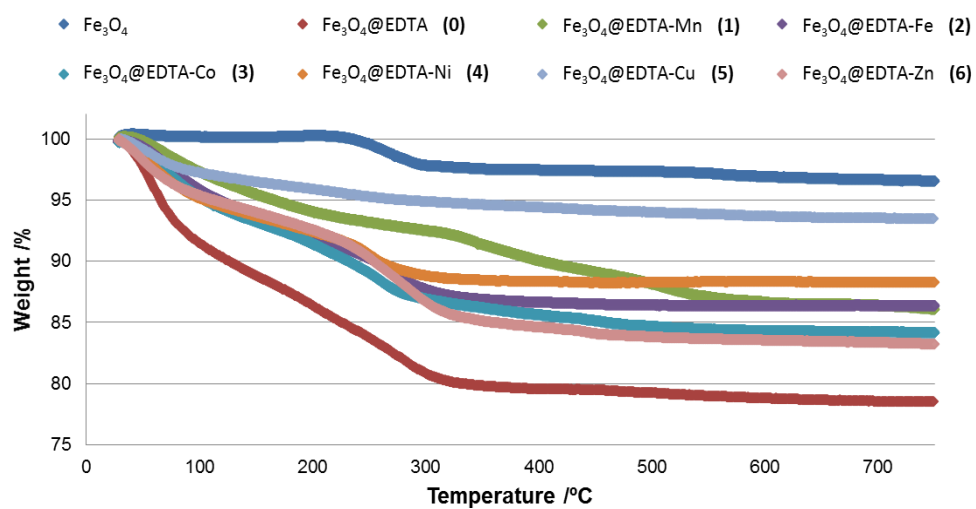


Figure S10. TGA analysis of Fe_3O_4 and 0–6 MNPs.

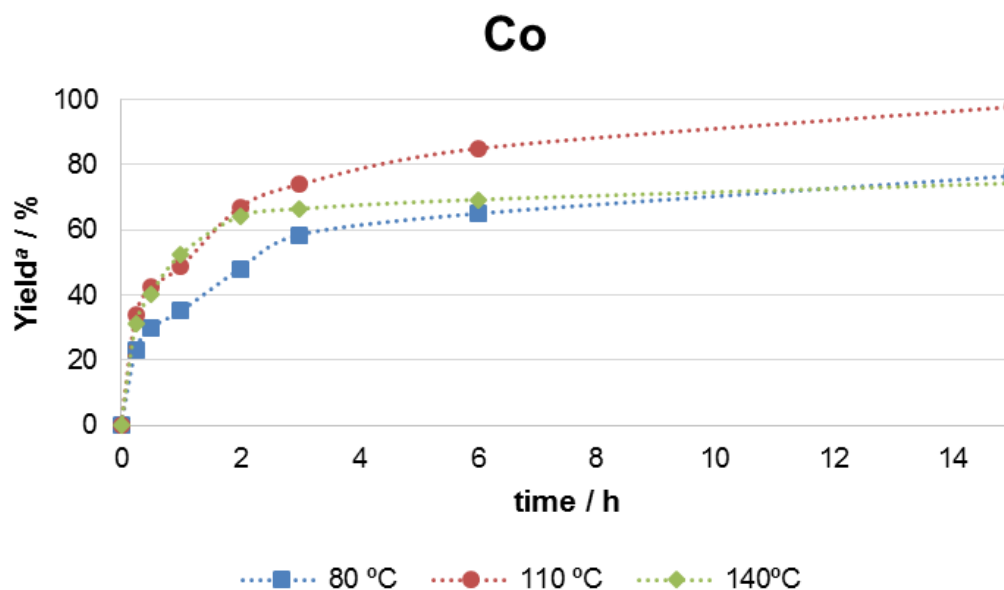


Figure S11. Acetophenone yields vs. reaction time in the solvent-free traditional heating oxidation of 1-phenylethanol using $\text{Fe}_3\text{O}_4\text{@EDTA-Co}^{2+}$ (3) as catalyst. Reaction conditions: catalyst (30 mg), 1-phenylethanol (2.5 mmol), *t*-BuOOH 70% (5.0 mmol). ^a Moles of acetophenone per 100 mol of 1-phenylethanol (GC yield), >99% selectivity.

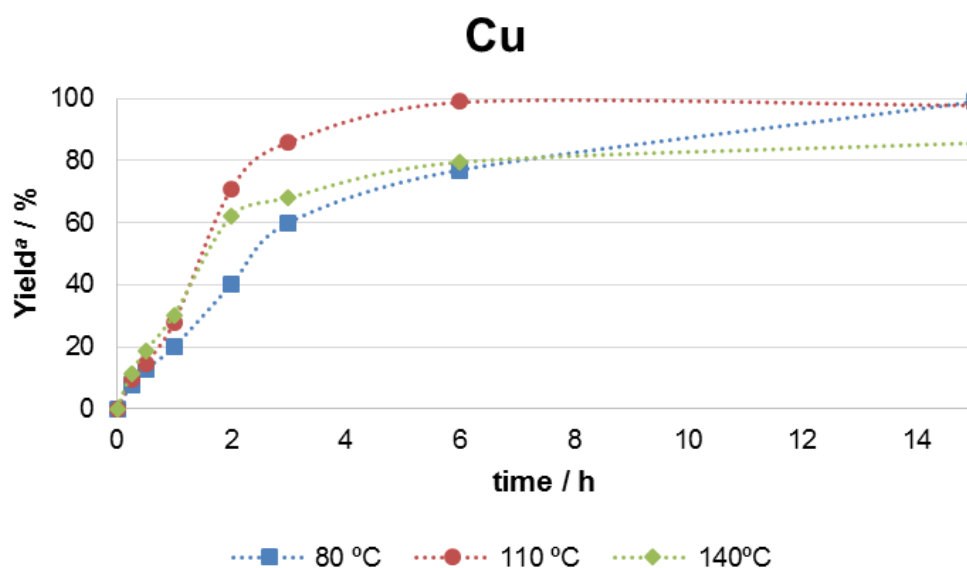


Figure S12. Acetophenone yields vs. reaction time in the solvent-free traditional heating oxidation of 1-phenylethanol using $\text{Fe}_3\text{O}_4\text{@EDTA-Cu}^{2+}$ (5) as catalyst. Reaction conditions: catalyst (30 mg), 1-phenylethanol (2.5 mmol), *t*-BuOOH 70% (5.0 mmol). ^a Moles of acetophenone per 100 mol of 1-phenylethanol (GC yield), >99% selectivity.

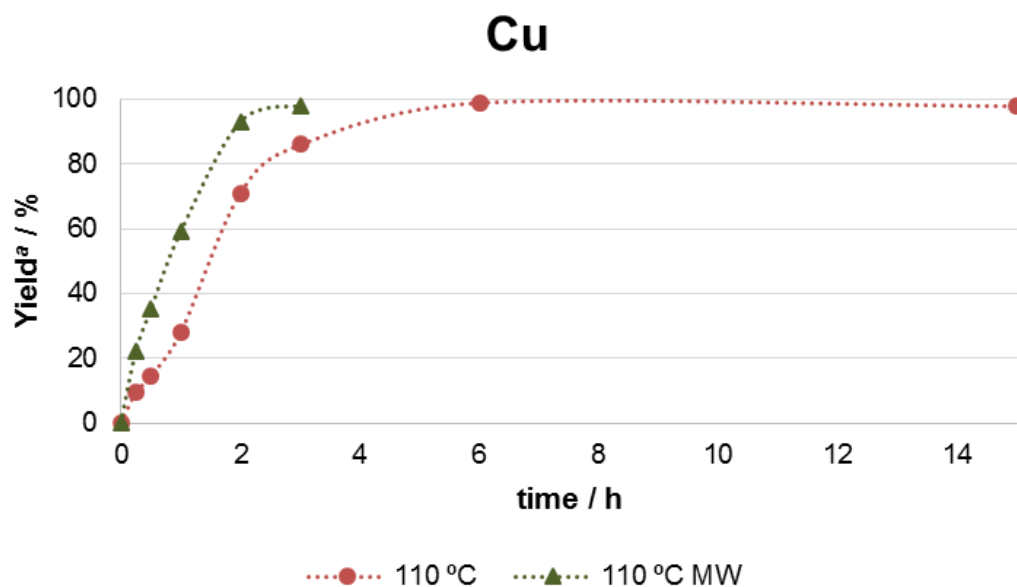


Figure S13. Acetophenone yields vs. reaction time in the solvent-free traditional heating and MW-assisted oxidation of 1-phenylethanol using $\text{Fe}_3\text{O}_4\text{@EDTA-Cu}^{2+}$ (5) as catalyst. Reaction conditions: catalyst (30 mg), 1-phenylethanol (2.5 mmol), *t*-BuOOH 70% (5.0 mmol), $T = 110\text{ }^\circ\text{C}$. ^a Moles of acetophenone per 100 mol of alcohol substrate (GC yield), >99% selectivity.

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