

# Magnetically Induced Iron-Catalyzed Hydrodeoxygenation of Benzylic Esters and Polyesters

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## Highlights

- ICNPs are active and selective for the hydrodeoxygenation of benzylic esters to tolyl derivatives using mild H<sub>2</sub> pressure
- ICNPs catalysts are stable under magnetic induction heating and adaptive to fluctuations in electricity supply
- Versatile approach, showcased with the selective depolymerization of real PET waste

## 1. Introduction

The exhaustive reduction of esters all the way to methyl-containing compounds is challenging but of fundamental importance to enable degradation and recycling of polyesters, as well as to synthesize methyl and tolyl derivatives in synthetic chemistry.<sup>[1-2]</sup> However, this transformation is typically carried out following non-sustainable pathways employing excess of strong and often hazardous reducing agents (e.g. metal hydrides, hydrosilanes, ammonia borane) under harsh conditions.<sup>[2-3]</sup> As a result, the development of catalytic and atom-economical ester reduction pathways using H<sub>2</sub> as a reducing agent under mild conditions is highly desired, but remains a challenge. In this context, we explore here the possibility to achieve selective ester reduction with H<sub>2</sub> using iron-based nanoparticles (NPs) with magnetic heating capabilities.<sup>[4]</sup> Indeed, magnetic induction heating has been demonstrated by our group and others to heat suitable catalyst materials in a very rapid, localized, and energy efficient manner.<sup>[5-7]</sup> In particular, this technology obviates the necessity of heating the entire reactor environment, potentially leading to lower overall process temperatures and reduced energy consumption. In the present work, we prepare and characterize iron carbide nanoparticles (ICNPs) with exceptional induction heating capabilities, and apply them to the magnetically induced reduction of esters using H<sub>2</sub>.

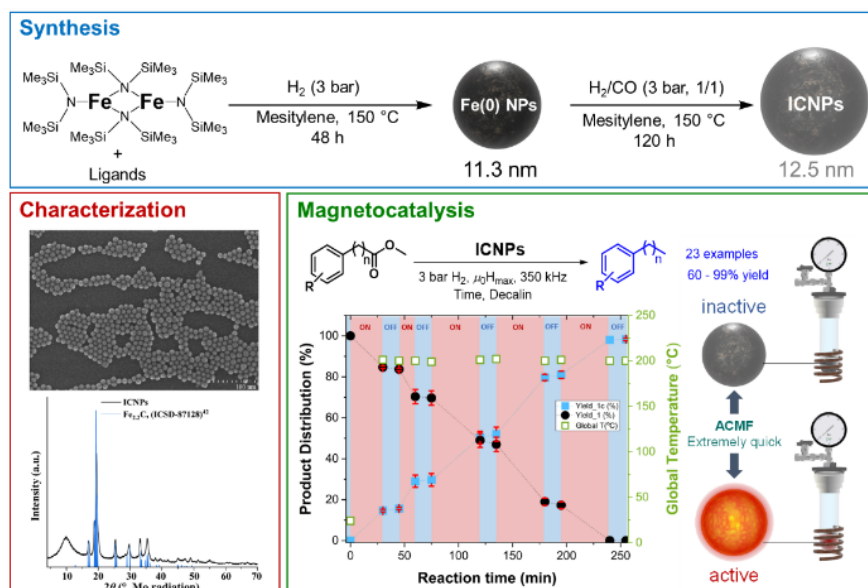
## 2. Methods

Iron carbide nanoparticles (ICNPs) were prepared following an organometallic approach,<sup>[6]</sup> and characterized by various techniques including electron microscopy, XRD, Mössbauer spectroscopy, vibrating sample magnetometry. These nanoparticles exhibit excellent heating power under an alternating current magnetic field (ACMF) (specific absorption rate (SAR) of ca. 2500 W g<sup>-1</sup> at  $f = 100$  kHz and  $\mu_0 H_{\max} = 66$  mT). The catalytic performance of ICNPs was investigated for the hydrodeoxygenation of methyl benzoate to toluene as a model reaction. Catalytic experiments were conducted under batch conditions using Fisher-Porter bottles as reactors placed inside a commercial coil for the generation of the ACMF. The reactions were started by switching on the ACMF generator to a standard set of parameters ( $f = 350$  kHz,  $\mu_0 H_{\max} = 70$  mT). An infrared camera was used to determine the “global temperature” reached by the Fisher-Porter bottle as a result of the dissipation of thermal energy from the ICNP catalyst under the reaction conditions. For reactions conducted under conventional heating, the reaction time monitoring was started once the reaction solution reached the desired temperature. No stirring was implemented, and mixing was ensured only through convection.

## 3. Results and discussion

Activated by magnetic induction, ICNPs reached high local temperatures (estimated to ca. 330 °C) and exhibited high activity, selectivity, and stability for the reduction of a large scope of esters (including PET models) under mild reactor conditions (3 bar H<sub>2</sub>, 200 °C).<sup>[4]</sup> Strikingly, ICNPs heated conventionally at 200 °C showed no activity. The catalyst's adaptivity to intermittent power supply was

demonstrated by regularly stopping and re-starting the AC magnetic field. This work may pave the way toward a greatly enhanced practical implementation of ester reduction in research and industry, and demonstrates more generally the broad potential of the emerging field of magnetically induced catalysis for synthetic transformations typically requiring demanding operating conditions (Figure 1).



**Figure 1.** Illustration of the approach, with the synthesis of ICNPs, their characterization, and their application to the magnetically induced catalytic reduction of benzylic esters.

#### 4. Conclusions

ICNPs are heated locally at high temperature by magnetic induction to catalyze the hydrodeoxygenation of benzylic esters in a highly active and selective manner, paving the way toward valuable synthetic pathways to methyl-substituted aromatic compounds under mild H<sub>2</sub> pressure (3 bar) and moderate reactor temperature (ca. 200 °C). ICNPs show excellent stability under magnetocatalytic conditions, superior energy efficiency, and adaptivity to intermittent power supply as provided by renewable energies. This work may pave the way toward practical ester and polyester hydrodeoxygenation with magnetically activated earth-abundant Fe-based catalysts using renewable H<sub>2</sub> at the laboratory and production scales. In addition, the observed chemical and process benefits are of significant general interest, further encouraging the exploration of the emerging field of magnetically induced catalysis in research and industry.

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#### Keywords

magnetically induced catalysis; iron carbide nanoparticles; ester hydrodeoxygenation ; PET recycling