

## Unprecedented synthesis of iron NHC complexes by C-H activation of imidazolium salts. Mild catalysts for reduction of sulfoxides

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### Electronic Supplementary Information:

#### Preparation of (Cp\*-NHC)Fe(CO)I (**3**) (Cp\* = $\eta^5$ -C<sub>5</sub>Me<sub>4</sub>)

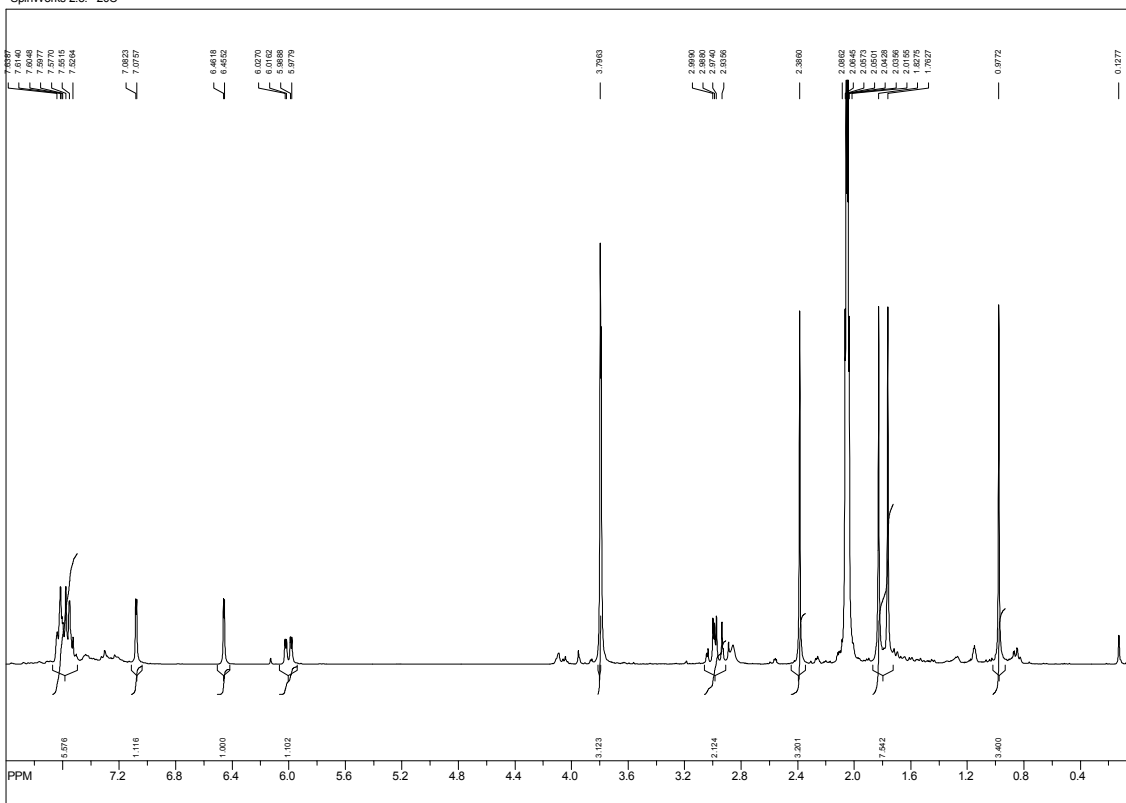
A mixture of proligand **1** (600 mg, 1.38 mmol) and Fe<sub>3</sub>(CO)<sub>12</sub> (180 mg, 0.46 mmol) is refluxed in toluene (15 mL) overnight. Filtration and removal of the toluene gave a green solid, which was washed with hexane to yield the iron complex **3** (523 mg, 0.94 mmol, 85 %).

#### Preparation of (Cp-NHC)Fe(CO)I (**4**) (Cp = $\eta^5$ -C<sub>5</sub>H<sub>4</sub>)

This was obtained following a similar procedure using proligand **2** (600 mg, 1.38 mmol) and Fe<sub>3</sub>(CO)<sub>12</sub> (180 mg, 0.46 mmol). Yield 83 %.

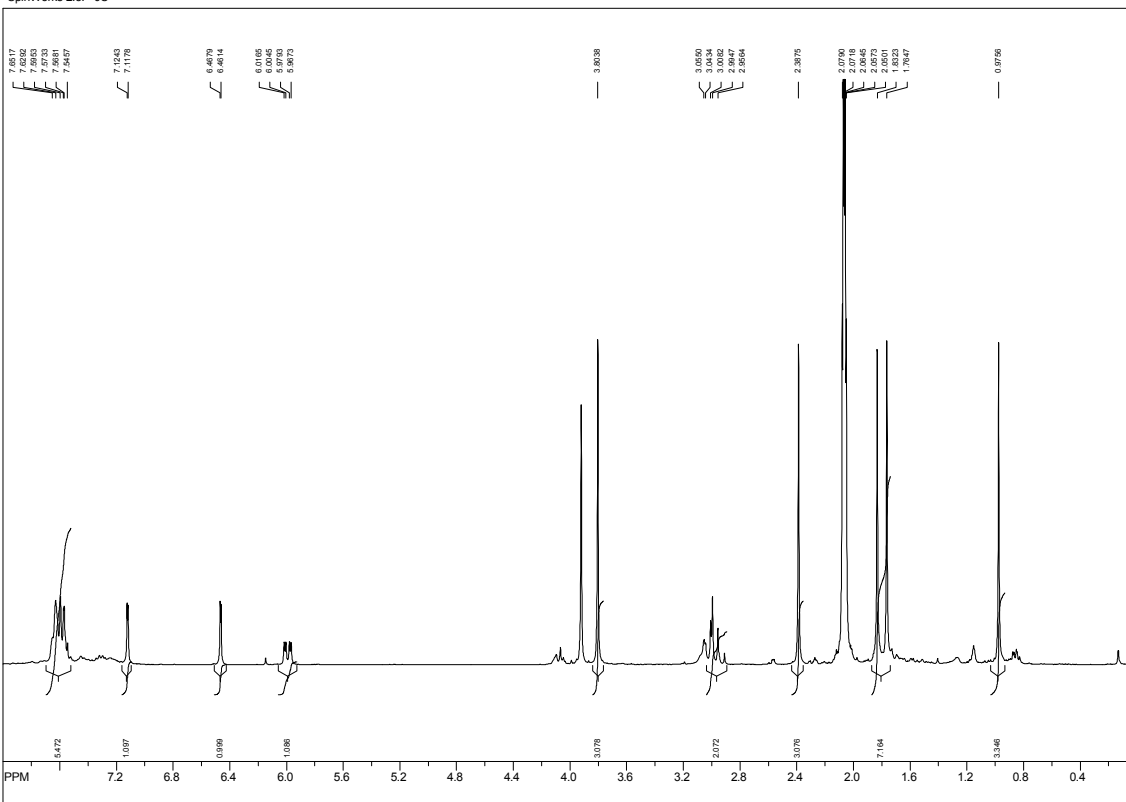
### $^1\text{H}$ NMR spectrum of **3** at 20 °C in acetone- $\text{d}_6$

SpinWorks 2.5: 20C



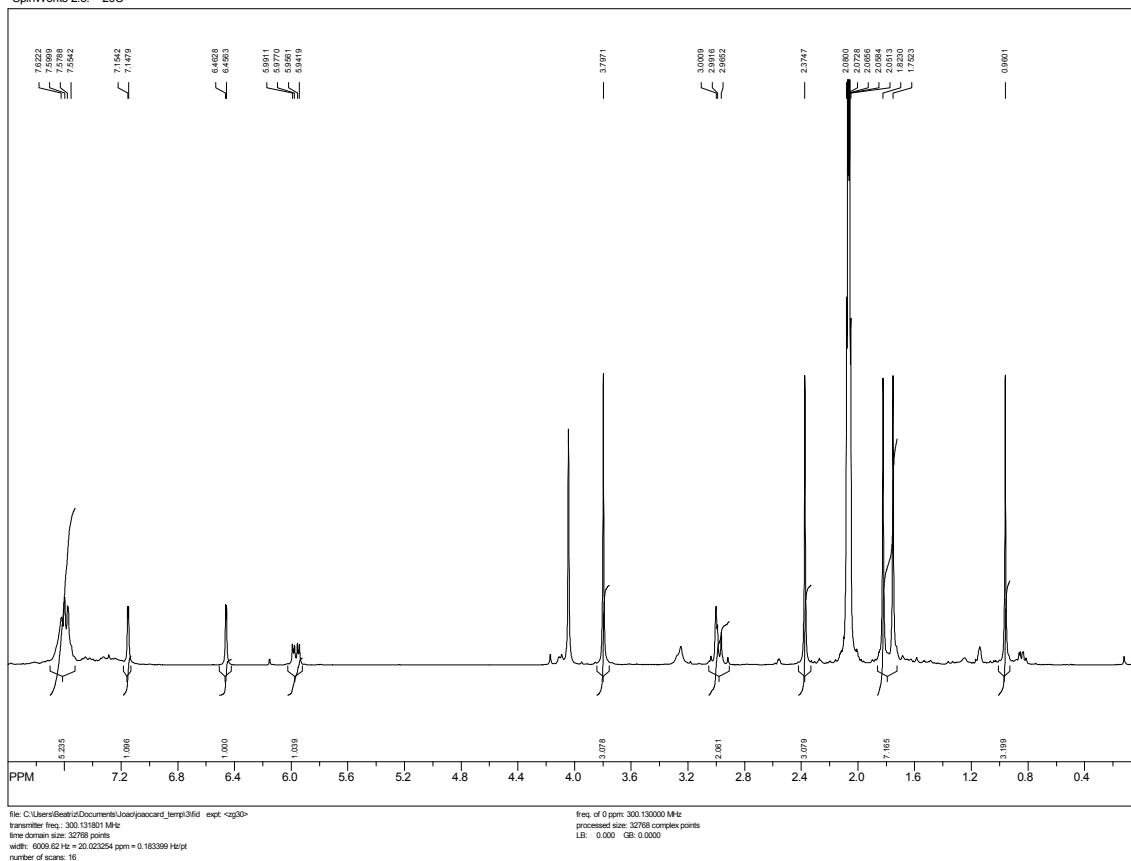
### $^1\text{H}$ NMR spectrum of **3** at 0 °C in acetone- $\text{d}_6$

SpinWorks 2.5: 0C



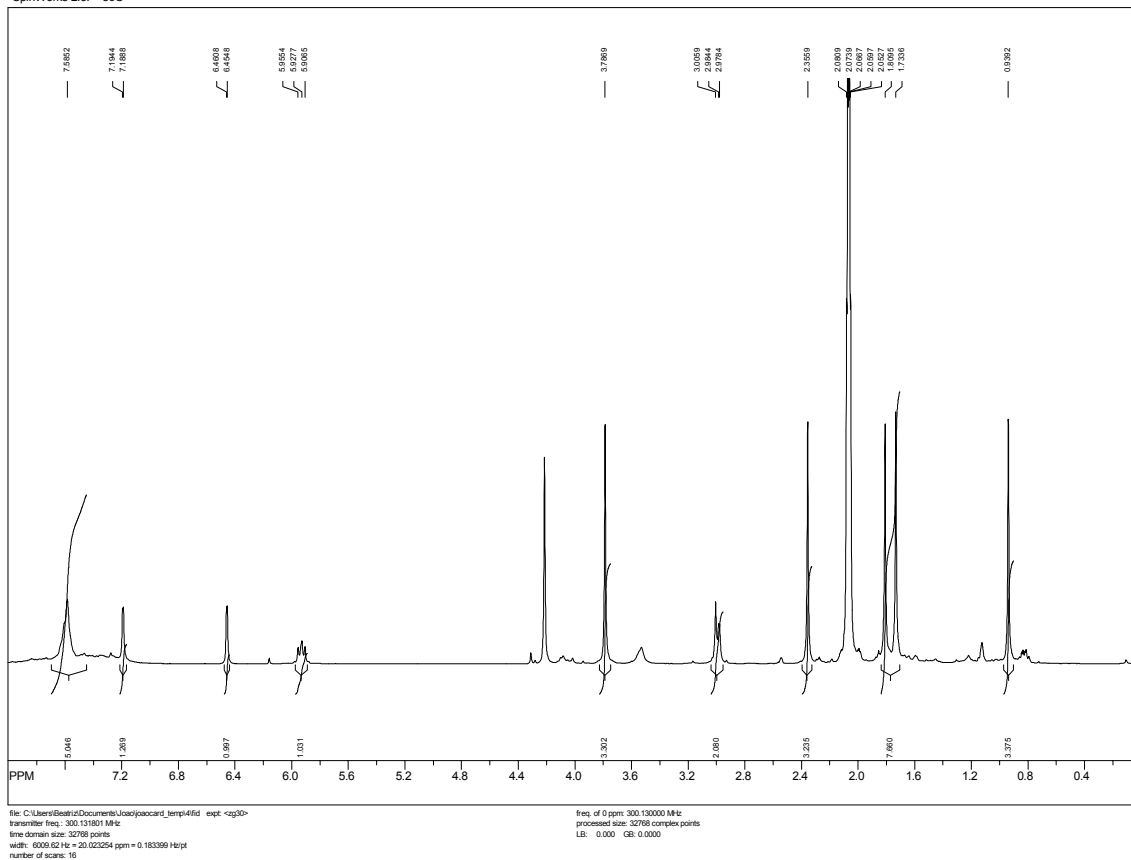
### <sup>1</sup>H NMR spectrum of **3** at -20 °C in acetone-d<sub>6</sub>

SpinWorks 2.5: -20C



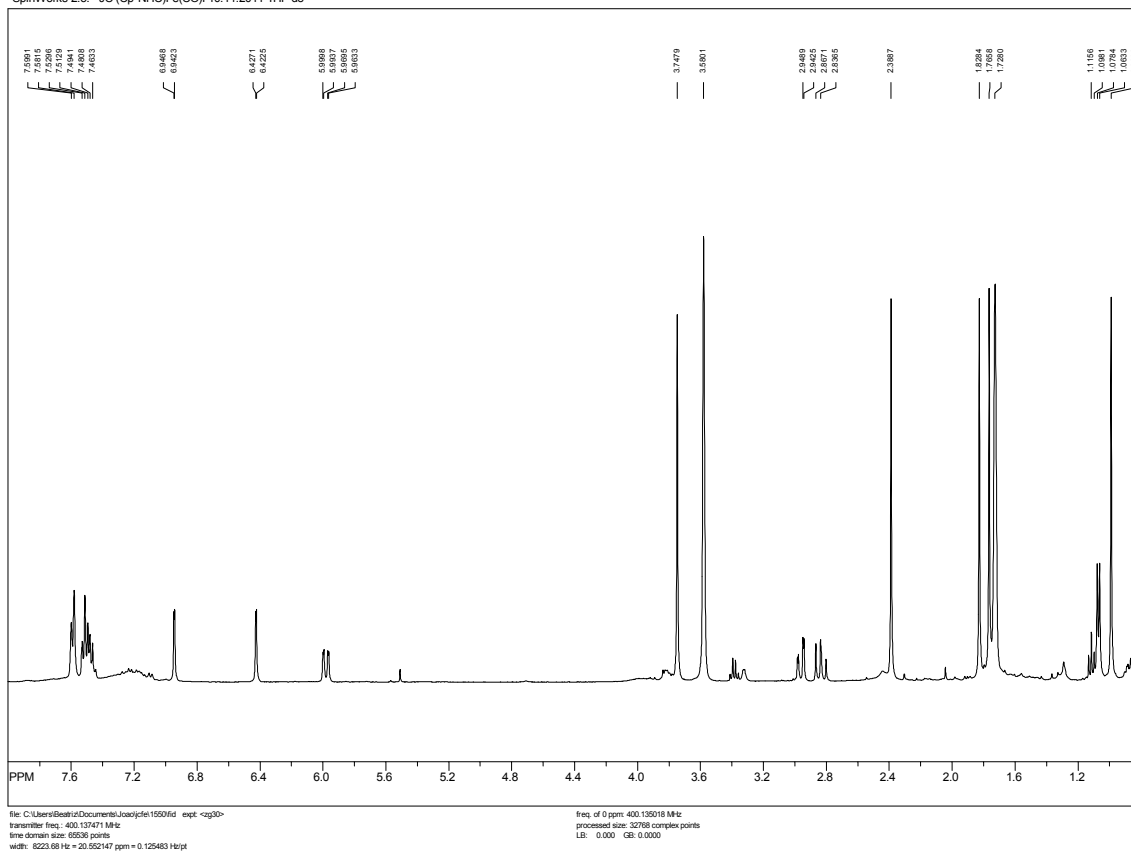
### <sup>1</sup>H NMR spectrum of **3** at -50 °C in acetone-d<sub>6</sub>

SpinWorks 2.5: -50C



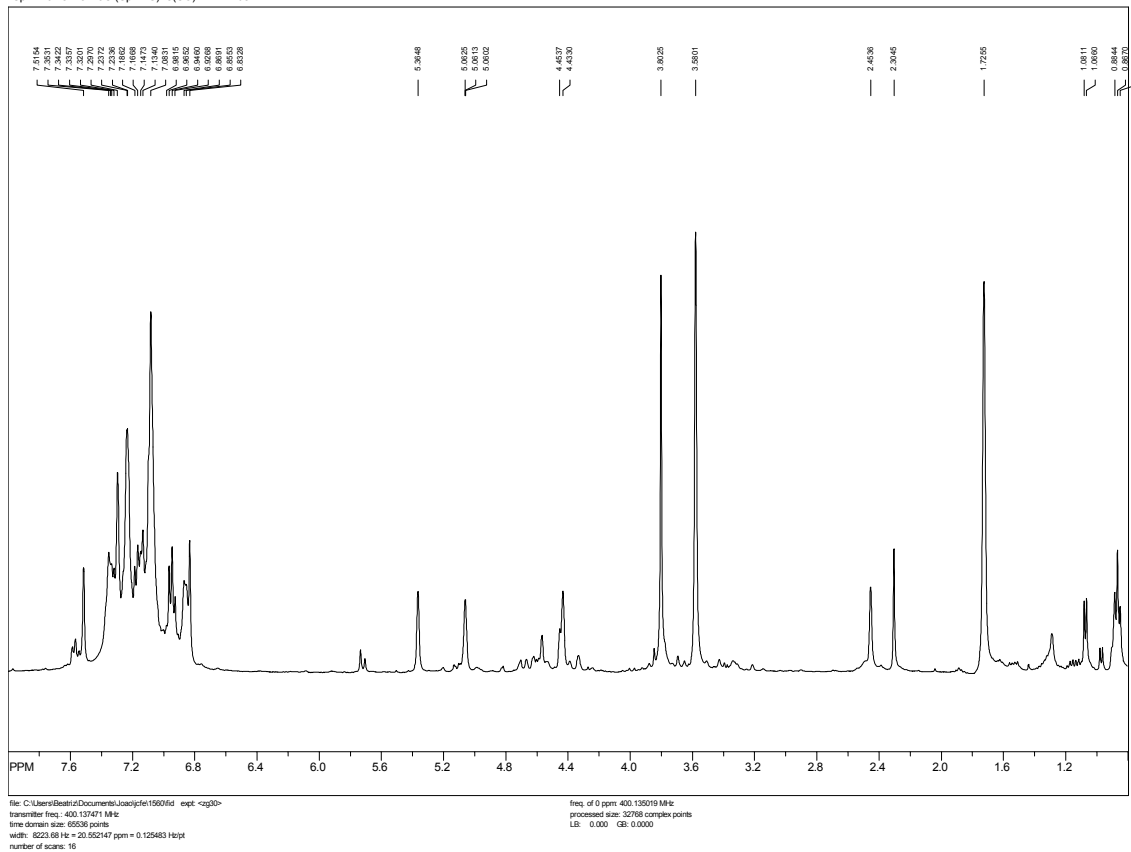
### <sup>1</sup>H NMR spectra of **3** in THF-d<sub>8</sub> at 25 °C

SpinWorks 2.5: JC (Cp\*NHC)Fe(CO) 10.11.2011 THF-d8



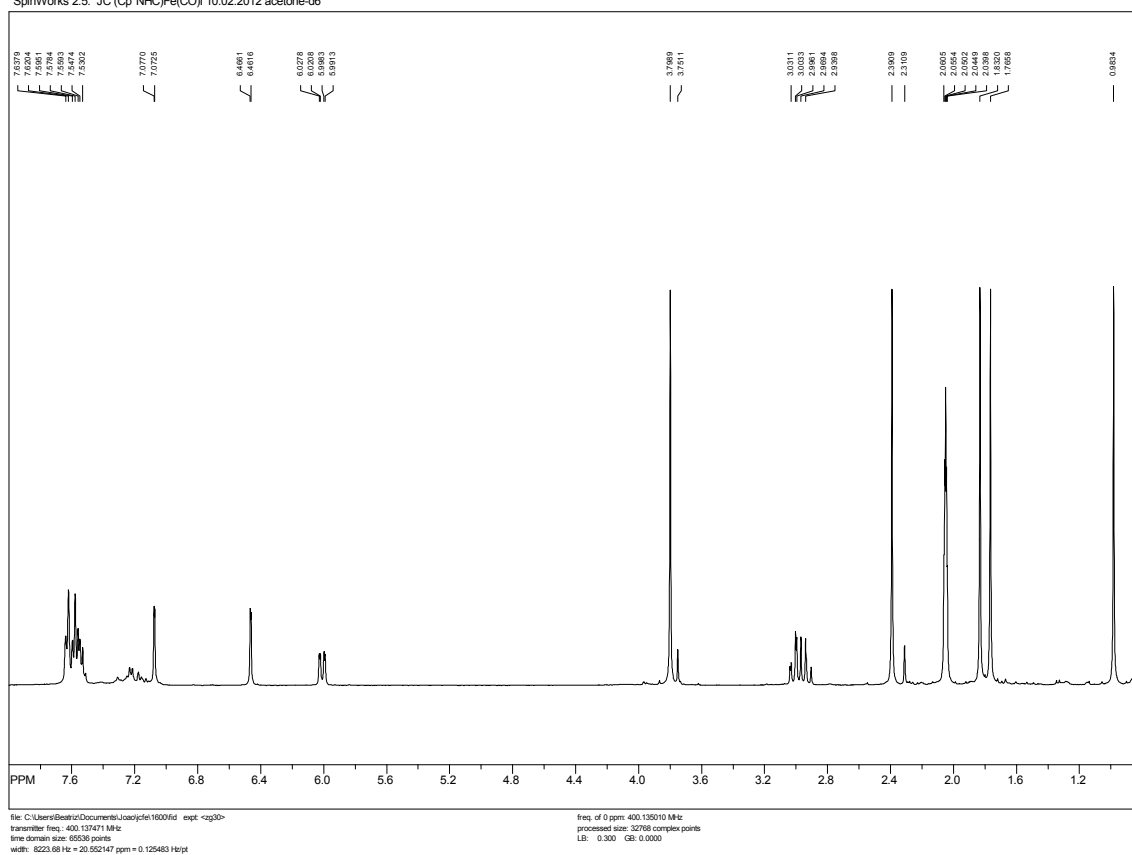
### <sup>1</sup>H NMR spectra of **4** in THF-d<sub>8</sub> at 25 °C

SpinWorks 2.5: JC (Cp\*NHC)Fe(CO) in THF-d8



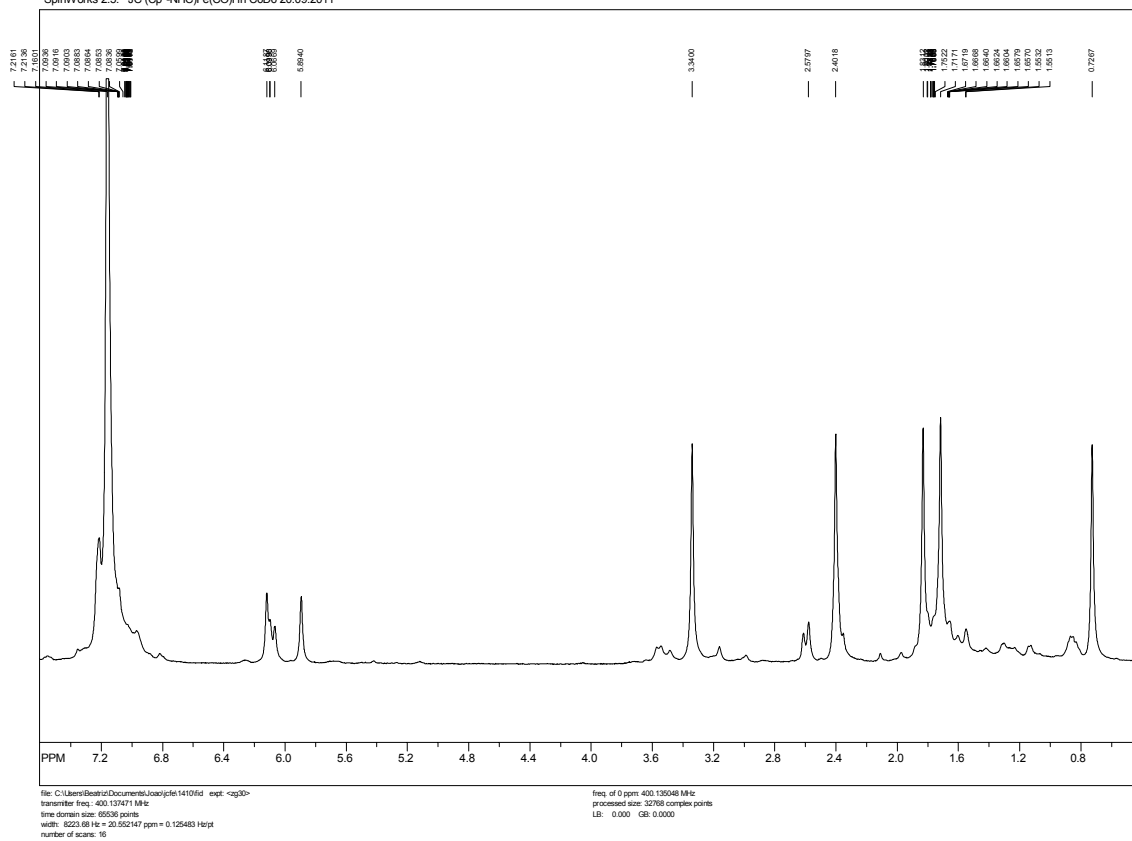
### $^1\text{H}$ NMR spectra of **3** in acetone- $d_6$ at 25 °C

SpinWorks 2.5: JC (Cp\* $\text{NHC}$ )Fe(CO) 10.02.2012 acetone- $d_6$



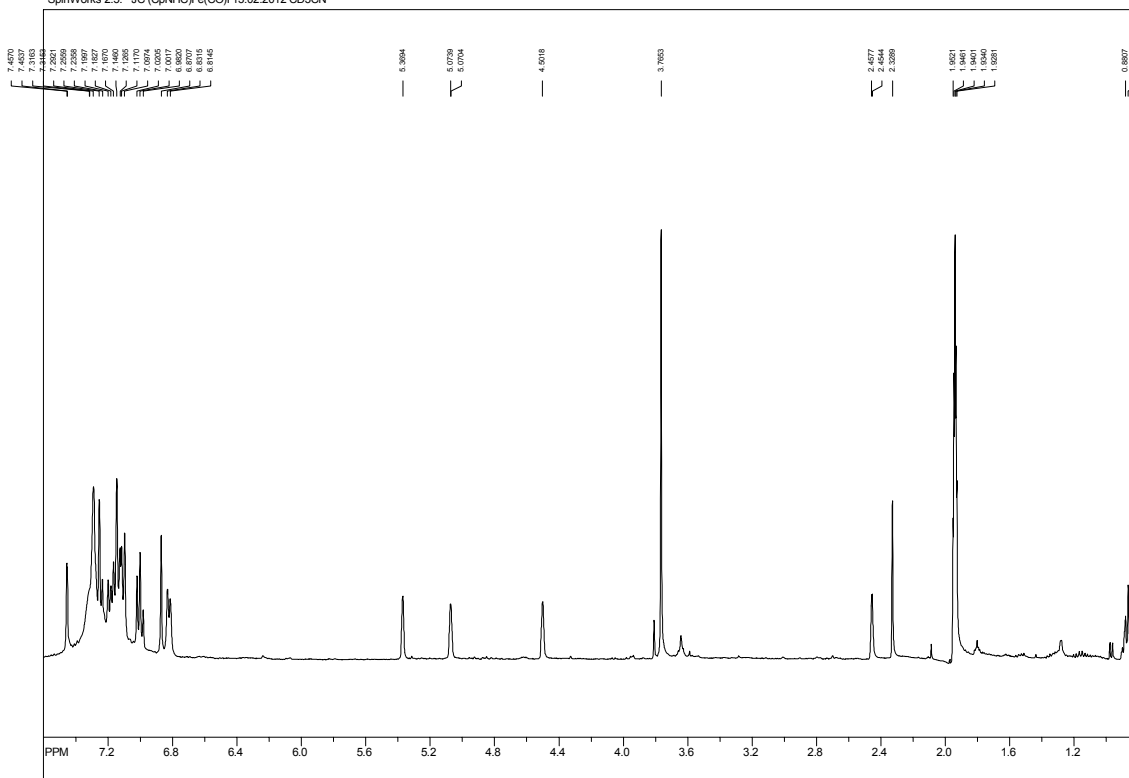
### $^1\text{H}$ NMR spectra of **3** in $\text{C}_6\text{D}_6$ at 25 °C

SpinWorks 2.5: JC (Cp\* $\text{NHC}$ )Fe(CO) in  $\text{C}_6\text{D}_6$  20.09.2011



# <sup>1</sup>H NMR spectra of 4 in NMe-d<sub>3</sub> at 25 °C

SpinWorks 2.5: JC (Cp)H(C)Fe(CO) 13.02.2012 CD3CN



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time domain size: 65536 points  
width: 6223.98 Hz = 20.662147 ppm = 0.125483 Hz/pt  
number of scans: 16

freq: of 0 ppm: 400.139214 MHz  
processed size: 32768 complex points  
LB: 0.000 GB: 0.0000