Supporting Information

Figure S1. Ir L_{III}-edge XANES spectra for $(Ir^{3+})_{40}$G4OH complex and $IrCl_3$ aqueous solutions before and after reduction with $NaBH_4$.

Figure S2. CO adsorption after a) H_2 at different temperatures, b) H_2 at 400 °C for different times.

Figure S3. HRTEM micrographs and particle size distribution histograms of 1 wt.% a) Ir_{40}G4OH/γ-Al_2O_3 , b) Ir/γ-Al_2O_3 treated with reduction treatment and c) Ir_{40}G4OH/γ-Al_2O_3 , d) Ir/γ-Al_2O_3 treated with oxidation/reduction treatment.

Figure S4. Typical benzonitrile concentration versus time plot obtained for the hydrogenation of benzonitrile over supported Ir catalysts.

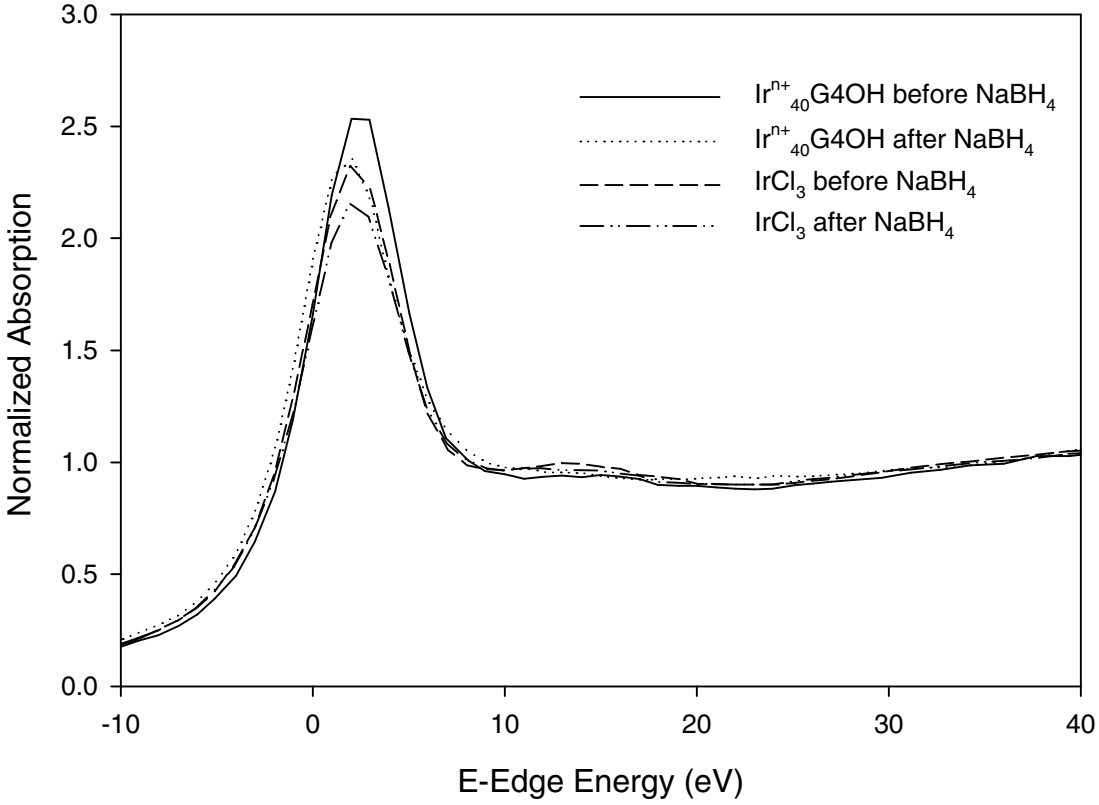

3.0
2.5
2.0
1.5
1.0
0.5
0.0
Normalized Absorption
-10
0
10
20
30
40
E-Edge Energy (eV)
Ir$^{n+}_{40}$G4OH before NaBH$_4$
Ir$^{n+}_{40}$G4OH after NaBH$_4$
IrCl$_3$ before NaBH$_4$
IrCl$_3$ after NaBH$_4$

Figure S1.

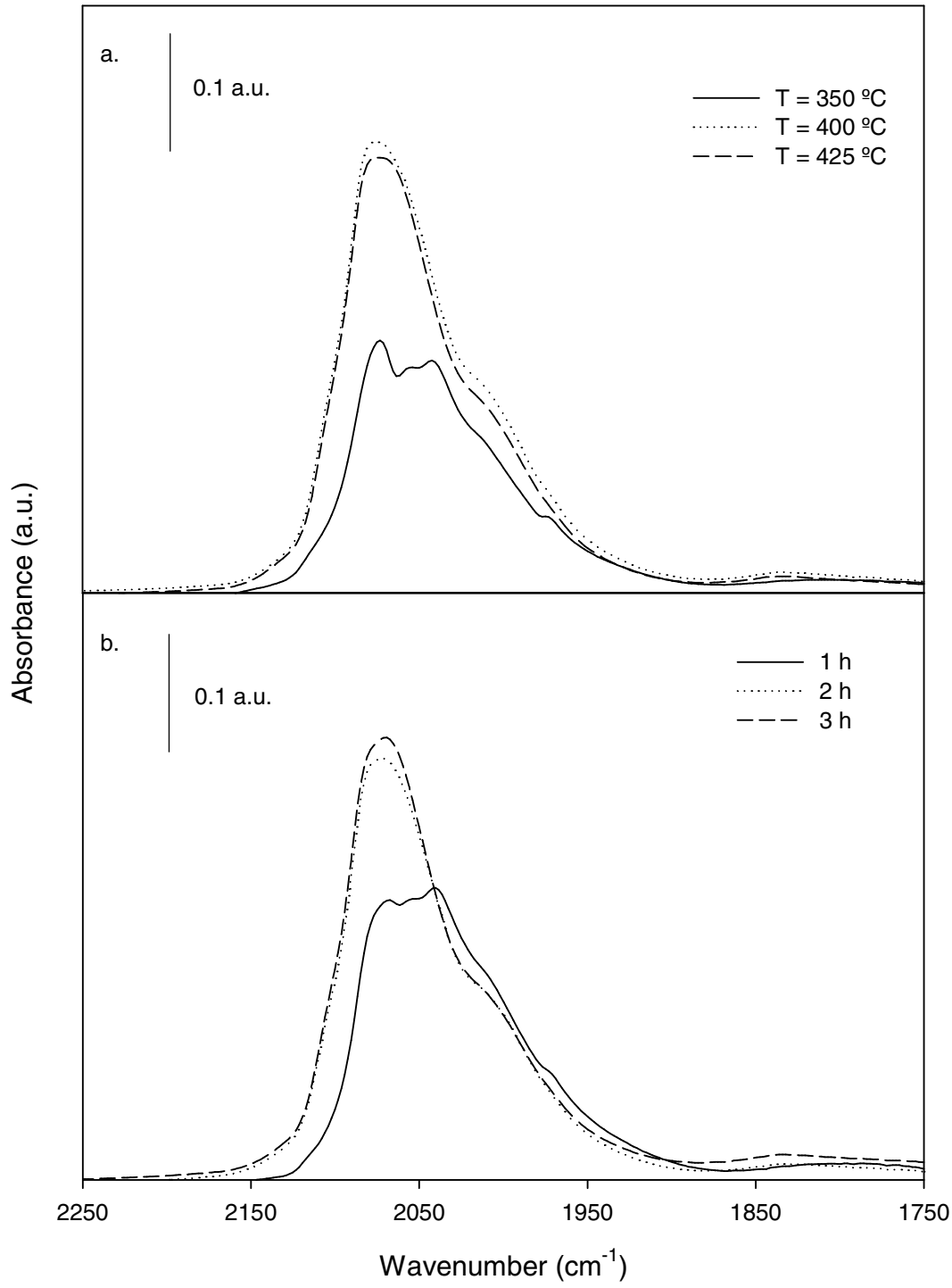

a.
0.1 a.u.
T = 350 ºC
T = 400 ºC
T = 425 ºC
b.
0.1 a.u.
1 h
2 h
3 h
Absorbance (a.u.)
2250
2150
2050
1950
1850
1750
Wavenumber (cm-1)

Figure S2.

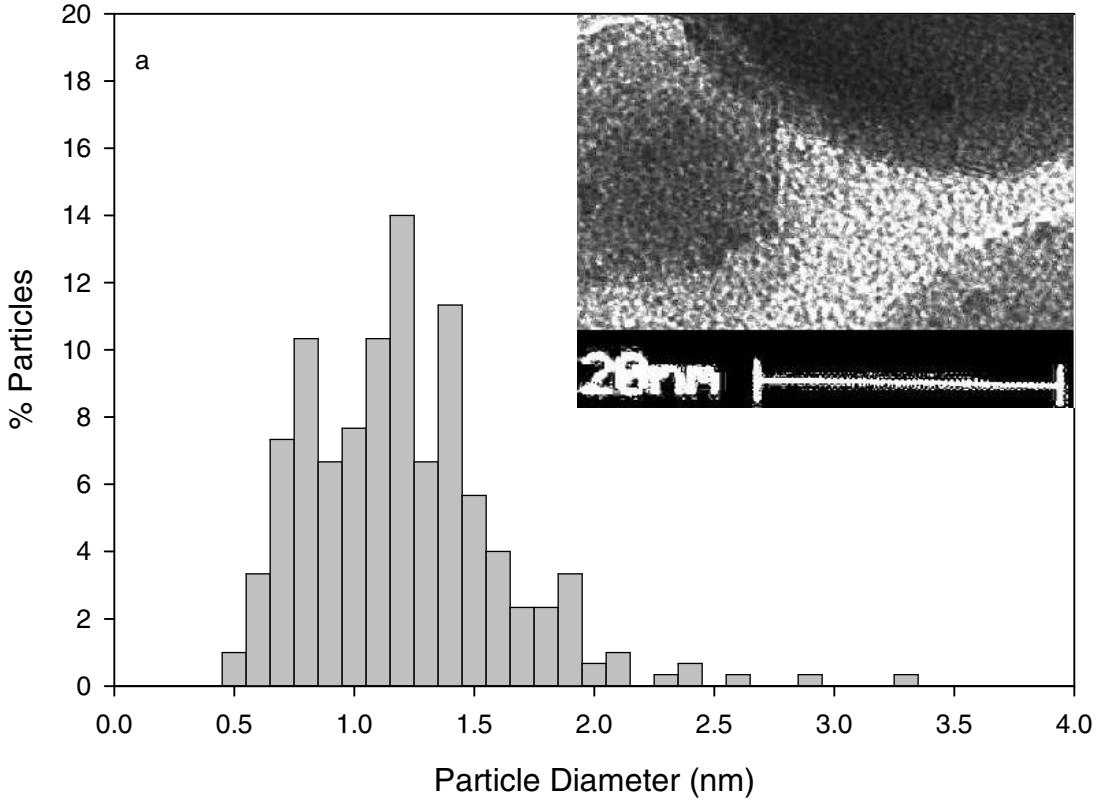

a
% Particles
Particle Diameter (nm)
0
2
4
6
8
10
12
14
16
18
20
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0

Figure S3.

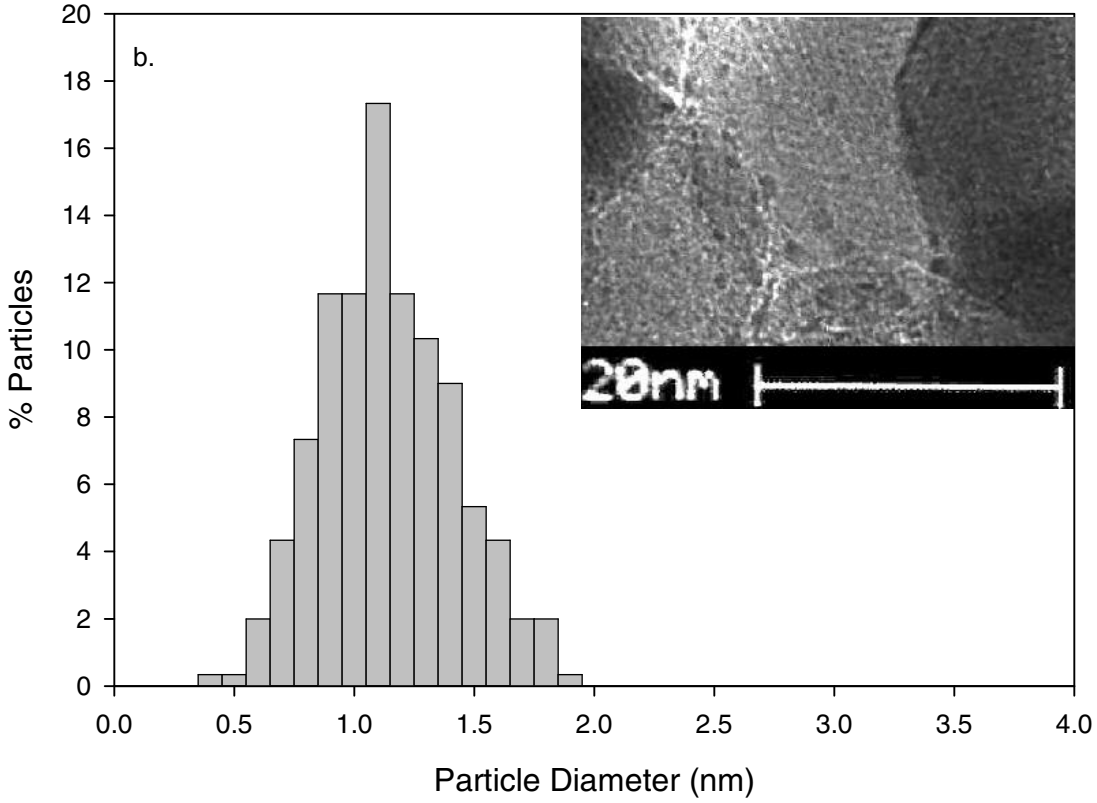


Figure S3. (cont.)

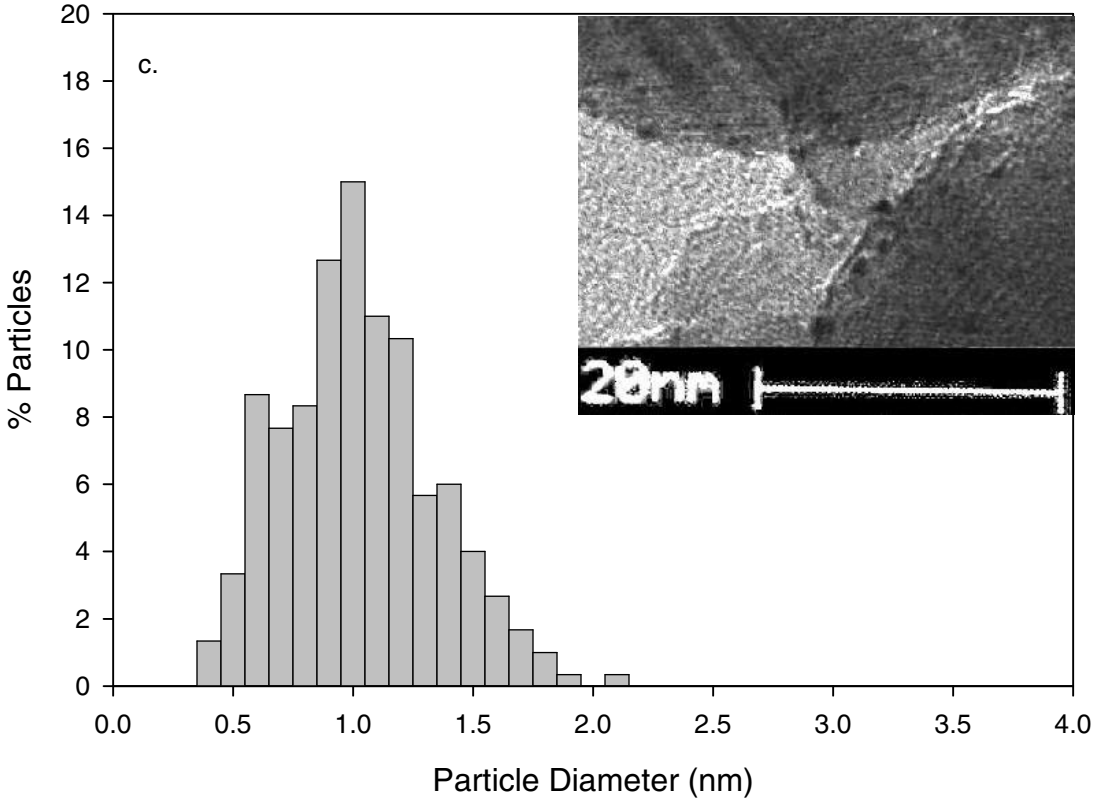


Figure S3. (cont.)

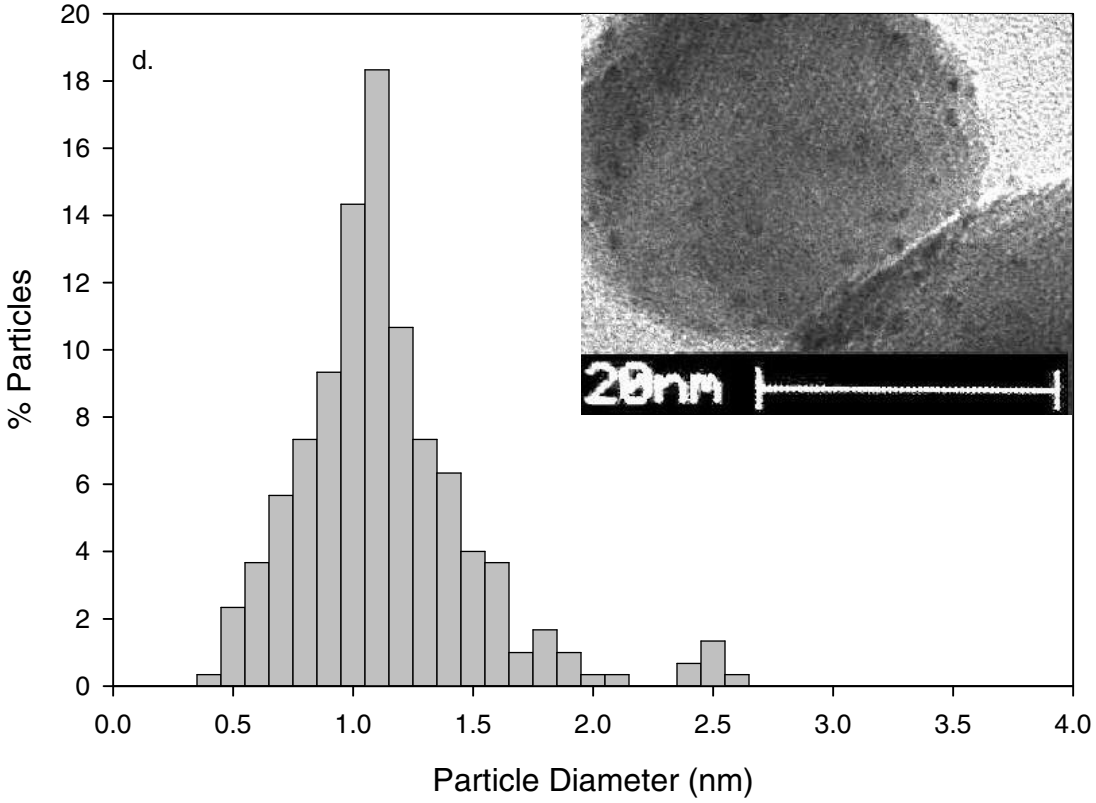
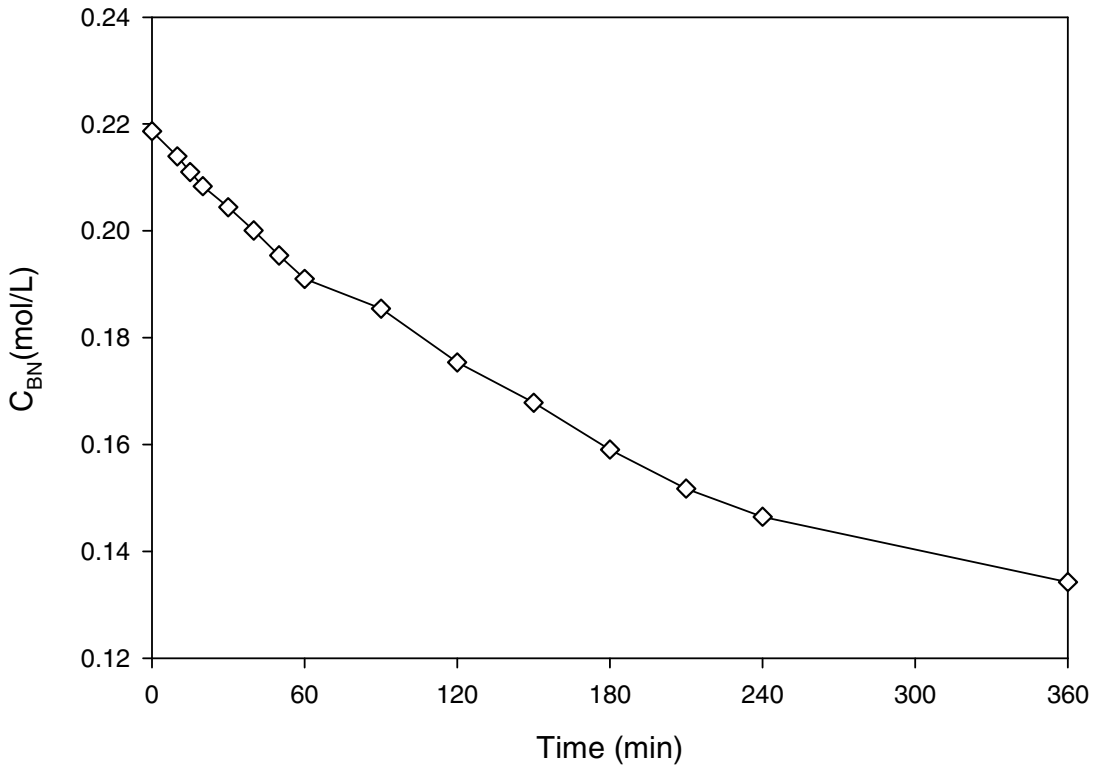


Figure S3. (cont.)



Initial rate was calculated by fitting the benzonitrile concentration versus time with an appropriate polynomial during the initial stages of the reaction and determining $-\left(\frac{dC_{BN}}{dt}\right)_{t=0}$.

Selectivity toward dibenzylamine (DBA) was calculated at 20 % benzonitrile conversion using the following formula:

$$S_{DBA} = \frac{n_{DBA}}{\sum v_i n_i}$$

where, n_i is the moles of the product, v_i is the stoichiometric number of the product

Figure S4.