Electronic Supplementary Material (ESI) for RSC Advances.

Hydrogenation by nanoscale ruthenium embedded into the nanopores of K-10 Clay

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(Electronic Supplementary Information)

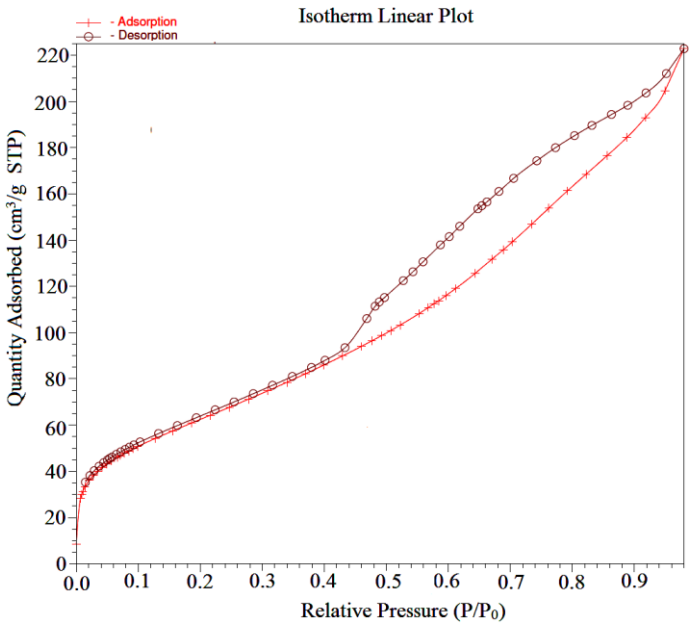

Figure S1 N_2 adsorption-desorption isotherm linear plot of K-10 clay

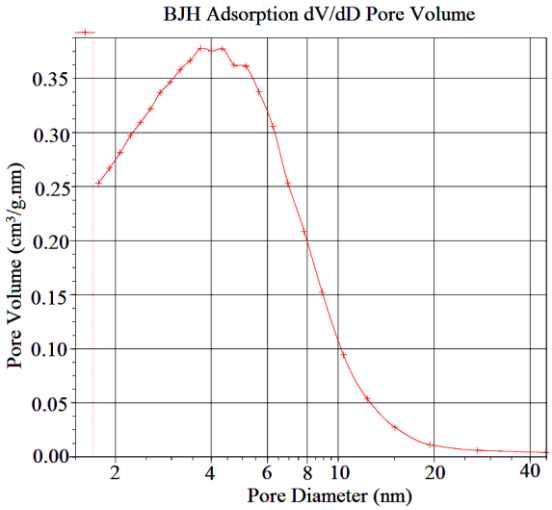

Figure S2 BJH dV/dD Pore Volume of K-10 clay

1. Calculations of TOF considering true active sites in case of "Ru (0) nano Mont K-10 " catalysed hydrogenation of Cyclohexene

Calculations of true active sites:

For hcp Ruthenium, average diameter of the particle obtained from TEM = 2.34 nm

Therefore, radius of 1 Ru nanoparticle = 1.17 nm

Atomic radius of 1 Ru atom = 0.134 nm.

Volume of 1 Ru nanoparticle,

$= 4/3 \times 22/7 \times (1.17)^3 \text{ nm}^3$

$= 6.711 \text{ nm}^3$

Volume of 1 atom of Ru

$= 4/3 \times 22/7 \times (0.134)^3 \text{ nm3}$

$= 0.01 \text{ nm}^3$

Since only 74% of the total volume of a hcp Ru is occupied by Ru atoms and rest is free space,

Actual volume of total Ru atoms present = 74% of 6.71 nm^3 = 4.96 nm^3

Therefore, total number of Ru atoms in each nanoparticle = 496.65 which approaches 561 of full shell magic number cluster. Considering 2.37asmeandiameter of Ru nanoparticles, total number of Ru atoms in each nanoparticle is calculated to be 515 and considering 2.41 as diameter ofRu total number of Ru atoms is calculated to be 542. Each of the two values 515 and 547 approaches 561 of full shell magic number cluster. So it can be concluded that the 45% of the total atoms are on the surface. That is 45% of 561 = 252 are surface atoms. After calculating the number of face atoms and subtracting from total surface atoms, true active sites are found to be 33.27%.

For hydrogenation of 1mM substrate (cyclohexene) by 0.05 g of Ru (0) nano Mont K-10 (Ru loading being 0.25 mM/g of the clay),

TOF = 411 h^{-1}.

2. Calculations of TOF considering true active sites in case of "Ru (0) nano Mont K-10" catalysed hydrogenation of Dextrose

For hydrogenation of 1mM substrate (dextrose) by 0.05 g of Ru (0) nano Mont K-10 (Ru loading being 0.25 mM/g of the clay), TOF was calculated by dividing the moles of dextrose converted to sorbitol by true active sites available from the catalyst taken and multiplying the ratio obtained by the inverse of the time taken for the reaction.

$$TOF = 8.3 \times 10^{-2}\ s^{-1} = 4.98\ h^{-1}$$

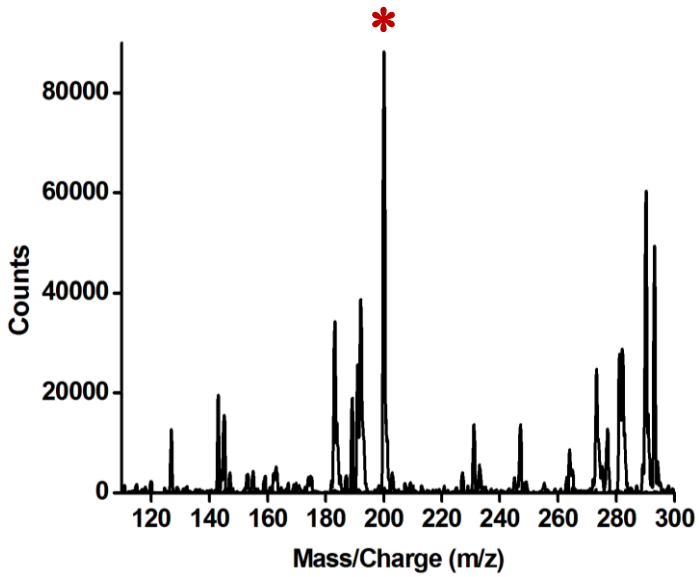

Figure S3 Mass Spectra (LCMS) of Sorbitol (*) obtained by hydrogenation of dextrose using Ru (0) nano Mont K-10 as catalyst.

Figure S4. Mass Spectra of the Product (Cyclohexane) obtained from catalytic hydrogenation reaction of cyclohexene

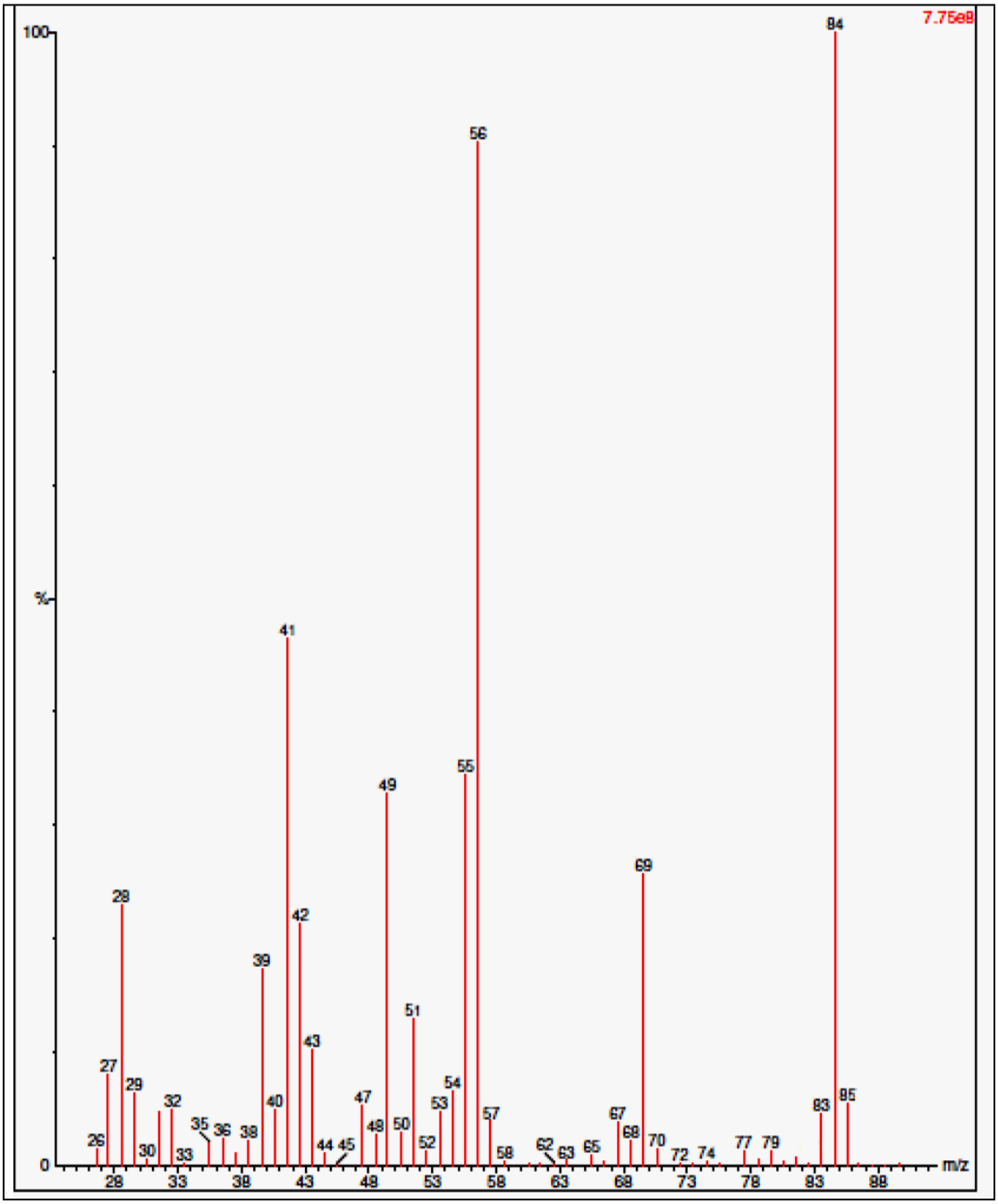

Figure S5 **Mass Spectra of the Product (Cyclohexanol) obtained from catalytic hydrogenation reaction of phenol**

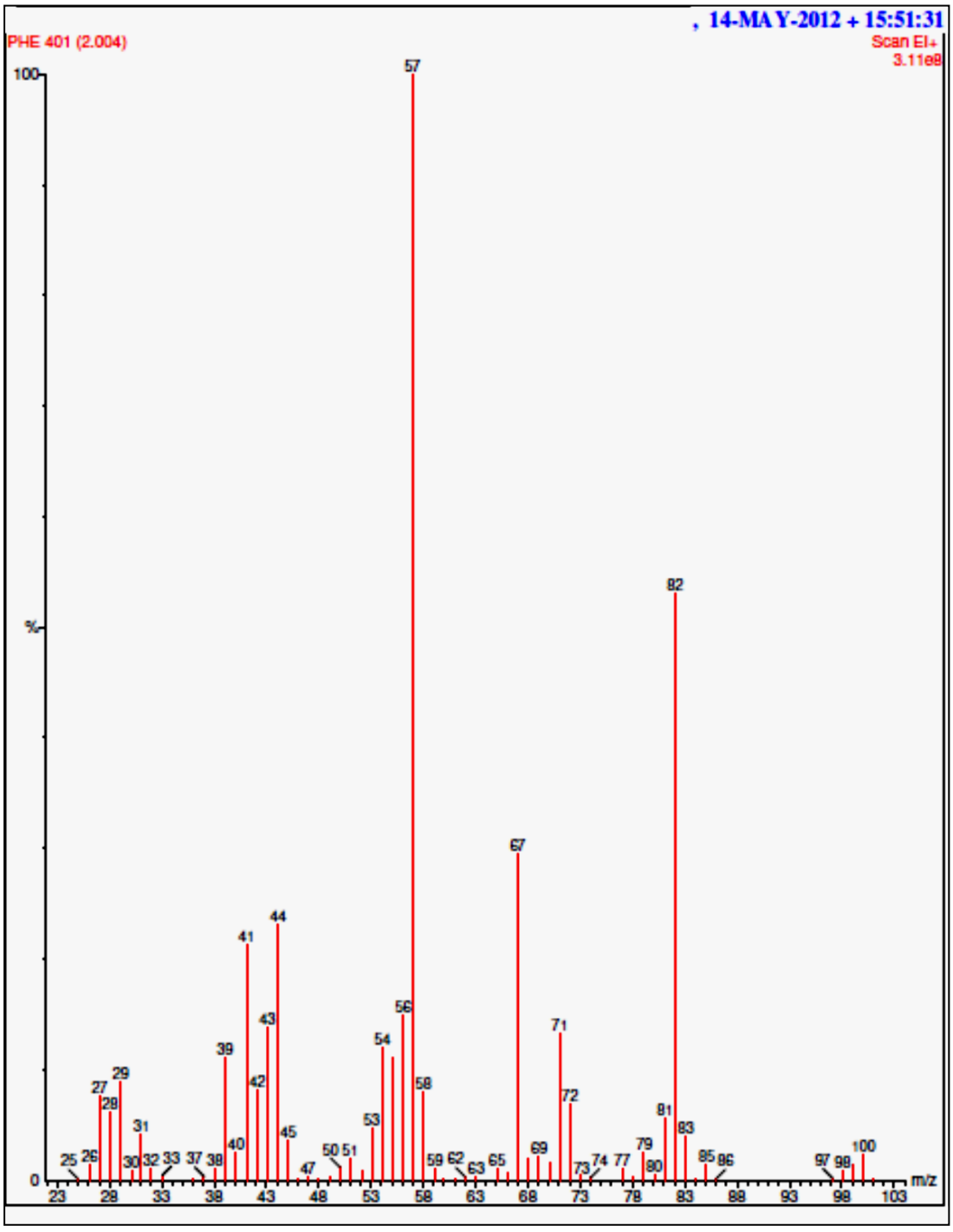

Figure S6 Mass Spectra of the Product (Cyclohexanone) obtained from catalytic hydrogenation reaction of phenol