New Journal of Chemistry

ARTICLE

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

www.rsc.org/

Supplementary Information

Intrinsic Role of pH in altering Catalyst Properties of NiMoP/Alumino-Silicate for the Vapour phase Hydrodeoxygenation of Methyl Heptanoate

Arumugam Ramesh, Perumal Tamizhdurai, Krishnan Suthagar, kandhasamy Sureshkumar, Gubert Sonia Theres, Kannan Shanthi *

[a]Department of Chemistry, Anna University, Chennai-600025, Tamil Nadu, India

*Corresponding Author: shanthiramesh@annauni.edu.in and kshanthiramesh@yahoo.com

Figure S1

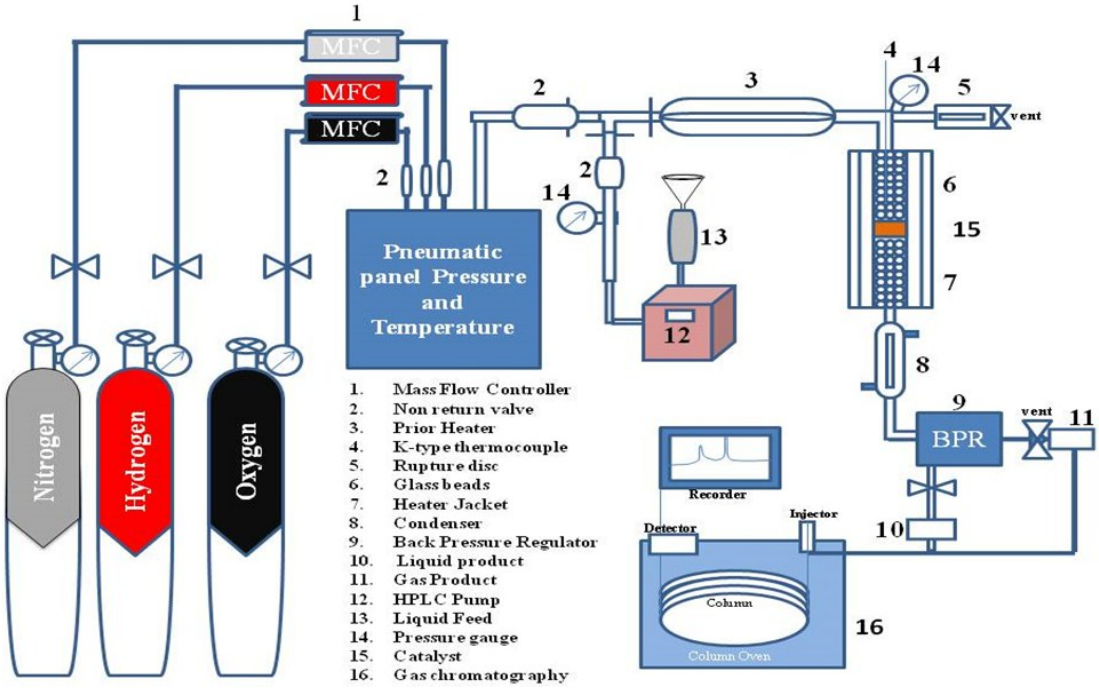

Figure S1 Schematic Diagram of Stainless steel high pressure fixed bed reactor

Figure S2

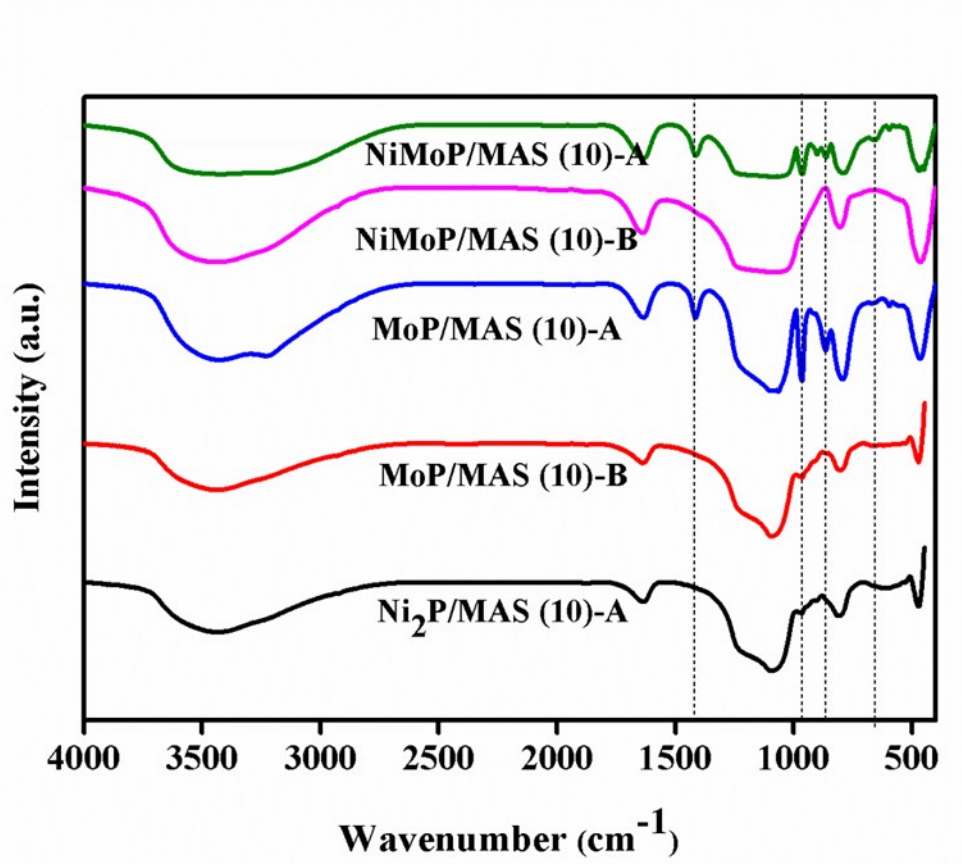

Figure S2 FT-IR spectra of catalysts Vis spectroscopy

Figure S3

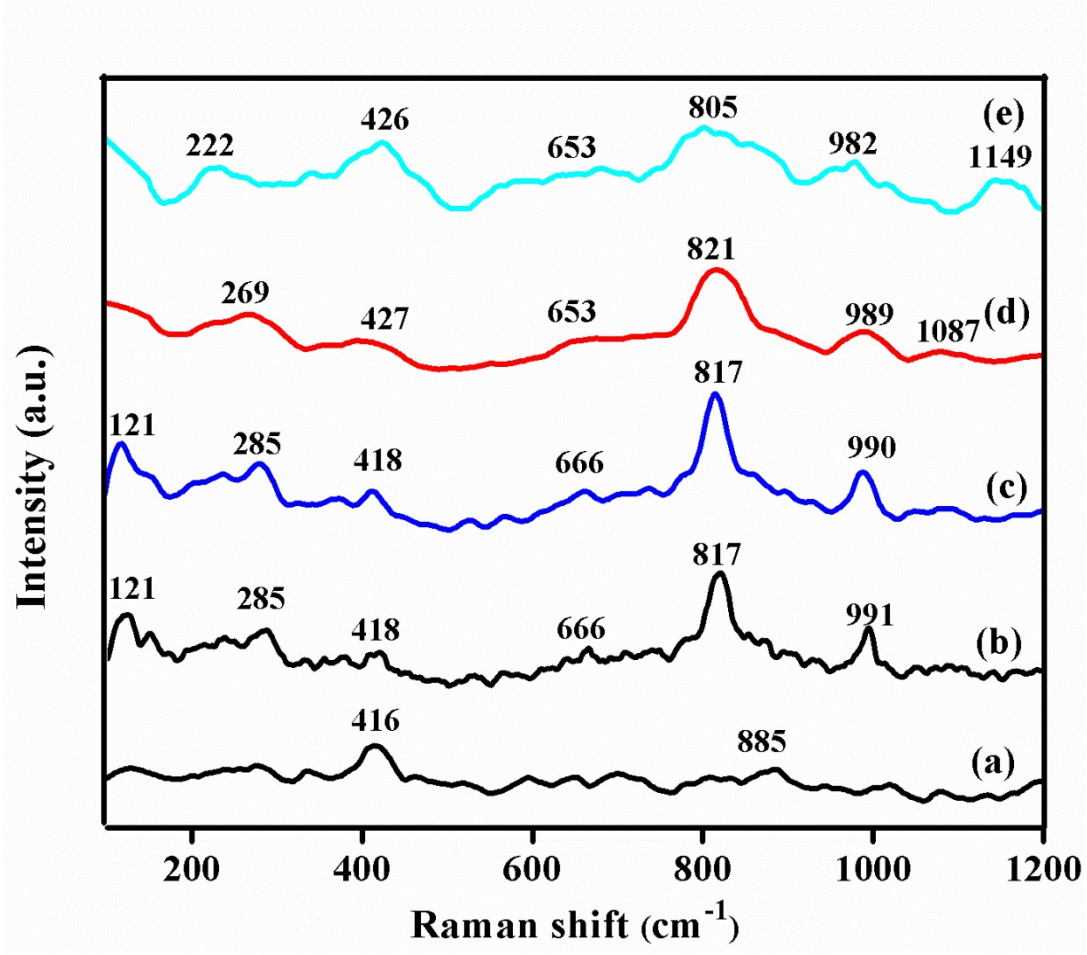

Figure S3 FT-Raman spectra of catalysts (a) Ni2P/MAS (10)-A, (b) MoP/MAS (10)-A, (c) MoP/MAS (10)-B, (d) NiMoP/MAS (10)-A, (e) NiMoP/MAS (10)-B catalysts

Figure S4

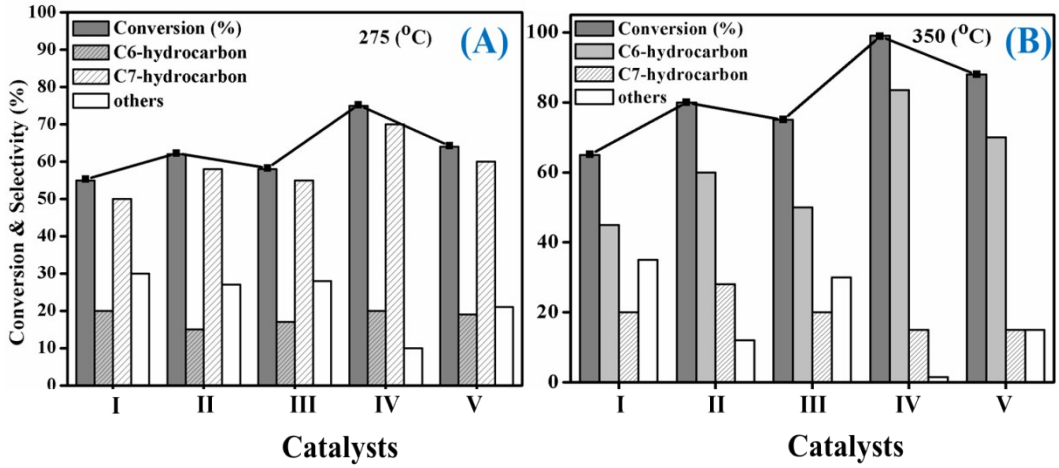

Figure S4 Comparison of activity of catalysts for HDO of Methyl heptanoate, towards the conversion (%) and selectivity (%) of hydrocarbons (A) Reaction temperature at 275 °C (B) Reaction temperature at 350 °C; catalysts (I) Ni_2P/MAS (10)-A, (II) MoP/MAS (10)-A, (III) MoP/MAS (10)-B, (IV) NiMoP/MAS (10)-A and (V) NiMoP/MAS (10)-B (Reaction conditions; 30 bar H_2 Pressure, Methyl heptanoate 7 % in m-xylene, WHSV= 3.42h^{-1}, and H_2 flow rate = 1200 ml/h) Raman spectroscopy

Figure S5

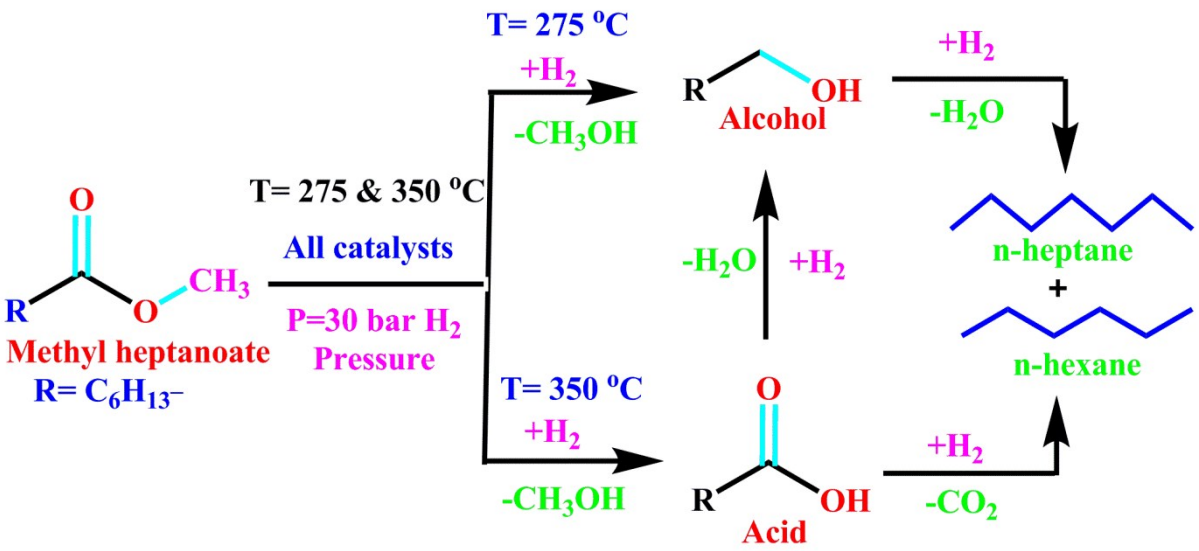

Figure S5 HDO reaction pathways of Methyl heptanoate

Figure S6

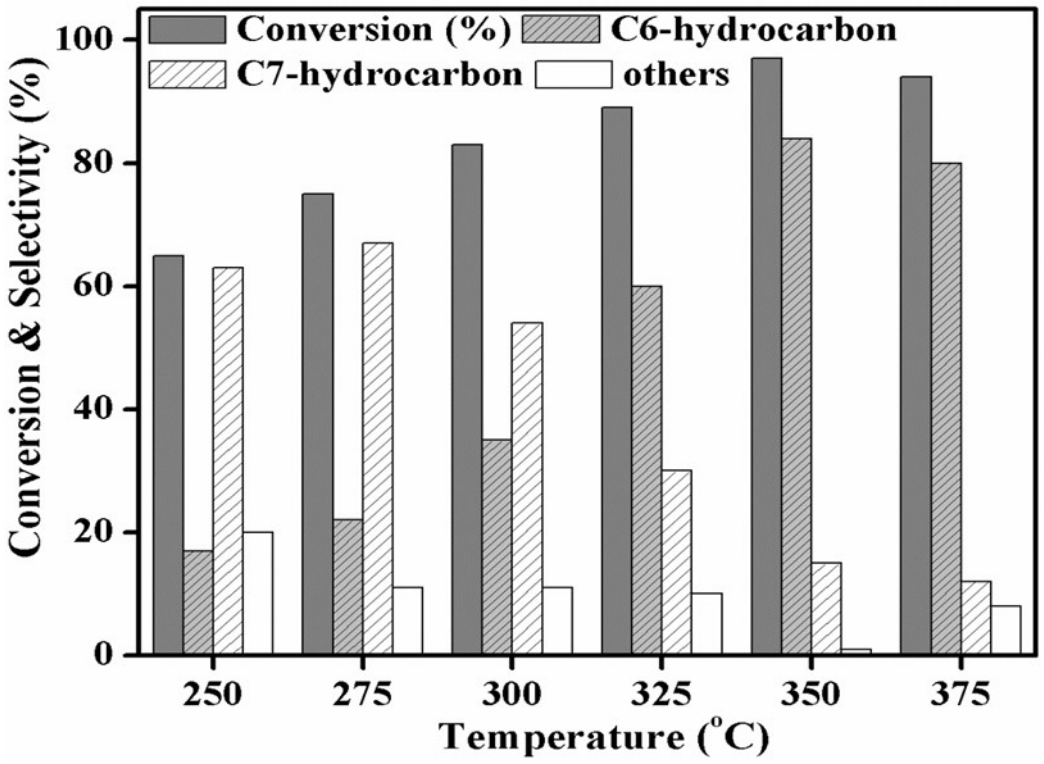

Figure S6 Effect of reaction temperature on HDO of Methyl Heptanoate towards conversion (%) and selectivity (%) of hydrocarbons on NiMoP/MAS (10)-A catalyst. (Reaction conditions: 250 °C - 375 °C under 30 bar H2 Pressure, reactant: Methyl heptanoate 7 % in m-xylene, time = 5h, WHSV= 3.42h^{-1}, H_2 flow rate = 1200 ml/h)

Table S1 Mass Transfer Considerations of Ni_2P/MAS (10)-A, MoP/MAS (10)-A, MoP/MAS (10)-B, NiMoP/MAS (10)-A, and NiMoP/MAS (10)-B Catalysts

S.N	Catalysts	Catalysts weight (g)	Flow rate (mL/min)	Reactant (mL/h)	TOF s^{-1}	Catalysts pellet size (mm)	TOF s^{-1}
1	**Ni_2P/MAS (10)-A**	2	0.113	6.8	2.1	0.5-1	2.1
		4	0.227	13.6	2.2	3-4	2.27
2	**MoP/MAS (10)-A**	2	0.113	6.8	4.34	0.5-1	4.34
		4	0.227	13.6	4.39	3-4	4.18
3	**MoP/MAS (10)-B**	2	0.113	6.8	4.07	0.5-1	4.07
		4	0.227	13.6	4.23	3-4	4.07
4	**NiMoP/MAS (10)-A**	2	0.113	6.8	8.17	0.5-1	8.17
		4	0.227	13.6	8.16	3-4	7.83
5	**NiMoP/MAS (10)-B**	2	0.113	6.8	6.78	0.5-1	6.78
		4	0.227	13.6	6.86	3-4	6.70

Reaction conditions: 7% Methyl heptanoate, temperature 350 ^oC, 30 bar H_2 pressure, reaction time: 5 h and H_2 flow rate = 1200 ml/h WHSV= 3.4 h^{-1}