

ELECTRONIC SUPPLEMENTARY INFORMATION

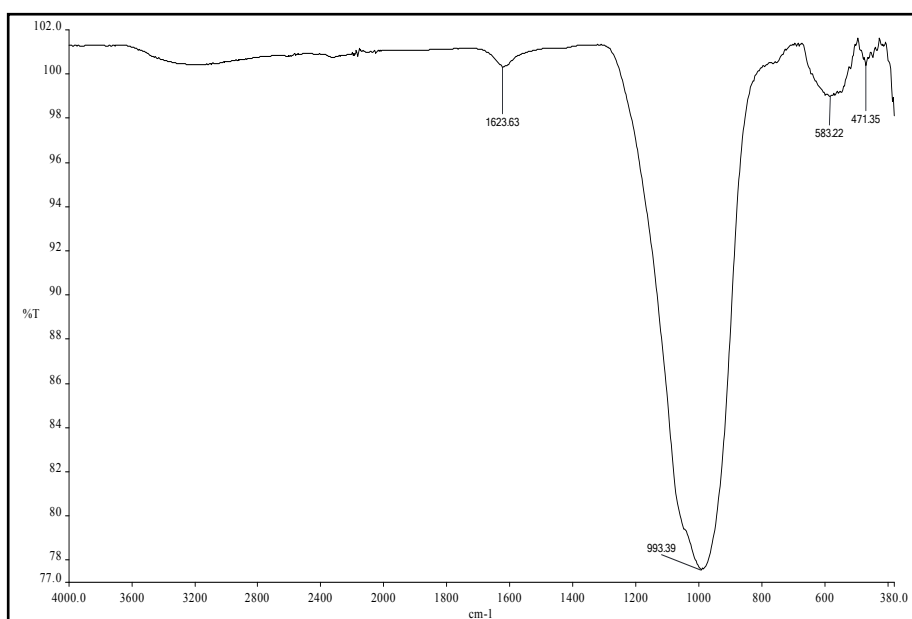


Figure S1 : IR spectra of FePO₄ catalyst

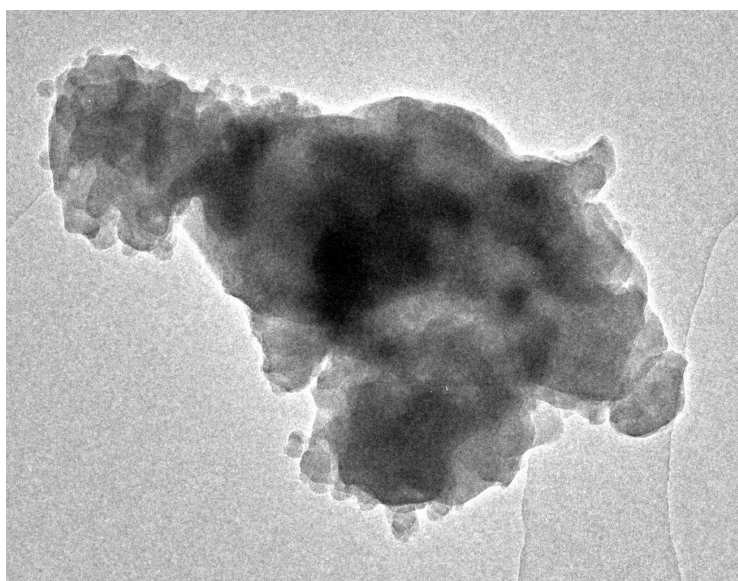


Figure S2 : TEM micrograph (scale = 100 nm) of FePO₄ catalyst

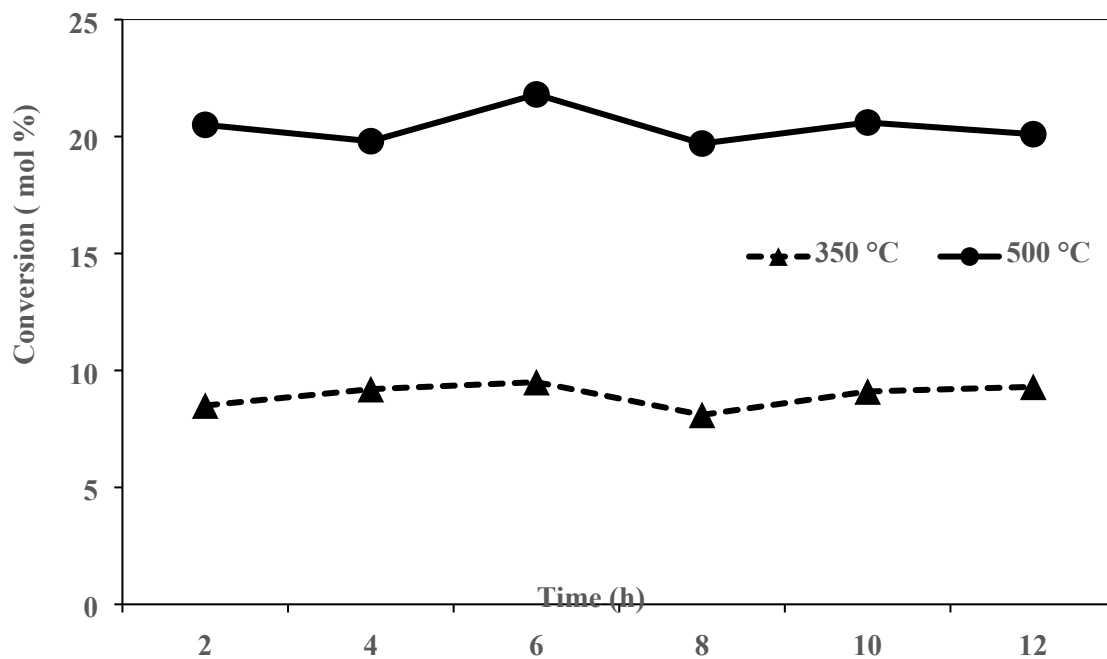


Figure S3 : Time on line studies over the fresh catalysts at a temperatures of 350 °C and 550 °C at a carbon to oxygen ratio of 8:3, GHSV = 5000 h⁻¹

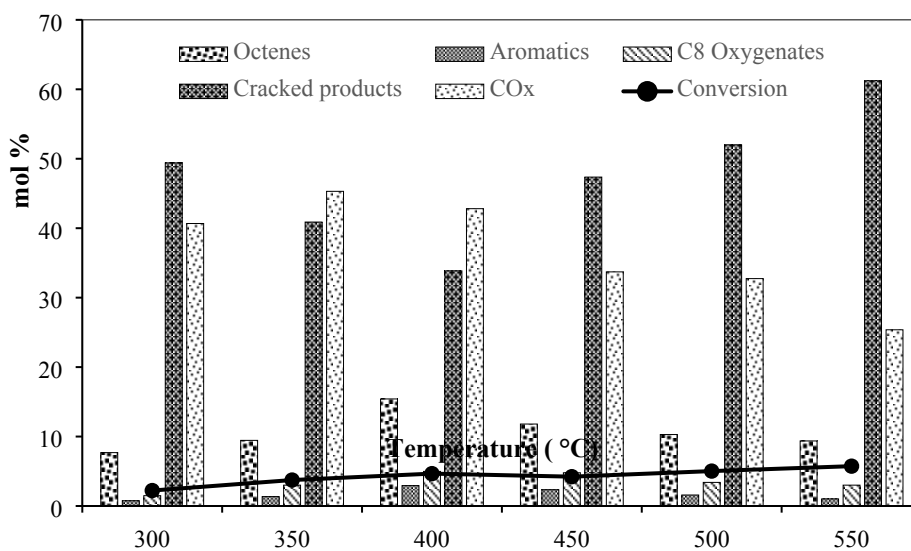


Figure S4 : Effect of temperature on the conversion of *n*-octane and selectivity towards products over Fe₂P₂O₇ phase at a carbon to oxygen ratio of 8:3, GHSV = 5000 h⁻¹

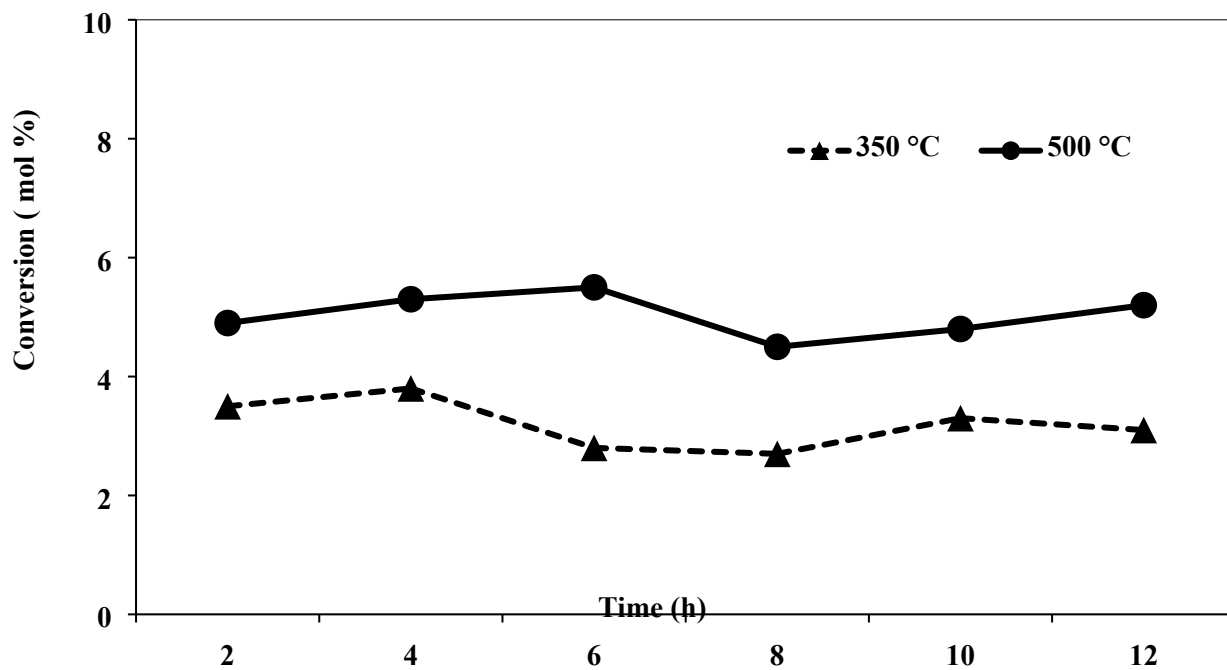


Figure S5 : Time on line studies over the “deactivated” catalyst catalysts at a temperatures of 350 °C and 550 °C at a carbon to oxygen ratio of 8:3, GHSV = 5000 h⁻¹

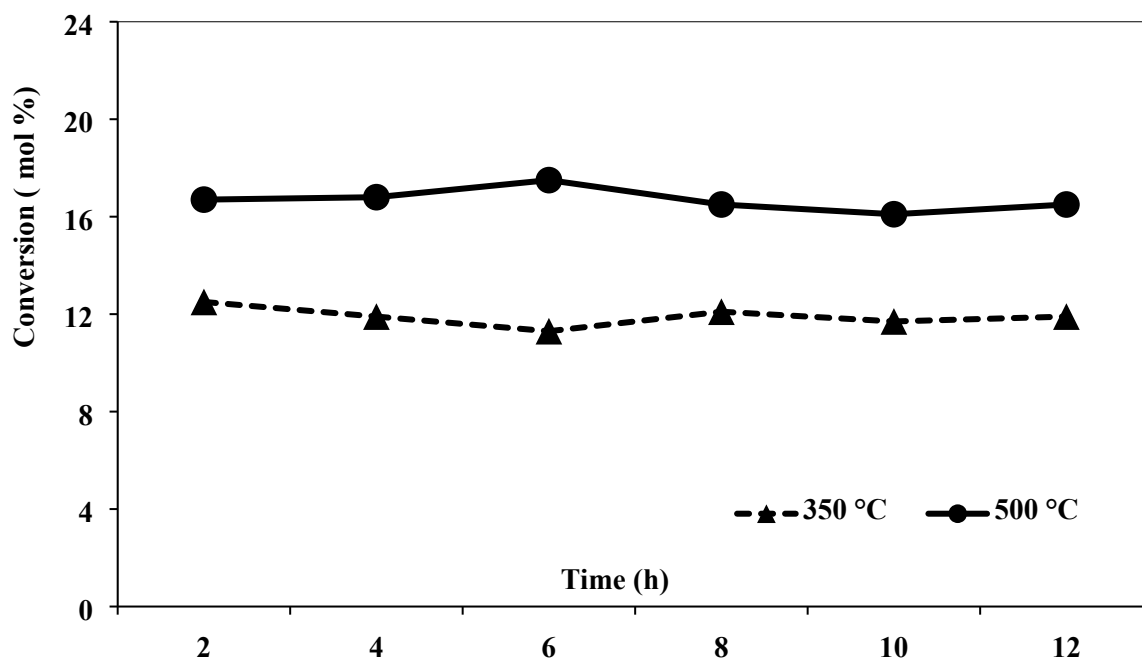


Figure S6 : Time on line studies over the “regenerated” catalyst catalysts at a temperatures of 350 °C and 550 °C at a carbon to oxygen ratio of 8:3, GHSV = 5000 h⁻¹

S1: Analysis of products and Calculations:

The products of the catalysed reactions were expressed as conversion, selectivity and yield. Conversion is a measure of the amount of feed introduced into the reactor that is converted into products:

$$\text{Conversion (mol \%)} = \frac{\text{moles of } n\text{-octane in} - \text{moles of } n\text{-octane out}}{\text{moles of } n\text{-octane in}} \times 100$$

The selectivity towards a product may be defined as the ratio of that product formed to the total moles of products formed, based on carbon atoms:

$$\text{Selectivity (mol \%)} = \frac{\text{total moles carbon of product component}}{\text{total moles carbon of all product components}} \times 100$$

The yield is the molar fraction of a particular product formed to the total number of moles of feed introduced:

$$\text{Yield (mol \%)} = \frac{\text{Selectivity of product component} \times \text{conversion}}{100}$$

The gas hourly space velocity (GHSV) was calculated as follows:

$$\text{Gas hourly space velocity, GHSV (h}^{-1}\text{)} = \frac{\text{total flow rate into the reactor}}{\text{volume of the catalyst used}}$$

The carbon balance of each reaction was determined as below :

$$\text{Carbon balance} = \frac{\text{moles of carbon in}}{\text{moles of carbon out}} \times 100$$

S2. Calculation of response factors (RF):

Assign *n*-octane a RF of 1 and calculate all other Response Factors relative to this:

Mass of *n*-octane in standard solution = 0.0073 g

Mass of *trans*-2-octene in standard solution = 0.00715g

Injection volume = 0.1 μ l

Peak area of *n*-octane = 46684.56

Peak area of *trans*-2-octene = 51712.54

The RF of *n*-octane was considered as 1 and Response Factor calculations was carried out relative to *n*-octane

Mass of *n*-octane in standard solution = 0.0075

Mass of *trans* 2-octene in standard solution= 0.00715

Injection volume= 0.1 μ L

Peak area of *n*-octane= 46684.56

Peak area of *trans*-2-octene= 50712.21

$$\text{Response factor of trans-2-octene} = \frac{\text{peak area of trans-2-octene} \times \text{mass of n-octane}}{\text{mass of trans-2-octene} \times \text{peak area of n-octane}}$$

Table A2.4 Relative response factor of *trans* 2-octene

Injection volume (μ l)	Amount of <i>trans</i> 2-octene	Peak area of <i>trans</i> 2-octene	Amount of <i>n</i> -octane injected	Peak area of <i>n</i> -octane	Relative response factor (RF)
0.1	0.00071	51714,89	0.000703	46684.56	0.91
0.2	0.00153	113606.4	0.001416	94552.7	0.9
0.3	0.00225	158300.4	0.002109	136843.9	0.91
0.4	0.00285	229129.7	0.002813	205058.5	0.91

Average response factor of *trans* 2-octene= 0.91

Table S1. Retention times, Response factors and gradient of the calibration graph of compounds

Component	R. T. (min)	R.F	Equation (y=..)
1-pentene	2.432	0.93	1.01E+14
2-methyl-2-propanol	2.477	0.72	8.13E+14
<i>n</i> -Pentane	2.37	0.76	8.81E+14
1-hexene	3.52	0.95	1.36E+14
<i>n</i> -Hexane	3.692	0.93	1.32E+14
Methylcyclopentane	4.311	0.92	1.24E+14
<i>n</i> -Heptane	6.98	0.91	1.63E+14
2, 4-dimethylhexane	8.97	0.94	1.79E+14
Toluene	10.47	1.12	1.57E+14
4-methylheptane	11.72	1.14	1.83E+14
1, 7-octadiene	12.52	0.90	1.85E+14
1-octene	13.8	0.98	1.90E+14
3-octene	14.9	0.98	1.75E+14
Trans-4-octene	14.53	0.97	1.83E+14
<i>n</i> -Octane	15.26	1	1.82E+14
Trans-2-octene	15.59	0.94	1.79E+14
1,3-octadiene	16.523	0.92	1.54E+14
Ethyl cyclohexane	16.92	0.90	1.87E+14
Propyl cyclopentane	16.93	1 0.95	1.75E+14
Ethyl benzene	17.58	1.13	1.93E+14
Styrene	18.34	1.17	1.75E+14
xylene	18.49	1.15	1.92E+14

cis-cyclooctene	18.829	1.20	1.78E+14
cyclooctane	19.16	1.16	1.90E+14
cis.cis-1,5-cyclooctadiene	19.52	1.12	1.84E+14
4-octanone	20.839	0.73	1.32E+14
3-octanone	21.28	0.91	1.87E+14
2-octanone	21.394	0.84	1.80E+14
3-octanol	21.83	0.76	1.51E+14
octanal	21.84	0.71	1.40E+14
2-octanol	21.992	0.78	1.46E+14
octene oxide	22.244	0.85	1.61E+14
benzyl alcohol	22.765	0.89	1.28E+14
1-octanol	24.446	0.85	1.86E+14
octanoic acid	26.396	0.61	1.23E+14

S2. Determination of moles of *trans* 2-octene from a liquid organic sample

Mass of the organic layer = 1.786 g Percentage peak area of *trans* 2-octene = 0.91 Calculated

Response Factor = 1.0519

Corrected area = Percentage peak area \div Response factor = $0.91 \div 1.0519 = 0.9677$

$$\text{Normalised area (\%)} = \frac{\text{corrected area}}{\text{Sum of corrected areas of all the products in sample}} \times 100$$
$$= 0.866$$

$$\begin{aligned} \text{Mass Component} &= \frac{\text{(g)} \\ &= \text{normalised area}}{100} \times \text{mass of organic layer} \\ &= \frac{(0.8601 \times 1.786)}{100} = 0.01525 \text{ gm} \end{aligned}$$

$$\begin{aligned} \text{Moles component out (moles)} &= \frac{\text{mass of component}}{\text{molar mass of component}} \\ &= \frac{0.01525}{112.21} = 0.000135 \end{aligned}$$

$$\begin{aligned} \text{Moles of carbon out} &= \text{moles component out} \times \text{carbon number} \\ &= 0.001087 \text{ moles of carbon} \end{aligned}$$

S3. Determination of moles of butane from a gaseous organic sample

The gaseous samples were identified with the help of GCMS and their quantification was carried out by using methane as a standard gas by using the equation below

Initially, the constant was derived by using equation

$$\text{Constant} = (\text{Rf of methane} / \text{Area of methane}) \times \text{Vol. \% of methane}$$

The values obtained by injecting 0.2 μL in the GC-FID are

Injection volume = 0.2 μL Methane area = 90000

Methane Rf = 1

$$\text{Constant} = (1/90000) \times 0.02$$

$$= 2.22 \times 10^{-7}$$

Ethylene area from gaseous sample from reaction = 17629.91 Corrected area =

Area / Rf

$$= 17629.91/1$$

$$= 17629.91$$

Further, the corrected area was entered in the following formula to get the Mol. %, Mol. % = Corrected area \times constant \times (molecular weight of methane / molecular weight of unknown)

$$\text{Mol. \%} = 17629.91 \times 2.22 \times 10^{-7} \times (16/28) \text{ Mol \%} = 0.223871\%$$

Then, the volume of gas out was calculated from Mol. % Volume of gas out = Mol.

% \times gas out/min

$$= 0.223 \% \times 67 \text{ mL/min}$$

$$= 0.0538 \text{ mL/min}$$

Moles out were calculated by using ideal gas equation

$$PV=nRT$$

Where,

$$P= 10000 \text{ Pa}$$

$$V= 0.0538 \text{ ml/min}$$

$$R= 8.314 \text{ L kPa K}^{-1} \text{ mol}^{-1} \quad T= 298 \text{ K}$$

$$\text{Number of moles of ethylene} = 100000 \text{ Pa} \times 0.0538 \text{ ml/min} \times 0.000001 / (8.314 \text{ kPa K}^{-1}$$

$$\text{mol}^{-1} \times 298 \text{ K})$$

$$= 0.00000217$$

$$\text{Moles of Carbon} = 0.00000217 \times 2$$

$$= 0.00000434$$

$$\text{Total moles of Carbon} = 0.00000434 \times \text{Reaction time (min.)}$$

$$= 0.00000434 \times 120 \text{ min.}$$

$$= 0.00052$$