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Optimization of Reaction Parameters for Production of Hydrogenated Soya Bean Oil with Least Trans Isomer Content

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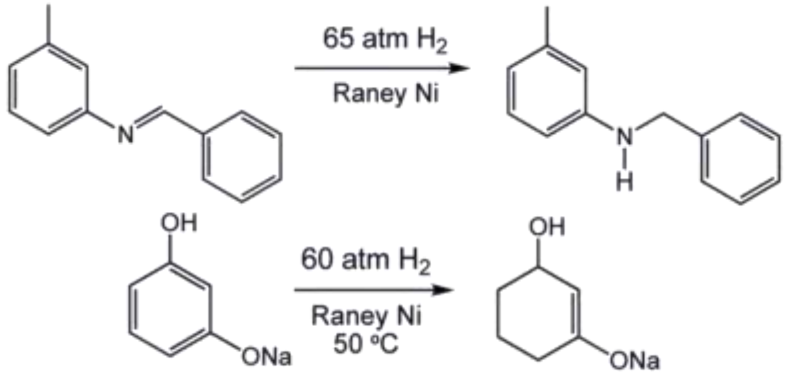
ABSTRACT:
Hydrogenation is a chemical reaction between molecular hydrogen (H_2) and another compound or element, usually in the presence of a catalyst. The process is commonly employed to reduce or saturate organic compounds. Hydrogenation typically constitutes the addition of pairs of hydrogen atoms to a molecule, generally an alkene. Catalysts are required for the reaction to be usable. Also non-catalytic hydrogenation takes place only at very high temperatures. In this study hydrogenation of Soya bean oil was conducted with Nickel catalyst at different temperatures and pressures. The iodine values of the oil samples were determined. The optimum conditions for hydrogenation were obtained as 170^{o}C and 4 atmospheres. At these optimum conditions the hydrogenation was again carried out with the Copper-chromium catalyst. The gas chromatographic analysis was conducted to analyze the samples for trans fat content. It is observed that the trans fat content in the later process is very less even though the drop in iodine value is more with Nickel catalyst.

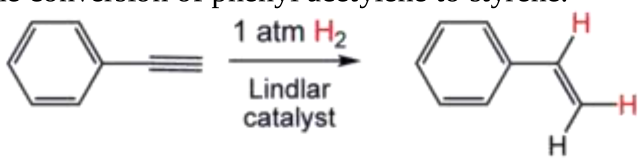
KEYWORDS: Hydrogenation, Catalyst, Optimum Conditions, Trans fats.

INTRODUCTION:

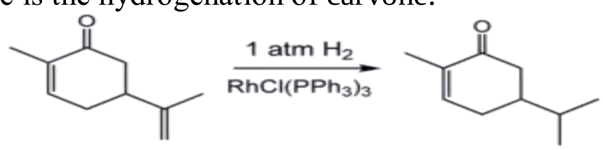
Hydrogenation is a chemical reaction between molecular hydrogen (H_2) and another compound or element, usually in the presence of a catalyst. The process is commonly employed to reduce or saturate organic compounds. Hydrogenation typically constitutes the addition of pairs of hydrogen atoms to a molecule, generally an alkene. Catalysts are required for the reaction to be usable. Also non-catalytic hydrogenation takes place only at very high temperatures. Hydrogenation of unsaturated fats produces saturated fats. In the case of partial hydrogenation, Tran's fats may be formed as well. Hydrogenation has three components, the unsaturated substrate, the hydrogen (or hydrogen source) and, invariably, a catalyst. The reduction reaction is carried out at different temperatures and pressures depending upon the substrate and the activity of the catalyst. With rare exceptions, no reaction below 480 °C (750 K or 900 °F) occurs between H_2 and organic compounds in the absence of metal catalysts. The catalyst binds both the H_2 and the unsaturated substrate and facilitates their union. Platinum, palladium, rhodium, and ruthenium form highly active catalysts, which operate at lower temperatures and lower pressures of H_2. Non-precious metal catalysts, especially those based on nickel (such as Raney nickel and Urushibara nickel) have also been developed as economical alternatives, but they are often slower or require higher temperatures. The trade-off is activity (speed of reaction) vs. cost of the catalyst and cost of the apparatus required for use of high pressures. Notice that the Raney-nickel catalyzed hydrogenations require high pressures.



Two broad families of catalysts are known - homogeneous catalysts and heterogeneous catalysts. Homogeneous catalysts dissolve in the solvent that contains the unsaturated substrate. Heterogeneous catalysts are solids that are suspended in the same solvent with the substrate or are treated with gaseous substrate. Heterogeneous catalysts for hydrogenation are more common industrially. As in homogeneous catalysts, the activity is adjusted through changes in the environment around the metal, i.e. the coordination sphere. Different faces of a crystalline heterogeneous catalyst display distinct activities. Similarly, heterogeneous catalysts are affected by their supports, i.e. the material upon with the heterogeneous catalyst is bound. In many cases, highly empirical modifications involve selective "poisons". Thus, a carefully chosen catalyst can be used to hydrogenate some functional groups without affecting others, such as the hydrogenation of alkenes without touching aromatic rings, or the selective hydrogenation of alkynes to alkenes using Lindlar's catalyst. For example, when the catalyst palladium is placed on barium sulfate and then treated with quinoline, the resulting catalyst reduces alkynes only as far as alkenes. The Lindlar's catalyst has been applied to the conversion of phenyl acetylene to styrene.



Homogeneous catalysts dissolve in the solvent that contains the unsaturated substrate. Homogeneous catalysts include the rhodium-based compound known as Wilkinson's catalyst and the iridium-based Crabtree's catalyst. An example is the hydrogenation of carvone:

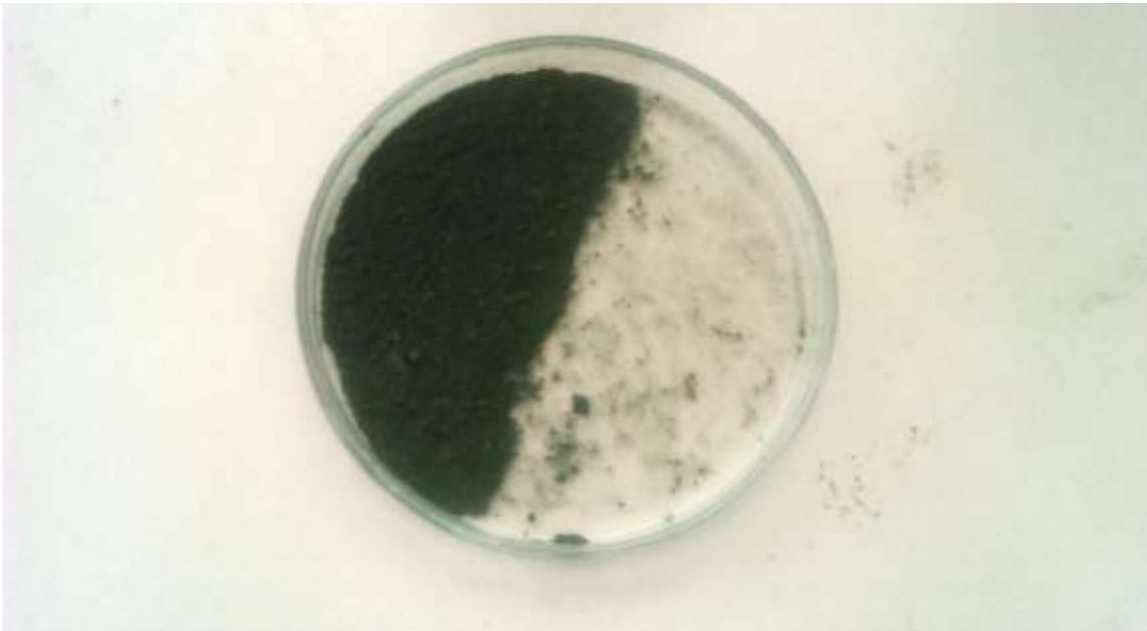


Hydrogenation is sensitive to steric hindrance explaining the selectivity for reaction with the exo cyclic double bond but not the internal double bond. The activity and selectivity of homogeneous catalysts is adjusted by changing the ligand. For prochiral substrates, the selectivity of the catalyst can be adjusted such that one Enantiomeric product is favored. Asymmetric hydrogenation is also possible via heterogeneous catalysis on a metal that is modified by a chiral ligand.

MATERIALS AND METHODS:

Preparation of Copper-Chromium catalyst:

First 6.057g of copper nitrate and 1.361g of chromium nitrate were weighed accurately and dissolved in 250ml distilled water. Then to the mixture 250ml of aqueous solution containing 14g of urea was added. Then the total 500ml prepared solution is kept on water bath and heated for about 5 hours, which leads to formation of dark-green precipitate. The resulting dark-green precipitate was filtered, washed thoroughly with distilled water, dried at 110^0C and ground to fine powder. Heating the fine powder to 350^0C in a muffle furnace yields around 2 grams of black powder, which is the required copper-chromium catalyst as shown in the figure.



HYDROGENATION OF SOYA BEAN OIL:

One litre of the Soya bean oil was taken into the autoclave and heat it by the means of an electrical heater under vacuum conditions. After Heating collect a minimum of 200 ml of oil and add 2 gm. of nickel catalyst to the oil beaker and mix it thoroughly. The mixture was transferred to an autoclave and vacuum is applied using a vacuum pump. The process conditions where the hydrogenation has to conduct are pressures of 3atm to5atm with temperatures of 160^0C to 180^0C. After attaining the desired temperature in the autoclave the hydrogen gas was introduced. Allow the oil to undergo hydrogenation for about three hours and collect some sample to conduct iodine value test. If there is decrease in iodine value the total sample is collected, filtered and its iodine value is calculated. Repeat the same procedure by using copper-chromium catalyst and the samples are analyzed by gas chromatography.

RESULTS& DISCUSSIONS:

The hydrogenation of soya bean oil is carried out at 160^0C to 180^0C temperaturesand 3 to 5 atmosphere pressures and the iodine value tests for the sample have been conducted and the contents in the samples were determined by Gas Chromatography.

HYDROGENATION OF SOYA BEAN OIL WITH NICKEL CATALYST:

EFFECT OF PRESSURE ON IODINE VALUE:

Temperature is fixed to 170^0C and the soya bean oil was hydrogenated at different pressures, the results are shown below.

SL.NO	PRESSURE(atm)	IODINE VALUE
1	3	105.70
2	4	99.00
3	5	98.90

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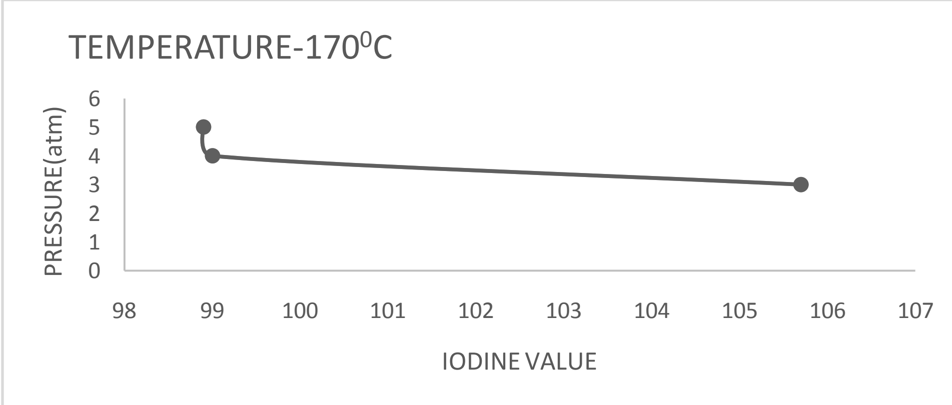
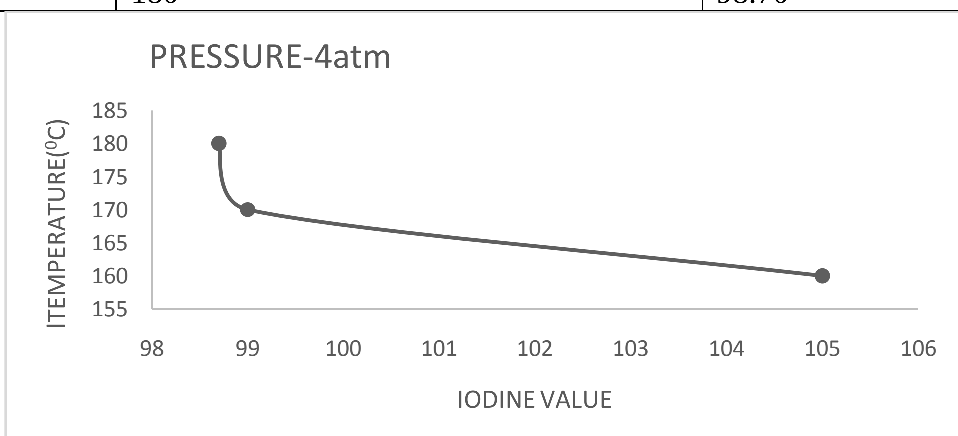


It is observed that the iodine value of sample decreases with increase in pressure. The change in iodine value is negligible from 4 to 5atm, so 4 atm pressure was considered as optimum pressure.

Effect of temperature on iodine value:

Pressure is fixed to 4atm and the soya bean oil is hydrogenated at different temperatures, the results are as shown,

SL.NO	TEMPERATURE(^{0}C)	IODINE VALUE
1	160	105.00
2	170	99.00
3	180	98.70



It is clear that as the temperature increases the iodine value decreases. The change in iodine value is marginal when the temperature goes from 170^{0}C to180^{0}C, therefore 170^{0}C temperature was considered as optimum temperature.

From the above data 170^{0}C temperature and 4atm pressure are considered as optimum conditions. The soya bean oil is again hydrogenated at same optimum conditions using copper-chromium catalyst and its iodine value is determined to be 105.00.

Both the samples are analysed by Gas chromatography, and various isomer contents are tabulated as shown below:

Property	Nickel catalyst	Copper-chromium catalyst
Iodine value	99	105
Drop in Iodine value	33	27
Trans isomer content	5.45	2.71

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From the gas chromatographic analysis it was observed that the drop in Iodine value is more when hydrogenation was carried out with the nickel catalyst as compared to copper-chromium catalyst. But the trans isomer content in the hydrogenated oil was less in case of copper-chromium catalyst. Therefore the copper-chromium catalyst is superior to nickel catalyst when the hydrogenated oil is used for human consumption.

CONCLUSIONS:

1. The optimum conditions for hydrogenation of soya bean oil were determined. The temperature and pressure recommended were 170^{o}C and 4 atmospheres.
2. The hydrogenation was carried out with nickel and copper-chromium catalyst.
3. The drop in iodine value was more with the nickel catalyst but the trans isomer content of the product was more as compared to those with copper-chromium catalyst.
4. Hydrogenation with copper-chromium catalyst was recommended in order to use the hydrogenated product for human consumption as its trans isomer content is less.

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