

**Birla Institute of Technology & Science, Pilani**  
**Pilani Campus, Rajasthan - 333 031**

I Semester 2017-2018, Comprehensive examination

Course: CHEM F337

**Model Solution: Part A: Closed Book**

Time: 90 min.

Course Title: Green Chemistry and Catalysis

Max. Marks: 40

Instruction to students: Answer all questions and answer all parts of a question together

---

- Q. 1** Give a reasonable working definition of green chemistry. Prof. Anastas has given 12 principles of green chemistry, mention any four which are more appropriate in synthetic organic chemistry. 3
- Q. 2** Write reaction for the hydroformylation of propene with appropriate reagents. Comment on the product distribution and give mechanism of the reaction? 4
- Q. 3** Catalysis can address many aspects of green chemistry, how? 2
- Q. 4** Mention two approaches for the preparation of basic zeolites. 2
- Q. 5** Using microwaves solvents can be heated well above their boiling points for extended time. Explain. 2
- Q. 6** Fill in the blank with appropriate option. 4
- a) In zeolite process, the exchange of ... .. takes place (anions/ cations/ both cations and anions).
  - b) The chemical formula of zeolite is .....
  - c) In zeolites Lewis basicity is associated with the ... ..
  - d) Heteropoly acids with general formula .....is called Dawson structure.
  - e) ... .. are suitable solid base catalysts for the conversion of bulky molecules which cannot access the pores of zeolites.
  - f) Fluorous chemistry is associated with the ..... to aqueous and organic solvents at room temperature.
  - g) In hydrotalcites, each OH group in the layer is coordinated to ..... (one/two/three) metals.
  - h) The edge sharing of  $MO_6$  can occur to a ..... extent in the isopoly anions of small sized  $Mo^{6+}$  than bigger sized  $W^{6+}$  ion.
- Q. 7** Define adsorption isotherm? What are the basic assumption in Langmuir theory of adsorption? 3
- Q. 8** Define phase transfer catalysis. Give an example of PTC and write at least two advantages of PTC. 3
- Q. 9.** Distinguish between physisorption and chemisorption? 2
- Q. 10** What information can be gained from TPR curves. What does a higher reduction temperature in TPR indicate about nature of the solid metal? 3
- Q. 11** It has been observed that in case of cracking reactions, n-heptane undergoes preferential cracking over dimethylhexane using zeolite as catalyst. Similarly, alkylation of methylbenzene over pentasil zeolites produces p-xylene preferentially over *ortho* and *meta* forms. Provide appropriate reason for these observations. 3
- Q. 12** Draw schematic diagram for the preparation of primary amine functionalized mesoporous silica by grafting and co-condensation methods. 4
- Q. 13** Write different type of metal species immobilized hydrotalcites. How these can be achieved. 3
- Q. 14** Draw Lineweaver-Burk plot (with appropriate labelling) to show competitive and uncompetitive inhibition of an enzyme. 2

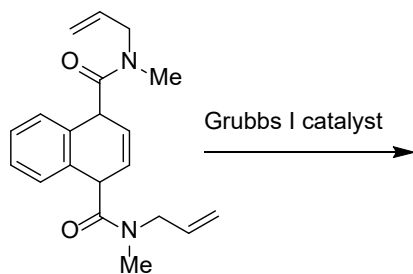
**-End of the examination-**

**Q. 1** Butyl ethanoate is an ester used in flavoring agent. This ester can be prepared from 1-butanol by two different processes. **Process A** is a one-step reversible process where acetic acid reacts with butanol to form butyl ethanoate. In this process 6.25 g of 1-butanol forms 6.57 g of butyl ethanoate. **Process B** is a two-step process where acetic acid first reacts with  $\text{SOCl}_2$  to give acetyl chloride which then reacts with butanol to form butyl ethanoate. In this process 5.45 g of acetic acid forms 9.806 g of butyl ethanoate.

Write chemical equations for both the processes and calculate percent yield, atom economy for each process. With at least two appropriate reason suggest which of the two process is more suitable for the synthesis of this flavoring agent. 6

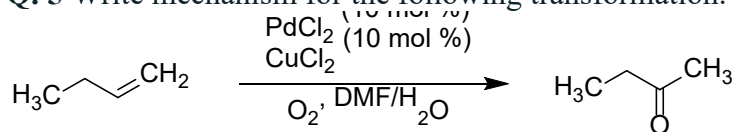
**Q. 2** A certain reaction is a single-step reaction. If a catalyst is added to the reaction it becomes two-step reaction with first step being faster than the second one. Draw energy profile diagram with proper labelling to show the progress of the two reaction. 3

**Q. 3** The reaction of the given compound proceeds readily with Grubbs 1 catalyst. Write the structure of the product formed. 2

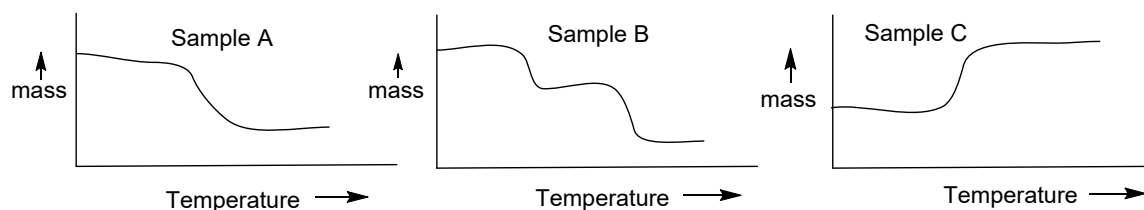


**Q. 4** Draw a schematic diagram with proper labelling depicting fluororous biphasic catalysis. 3

**Q. 5** Write mechanism for the following transformation. 4



**Q. 6** The TGA diagram for three samples (A, B and C) is given below. What information we can get from these TGA analysis about the type of the reaction or any changes? 3



**Q. 7** Nitrogen was employed to determine the surface area of a 1 g sample of alumina, the following results were obtained. The sample of alumina was maintained at normal boiling point of nitrogen (77.3K). Calculate the specific area of the silica gel by BET method. At 77.3 K, saturation pressure,  $P^* = 733.59$  torr. **8**

P/ (torr)	37.67	74.20	114.54	142.0	185.34
V (cm <sup>3</sup> /g: STP)	23.14	28.1	33.1	36.35	41.49

**Q. 8** A cubic crystal was placed in an X-ray diffractometer using incoming X-rays with a wavelength  $\lambda = 0.154$  nm. The various peak intensities recorded at different  $2\theta$  values are given in following table. A) Calculate the crystal size and the value for the lattice constant assuming first order diffraction with  $n = 1$ . (Given:  $k=0.9$ ;  $\beta = 0.0098$ ; and  $\sin 20.15 = 0.3436$ ). **8**

$2\theta$ (deg.)	40.3	58.3	73.2	131.2	154.2
hkl	110	200	211	321	400
Relative intensity	100	15	23	18	2

**Q. 9** Organocatalysts can be used for a wide array of synthetically useful transformations, however their recycling is difficult. Suggest ways in which organocatalytic methods could be modified in accord with the principles of green chemistry. **3**

***-End of the examination-***