Uva Wellassa University of Sri Lanka
Faculty of Science and Technology
Department of Science and Technology
300 Level 2nd Semester Examination – Dec./Jan. 2017
SCT 332-3 Material Chemistry II

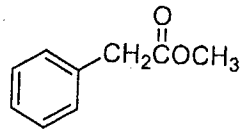
Uva Wellassa University

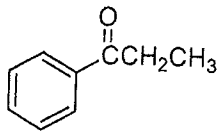


(71)

## Part III – Essay Questions

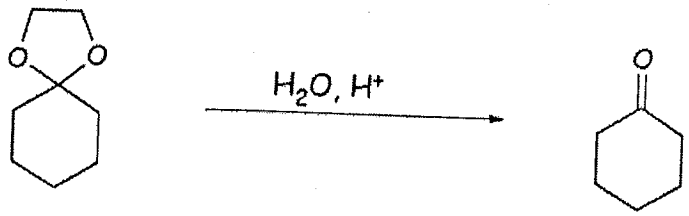
1. IR spectroscopy generally determines the vibrational changes of electrons. Hence, IR spectroscopy is also known as vibrational spectroscopy.
   a. Categorize the possible molecular vibrations (10 Marks)
   b. Briefly explain each category. Use schematics if necessory (30 Marks)
   c. Explain how $^{1}$H-NMR spectroscopy could be used to distinguish between the following two compounds (10 Marks)



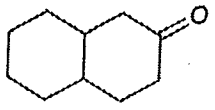

2. For trans-1,2-dichloroethylene,
   a. List all the symmetry operations for this molecule (20 Marks)
   b. Determine the point group of trans-1,2-dichloroethylene belongs to (10 Marks)
   c. Write a set of transformation matrices that describe the effect of each symmetry operation of the above molecule on a set of coordinates x, y, z for a point. (10 Marks)
   d. Using the character table of this molecule belongs to, verify that the irreducible representations are mutually orthogonal. (10 Marks)

3.
   a. Show all the steps of the mechanism for the reaction shown below using curved arrows to represent movement of electron pairs. (16 Marks)

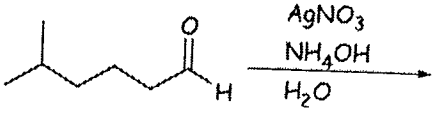



   b. Draw the major product for each of the following reactions (12 Marks)

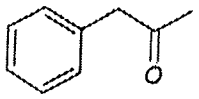
i



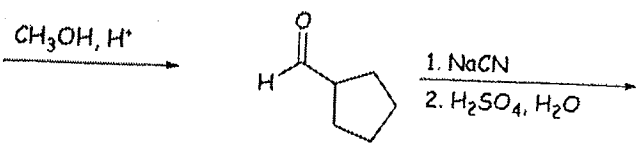

ii




iii



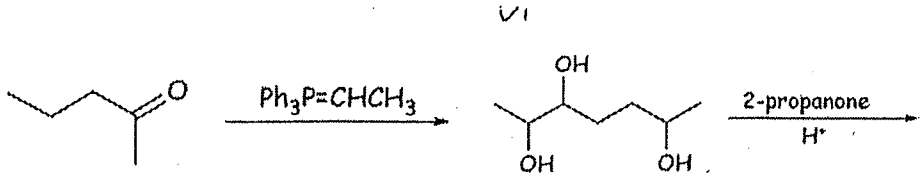

iv




v

vi

v

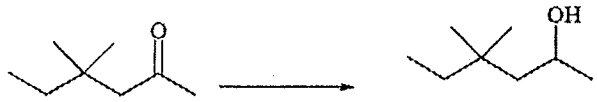



vi

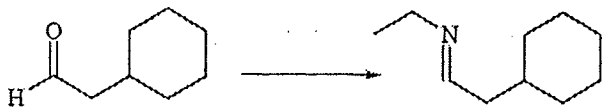
c. Write down the necessary reagents for the following conversion. Note that all are one-step reactions. (12 Marks)

i


ii



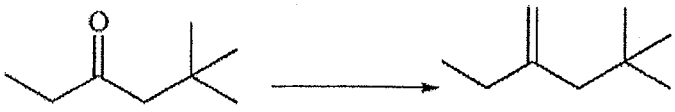

iii




iv

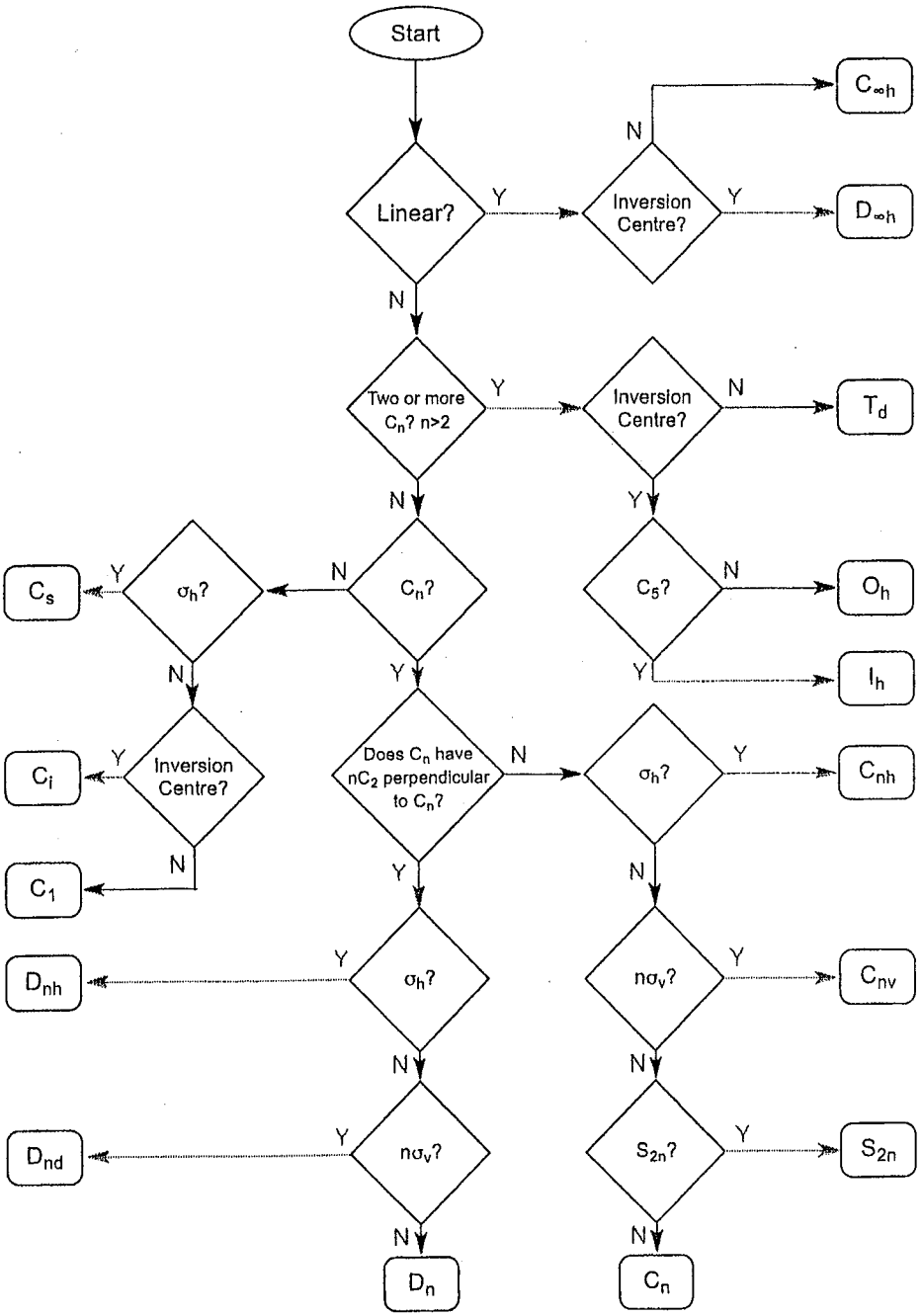

v


vi



d. Sterically, aldehydes react faster than ketones because they only have one alkyl group attached to the carbonyl carbon, making the carbonyl less sterically hindered. What is the other reason that aldehydes react faster than ketones?

(10 Marks)




The decision tree for identifying a molecular point group

| $C_{3v}$ (3m) | $E$ | $2C_3$ | $3\sigma_v$ | $h = 6$ | |
|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | $z$ | $x^2 + y^2, z^2$ |
| $A_2$ | 1 | 1 | −1 | $R_z$ | |
| E | 2 | −1 | 0 | $(x, y)$ $(R_x, R_y)$ | $(x^2 - y^2, xy)(zx, yz)$ |

| $T_d$ (43m) | $E$ | $8C_3$ | $3C_2$ | $6S_4$ | $6\sigma_d$ | $h = 24$ | |
|---|---|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | 1 | | $x^2 + y^2 + z^2$ |
| $A_2$ | 1 | 1 | 1 | −1 | −1 | | |
| E | 2 | −1 | 2 | 0 | 0 | | $(2z^2 - x^2 - y^2, x^2 - y^2)$ |
| $T_1$ | 3 | 0 | −1 | 1 | −1 | $(R_x, R_y, R_z)$ | |
| $T_2$ | 3 | 0 | −1 | −1 | 1 | $(x, y, z)$ | $(xy, yz, zx)$ |

| $D_{3h}$ (6m2) | $E$ | $2C_3$ | $3C_2$ | $\sigma_h$ | $2S_3$ | $3\sigma_v$ | $h = 12$ | |
|---|---|---|---|---|---|---|---|---|
| $A_1'$ | 1 | 1 | 1 | 1 | 1 | 1 | | $x^2 + y^2, z^2$ |
| $A_2'$ | 1 | 1 | −1 | 1 | 1 | −1 | $R_z$ | |
| E' | 2 | −1 | 0 | 2 | −1 | 0 | $(x, y)$ | $(x^2 - y^2, xy)$ |
| $A_1''$ | 1 | 1 | 1 | −1 | −1 | −1 | | |
| $A_2''$ | 1 | 1 | −1 | −1 | −1 | 1 | $z$ | |
| E'' | 2 | −1 | 0 | −2 | 1 | 0 | $(R_x, R_y)$ | $(zx, yz)$ |

| $O_h$ (m3m) | $E$ | $8C_3$ | $6C_2$ | $6C_4$ | $3C_2(=C_4^2)$ | $i$ | $6S_4$ | $8S_6$ | $3\sigma_h$ | $6\sigma_d$ | $h = 48$ | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $A_{1g}$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | $x^2 + y^2 + z^2$ |
| $A_{2g}$ | 1 | 1 | −1 | −1 | 1 | 1 | −1 | 1 | 1 | −1 | | |
| $E_g$ | 2 | −1 | 0 | 0 | 2 | 2 | 0 | −1 | 2 | 0 | | $(2z^2 - x^2 - y^2, x^2 - y^2)$ |
| $T_{1g}$ | 3 | 0 | −1 | 1 | −1 | 3 | 1 | 0 | −1 | −1 | $(R_x, R_y, R_z)$ | |
| $T_{2g}$ | 3 | 0 | 1 | −1 | −1 | 3 | −1 | 0 | −1 | 1 | | $(xy, yz, zx)$ |
| $A_{1u}$ | 1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 | | |
| $A_{2u}$ | 1 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | | |
| $E_u$ | 2 | −1 | 0 | 0 | 2 | −2 | 0 | 1 | −2 | 0 | | |
| $T_{1u}$ | 3 | 0 | −1 | 1 | −1 | −3 | −1 | 0 | 1 | 1 | $(x, y, z)$ | |
| $T_{2u}$ | 3 | 0 | 1 | −1 | −1 | −3 | 1 | 0 | 1 | −1 | | |

| $C_{2h}$ (2/m) | $E$ | $C_2$ | $I$ | $\sigma_h$ | | |
|---|---|---|---|---|---|---|
| $A_g$ | 1 | 1 | 1 | 1 | $R_z$ | $x^2, y^2, z^2, xy$ |
| $B_g$ | 1 | −1 | 1 | −1 | $R_x, R_y$ | $xz, yz$ |
| $A_u$ | 1 | 1 | −1 | −1 | $z$ | |
| $B_u$ | 1 | −1 | −1 | 1 | $x, y$ | |