

CHE320; TIMED TEST
TO BE DONE ON 16TH JANUARY 2013
(COME WITH THIS QUESTION PAPER FREE FROM ANY HAND WRITINGS)

QN 1

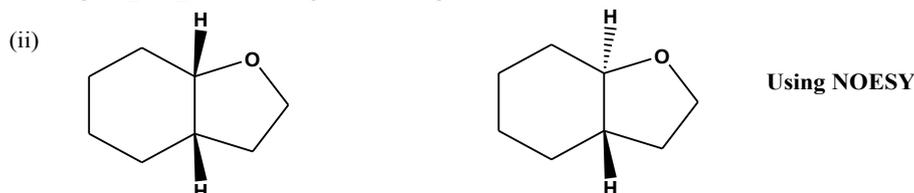
(A) Define (or give the meaning of the following terminologies as organic spectroscopy is concerned.

(i) Chemical equivalence (ii) magnetic equivalence (iii) rule of thirteen (iv) anisotropy

(B) Why all hydrogen isotopes can be observed using NMR while the only carbon isotope that is measurable is carbon-13?

(C) Explain how the following compounds can be distinguished using the named NMR techniques

(i) $\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$ and $\text{CH}_3\text{CH}(\text{Cl})\text{CH}_3$ using DEPT experiment



QN 2

(A) (i) Base peak (ii) molecular ion peak (iii) McLafferty rearrangement

(B) You are given a sample of an unknown compound **Q** and asked to identify it.

(i) MS (EI): m/z 111 (10%), 96 (5%), 68 (14%), 54 (3%), 43 (100%).

(ii) IR (neat): 2219, 1715 cm^{-1} .

(iii) ^{13}C NMR (100 MHz, CDCl_3): δ 207.6, 118.3, 43.2, 27.8, 19.5, 16.2 ppm.

(iv) ^1H NMR (400 MHz, CDCl_3): δ 2.80 (m, 1H), 2.52 (dd, 16.9 Hz, 5.8 Hz, 1H), 2.36 (dd, 16.9 Hz, 7.7 Hz, 1H), 2.17 (s, 3H), 1.27 (d, 7.3 Hz, 3H) ppm

QN 3

(A) Give explanation to each of the following

(i) J -resolved spectroscopy (ii) Off-diagonal peaks (iii) Long-Range COSY

(B) Following is the ^1H -NMR spectrum of compound **O**, molecular formula C_7H_{12} . Compound **O** reacts with bromine in carbon tetrachloride to give a compound of molecular formula $\text{C}_7\text{H}_{12}\text{Br}_2$. The ^{13}C -NMR spectrum of compound **O** shows signals at 150.12, 106.43, 35.44, 28.36, and 26.36.

(i) Deduce the structural formula of compound **O**.

(ii) Propose the main fragments ions and m/z of compound **O**.

QN 4

(A) Briefly explain what structural information can be obtained from the following techniques. Use structural examples of your explanation

(i) NOESY (ii) HMQC (iii) HMBC (iv) DEPT (v) COSY

(B) Compound **Z** has been found to exist in dimeric form **5** and **6** and the following are the possible structure isomers. Explain how the two isomers can be differentiated using NMR spectroscopic techniques

