CHEM1902/4 Worksheet 2 – Answers to Critical Thinking Questions

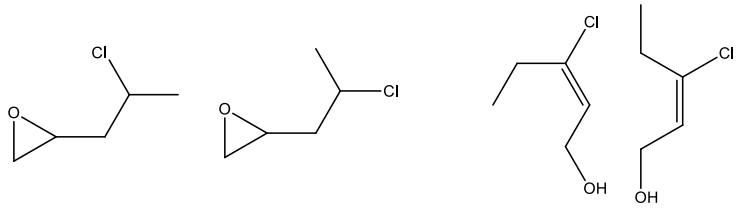
The worksheets are available in the tutorials and form an integral part of the learning outcomes and experience for this unit.

Model 4: Isomerism

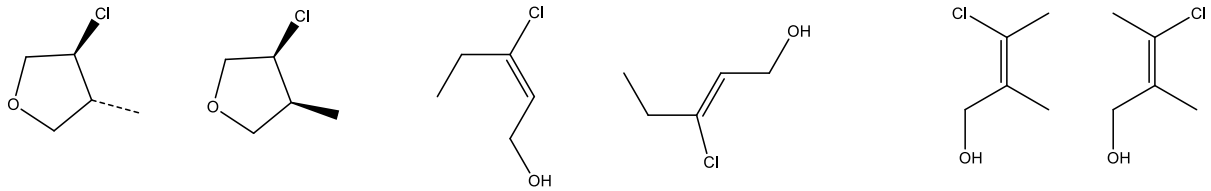
The three pairs of isomers are constitutional, conformational and configurational (from left to right).

1. All of the molecules are constitutional isomers except those are conformational (see Q2) or configurational / stereoisomers (see Q3).

2.



3.



trans *cis* (*E*) (*Z*) (*Z*) (*E*)

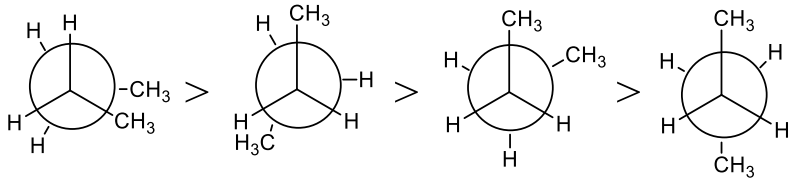
Extension:

Top row: (i) cyclic ether & chloride, (ii) cyclic ether (epoxide) & halide, (iii) alkene, chloride & alcohol and (iv) cyclic ether (epoxide) and halide.

Second row: (i) ketone & chloride, (ii) cyclic ether & chloride, (iii) alkene, chloride & alcohol and (iv) acid chloride

Third row: (i) alkene, chloride & alcohol, (ii) alkene, chloride & alcohol, (iii) enol & chloride, (iv) alkene, chloride & alcohol and (v) cyclic ether & chloride

4. From highest to lowest energy:



5. No. At room temperature, the molecules have more than enough energy to rotate around a C-C bond. Conformers can only be isolated at (very) low temperature, in the solid phase.

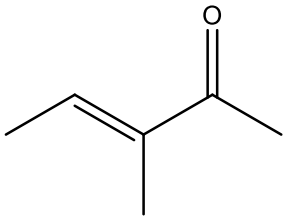
Model 5: Structure Elucidation

1. Mass Spectrometry.

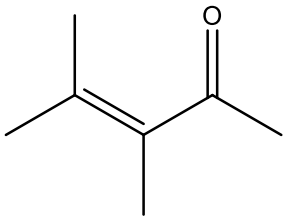
The loss of an ethyl group would lead to a peak with an *m* / *z* value 29 *less* than the molecular ion peak.

m / *z*	Fragment
99	M+ peak: containing one ^{13}C (1% chance).
98	**Molecular ion** – $C_6H_{10}O$
83	C_5H_7O (loss of $–CH_3$ - 15 mass units)
55	C_4H_7 (loss of $–CH_3CO$ - 43 mass units)
43	C_3H_7 (loss –of CH_3COC – 45 mass units)
39	C_3H_3
29	CHO or C_2H_5

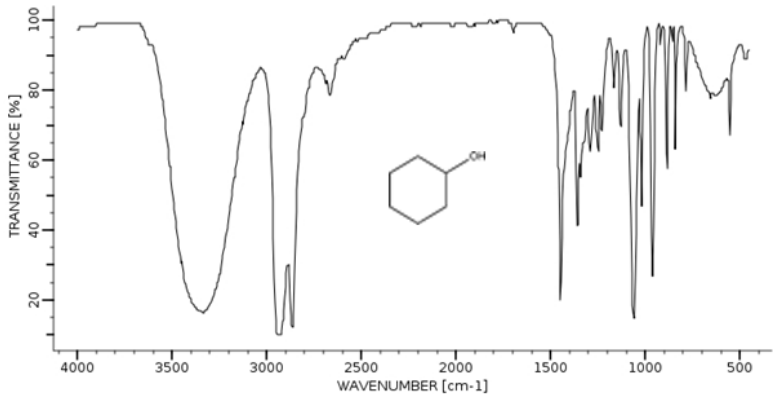
3-methyl-pent-3-enone (see below) is an isomer of 4-methyl-pent-3-enone: the molecular ion peak will occur in the same place. The fragmentation pattern will be slightly different.

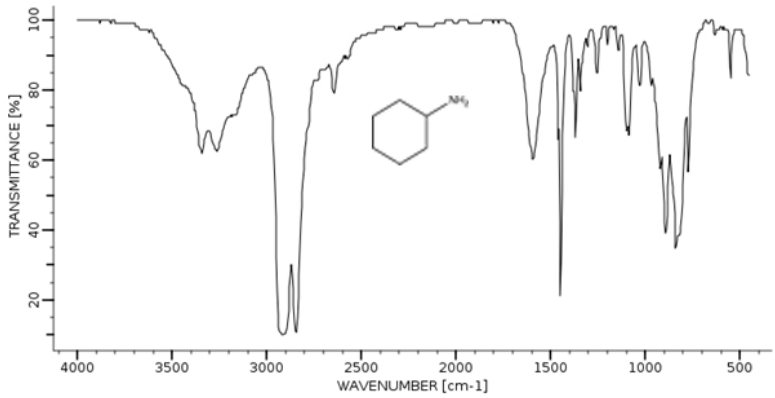


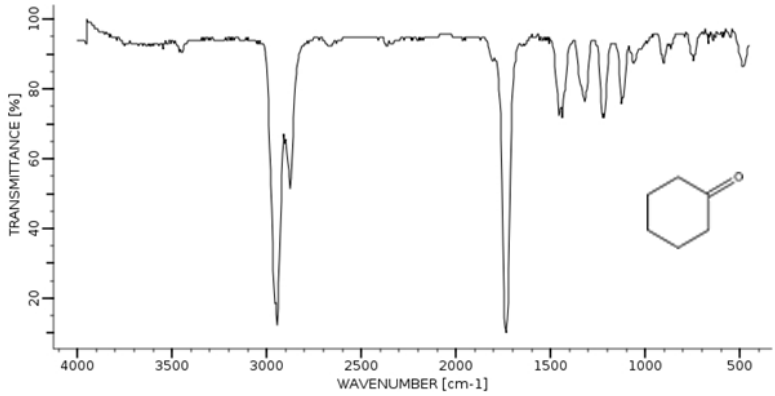
3,4-dimethylpent-3-enone (see below) will show a molecular ion peak at 112 and will have a different (but similar) fragmentation pattern.

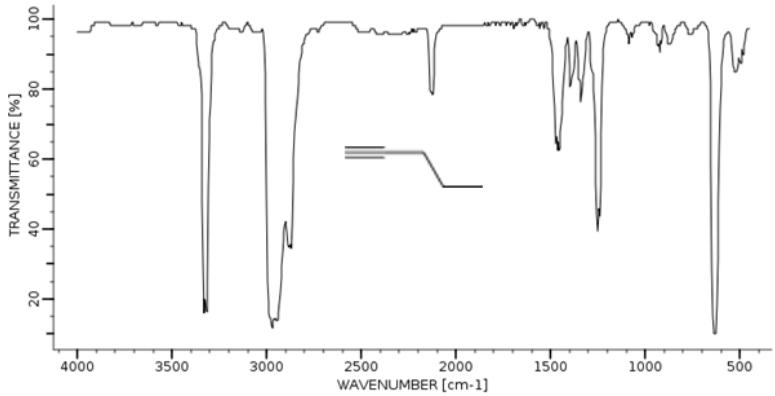


2. Infrared Spectroscopy (IR)



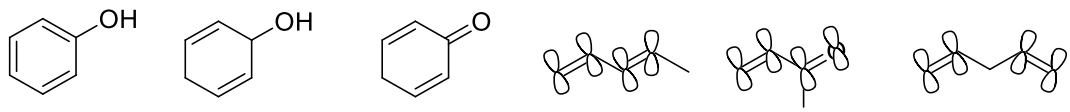






3. UV-Vis.

Each carbon atom in benzene is sp^2 hybridized.



yes no yes yes yes no

In conjugated compounds, there is an unhybridized p orbital on ≥4 adjacent atoms.

The usefulness of UV-Vis spectroscopy in organic chemistry is restricted to identifying conjugation.

Key to success: practice further by completing this week's tutorial homework

Key to even greater success: practice even further by completing this week's suggested exam questions.

For additional help on structure elucidation, see

https://scilearn.sydney.edu.au/OrganicSpectroscopy/