1. nomen /12
2. chairs1 /25
3. Newmans /6
4. Newmans 2 /25
5. IR spectra /22
6. resonance /25
7. res/NMR /22
8. IR concept /12

Extra Credit /5
Total (incl Extra) /175+5

Interaction Energies, kcal/mol

<table>
<thead>
<tr>
<th>Interaction</th>
<th>Energy (kcal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H/H</td>
<td>-1.0</td>
</tr>
<tr>
<td>He/He</td>
<td>0.9</td>
</tr>
<tr>
<td>Ne/Ne</td>
<td>-0.9</td>
</tr>
<tr>
<td>H/He</td>
<td>-1.4</td>
</tr>
<tr>
<td>He/He</td>
<td>-0.95</td>
</tr>
<tr>
<td>Me/Me</td>
<td>-2.6</td>
</tr>
<tr>
<td>Pr/Pr/Me</td>
<td>-1.1</td>
</tr>
<tr>
<td>Et/Pr/Me</td>
<td>-3.1</td>
</tr>
<tr>
<td>t-Bu/Me</td>
<td>-2.7</td>
</tr>
</tbody>
</table>

Infrared Correlation Chart

Approximate Coupling Constants, J (Hz), for

<table>
<thead>
<tr>
<th>Coupling Constant (J)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>H-H</td>
<td>~7</td>
</tr>
<tr>
<td>H-C</td>
<td>~10</td>
</tr>
<tr>
<td>C=C</td>
<td>~15</td>
</tr>
<tr>
<td>C-C</td>
<td>~16</td>
</tr>
<tr>
<td>O-C</td>
<td>~15</td>
</tr>
</tbody>
</table>

NMR Correlation Charts

<table>
<thead>
<tr>
<th>Chemical Shift (δ, ppm)</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-CH₃</td>
<td>~2.1</td>
</tr>
<tr>
<td>R-CH₂</td>
<td>~2.3</td>
</tr>
<tr>
<td>R-CH₃</td>
<td>~2.5</td>
</tr>
<tr>
<td>R-CH₂</td>
<td>~2.6</td>
</tr>
</tbody>
</table>

Aromatic

R-C=CH₂

R-C≡CH

R-C=CR₂

R-C≡CR

C=N

C-R

C-C

C-O

C-N
Question 1 (12 pts) Give the IUPAC name for the following structure.

3,4-diethyl-2,7-dimethyloctane

Question 2 (25 pts) For the following structure:

a) Draw both chair conformations.

b) Determine the energy difference between the two chair conformations using the tables on the front page of this test. **Be sure to clearly show each energy contribution that you take into account when answering this question.**

c) Indicate the lower energy chair.

EXTRA CREDIT (5 pts) Which of these techniques forms the basis for the device that is used to detect traces explosives and/or narcotics at airport security checkpoints?

- mass spectrometry
- infrared spectroscopy
- proton nmr spectroscopy
- carbon nmr spectroscopy
Question 3 (6 pts.) Convert the following Newman projection into a 3-D/sawhorse structure

Question 4 (25 pts.) For 3-methylhexane
a) Draw a line-angle structure
b) Draw Newman projections (only, no 3-D/sawhorse structures) corresponding to the lowest AND highest energy conformations for rotation around the C3-C4 bond, draw the Newmans looking FROM THE C4 CARBON TO THE C3 CARBON (i.e. with the C4 carbon in "front")
c) Determine the energy difference between these conformations (use the data in the tables on the front page of this test), be sure to clearly show each energy contribution that you take into account when answering this question

1 x Et/Me gauche interaction = 0.95 kcal/mol
energy difference = 4.55 kcal/mol

1 x Et/Et eclipse interaction = 3.1 kcal/mol
1 x Me/H eclipse interaction = 1.4 kcal/mol
1 x H/H eclipse interaction = 1.0 kcal/mol
total = 5.5 kcal/mol
Question 6 (25 pts.) This anion is inadequately represented by the provided Lewis structure.

a) Draw additional resonance contributors that show how the negative charge is delocalized, include curved arrow-pushing and resonance arrows/brackets.

b) Indicate the major contributor or contributors and give a BRIEF justification for your choice that includes the phrase "energy of the electrons".

c) Draw an "actual" or resonance hybrid anion and on this structure AND, clearly indicate the atom or atoms where the greatest partial negative charge would be found (you can use the δ notation to indicate partial charges).

d) The hybridization of the NITROGEN ATOM is \( \text{sp}^2 \)

![Resonance contributors and atomic charges](image)

The major contributors have the formal negative charge on the more electronegative oxygen atoms, which results in the lowest formal energy of the electrons.

Question 7 (22 pts.) This is benzoic acid. Draw MINOR RESONANCE contributors as necessary to explain why the nmr chemical shift of carbon A is larger than that of carbon B. Give a brief explanation that includes the terms "deshielding" and "electron density".

![Resonance contributors and carbon shifts](image)

nuclei are shielded by their associated electron density, removal of electron density results in deshielding which results in an increase in chemical shift, the minor resonance contributors show a partial positive charge (reduced electron density) on carbon A but not on carbon B.

Question 8 (12 pts.) Briefly explain (2-3 sentences maximum) why the intensity of a absorption signal due to a single O-H stretching vibration is often larger than the sum of many C-H stretching vibration absorptions in an infrared spectrum of an alcohol. Include the term "electric field vector" in your explanation.

absorption of IR light by a molecule requires interaction of the electric field vector with the dipole moment of a vibrating bond, the larger the bond dipole moment the larger the interaction and the larger the absorption, an O-H bond has a much larger dipole moment than a C-H bond.
Question 5 (22 pts.) Assign the BOTH IR spectra to ONE of the THREE provided structures A - C. ONE of the structures does not have a provided spectrum. On each spectrum, identify the peaks that are associated with a specific functional group or type of C-H bond by drawing the functional group or bond and drawing an arrow from the specific bond in the functional group that vibrates to the absorption peak, as appropriate.

the spectrum below corresponds to structure A

the spectrum below corresponds to structure B
Question 9 (26 pts) Provided are spectra for a compound with molecular formula $\text{C}_{10}\text{H}_{14}$

a) Give the degrees of unsaturation

4 degrees of unsaturation

b) On the infrared spectrum, indicate which peaks correspond to which functional groups

![Infrared spectrum with labeled peaks](image)

- 3094 cm$^{-1}$
- 1941 cm$^{-1}$
- 1803 cm$^{-1}$
- 1598 cm$^{-1}$
- 1354 cm$^{-1}$
- 1031 cm$^{-1}$
- 779 cm$^{-1}$
- 762 cm$^{-1}$

![Functional group assignments](image)

- $\text{C} = \text{H}$ sp$^2$
- $\text{C} - \text{H}$ sp$^3$
- $\text{C} - \text{H}$ sp$^3$
- $\text{C} - \text{H}$ sp$^3$
- $\text{C} - \text{H}$ sp$^3$

(c) draw the structure and clearly indicate which hydrogens correspond to which signals in the proton nmr spectrum

![Proton NMR spectrum with labeled hydrogens](image)

- 1H
- 2H
- 3H
- 5H

![Structure with hydrogen assignments](image)