Interaction Energies, kcal/mol

<table>
<thead>
<tr>
<th></th>
<th>Eclipsing</th>
<th>Gauche</th>
</tr>
</thead>
<tbody>
<tr>
<td>H/H</td>
<td>~1.0</td>
<td>0.9</td>
</tr>
<tr>
<td>He/He</td>
<td>~1.4</td>
<td>~0.95</td>
</tr>
<tr>
<td>Me/Me</td>
<td>~2.6</td>
<td>~1.1</td>
</tr>
<tr>
<td>Et/Me</td>
<td>~3.1</td>
<td>~2.7</td>
</tr>
<tr>
<td>i-Pr/Me</td>
<td>~3.1</td>
<td>~2.7</td>
</tr>
<tr>
<td>t-Bu/Me</td>
<td>~3.1</td>
<td>~2.7</td>
</tr>
</tbody>
</table>

Approximate Coupling Constants, J (Hz), for \(^1\)H NMR Spectra

- C–C ~7
- C–C ~10
- C–C ~15
- C–H ~15
- C–H ~15
- C–H ~15
- C–H ~15

**Infrared Correlation Chart**

- **3000–3150** broad with spikes ~3300
- **2800–2999** broad ~3000
- **1725** 2 peaks
- **1710** broad ~3000
- **1650** ~2730–2820
- **1680** ~2200
- **1600–1660** 2 peaks
- **1500** 3 peaks
- **1460** ~2200
- **1450** ~3300

**NMR Correlation Charts**

- **3000–3150** broad with spikes ~3300
- **2800–2999** broad ~3000
- **1725** 2 peaks
- **1710** broad ~3000
- **1650** ~2730–2820
- **1680** ~2200
- **1600–1660** 2 peaks
- **1500** 3 peaks
- **1460** ~2200
- **1450** ~3300

**Aromatic**

- δ, ppm: **11** 10 9 8 7 6 5 4 3 2 1 0
- **1400–1500**
- **1500** 3 peaks
- **1600** ~2200
- **1650** ~3300
- **1710** broad ~3000
- **1725** 2 peaks
- **1750** broad ~3000
- **1800** ~2200
- **1900** ~3300
- **2000** ~4400

**Alkyl**

- 3° > 2° > 1°

**Alkoxy**

- **3° > 2° > 1°

**amide**

- 3° > 2° > 1°

**amine**

- R–NH₂ variable and condition dependent, ca. 2 – 6 δ

**alcohol**

- R–OH dependent, ca. 2 – 6 δ

**Molecular Models Are Allowed**

- **DO NOT USE RED INK**
- **DON'T CHEAT, USE COMMON SENSE!**
Question 1 (12 pts) Give the IUPAC name for the following structure.

Question 2 (24 pts)

a) Which of the following two anions A or B would be more chemically reactive? Give a brief explanation that includes drawings of all important resonance contributors, including curved arrow pushing and resonance arrows/brackets as appropriate, and IDENTIFY the major contributor if there is one.

b) For EACH of the ions above, draw the "actual" structures, use either the delta charge symbol or an exact fractional charge as appropriate, AND, CIRCLE EACH ATOM that is PART OF THE CONJUGATED SYSTEM in each actual structure.

EXTRA CREDIT (5 pts) Which types of structures are the primary constituent of gasoline?

alkenes   ketones   alkanes   aromatics
Question 3 (24 pts) For the following structure
a) draw both chair conformations
b) determine the energy difference between the two chair conformations
c) indicate the lower energy chair and CLEARLY indicate the energy factors that you include in your calculation of this energy difference

Question 4 (18 pts) Shown are chair structures for cis-1,4-dimethycyclohexane and trans-1,4-dimethycyclohexane. Indicate which is the trans-isomer and which is the cis-isomer. Considering these chairs only, explain WHICH would have the LARGER heat of combustion. Your explanation MUST include the phrase "1,3-diaxial interaction" (it is not necessary to know or draw the chemical equations for combustion for these structures to answer this question).
Question 5  (20 pts.) Assign EACH IR spectrum to ONE of the TWO provided structures. On each spectrum, identify the peaks that are associated with specific a functional group (including all C-H bond types) by drawing the functional group and drawing an arrow from the specific bond in the functional group that vibrates to the absorption peak, as appropriate.
Question 6 (31 pts.)

a) Explain which of the bonds C-Ha or C-Hb has the larger homolytic bond dissociation energy. Give an explanation that includes drawings of the products of EACH bond dissociation, including all relevant resonance contributors as appropriate. As usual, include the curved arrow pushing showing how the electron distributions "move" between each contributor and resonance arrows/brackets.

b) Draw an ENERGY DIAGRAM with properly labelled axes for cleavage of the C-Ha and C-Hb bonds ON THE SAME DIAGRAM, clearly indicating which diagram refers to which bond cleavage and indicate the MAGNITUDES of the two bond dissociation energies on your diagrams. Deciding where to normalize the diagrams is part of the problem so oleae do not ask fro help with this part.
Question 7 (18 pts.) Explain which you would expect to have the higher vibration frequency, the C=O bond of a ketone or the C=N bond of an imine (examples are shown below), AND, explain which of the absorption bands would be stronger or more intense in an IR spectrum, that for the C=O bond or the C=N bond.

![Imine and Ketone Structures]

Question 8 (28 pts.) For rotation around the C2-C3 bond of 2,3-dimethylbutane:

a) Draw Newman projections for BOTH the HIGHEST and the LOWEST energy conformations, (clearly indicate which is which)

b) Draw 3D (sawhorse) structures for these two conformations (clearly indicate which is which)

c) Determine the energy difference between these two conformations. CLEARLY indicate the energy factors that you include in your calculation of this energy difference