Interaction Energies, kcal/mol

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

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

NMR Correlation Charts
Question 1 (14 pts.)
a) Give a line-angle structure for the following condensed formula. Do not forget to add all non-bonding electrons where appropriate.

\[(\text{CH}_3\text{CH}_2)_2\text{CH}(\text{CH}_2)_2\text{COCH}_2\text{CCCHO}\]

the graders do not get an absolute grading rubric for my tests, there are always too many possible ways to get partial credit in my exams, the guidelines in blue therefore are guidelines ONLY

~3 pts each for the functional groups
-2pts for incorrect alkyl groups
-3pts for this at the end:

Question 2 (30 pts.) Directly ON TOP of the structures below
a) Draw a picture of the $\Psi$ or $\Psi^2$ as requested, for the indicated orbitals
b) Clearly indicate the atomic orbital or orbitals that you used to construct the requested orbitals
c) For each drawing, clearly indicate the positions of any nodes, or locations of zero probability of finding the electrons, as appropriate to the question

$\Psi^2$ for the C-O $\pi^*$ M.O.
- incorrect sizes -2pts
- p A.O. (carbon)
- p A.O. (oxygen)

$\Psi$ for the C-Cl $\sigma^*$ M.O.
- p A.O. (carbon)
- p A.O. (oxygen)

$\Psi$ for the C-C $\sigma$ M.O.
- sp (C)
- sp3 (C)

forgot A.O.s = -2pts
- did the wrong question (wrong bond) = 7 pts maximum
- did bonding instead of anti-bonding or vica versa 7pts max

Extra Credit (5 pts). One of the factors that contributes to the "stiffness" of the poly-peptide chains in proteins is...........

the wavefunctions
- the geometrical isomers
- resonance
- the ester functional groups
Question 3 (24pts.) For the structure shown on the right:

a) give the hybridization for the nitrogen atom
b) list all of the valence atomic orbitals formally associated with this nitrogen atom and give a brief description of how the nitrogen atom uses each orbital, e.g. p atomic orbital used to make a sigma bond to chlorine (this is obviously not correct, it is just to indicate how to answer this question)

too many options for a rubric, generally half correct = half points
there were 4 questions JUST LIKE THIS ONE on the problem set
the N has an sp2 hybrid A.O. containing one pair of non-bonding electrons

the N has an sp2 hybrid A.O. that is used to build the $\sigma$-bond to the hydrogen atom

the N uses an sp2 hybrid A.O. to build the $\sigma$-bond to carbon, which contains one of the pairs of electrons in the C=C double bond

the N uses an unhybridized p A.O. to build the $\pi$-bond to carbon, which contains the second of the pairs of electrons in the C=N double bond

c) Give the approximate C-N-H bond angle indicated in the structure above with the arrow, assign the geometry around the nitrogen atom, AND, give a BRIEF explanation (2-3 sentences MAX.) for your choice of geometry that includes the terms "energy of the electrons", "VSEPR", "electron domains".

there are 3 domains of electrons around the nitrogen, VSEPR requires a trigonal planar-like geometry to minimize the total energy of the electrons, HOWEVER, the nitrogen only has 2 atoms attached to it and the position of the non-bonding electrons cannot be determined with certainty, the geometry can only be defined as bent

students will probably give a less detailed explanation than this, which is OK, just so long as it is correct and includes the FOUR required items in bold above

Question 4 (15 pts.) Circle and identify all functional groups in the following structures, ignore alkyl groups.

ibuprofen
the active ingredient in Motrin

acetaminophen
the active ingredient in Tylenol
Question 5) (48 pts.) For the molecular formula \( C_3H_6O_2 \)

a) Give the degrees of unsaturation  

1 degree of unsaturation

b) Draw EIGHT structural isomers for \( C_3H_6O_2 \) that obey the normal rules of valence for each atom. Include all non-bonding electrons. You can draw Lewis structures or line-angle structures (your choice). If you draw line-angle structures, don't forget to include the H atoms that are normally included as part of the functional groups.

![Structural Isomers](image)

there are MANY more than these!

c) Draw TWO PAIRS of stereoisomers for \( C_3H_6O_2 \) that obey the normal rules of valence for each atom. Include all non-bonding electrons. You can draw Lewis structures or line-angle structures (your choice). If you draw line-angle structures, don't forget to include the H atoms that are normally included as part of the functional groups.

DO NOT INCLUDE ANY STRUCTURES in part c) THAT WERE DRAWN AS PART OF YOUR ANSWER TO PART b) OF THIS QUESTION!!

![Stereoisomers](image)

etc.
Question 6) (30 pts) For the structure provided:

a) Draw ALL reasonable missing resonance contributors
b) Draw the curved arrow-pushing that indicates how the electrons are delocalized
c) give the NUMBER OF ELECTRONS that are delocalized
d) Indicate which is the MAJOR resonance contributor and give a BRIEF EXPLANATION for your choice. If there are equal major contributors, indicate so.
e) Include resonance arrows and brackets to complete your description of the final structure
f) Based on the resonance contributors you drew, give the "actual" resonance hybrid structure. Indicate the atoms that have a partial charge, do not worry about determining absolute partial charges, just use the $\delta$ charge notation.

\[ \text{SIX electrons delocalized} \]

the major resonance contributor has the negative charge in the more electronegative nitrogen atom

"actual" hybrid structure

1pt each

g) On the structure below (same one as above), give the hybridization of EVERY CARBON ATOM and also the NITROGEN ATOM. Take ALL of the resonance contributors your drew above into account when determining hybridizations.

Question 7) (14 pts) One of the two carbon atoms in the C=C double bond in the structure below has a small partial negative charge. Draw a MINOR resonance contributor that illustrates which carbon this is, and clearly indicate the carbon that has this small partial negative charge. Include curved arrow pushing, resonance arrows and resonance brackets.

THIS carbon has the small partial negative charge