Question 1

Which best describes the relationship between the following two structures?

\[ \text{trans-1,3-diethylcyclohexane} \]

A. structural isomers  
B. different structures and not isomers  
C. stereoisomers  
D. the same thing

\[ \text{trans-1,3-diethylcyclohexane} = \begin{array}{c} \text{ Et} \\ \text{ Et} \end{array} \quad \text{OR} \quad \begin{array}{c} \text{ Et} \\ \text{ Et} \end{array} \]

\[ = \text{cis-1,3-diethylcyclohexane} \]
**Question 2**
MC19l

What is the energy difference between the two chair conformations of the following molecule?

<table>
<thead>
<tr>
<th></th>
<th>A 1.5 kcal/mol</th>
<th>B 3.7 kcal/mol</th>
<th>C 0.55 kcal/mol</th>
<th>D 3.15 kcal/mol</th>
</tr>
</thead>
</table>

**Energy Cost Calculation**

- **1 Et group axial, energy cost = 2 x (Me/Et) = 1.9 kcal/mol**
- **1 Me group axial, energy cost = 2 x (Me/Me) = 1.8 kcal/mol**
- **1 i-Pr group axial, energy cost = 2 x (Me/i-Pr) = 2.2 kcal/mol**
- **1 Me/Et gauche, energy cost = 0.95 kcal/mol**

**TOTAL energy cost = 3.7 kcal/mol**

**DIFFERENCE = 3.7 - 3.15 = 0.55 kcal/mol**
Question 3
MC23h

which of the provided compounds has this IR spectrum?

B would have 2 peaks due to N-H at ca. 3300, and also a broad weak band around 3000 (not observed), and would also not have C=O etc.

C would also have O-H (not observed), would not have benzene peak at ca. 1600

D would not have carboxylic acid O-H at ca. 3000 cm⁻¹
Question 4
MC 23d

Determine how many reasonable molecular formulas correspond to the mass spectrum below. Assume that only carbon, hydrogen and possibly oxygen atoms are present. For the purpose of this question you should assume that all reasonable molecular formulae will have hydrogens and will not have more carbon atoms than hydrogen atoms or more oxygens than hydrogens.

- \( \frac{72}{12} = 6 \) (Remainder = 0), i.e. \( C_6 \) (unreasonable)
- replace 1 C by 12 H's: \( C_5H_{12} \) (0° of unsaturation, possible)
- replace another C by 12 H's: \( C_4H_{24} \) (impossible)
- replace 1C & 4H's by 1 O, \( C_5H_{12} \) becomes \( C_4H_8O \) (1°, possible)
- replace 1C & 4H's by 1 O, \( C_4H_8O \) becomes \( C_3H_4O_2 \) (2°, possible)
- replace 1C & 4H's by 1 O, \( C_3H_4O_2 \) becomes \( C_2O_3 \) (unreasonable)
Question 5

Use minor resonance contributors to determine which compound from the following has the LOWEST frequency for the C=O stretching vibration.

MC23i

Hint: the way to think about this question is to remember why the amide C=O has a low vibration frequency, and remember that the explanation for that was also on the basis of minor resonance contributors.

Several minor resonance contributors can be drawn for these ketones. Remember, we used a minor resonance contributor to explain why the C=O bond in an amide has a relatively low vibration frequency. The more that resonance contributors with C-O single bond character contribute to the resonance hybrid, the weaker the C=O bond, the lower the vibration frequency. All of the above include resonance contributors with single C-O bond character, shown in red. However, those with the N, O and Cl substituents can also form the additional one in BLUE. This is not a small difference because the blue one has more electrons in bonds compared to the others. It also puts a positive charge on a substituent atom. Of N, O and Cl, Nitrogen is "happiest" with this formal positive charge (it is least electronegative). The blue resonance contributor is thus most important with the H$_2$N substituent, and B has the LOWEST vibration frequency. Oxygen is "next" happiest with the positive charge, C thus has the next lowest vibration frequency, followed by D. A has no blue resonance structure, the C=O bond in A thus has the highest double bond character and highest vibration frequency.
Question 6
MCir3

which of the provided compounds has this IR spectrum?

- not an alcohol RO-H centered at ca. 3300
- broad COO-H centered at ca. 3000
- C=O at ca. 1720
- not an aldehyde because it also has the broad -OH signal

A B C D
which of the provided compounds has this IR spectrum?

A would not have benzene peak at 1600 and no sp2 C-H

C would have N-H peaks at ca. 3300 and also strong C=O at ca. 1640

D would have carboxylic acid O-H centered ca. 3000
Identify the structure with the following IR spectrum

- 2 peaks ~3350 & 3200 cm⁻¹: probable -NH₂
- C=O, ~1650 cm⁻¹: probable amide
- No broad -OH observed at ca. 3300 cm⁻¹

Options:

- A: would not have C=O stretch
- B: no broad -OH observed at ca. 3300
- C: no broad -OH observed at ca. 3000
- D: