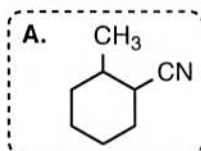


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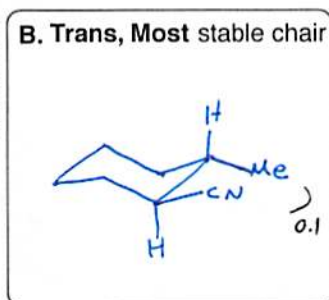
Consider the following: each 1,3-diaxial strain interaction between CH_3 and H is 1 kcal/mol; each 1,3-diaxial strain interaction between CN and H is 0.1 kcal/mol; each gauche strain interaction between CH_3 and CN is 0.1 kcal/mol; and the gauche strain interaction between CH_3 and CH_3 is 1 kcal/mol.

1a. 11 pts. Focus on the **cis** and **trans** stereoisomers of the molecule in box A. In B and C, draw the most stable chair conformer, as specified in the respective box (cis and trans). In boxes D and E, draw the least stable chair conformer.

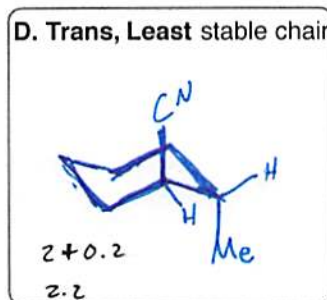
Then, calculate ΔG_0 for the chair-flip process in F and G.



B. Trans, Most stable chair

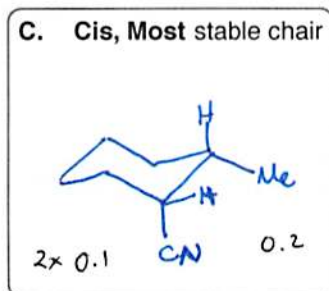


D. Trans, Least stable chair

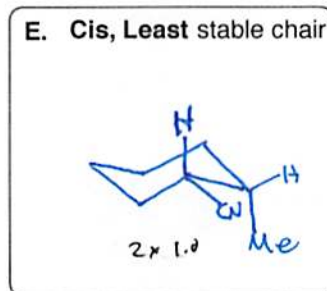


F. $\Delta G_0 = 2.1$ kcal/mol

C. Cis, Most stable chair

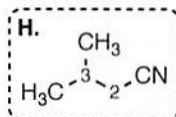


E. Cis, Least stable chair

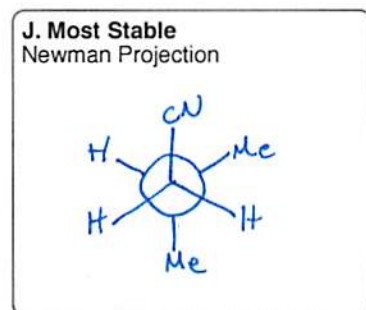


G. $\Delta G_0 = 1.8$ kcal/mol

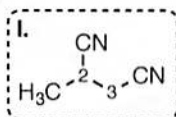
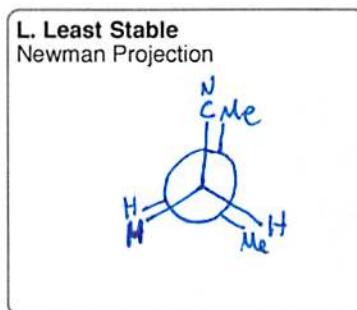
1b. 10 pts. Consider compounds H and I. Draw the **most** and **least** stable Newman projection of each molecule, putting carbon number 2 in the front. Note: exact strain energy values are not necessary to answer this question.



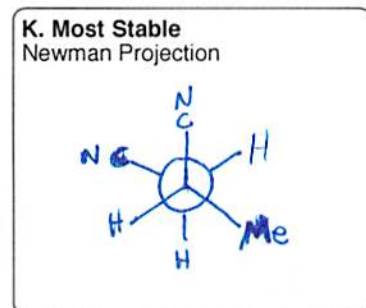
J. Most Stable
Newman Projection



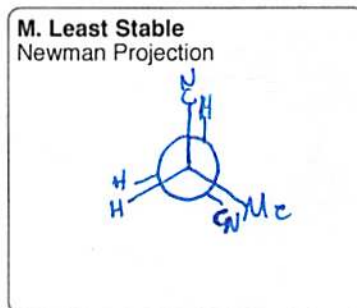
L. Least Stable
Newman Projection



K. Most Stable
Newman Projection



M. Least Stable
Newman Projection

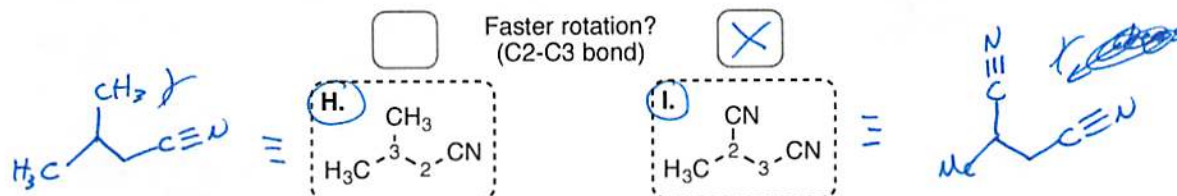


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Name: _____

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1c. 4 pts. Which compound would you expect to rotate faster about the C2-C3 bond? Mark an X in the box above the structure of the molecule that you expect to have a faster rotation.

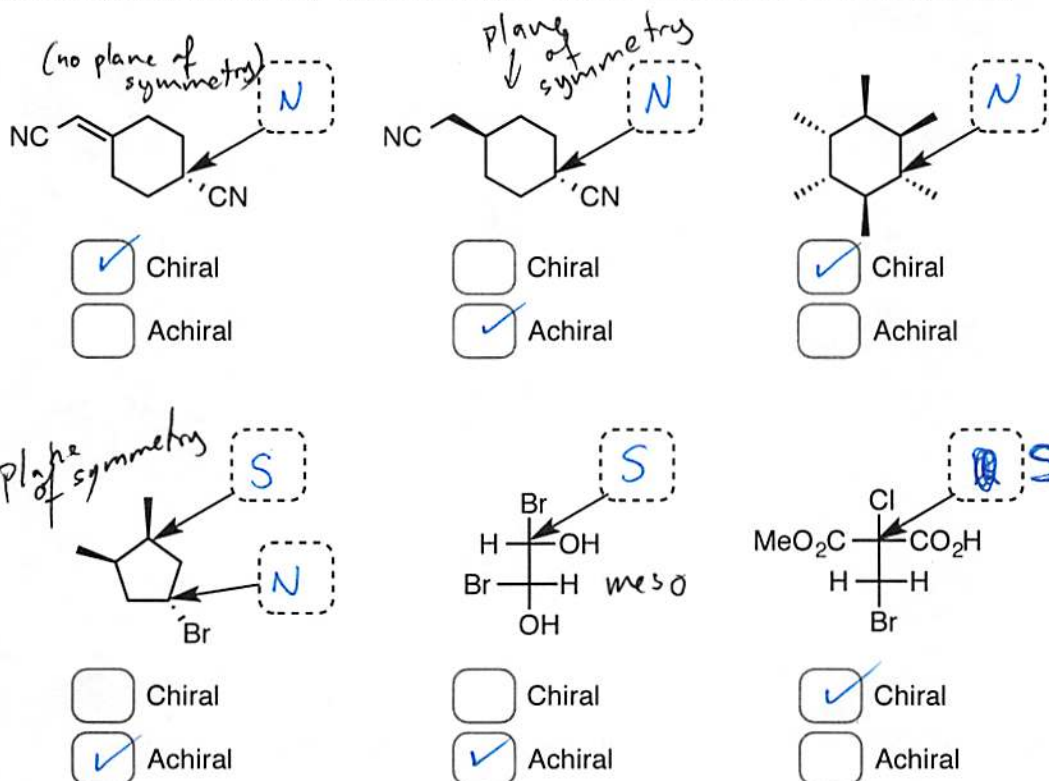


Briefly explain your answer in the box below:

There is more steric hindrance in the rotation in "H." between the cyano group and the methyl group, as opposed to "I" where there is less hindrance during rotation between the cyano groups. The less torsional strain in "I" leads to a lower energy for rotation, and \therefore a larger "k" rate of rotation.

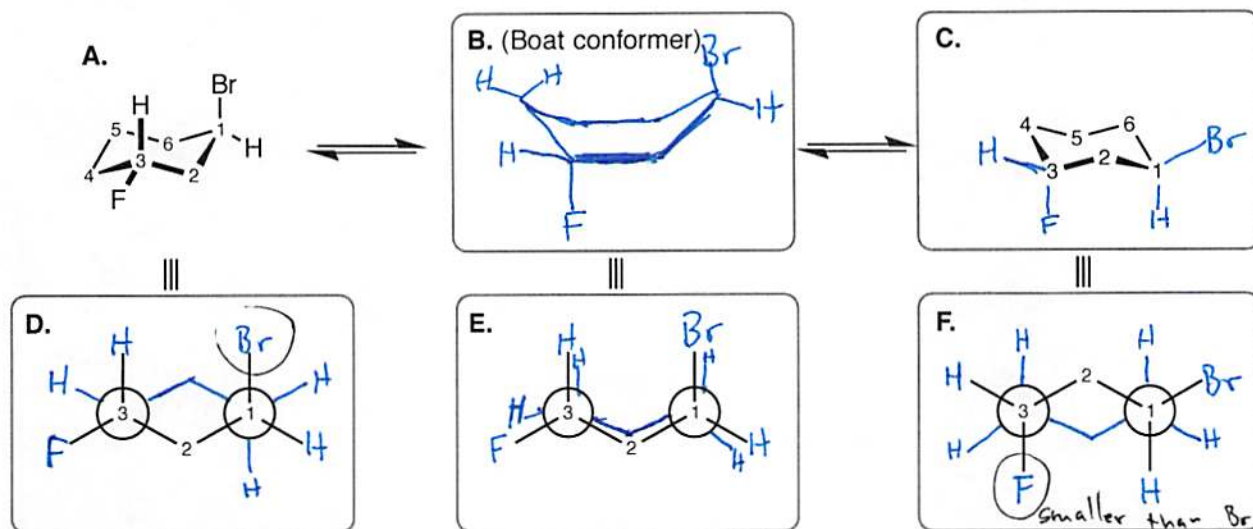
2. 18 pts. In the **dashed boxes**, label the **R/S** specific configuration of the carbon center indicated by the arrows. If the carbon is not a chiral center, enter the letter **N** (for "no chiral center").

In the solid boxes, put a check mark (☒) in the appropriate space if the **molecule is chiral or achiral**.



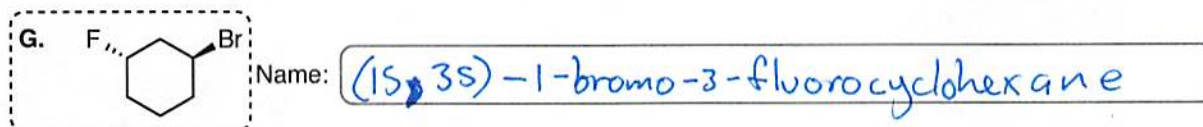
Name: _____

3a. 11 pts. The cyclohexane molecule containing two functional groups in box A is drawn as a chair, showing the carbons as numbers for easy labeling and tracking during the chair-flip process. In box B, draw the boat conformer, and in C, add the missing bonds and atoms that show the ring-flipped conformer. In boxes D, E, and F, complete the corresponding Newman projections with all missing bonds and atoms (C, H, Br, F).



Comparing **A**, **B**, and **C**, which conformer would you expect to be the most stable? Answer: **C** enter A, B or C

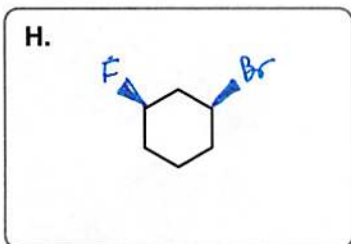
3b. 2 pts. What is the name of the molecule in box G. (Answer in the space provided).



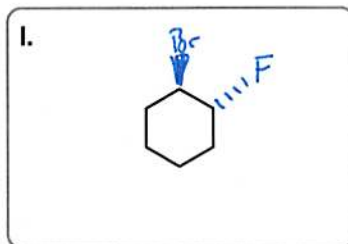
3c. 2 pts. Now consider the molecules in boxes A and G. What is their relationship? Mark an X in the boxes below. Check all that apply.

A and G are: ☐ same molecule ☒ enantiomers ☐ diastereomers

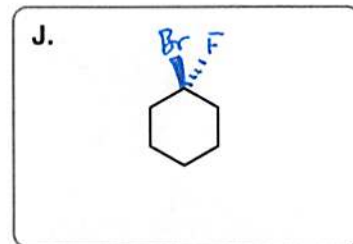
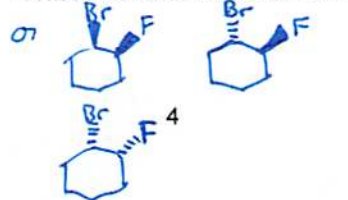
3d. 6 pts. In boxes H, I, and J, there may be more than one correct answer. Therefore, provide **one structure**, as specified by the following instructions: In box H, draw a **diastereomer** of A. In box I, draw a **chiral constitutional isomer** of $C_6H_{10}BrF$, where there's still a 6-membered ring (other than the ones shown above). In box J, draw an **achiral constitutional isomer** of $C_6H_{10}BrF$, where there's still a 6-membered ring.



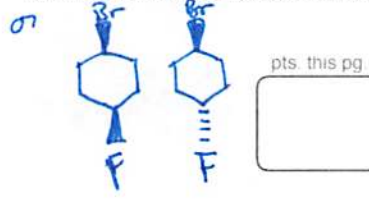
Diastereomer



Chiral constitutional isomer

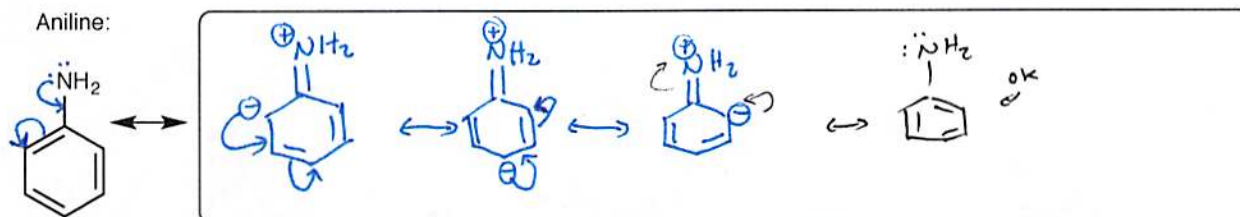


Achiral constitutional isomer

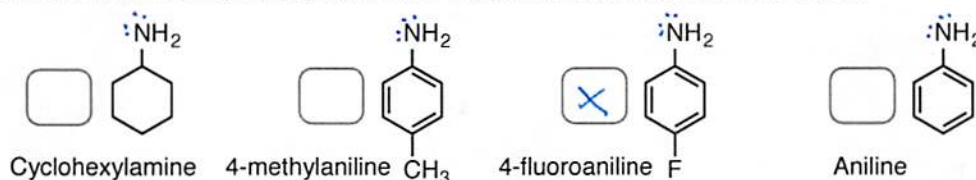


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4a. 5 pts. Draw all resonance structures for aniline (i.e. only the structures with full octets). Be sure to include lone pairs and arrow pushing to show the movement of electrons in the structure on the left and the ones within the box.



4b. 6 pts. Put an X in the box to indicate which one is the **weakest Brønsted base** below.



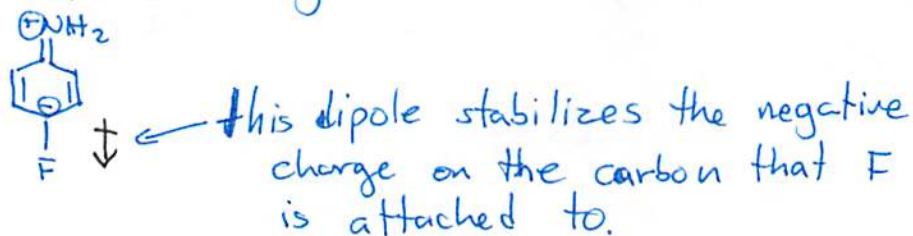
Briefly explain your answer, comparing and contrasting the different compounds, and include structures that are relevant to your explanation.

Be concise! Adding superfluous statements that are wrong will result in deduction of points, even if you have already written the correct explanation.

The anilines are weaker bases because the lone-pair electrons ~~to~~ than cyclohexylamine

that act as the Lewis base are delocalized over several resonance structures. These lone-pair electrons are more localized in cyclohexylamine.

Out of the three anilines, there is one resonance structure that is further stabilized by inductive effects:



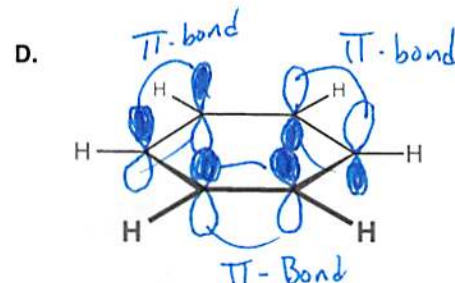
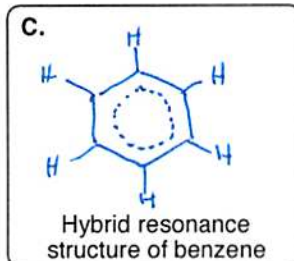
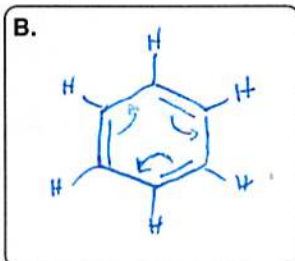
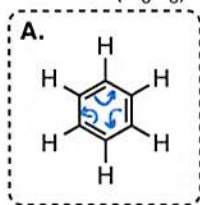
Because the other two anilines don't have such stabilization, that means that 4-fluoroaniline is the least reactive toward a proton ~~at~~ in the amine, therefore, it's less basic.

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Name: _____

5a. 5 pts. In box B, draw the best resonance structure of benzene (full octets, no formal charge), including the arrows that show the interconversion between both structures. In box C, draw the hybrid resonance structure of benzene. In the σ -bond skeleton of benzene (D. side view), draw the atomic orbitals and clearly label any π bonds. NOTE: exclude the s and sp^2 atomic orbitals and σ -bonds.

Benzene (C_6H_6)

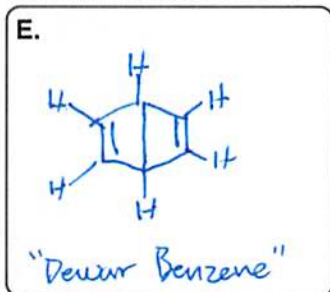


5b. 3 pts. The benzene structure in box A shows that benzene has alternating double bonds and single bonds in a cyclic fashion. A typical C-C single bond length is 1.54 Å. A typical C=C double bond length is 1.34 Å. However, the actual C-C bond distances in benzene are all equal (the C-C bonds in benzene are 1.40 Å). Briefly explain why: All bonds are the same because...

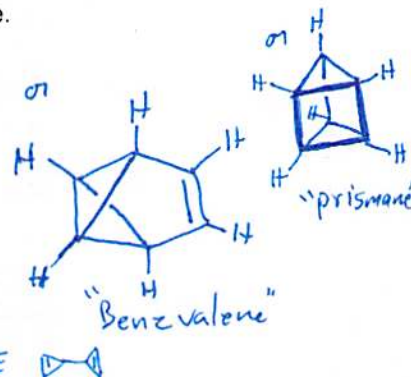
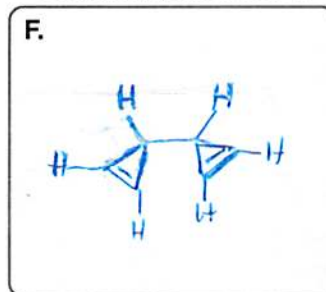
The hybrid resonance structure shows that the C-C bonds do not have differences in bond character. also, calculating the bond order leads to a value of 1.5 bonds, which is not single or double-bond character. Therefore, it is reasonable that the observed C-C distance in benzene is between the value of a single and double bond.

5c. 5 pts. In 1865, Kekulé proposed the structure of benzene (box A), which is one of the 217 constitutional isomers of the molecular formula C_6H_6 . Kekulé's structure contains each carbon bonded to one hydrogen. In boxes E and F, draw two other constitutional isomers of C_6H_6 that also have each carbon bonded to one hydrogen (excluding resonance structures of box A). Hint: Multicyclic structures are possible.

Constitutional isomer 1



Constitutional isomer 2



5d. 3 pts. Out of all the structures in boxes A, E, and F, which constitutional isomer do you expect to be the most stable (lower energy structure)? (Consider all factors contributing to the stability of the structure).

A Most stable constitutional isomer

Briefly explain your answer:

Benzene is the only structure that maintains all ideal bond angles and lengths. The other two isomers have: -ring strain -torsional strain -angle strain

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