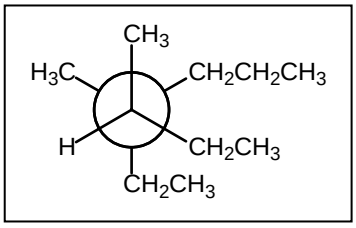
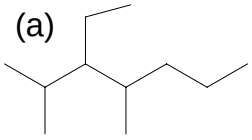


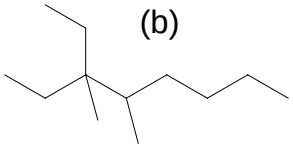
1. (11 Points) (a) Draw the skeletal structures (showing only C-C bonds) of all constitutional isomers of octane with only five carbon atoms in their main chain. Do not write extra or duplicate structures!

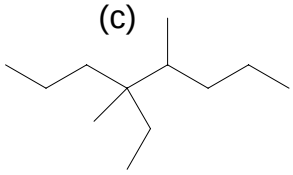
(b) Which of the following molecules is represented by the Newman projection:

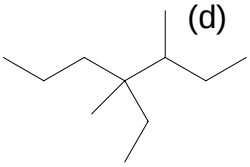


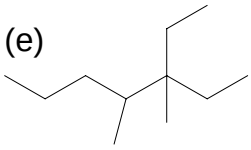
Answer =


(a)


(b)


(c)

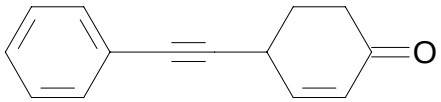

(d)


(e)

(f) None of these

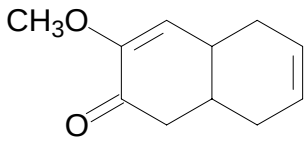
(c)

How many C atoms are in the sp^2 hybridization state



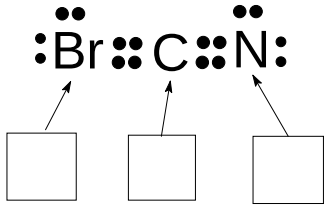
Answer:

How many C atoms are in the sp^3 hybridization state

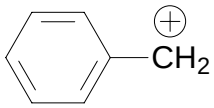


Answer:

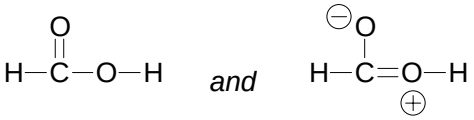
2. (12 Points) (a) What is the formal charge on each atom. Place each individual answer in the box provided at the end of the arrow.

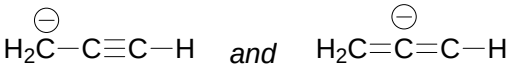


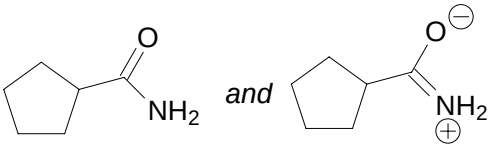
(b) Draw all the possible resonance forms for the benzyl cation.

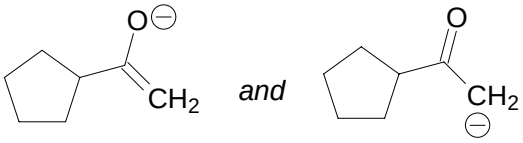


(c) Which of the following pairs are NOT resonance structures of each other?

A  *and*

B  *and*

C  *and*

D  *and*

E **All are pairs of resonance structures**

Answer(s):

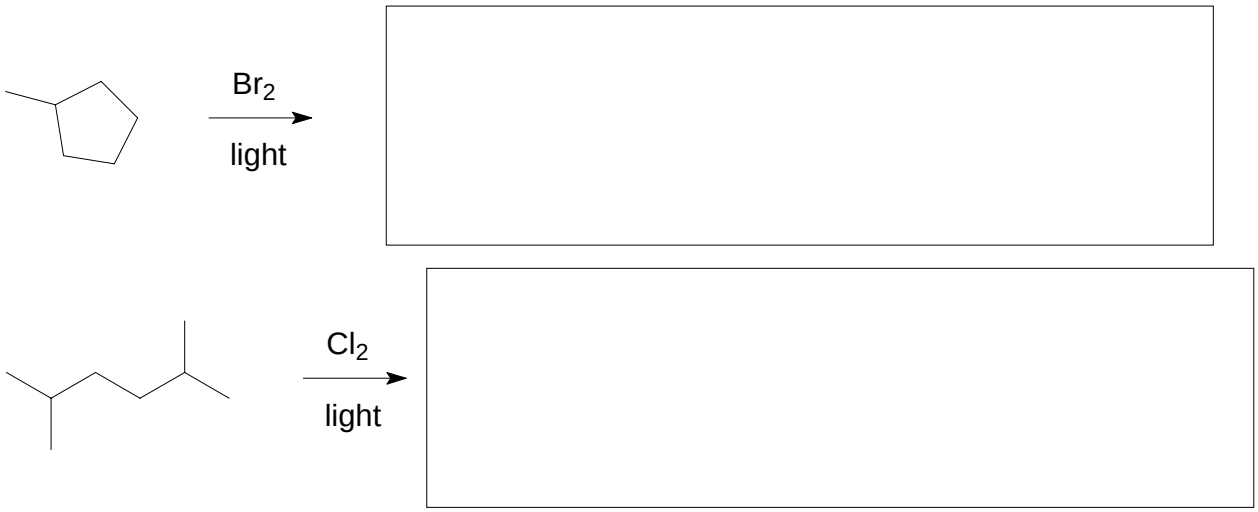
(d) Name the fuel used in jet engines

Answer:

(e) Name the catalyst mentioned in lecture used for cracking alkanes.

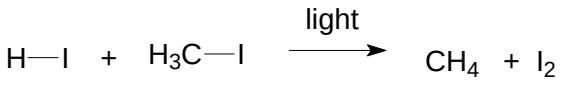
Answer:

3. (11 Points) (a) Show **the major product** for each of the monohalogenation reactions below



(b) Sketch a complete and fully labeled potential energy diagram for the formation of CH_3Cl from methane and chlorine. You can assume that chlorine radicals are always available to start the reaction. (make sure the diagram is fully legible, use all the space provided)

4. (13 Points). When exposed to light, a mixture of HI and CH_3I reacts to produce methane and iodine. (a) What is the enthalpy change for the overall reaction?



Answer: ΔH^o =

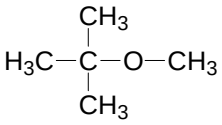
(b) Write a step-by-step mechanism for the reaction above showing the initiation and propagation steps only. For each step also show the enthalpy change associated with the specific step.

c) Show the structure of the compound used as a reference for diesel fuels with the cetane number of 100 and name it using IUAPC nomenclature.

5. (10 Points). (a) Explain briefly why water is not usually effective in extinguishing a gasoline fire.

Answer:

(b) MTBE (methyl-t-butyl ether, see structure below) was recently replaced by ethanol as a gasoline additive. Write a balanced equation for its complete combustion in oxygen.



(c) The heat of combustion of MTBE is $\Delta H^{o}_{comb} = -800$ Kcal mole^{-1} while that of ethanol is $\Delta H^{o}_{comb} = -330$ Kcal mole^{-1}. Calculate how many grams of ethanol would produce as much energy as 1 gram of MTBE in a combustion reaction. Show the detail of your calculation

Answer:

6. (10 Points)

(6a) Show the Newman projection of the conformation of Cl-CH_2-CH_2-Cl with the lowest dipole moment.

(6b) Show a clear structure for *cis*-1-cyclopentyl-3-methyl-cyclohexane

(6c) Arrange the following compounds in order of **increasing C-O bond length**. Explain your answer writing clear structures for each compound.

A Acetate ion CH_3COO^-

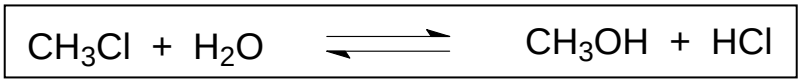
B Carbon monoxide CO

C Acetone CH_3COCH_3

D Methanol CH_3OH

ANSWER:

7. (10 Points) Consider the equilibrium shown below in which $\Delta H^o = 7.3$ kcal mole^{-1} and $\Delta S^o = 0.3$ cal K^{-1} mole^{-1}



(7a) calculate ΔG^o at 25^{o}C, show the equation you use and the details of your calculation.

ANSWER:

(7b) calculate the equilibrium constant $K_{eq.}$ show the equation you use and the details of your calculation. Which side of the equilibrium is favored?

ANSWER: K_{eq} = **Favored side is** …… side

(7c) What is the hybridization and shape of the methyl cation? Draw it .

Hybridization:

Shape:

8. (10 Points) (a) Write clear Newman projections for the three possible staggered conformations of 2,3-dimethylbutane (viewed along the bond between carbons 2 and 3). Two of these three conformations are equivalent, name them A and B and circle them. Name the other conformation C.

(b) Which of the two types (A/B or C) has the lowest energy Explain):

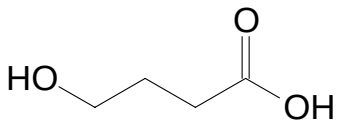
ANSWER:

(c) The two different types of conformations differ by 0.9 kcal mole^{-1}. Assume that $\Delta G^o = \Delta H^o$ and calculate the equilibrium composition at 25^{o}C (express this as % of A+B and % C). Show the equation you use and the details of your calculation.

ANSWER %C= % (A+B) =

9. (13 points) (a) Write a detailed mechanism for the formation of ethene $H_2C=CH_2$ by cracking of butane

(b) Circle and name each functional groups of the molecule below



(c) Show the electronic configuration of Si

(d) What is the length of each of the bonds shown below (choose your answer amongst the value provided below)

A: 103 pm; **B:** 124 pm; **C:** 133pm; **D:** 145 pm; **E:** 154 pm; **F:** 165 pm; **G:** 17876545 pm

Note: **There are no questions to be answered on this page**, it only contains data that may be of use in solving the questions contained in this exam. Not all of the data given is needed.

Value of gas constant: R = 2.0 cal K^{-1} mol^{-1} Value of absolute zero (kelvin) = $-273^{o}C$

Value of e (base for natural logarithms) e = 2.718

Density of gasoline : 0.8 g mL^{-1}

Bond dissociation energies (in kcal $mole^{-1}$): RCH_2-H 101; R_2CH-H 98.5; R_3C-H 96.5; Cl—Cl 58; Br—Br 46; I—I 36; H—Cl 103; H—Br 87; H—I 71; RCH_2-Cl 84; RCH_2-Br 70; RCH_2-I 56; R_2CH-Cl 85; R_2CH-Br 71; R_3C-Cl 85; R_3C-Br 71; CH_3-H 105; CH_3-I 57; CH_3-Br 70; CH_3-Cl 85;

Values of strain energies:

Each CH_3 - H eclipsing interaction: 1.5 kcal mol^{-1}

Each H - H eclipsing interaction: 1.0 kcal mol^{-1}

Each CH_3 - CH_3 eclipsing interaction: 2.5 kcal mol^{-1}

Each CH_3 - CH_3 gauche interaction: 0.9 kcal mol^{-1}

Each t-Butyl - CH_3 gauche interaction: 2.0 kcal mol^{-1}

Formulae used in solving quadratic equations:

$ax^2 + bx + c = 0$ $x = [-b \pm (\textit{square root of } (b^2 - 4ac)] / 2a$

Partial periodic table of the elements