Name: KEY

ID #: _____

4. An unknown compound, **X**, which contains 3 carbons (among other elements) was analyzed by a variety of spectroscopic techniques. The results of each of them are listed below. *(25 pts.)*

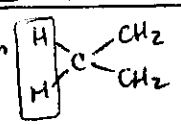
Mass Spec (MS)		IR	^{1}H NMR		
molecular ion at	m/z = 94/96	3200 cm^{-1} (broad)	2.00 ppm	multiplet (5 lines)	2H
fragments at	m/z = 76/78	several peaks below 850 cm^{-1}	2.80 ppm	singlet (broad)	1H
	m/z = 59		3.70 ppm	triplet	2H
			3.80 ppm	triplet	2H

(a) Explain what information each of these techniques tells you about the structure of **X**. In other words, analyze each of these pieces of information.

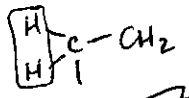
MS:
molec. ion 94/96 ∴ MW = 94/96
loses 18 = $-H_2O$
loses 35/37 = $-Cl$

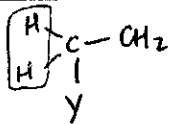
IR:
3200 cm^{-1} = O–H
<850 = some halogen (C–Cl)

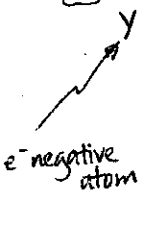
^{1}H NMR:
4 different H's

Ⓐ 2.00 ppm 

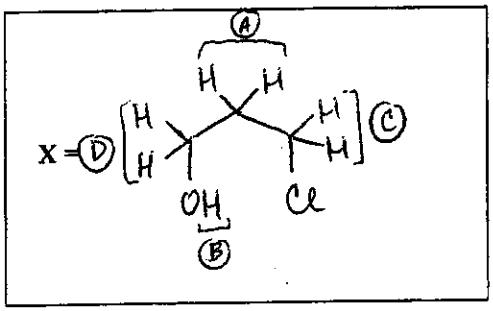
Ⓑ 2.80 O–H

Ⓒ 3.70 

Ⓓ 3.80 



(b) Give the structure of **X**.



Name: KEY

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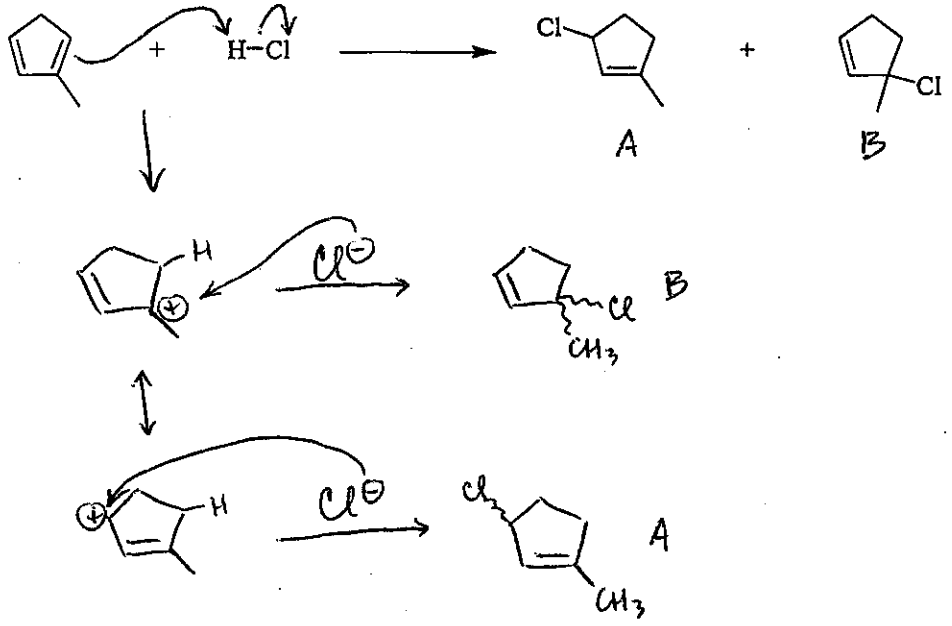
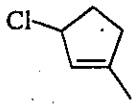
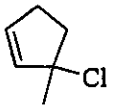
5. (a) Write a detailed mechanism for the reaction shown below. Use curved arrows to illustrate electron pushing. Show important resonance structures. *(20 pts.)*



(b) If possible, identify which of the products above is the kinetic product and which is the thermodynamic product.



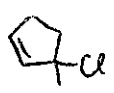
THERMODYNAMIC



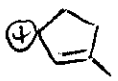
KINETIC

(c) Explain your reasoning for identifying each as either the kinetic or thermodynamic product.

THERMODYNAMIC: more stable alkene pdt.  trisubstituted ✓

(vs)  disubstituted

KINETIC: more stable carbocation IM  3° allylic ✓

(vs)  2° allylic