Dehydration and gc
lab report

Introduction In an E1 reaction, where E stands for elimination and 1 stands for unimolecular. The breaking of the C-LV bond is completed before any reaction occurs between the base to lose a hydrogen and form the carbon-carbon double bond [1]. When the more substituted alkene is the dominant product, the reaction follows Zaitsev's rule. Zaitsev's rule states that the major product of a ? -elimination reaction is the most stable alkene [1]. Acid-Catalyzed Dehydration is the elimination of a molecule of water from adjacent carbon atoms.

An alcohol can be converted to an alkene by dehydration, which is often brought on by heating the alcohol with either 85% phosphoric acid or concentrated sulfuric acid [1]. The objective of this experiment is to dehydrate 3-methyl-3-pentanol to obtain the product mixture of isomeric alkenes 3-methyl-2pentene and 2-ethyl-1-butene. Then use the gas chromatography to separate the product mixture and analyze the composition [2]. [pic] [pic] [pic] Figure1: Table of Reagents Name | Molecular Weight | Density | Melting Point | Boiling Point | | 2-methylcyclohexnol | 114. 19 g/mol | 0. 921 g/cm3 |-9. 5oC | 165oC | | Phosphoric Acid | 98 g/mol | 1. 88 g/cm3 | 42. 35oC | 158oC | | Calcium Chloride | 110. 98 g/mol | 2. 15 g/cm3 | 772oC | 1, 935oC |

Fig: The chart shows the reagents used in the laboratory experiment and information regarding the solvents. Experimental The experiment started by gathering the supplies for distillation. In the vial, 2mL of 2-methylcyclohexanol and 1mL of phosphoric acid is added. The solvents are thoroughly mixed and a few boiling chips is added to help with the boil. The sand bath is set up with the thermometer and the sand will be heated up to

100oC and the vial containing the solvents will be placed on the sand and let to boil. The process should take about 30 minutes to start boiling.

A beaker with a flask will be covered in ice and the water would be sucked out with the Pasteur pipette. When the distillation process is completed, the distillated liquid would be saved. CaCl2 would be added to the liquid to prevent evaporation and allows distillate to dry over drying agent. Then the little container will be weighed empty, and then the container with the liquid will be weight. Results ****** I can't figure out how to insert our graph. When I copy it my computer says it is too big to paste in a word document. So I'm going to pretend the graph is in this spot, and put the results of the graph under here.

Hopefully someone else in the group can use their computer to insert the graph or we can print it off and the graph will just have its own page. A gas chromatogram is a plot of a response against the retention time. Chemical substances as gases are retained on the liquid column (stationary phase) with a flow gas being the carrier (mobile phase) through the column. At the end of the column is some means of detection. The peak height or the peak area is used to quantitate the amount of substance. The number of peaks can also help determine whether or not one is dealing with a pure compound.

Peak one has a retention time of . 29 seconds and a peak area of 999. 00. Peak two was found to have a retention time of . 37 seconds and a peak area of 5067. 00. The percent composition for peak one is 16. 46884% and the percent composition for peak two is 83. 53116%. The percent yield is given by the ratio of the experimental yield to the theoretical yield, which was

found to be 52%. Discussion All possible products were observed. Under kinetic control, a significant yield of 3-methlycyclohexane is expected when 2-methylcyclohexane is dehydrated.

The kinetic product is known as Hofman product. The mechanism of this dehydration involves the formation of a tertiary carbocation intermediate. The observed products do support E1 mechanism. E1 mechanism indicates an elimination, unimolecular reaction, where rate = k [R-LG]. This implies that the rate determining step of the mechanism depends on the decomposition of a single molecular species. The pathway involves two critical steps, which are the loss of the leaving group to generate a carbocation intermediate, then the loss of a proton from the carbocation to form a pi-bond.

In this experiment the slow step in this elimination is the loss of a water molecule (the leaving group) from the oxonium ion to form the carbocation intermediate. This unimolecular rate-determining step makes this an E1 mechanism. The percent composition of a compound is a relative measure of the mass of each different element present in the compound. It gives the composition of the sample that was injected into the gas chromatograph, which ultimately helps determine alkene stability. In an error analysis of this experiment, peak resolution is critical.

In a good chromatographic separation, the components of the sample are completely separated from each other in the chromatogram. Unfortunately, an incomplete separation of the components in a sample gives poor peak resolution and there is an overlap between adjacent peaks in the chromatogram. When the peaks in a chromatogram are poorly resolved, it is

necessary to adjust one or more of the separation parameters until baseline resolution is obtained. Reference [1] Brown, William Henry. Organic Chemistry. Belmont, CA: Brooks/Cole Cengage Learning, 2009. Print. Page 149-157 2] Hill, Richard K. , and John Barbaro. Experiments in Organic Chemistry. Raleigh, NC: Contemporary Pub. of Raleigh, 2005. Print. Page E8-13 to E8-15 Questions (T8-9) 1)   When peaks in the gas chromatograms are poorly separated, it is best to change one or more separation parameters so the baseline resolution is obtained. 2)   Benzene > o-xylene > p-xylene > toluene 3)   Cyclohexyl methyl ether would have a shorter retention time because of the increase in temperature. 4)   A. Retention will increase when the temperature column is decreased

B. When you increase the length of a column, the retention time would increase because of the longer distance traveled. C. Increasing flow rate of carrier gas will decrease the retention time 5)   105oC 6)   Little to no partitioning of components in the sample will occur and therefore giving poor to no separation. 7)   29mm2, 210mm2, 136mm2 Mole %=(Area under individual Peaks)/(Total area under all the peaks) x 100% %= 29mm/375mm x100%= 7. 73% %= 210mm/375mm x100%= 56% %= 136mm/375mm x100%= 36. 27% Total area under peak= 29+210+136= 375mm