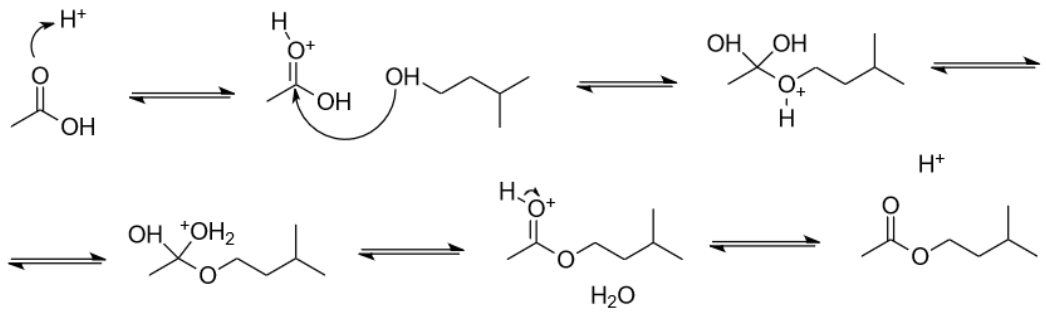
eman ta zabal zazu Universidad del País Vasco Euskal Herriko Unibertsitatea	EUSKAL HERRIKO UNIBERTSITATEA KIMIKAKO FAKULTATEA KIMIKA ORGANIKAKOA I SAILA
EXPERIMENTATION IN ORGANIC CHEMISTRY	**Practice number:**
FAMILY, FIRST NAME: Mirane Florencio Zabaleta	**DATE:** 28/04/2020

A	**MAIN FEATURES IN THE PRACTICE**
A.1	Main objective of the practice

To learn how to perform an esterification reaction. Basically, how to obtain an ester starting from an acid and an alcohol.

A.2	Mechanism of the reaction



A.3	Dangerous reagents	Preventive Measures; H and P phrases
	Acetic acid	H226: Flammable liquid and vapor. H314: Causes severe skin burns and eye damage. P241: Use explosion-proof electrical, ventilating, lighting equipment. P242: Use only non-sparking tools P243 :Take precautionary measures against static discharge.
	H_2SO_4 (con.)	H314: Causes severe skin burns and eye damage. P260 -Do not breathe mist, vapors, spray. P264 - Wash exposed skin thoroughly after handling.
	Isoamylic alcohol	H226: Flammable liquid and vapor H315:: Causes skin irritation. P210: Keep away from heat/sparks/open flames/hot surfaces. -No smoking. P233: Keep container tightly closed
	$NaHCO_3$(satur.)	H320:-Causes eye irritation P264: Wash exposed skin thoroughly after handling P305+P351+P338: If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
	Na_2SO_4 (anhy.)	H412: Harmful to aquatic life with long lasting effects. P273: Avoid release to the environment. P501: Dispose of contents/ container to an approved waste disposal plant.
A.4	Experimental procedure	

1. Place the acetic acid in a round bottom flask and then add isoamyl alcohol. Stir the mixture until it is homogeneous. After that add sulfuric acid carefully and slowly.
2. Attach the condenser to the neck of the flask connected to water and then start heating the solution for an hour.
3. When finished let the solution cool down. Then take it to the separation funnel and add a NaCl water solution.
4. Once the aqueous face is extracted, neutralize the organic phase solution three times with carbonate, so as to eliminate the excess of acetic acid.
5. After that if the pH of the organic phase is basic, the solution is washed with NaCl and dried with Na_2SO_4.
6. Finally, the solution is filtered and the final product placed into a Erlenmeyer flask.

<table>
<tr><td>B</td><td colspan="5">RESULTS</td></tr>
<tr><td rowspan="2">B.1</td><td>Molecular formula:
$C_7H_{14}O_2$</td><td>M.W. (g/mol):
130,18</td><td>Density:
0,876</td><td>State:
Liquid</td><td>Color:
Colorless</td></tr>
<tr><td colspan="2">Theoretical weight or volume of the final product:
$g = 0{,}0919 \times 130{,}18 = 11{,}95g$

Measured experimental weight or volume of the final product:
%70 yield of the starting product</td><td colspan="3">Theoretical melting point or boiling point (ºC):
- Boiling point: 142,5ºC
- Melting poin: -78,5ºC</td></tr>
<tr><td>B.2</td><td colspan="5">Yield. Analysis of the results</td></tr>
<tr><td></td><td colspan="5">
<table>
<tr><th>Reagent</th><th>g</th><th>MW</th><th>mol</th><th>δ</th><th>mL</th></tr>
<tr><td>$C_2H_4O_2$</td><td>52,5</td><td>60,052</td><td>0,874</td><td>1,05</td><td>50</td></tr>
<tr><td>$C_5H_{12}O$</td><td>8,1</td><td>88,15</td><td>0,0919</td><td>0,81</td><td>10</td></tr>
<tr><td>$C_7H_{14}O_2$</td><td>-</td><td>130,18</td><td>-</td><td>0,876</td><td>-</td></tr>
</table>
$\%Yield = \%70$ of the starting product:

In this case, we have a limitant reactant, isopentyl acetate, so we have a surplus of acetic acid. The quantity of mols of the final product will be the same as the value of isopentyl acetate moles.

Measured weight:

$$g_{practical} = \frac{70}{100} \times 11{,}95 = 8{,}365g$$
</td></tr>
</table>

B.3	Spectroscopic Data:

Isopentyl acetate:

- ^{1}H NMR:
  δ 3,97 this triplet belongs to the hydrogen in the α carbon.
  δ 1,91 this singlet has to do with the methyl group next to de carbonyl.
  δ 1,62-1,52 the multiplate belongs to the CH hydrogen of the isopropyl.
  δ 1,40 the quadruplet belongs to the hydrogens of the β carbon.
  δ 0,80 the doublet has to do with both methyls of the isopropyl group.
- ^{13}C NMR:
  δ 170,9 it belongs to the carbonilic carbon.
  δ 62,9 it belongs to the α carbon.
  δ 37,2 it belongs to the β carbon.
  δ 24,9 it belongs to the CH of the isopropyl.
  δ 22,3 it has to do with the methyl groups of the isopropyl.
  δ 20,8 it has to do with the methyl attached to de carbonyl.
- IR:
  We can observe some interesting signals, at approximately 1740 wavenumbers we can see a pointing big signal that refers to the carbonyl group. Apart from that, we can observe another peak at more or less 1330 wavenumbers that has to do with the ester bond.

B.4	Conclusions

In this practice we have learned how to do the esterification reaction, the mechanism of this and how can be shifted and a hydrolysis reaction can occur. As we haven't perform it practically is way more difficult to acquire the procedure, but we have learn useful things theoretically that will help us perform this practices better in the future..