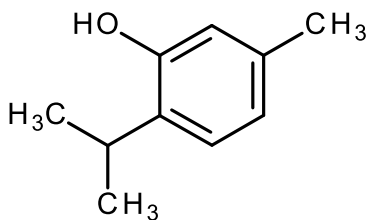


Experiment 41: Isomerization of a cyclic ketone

Analysis

- Final product structure



Carvacrol C₁₀H₁₄O

- Yield

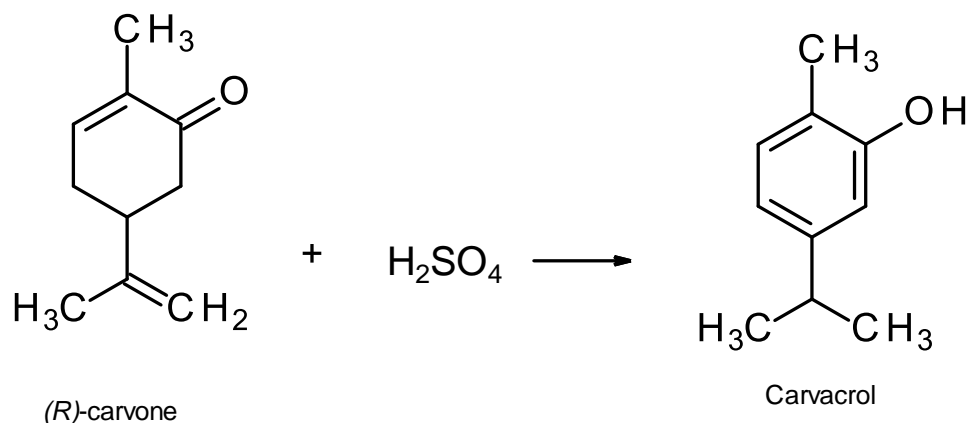


Table of experimental data.-

	(R)-carvone	Sulfuric acid	Carvacrol
Mass (g)	1.52	-	1.01
Volume (mL)	-	15 mL	-
Concentration (M)	-	6.0 M	-
Molar mass (g/mol)	150.22	98.08	166.26 g

- Theoretical yield

Limiting reagent:

$$\text{moles of R-carvone} = 1.52 \text{ g} \times \frac{1 \text{ mol}}{150.22 \text{ g}} = 10.12 \text{ mmol}$$

$$\text{Moles of sulfuric acid: } 15 \text{ mL} \times 6.0 \text{ mM} = 90 \text{ mmol}$$

(R)-carvone is the limiting reagent

Theoretical yield:

$$0.01012 \text{ mol (R) - carvone} \times \frac{1 \text{ mol Carvacrol}}{1 \text{ mol (R - carvone)}} \times \frac{166.26 \text{ g}}{1 \text{ mol}} = \mathbf{1.6626 \text{ g}}$$

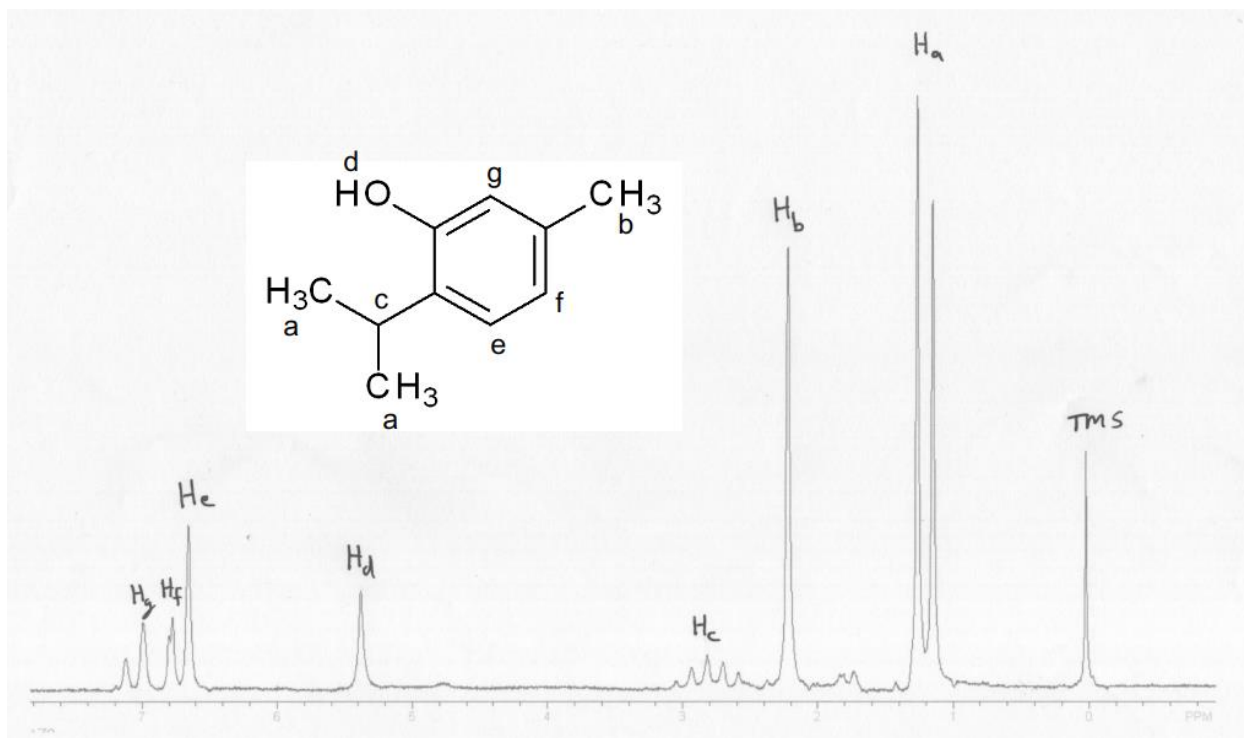
○ Percent yield

$$\% \text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% = \frac{1.01 \text{ g}}{1.66 \text{ g}} \times 100\% = \mathbf{61\% \text{ yield}}$$

- IR analysis

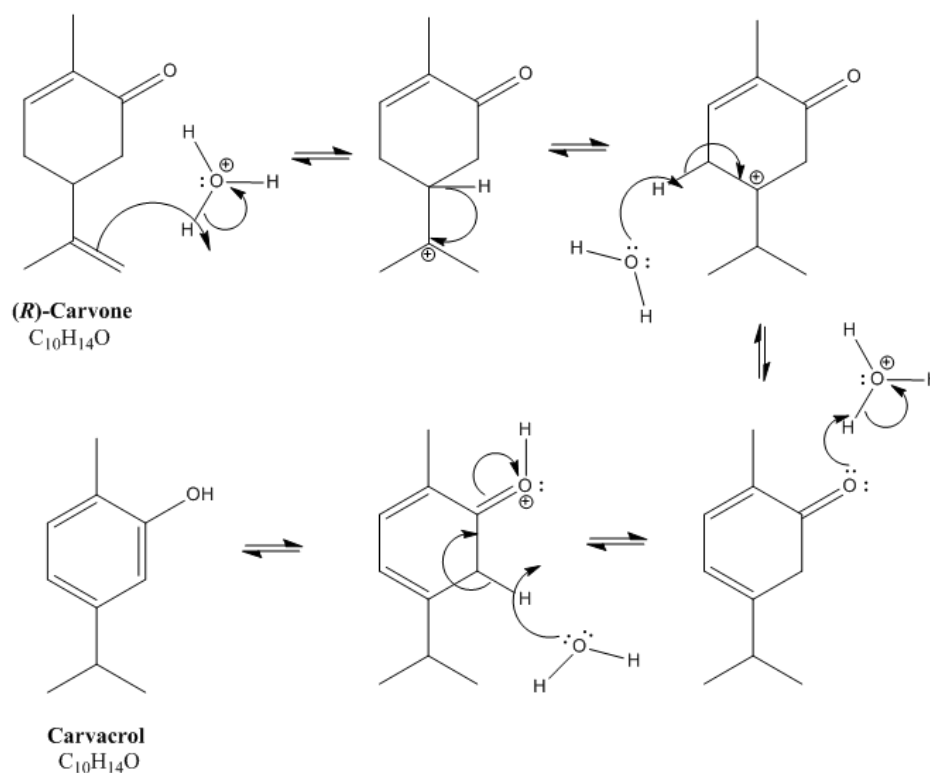
Bond type	Wavenumber (cm ⁻¹)
O-H stretch	3383.42
C-H (sp ³) stretch	2926.77 & 2960.23
C-H (sp ²) stretch	2869.30
C=C aromatic stretch	1421.57 & 1621.25
O-H bending (phenol)	1382.29

- NMR analysis



- Answer to exercises

1.



2. a) **IUPAC name:** 5-isopropyl-2-methylphenol **Common name:** Carvacrol

b) Numerous plants contains Carvacrol as the major metabolite, such as oregano, thyme, pepperwort, wild bergamont, among many others.

3. a) The removal of the product would be too difficult due to the relatively high boiling point. Even when this could be solved by increasing the temperature, this would lead to decomposition of the product. Thus, it is imperative to use a very volatile solvent.
- b) Sodium bisulfite is a very weak base compared to sodium bicarbonate and thus, not all of the Carvacrol product would be extracted, leading to a poor yield.
- c) Too much pressure would build up inside the funnel due to the formation of carbon dioxide and it could explode.