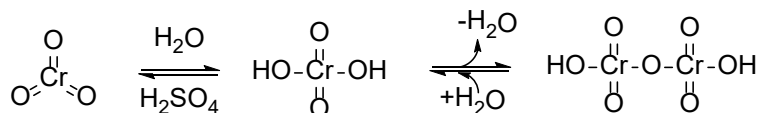


## THE VIRTUAL OXIDATION REACTION

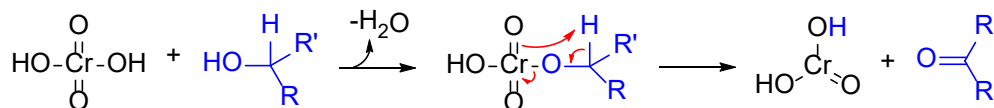
In this virtual experiment, you will explore the activity of various oxidants on primary, secondary, and tertiary alcohols. You will use this data to distinguish the relative susceptibility of various organic molecules to different oxidants.

### Introduction

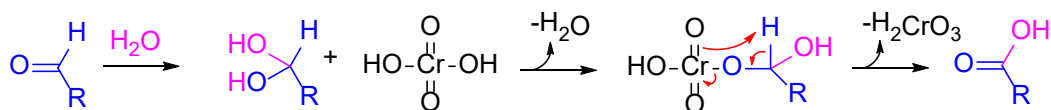
Chromium based reagents are useful in oxidation due to its stability in various oxidation states, particularly the +3 and +6 oxidation states. Both the Jones reagent and pyridinium chlorochromate (PCC) use a similar mechanism.



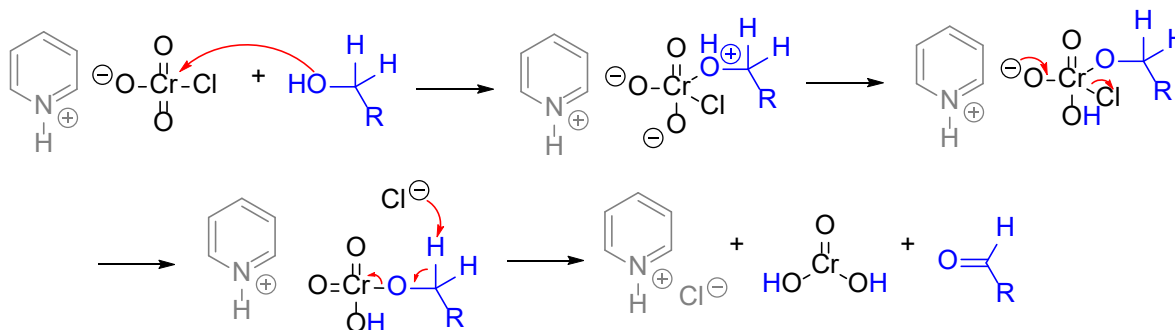
In the laboratory setting, there are a few different ways to prepare the Jones reagent. One such method is to dissolve chromic trioxide in diluted sulfuric acid which forms chromic acid *in situ*. The BeyondLabz platform labels Jones reagent as  $\text{H}_2\text{Cr}_2\text{O}_7$ , the dehydrated dimer of chromic acid.



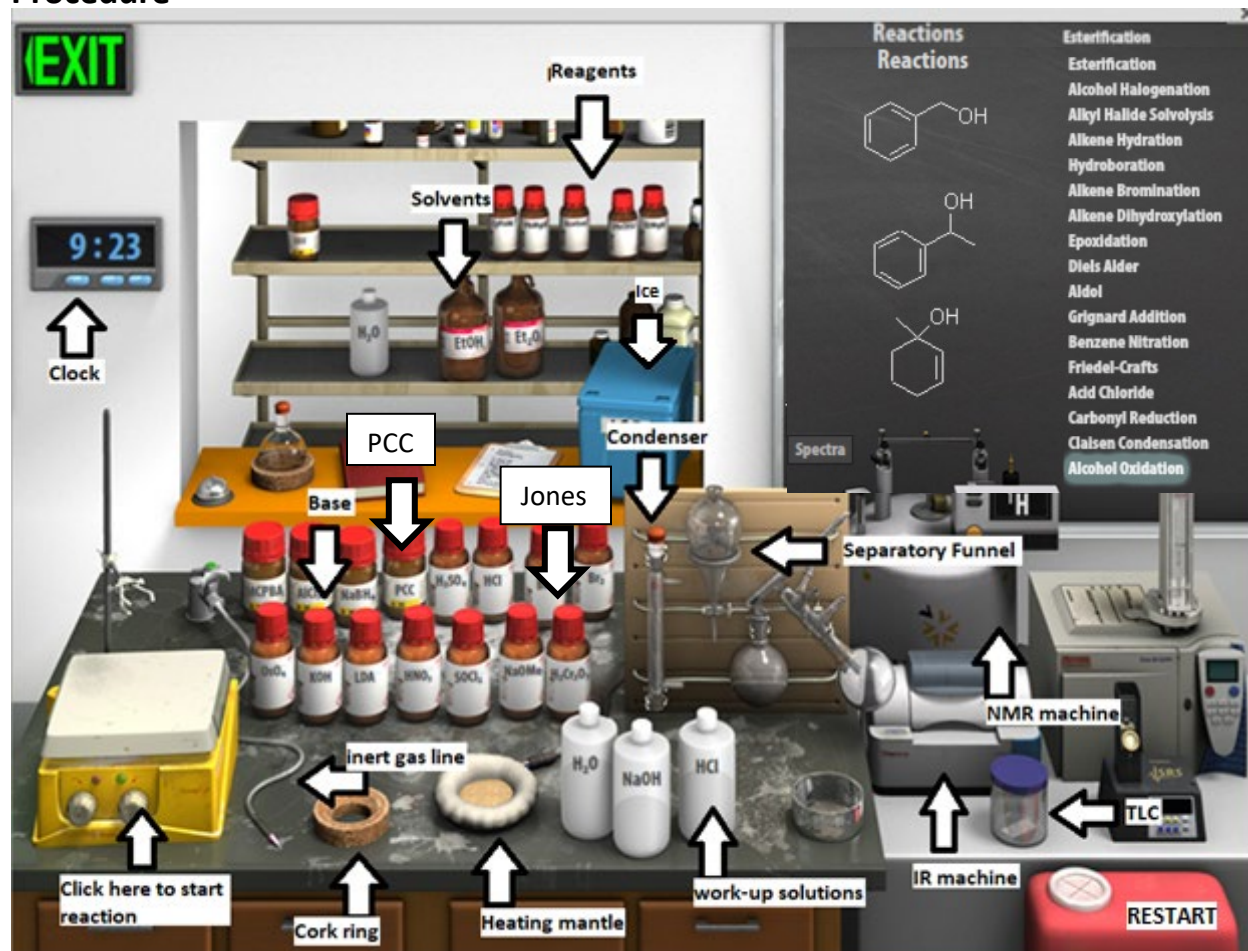
If  $\text{R}' = \text{H}$ , water can react with the aldehyde to form a diol



The Jones oxidation is capable of first oxidizing a primary alcohol to an aldehyde, and then further to the carboxylic acid. This is because aldehydes react with water to form a diol, which further reacts with chromic acid to oxidize it one step further. By looking at this mechanism, can you guess how we could stop the oxidation of a primary alcohol at the aldehyde? How would the reaction proceed if we could remove the presence of water from the reaction? To address this, PCC was developed for oxidations in the absence of water.



## Procedure



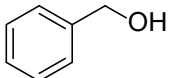
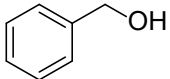
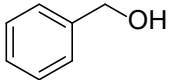
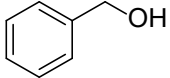
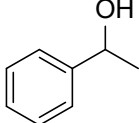
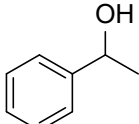
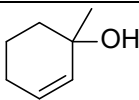
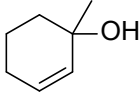
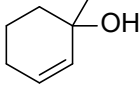
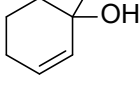
Using the BeyondLabz platform, enter the virtual organic chemistry lab. Click on the Synthesis button on the top left corner and select the Alcohol Oxidation reactions on the chalkboard to load the reaction specific reagents onto the stockroom shelves. Click and drag each solvent and reagent to the round bottom flask before moving the flask to the stir plate. Add a water cooled condenser, inert gas line, and heating mantle before turning the stir plate on and starting the reaction.

After the reaction has been completed, double click on the separatory funnel and add NaOH to work up the reaction. Drag the organic layer to the cork ring and if it is a singular compound, take  $^1\text{H}$  NMR and IR spectra of the compound by clicking on the NMR or FTIR machine and dragging it to the round bottom flask.



## Results & Discussion

Attach the labelled  $^1\text{H}$  NMR and IR spectra of the pure compounds (do not include ones with pyridine).

Alcohol	Solvent	Oxidant	Products
	Diethyl ether	PCC	
	Water	PCC	
	Diethyl ether	Jones	
	Water	Jones	
	Diethyl ether	PCC	
	Diethyl ether	Jones	
	Diethyl ether	PCC	
	Ethanol	PCC	
	Diethyl ether	Jones	
	Ethanol	Jones	
None	Ethanol	Jones	
None	Ethanol	PCC	



## Questions

What solvent should be used to run a PCC oxidation?

What solvent should be used to run a Jones oxidation?

Nitric acid will also bind to an alcohol in a similar way to the first step of the Jones oxidation. Why is nitric acid less reliable as an oxidant? (\*\*the reaction will explode after a few minutes in the BeyondLabz platform)

