

Reactions of Aldehydes and Ketones with Residual Disinfectants in the Drinking Water Distribution System

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Background

- Direct Potable Reuse treats wastewater to a potable standard and delivers it directly to the community.
- Low molecular weight aldehydes and ketones are not completely rejected by reverse osmosis, a common treatment step in advanced treatment intended for potable water reuse.
- These compounds react with the chlorine disinfection residual and related bromine present in water distribution systems to form unintended byproducts.

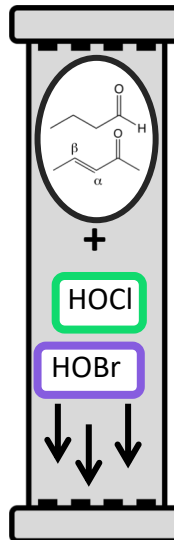
Objective: Determine the reaction rates of aldehydes and ketones in an excess of chlorine (HOCl) or bromine (HOBr).

Theory

Use the following pseudo first-order equation to determine the reaction rate (k).

$$d[Ald]/dt = -k_{obs} * [Ald]$$

- [Ald] : aldehyde concentration,
- $d[Ald]/dt$: rate of concentration change over time,
- k_{obs} : observed reaction rate.



Methods

Samples are made for each unique combination of compound, buffer of pH 5-10, and disinfectant.

Use a UV-vis Spectrophotometer (Fig. 1) to measure the absorbance of the sample before and each minute for 30 minutes after addition of chlorine.

The absorbance would be used directly to determine the reaction rate.

Each unique combination would be tested in duplicate, triplicate when possible.

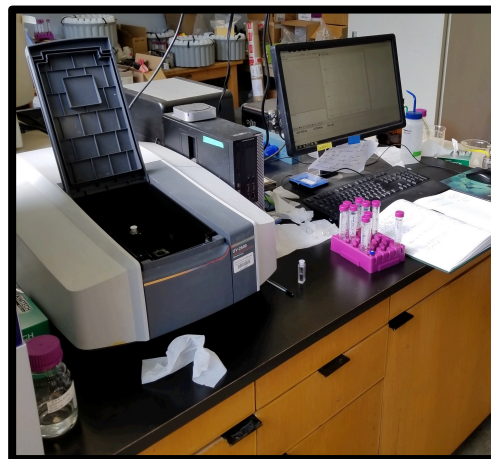
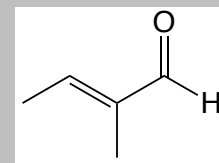
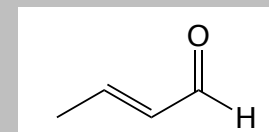


Figure 1. UV-vis Spectrophotometer setup

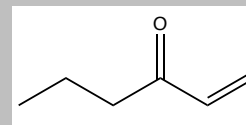
Notable Compound Structures



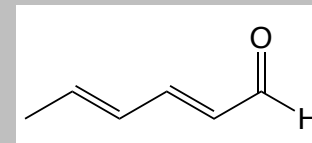
Tiglic aldehyde



Crotonaldehyde



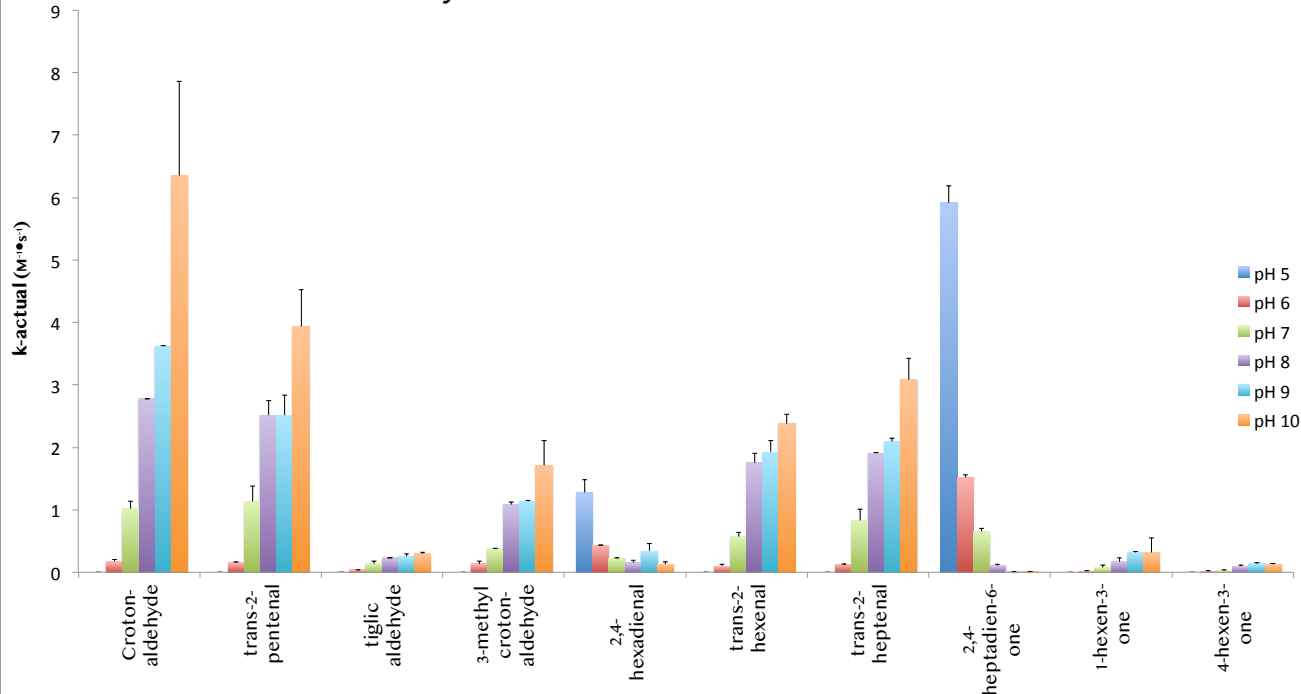
1-Hexen-3-one



2,4-Hexadienal

Results

Aldehyde and Ketone Reaction Rates with Chlorine

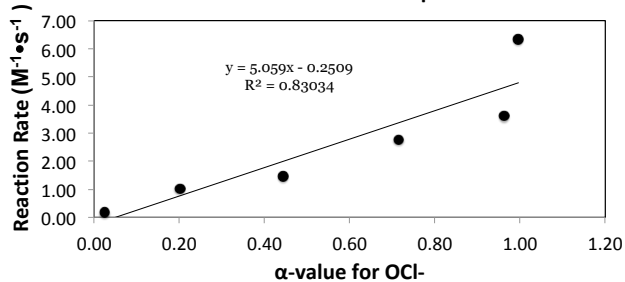


Discussion

The pH relationship suggests a possible reaction where the nucleophile OCl^- produced by the chlorine attacks the electrophilic compounds at a carbon in the double bond forming a chlorinated aldehyde or ketone.

A dosage of the compounds in a water distribution system with a residence time of 23.3 hours and a chlorine dosage of 1 mg/L in pH 7.5 water results in various amounts reacting away at the end of the system. Crotonaldehyde will have over 80% of its concentration react away while only 4% of 4-hexen-3-one will react away. All other compounds fall between this range.

Crotonaldehyde
Reaction Rate v. Fraction OCl^- Speciation



Conclusions

- Aldehydes and ketones can pass through RO membranes and react with chlorine and bromine to form unintended byproducts.
- Longer carbon chains and methyl groups decrease the reaction rate with HOCl .
- Ketones are slower reacting than aldehydes.
- The products of these reactions have yet to be identified.
- The threat to public health and the environment for the compounds and their products should be assessed.
- Reactions with bromine should be further studied.