

Kinetic Measurements and Modeling of OH Formation in Alkyl Oxidation

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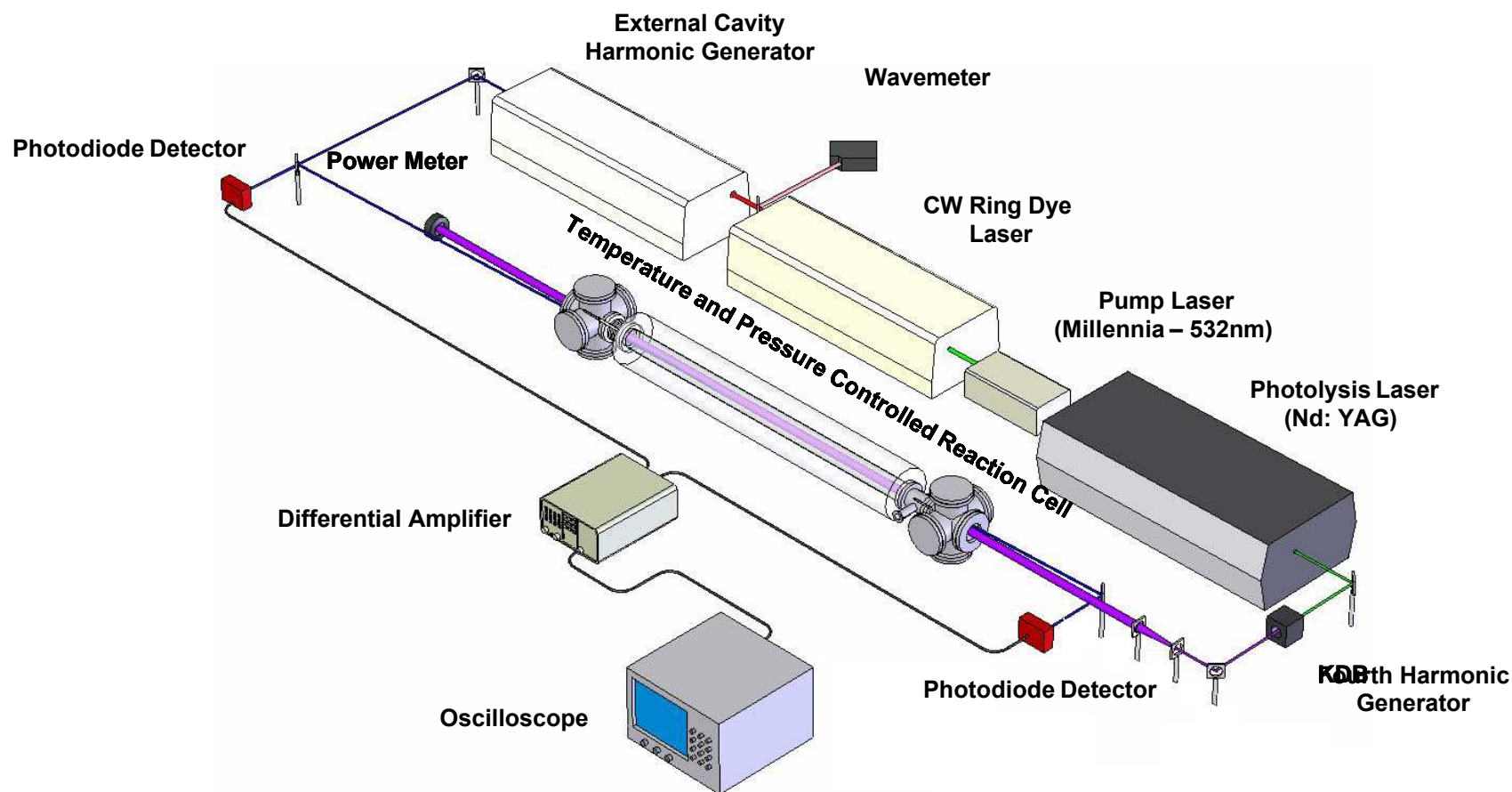
Outline

- Motivation
- Kinetics measurements
 - Experimental apparatus
- Modeling

Motivation

- Important in ignition chemistry
 - Autoignition
 - Enging knock
- Simple fuels

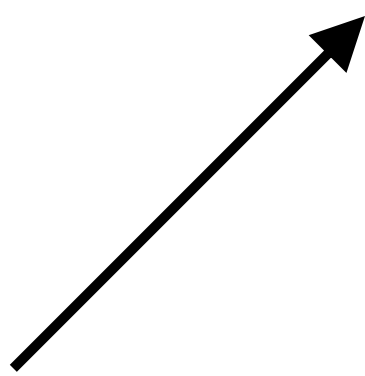
Experimental Apparatus



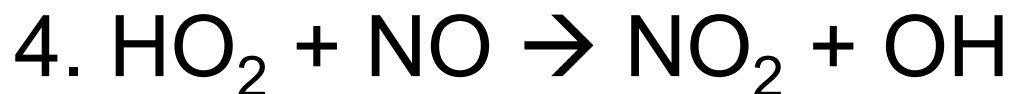
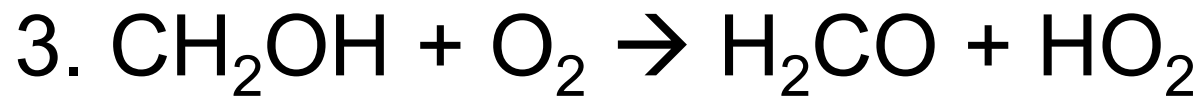
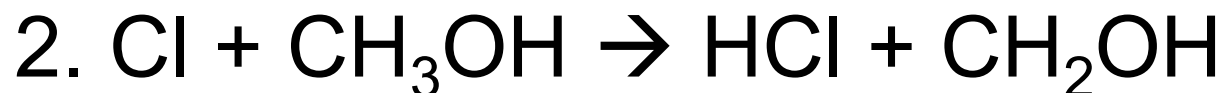
Experimental Reaction Pathway

1. $(\text{COCl})_2 + h\nu(266\text{nm}) \rightarrow 2 \text{ Cl} + 2 \text{ CO}$
2. $\text{Cl} + \text{Alkane} \rightarrow \text{HCl} + \text{Alkyl}$
3. $\text{Alkyl} + \text{O}_2 \rightarrow \text{Products} (\text{RO}_2, \text{QOOH}, \text{OH}, \text{+ Aldehyde, HO}_2 + \text{Alkene})$

$\text{A}^2\Sigma^+, v' = 0 \leftarrow \text{X}^2\Pi, v'' = 0$ at 308 nm

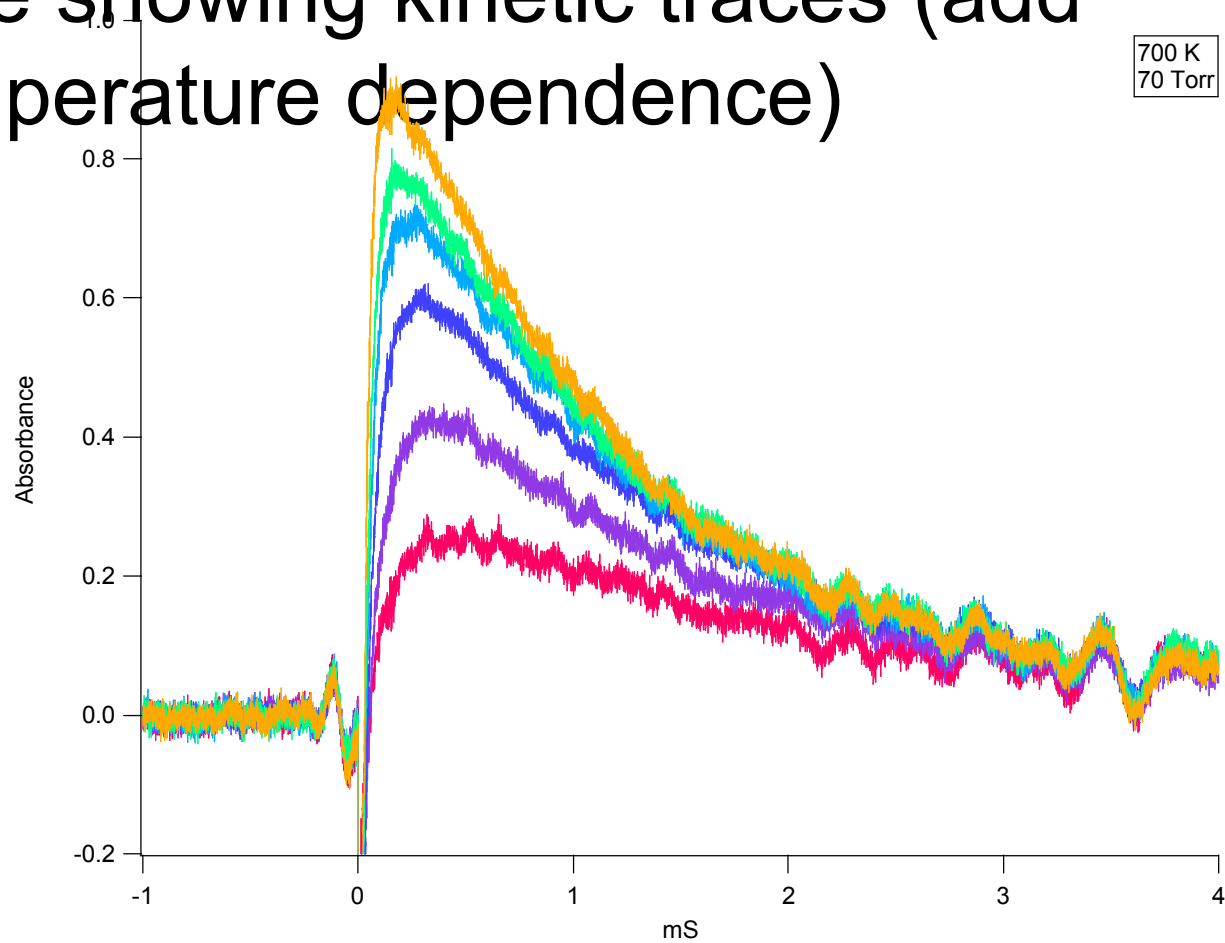


Reference Reaction Pathway



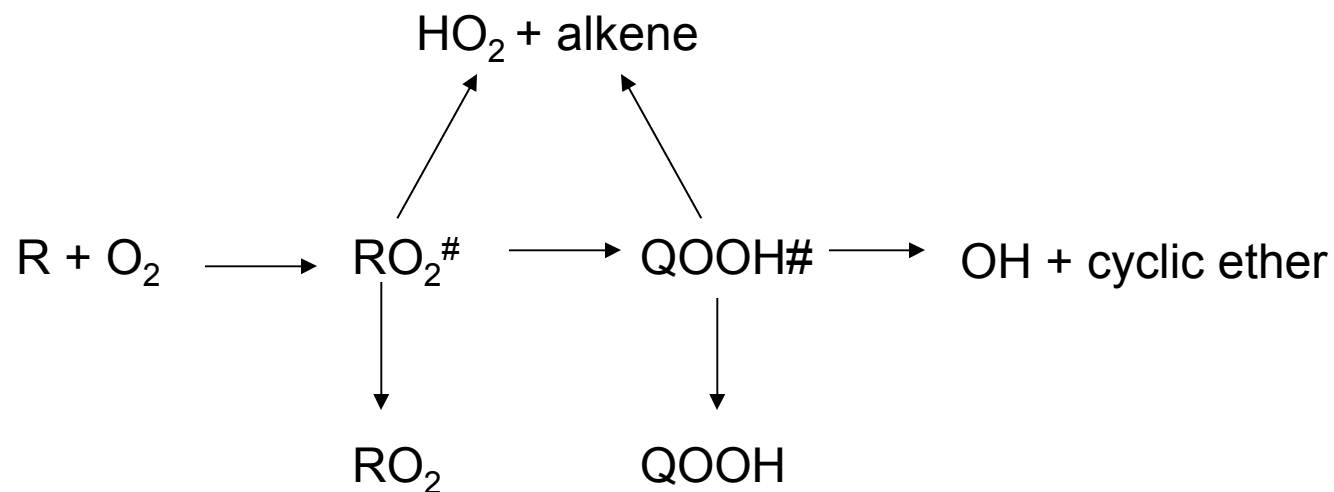
One OH formed for every CL

Figure showing kinetic traces (add temperature dependence)



Alkyl Oxidation

Reaction 3



Add figure: system potential energy surface

Modeling of system

List important reactions and where the rate constants came from

Figure of model overlaid on experimental data.

Conclusions

Acknowledgements

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