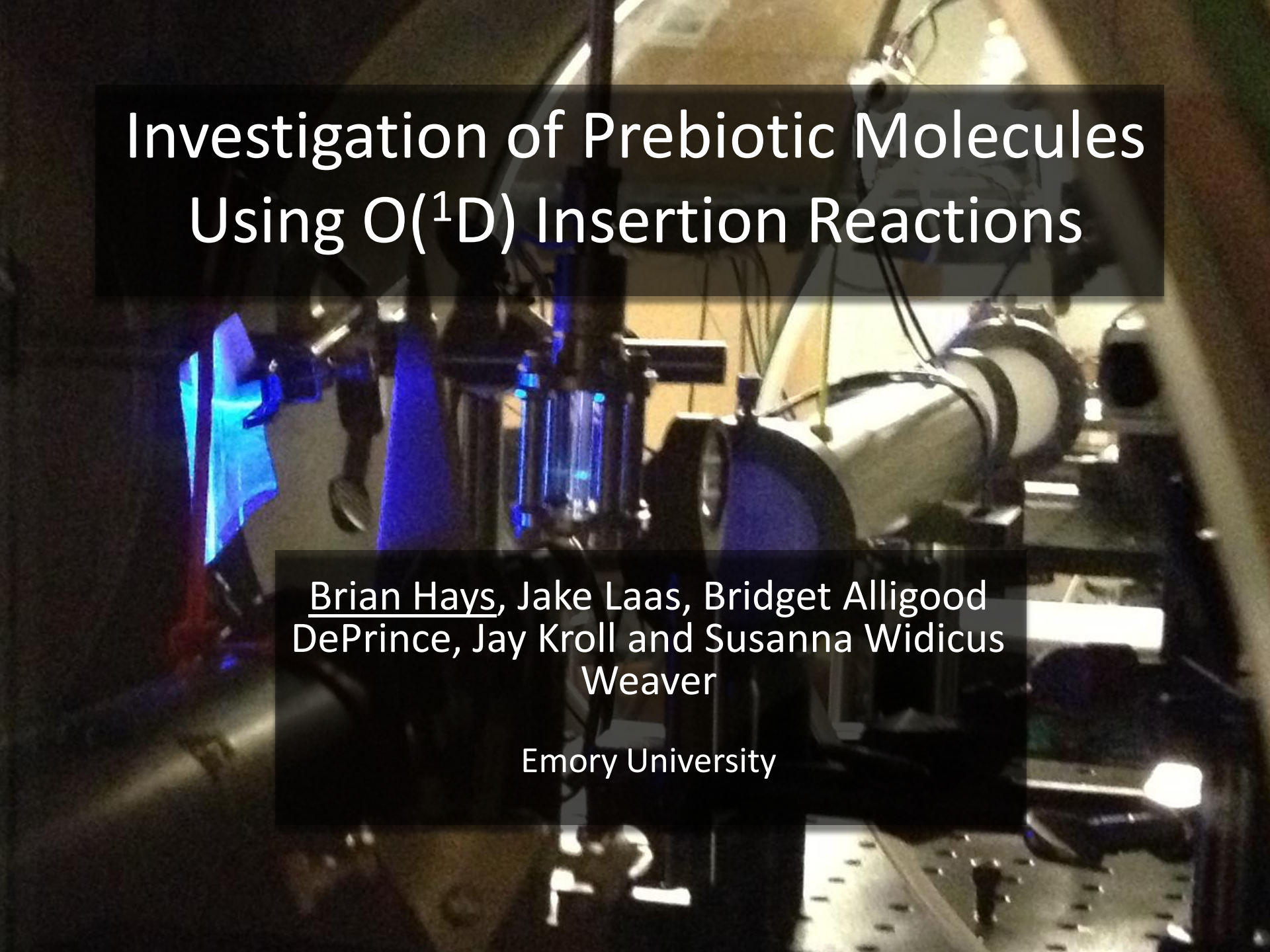
Investigation of Prebiotic Molecules Using O(^{1}D) Insertion Reactions



Brian Hays, Jake Laas, Bridget Alligood DePrince, Jay Kroll and Susanna Widicus Weaver

Emory University

Complex Chemistry in the ISM

$H_2O + h\nu \longrightarrow OH + H$

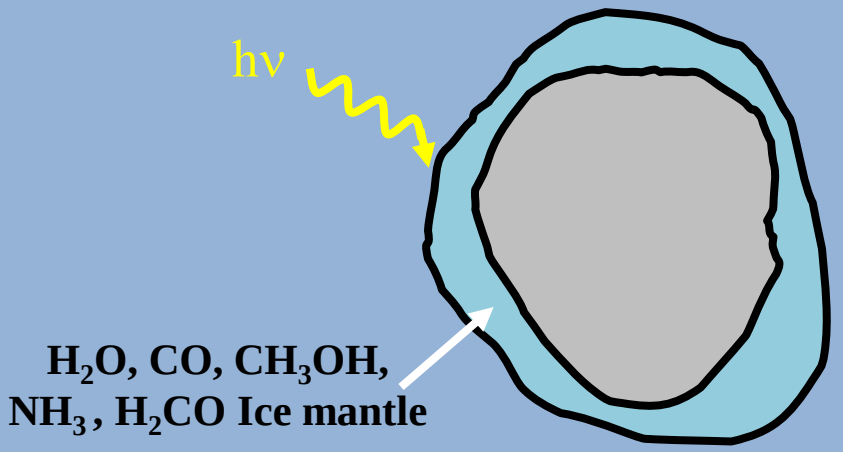
$\longrightarrow H_2 + O$

$CH_3OH + h\nu \longrightarrow CH_3 + OH$

$\longrightarrow CH_3O + H$

$\longrightarrow CH_2OH + H$

$NH_3 + h\nu \longrightarrow NH_2 + H$



Charnley, 2001

Garrod, Widicus Weaver, & Herbst, 2008

Complex Chemistry in the ISM

$H_2O + h\nu \longrightarrow OH + H$

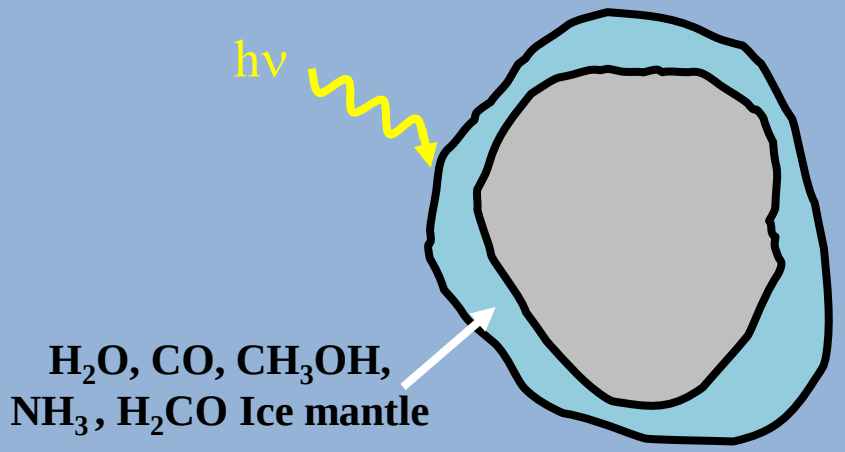
$\longrightarrow H_2 + O$

$CH_3OH + h\nu \longrightarrow CH_3 + OH$

$\longrightarrow CH_3O + H$

$\longrightarrow CH_2OH + H$

$NH_3 + h\nu \longrightarrow NH_2 + H$



$CH_2OH + OH \longrightarrow$	$CH_2(OH)_2$	Methanediol
$CH_2OH + CH_3O \longrightarrow$	CH_3OCH_2OH	Methoxymethanol
$CH_2OH + NH_2 \longrightarrow$	$HOCH_2NH_2$	Aminomethanol

Charnley, 2001
Garrod, Widicus Weaver, & Herbst, 2008

Complex Chemistry in the ISM

$H_2O + h\nu \longrightarrow OH + H$

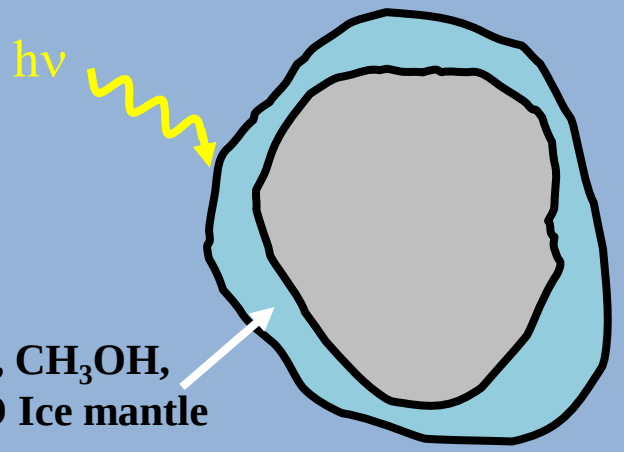
$\longrightarrow H_2 + O$

$CH_3OH + h\nu \longrightarrow CH_3 + OH$

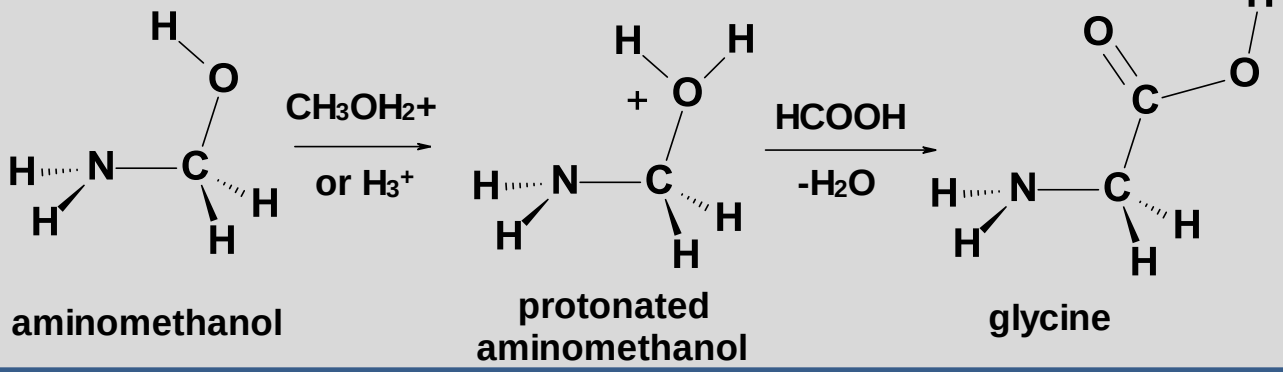
$\longrightarrow CH_3O + H$

$\longrightarrow CH_2OH + H$

$NH_3 + h\nu \longrightarrow NH_2 + H$



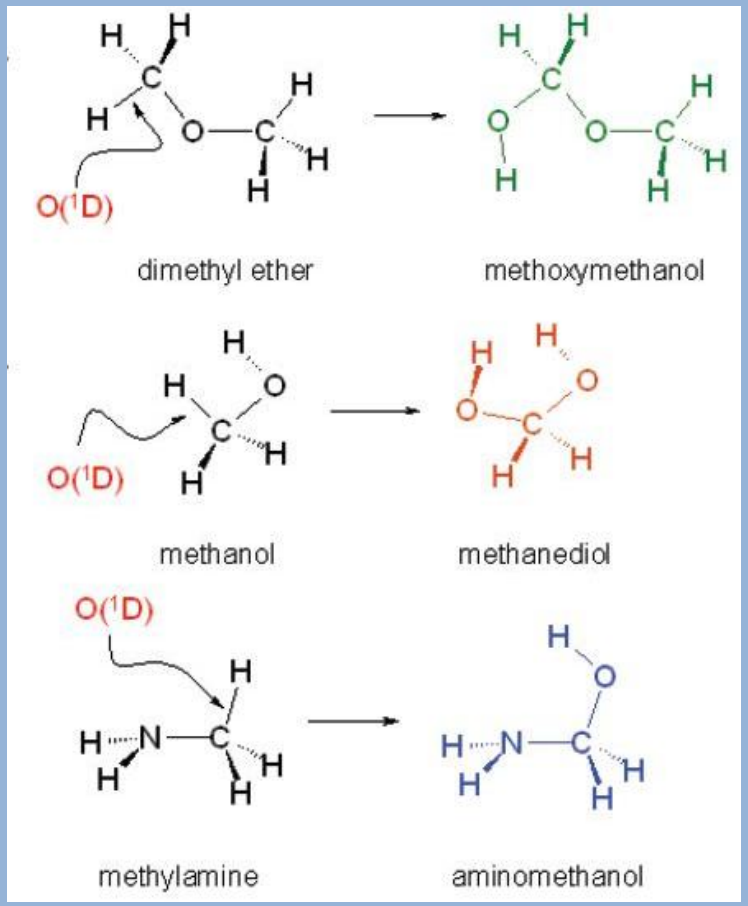
$CH_2OH + OH$	$\longrightarrow$	$CH_2(OH)_2$	Methanediol
$CH_2OH + CH_3O$	$\longrightarrow$	CH_3OCH_2OH	Methoxymethanol
$CH_2OH + NH_2$	$\longrightarrow$	$HOCH_2NH_2$	Aminomethanol



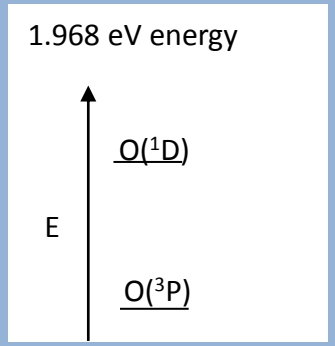
Charnley, 2001

Garrod, Widicus Weaver, & Herbst, ApJ 2008

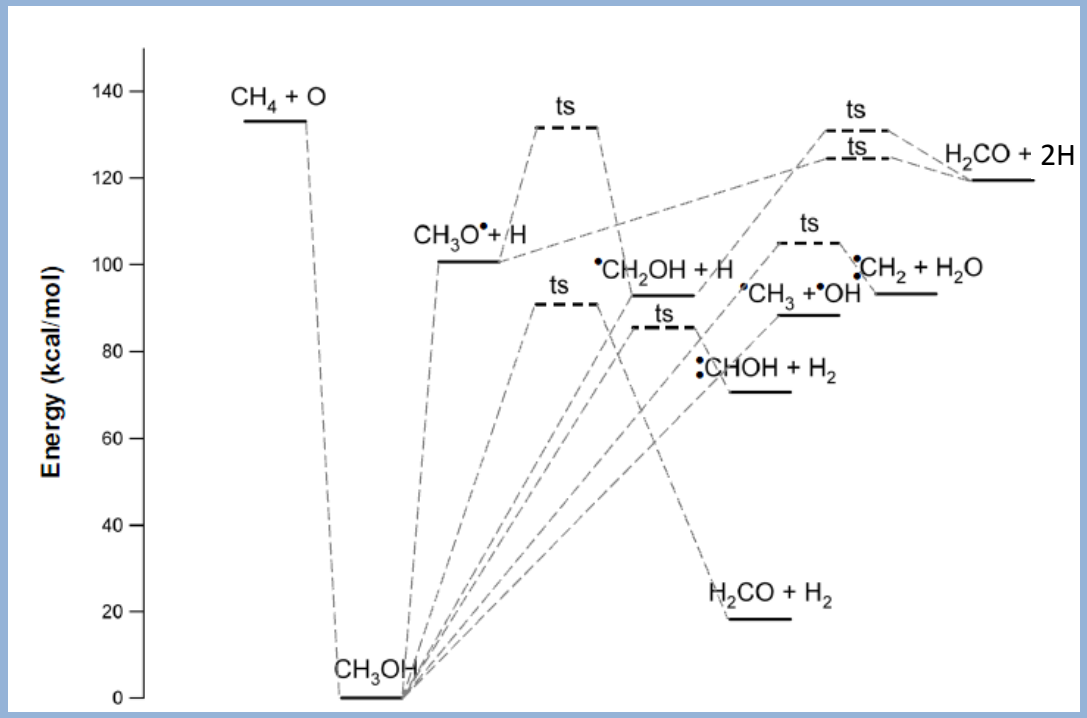
Proposed Formation Route for Laboratory Spectroscopy



- Molecules reactive under terrestrial conditions so no laboratory spectra exist
- Produce these molecules using barrierless $O(^1D)$ insertion reactions
- $O(^1D)$ primarily inserts into bonds that are H-X where X=C, N, O, H



O(^{1}D) Insertion into Methane

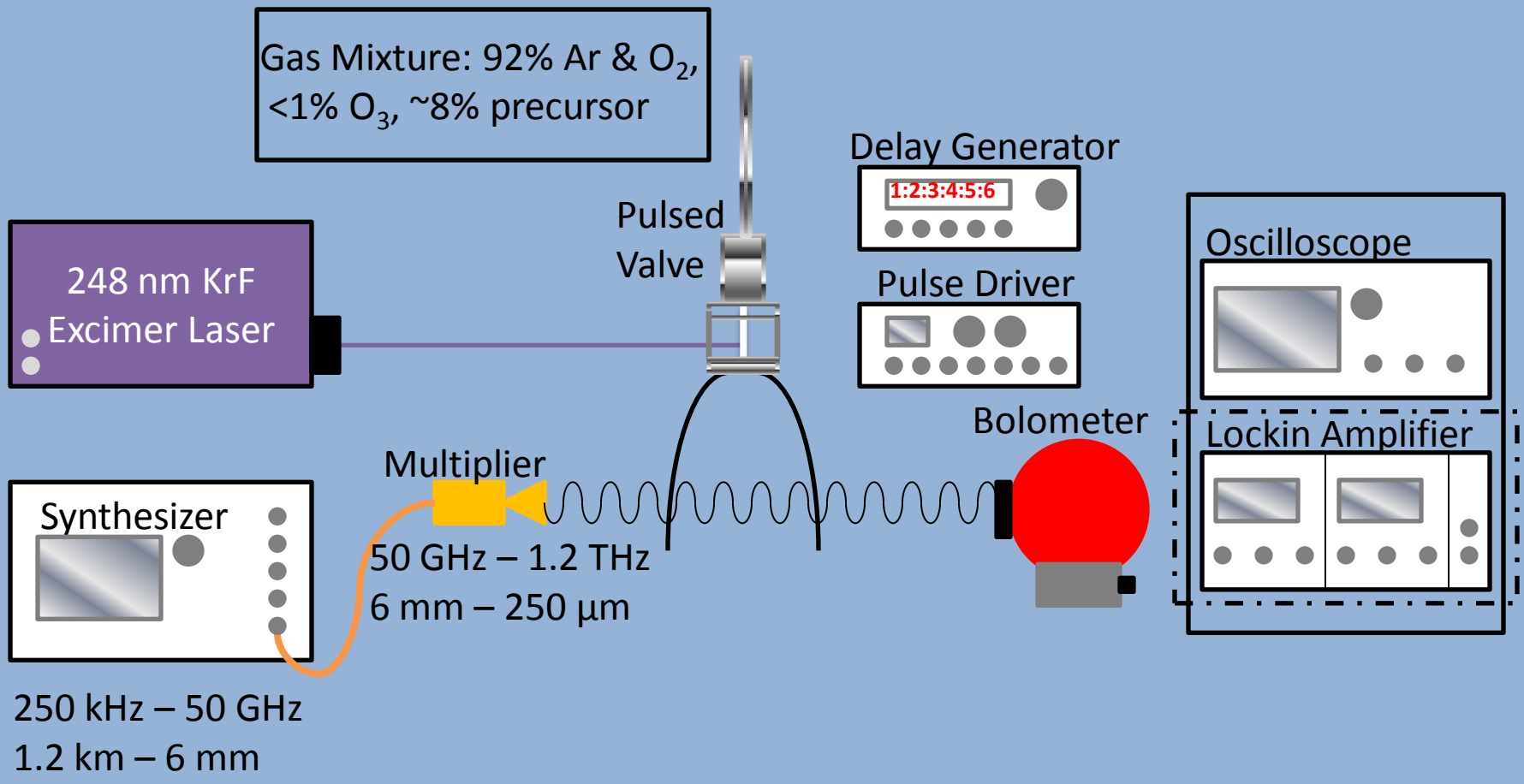


Chang and Lin, *Chem. Phys. Lett.* **363** (2002) 175-181

- O_3 + hν(248 nm) →
  $O_2(^1\Delta)$ + O(^{1}D) ~90%
  $O_2(^3\Sigma)$ + O(^{3}P) ~10%
- O(^{1}D) + CH_4 → CH_3OH

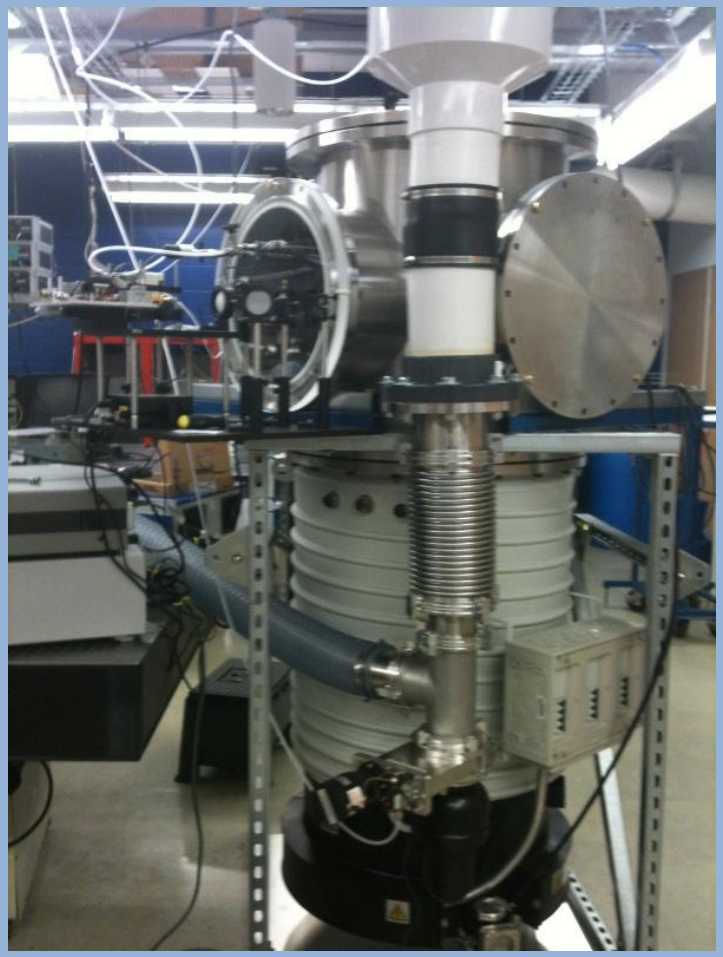
Unimolecular dissociation unless excess vibrational energy is quenched

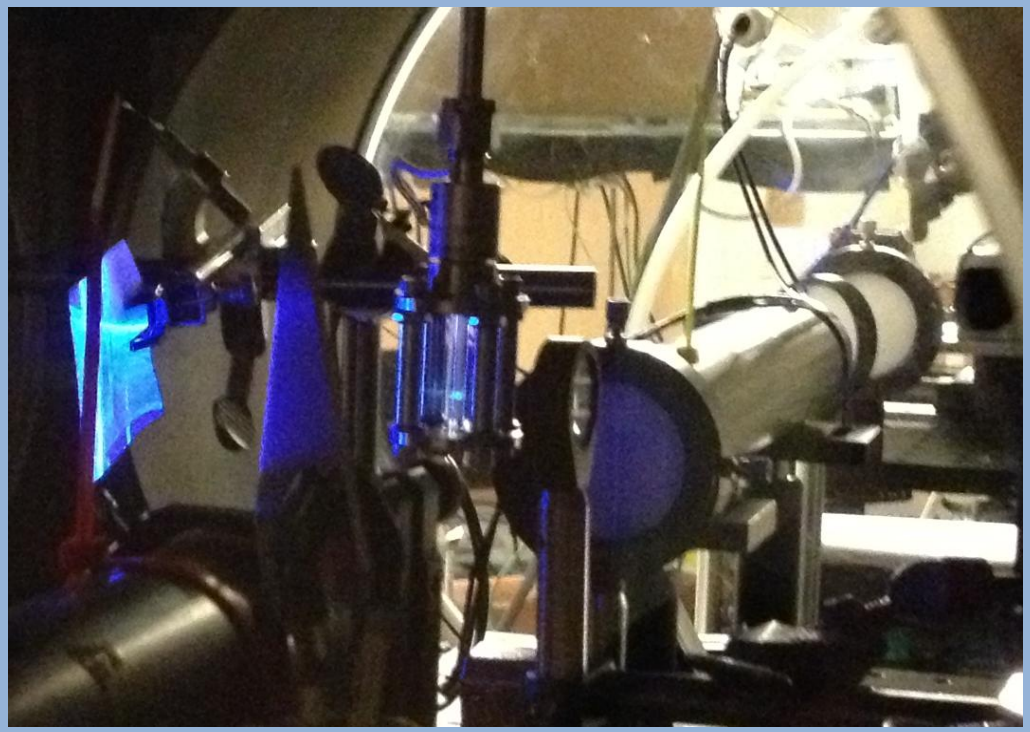
Experimental Design for O(^{1}D) Insertion Reactions



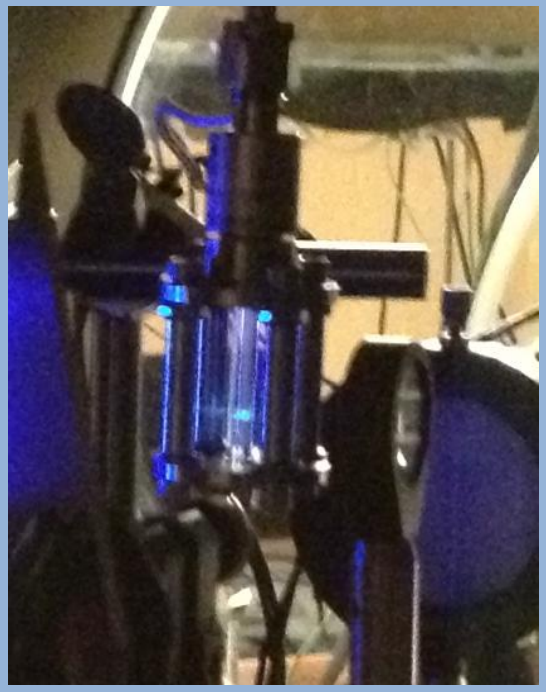
Cohen et al. *Chem. Phys. Lett.* 1989
Schuttenmaer et al. *Science* 1990
Duffy R*ev. Sci. Instr.* 2005

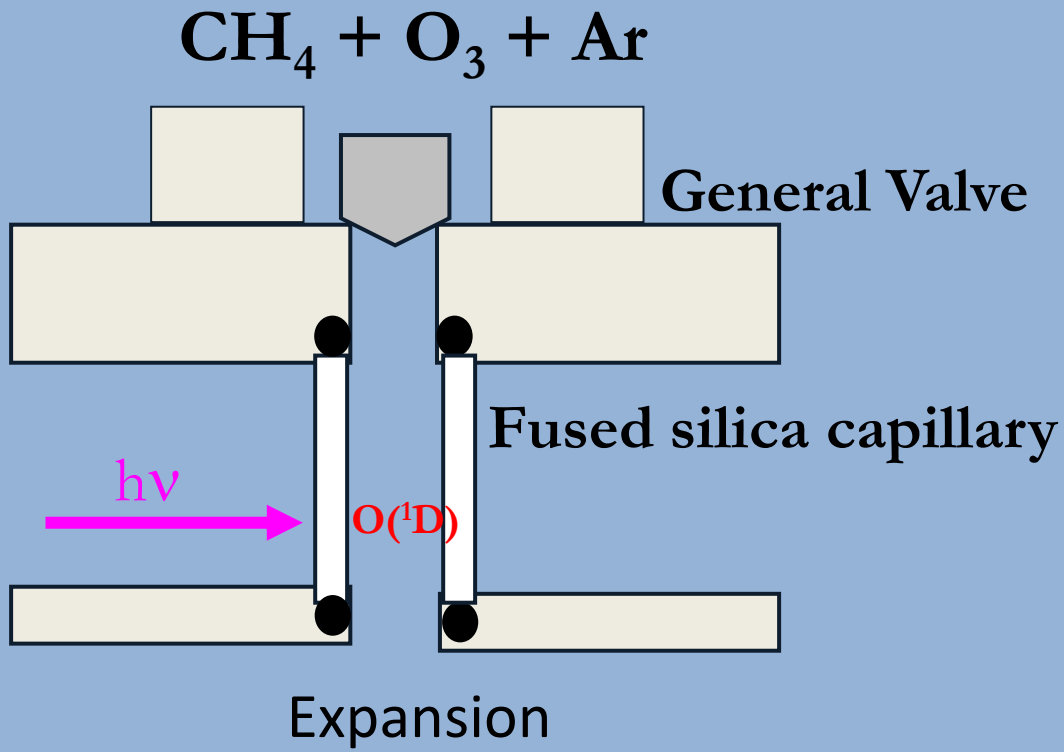
Experimental Design for O(^{1}D) Insertion Reactions





Experimental Design for $O(^1D)$ Insertion Reactions

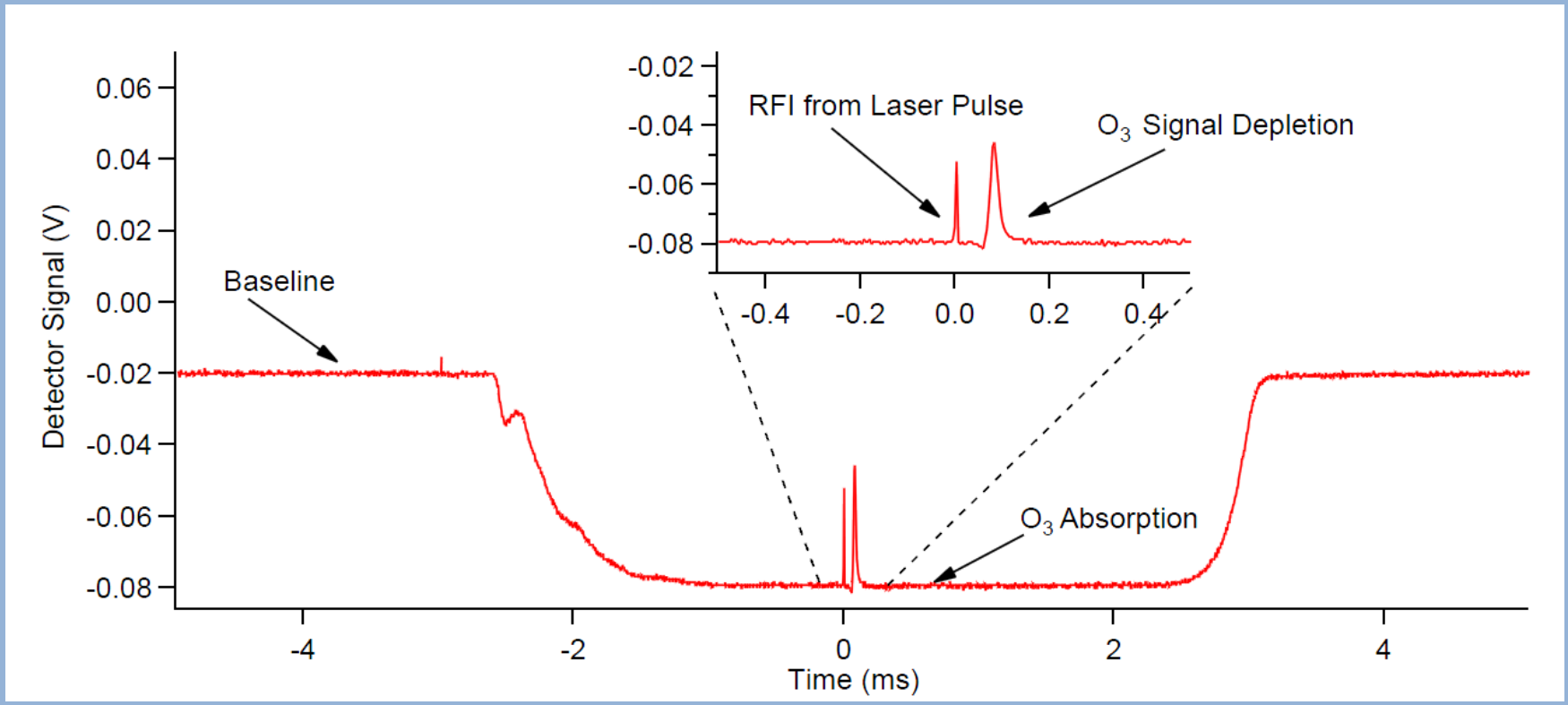




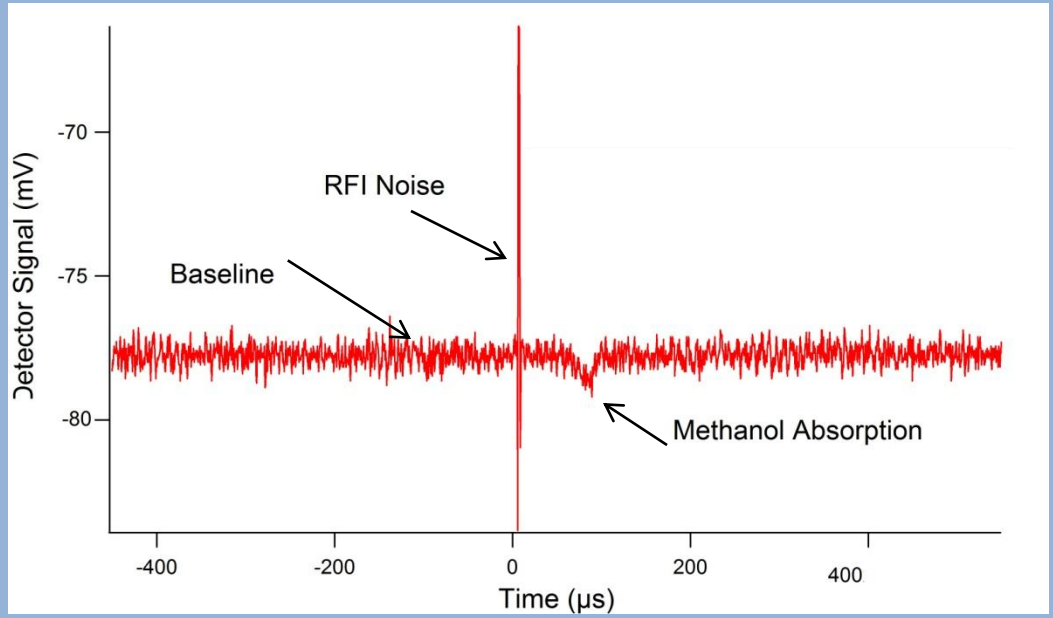
Similar to those used by Marsha Lester and coworkers

Ozone Depletion

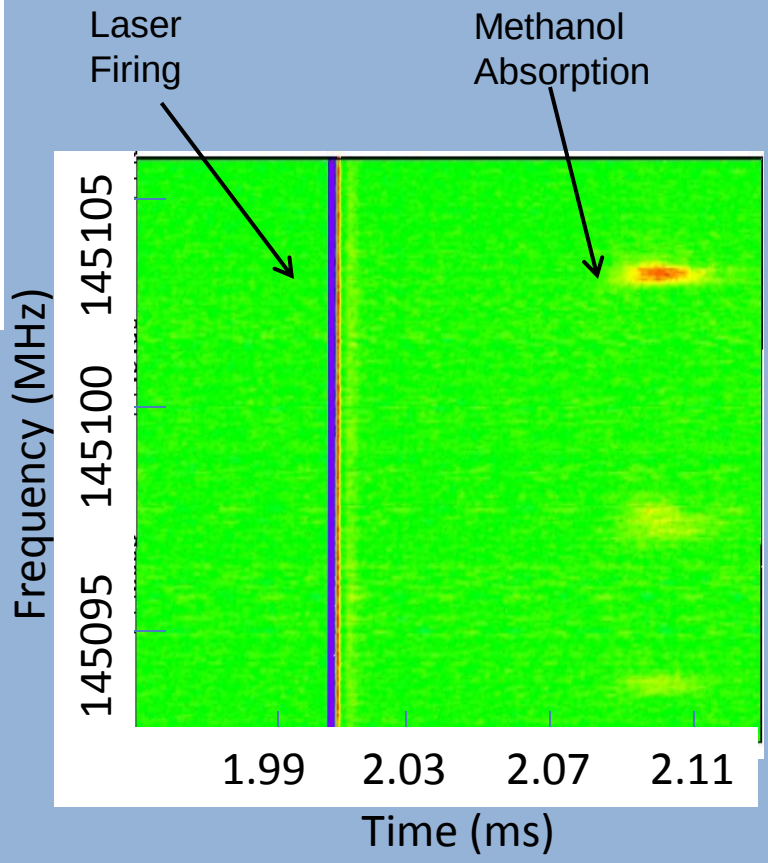
$O_3 + h\nu(248\ nm) \rightarrow O_2(^1\Delta) + O(^1D)$



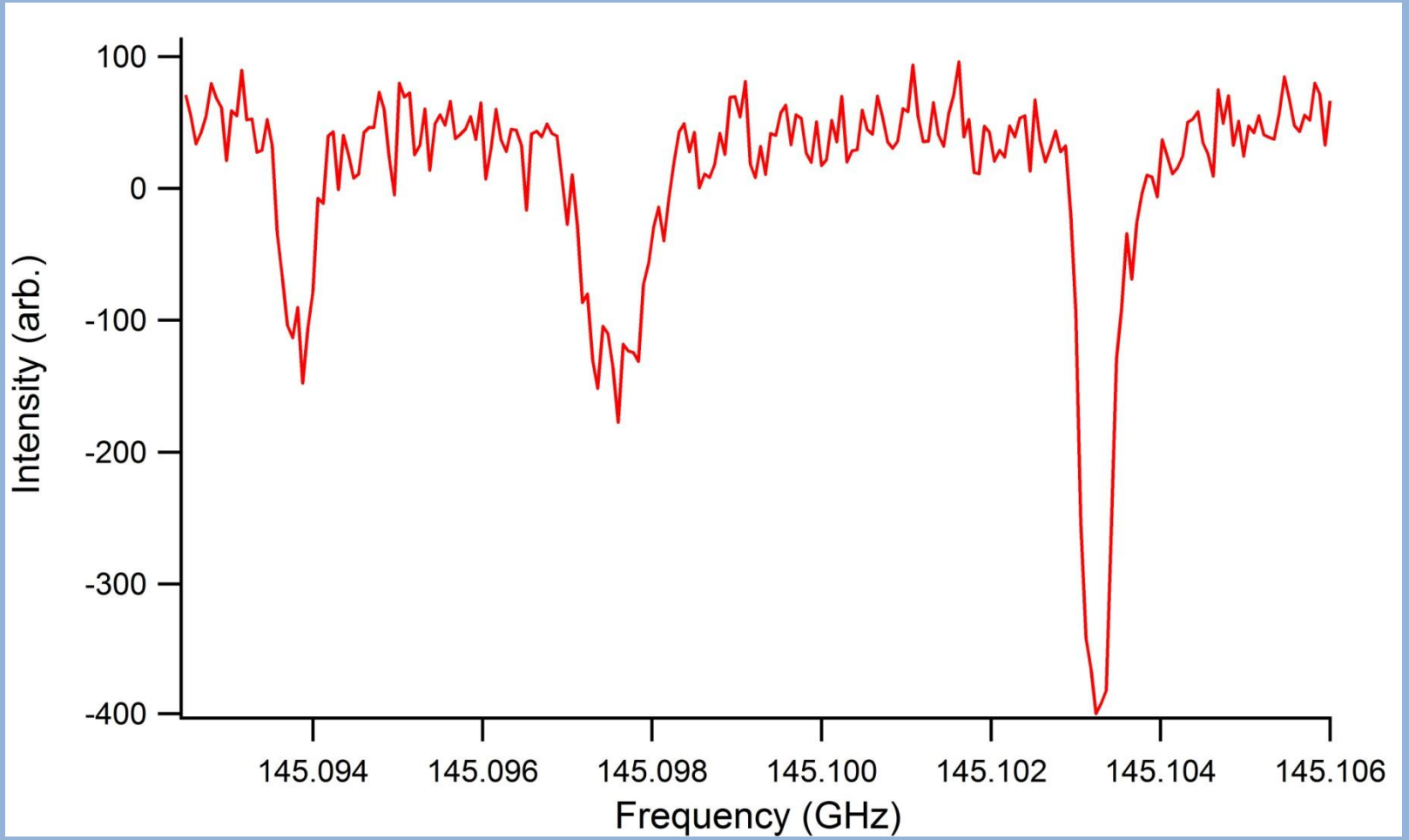
Methanol Production



$O(^1D) + CH_4 \rightarrow CH_3OH$

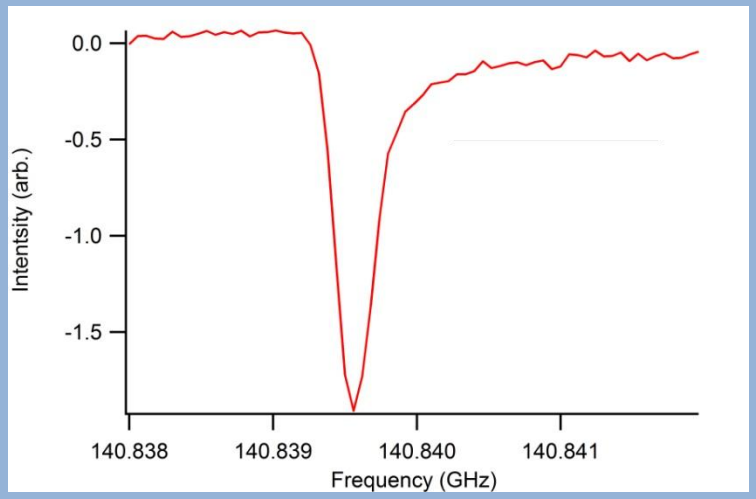


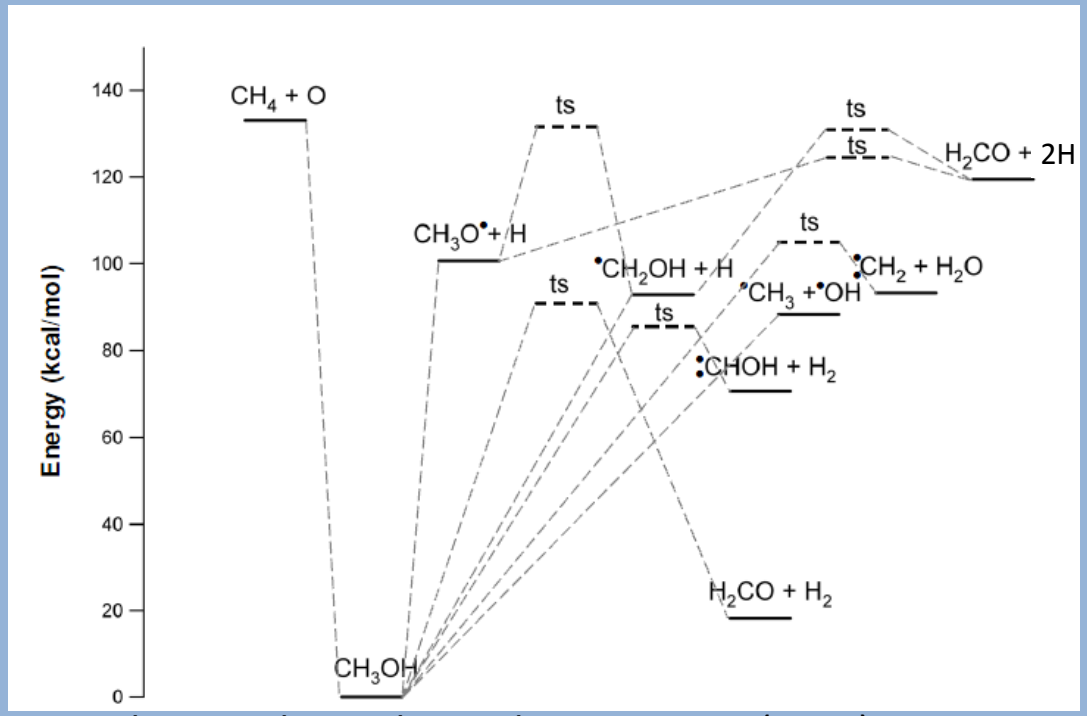
Methanol Production



Formaldehyde Formation

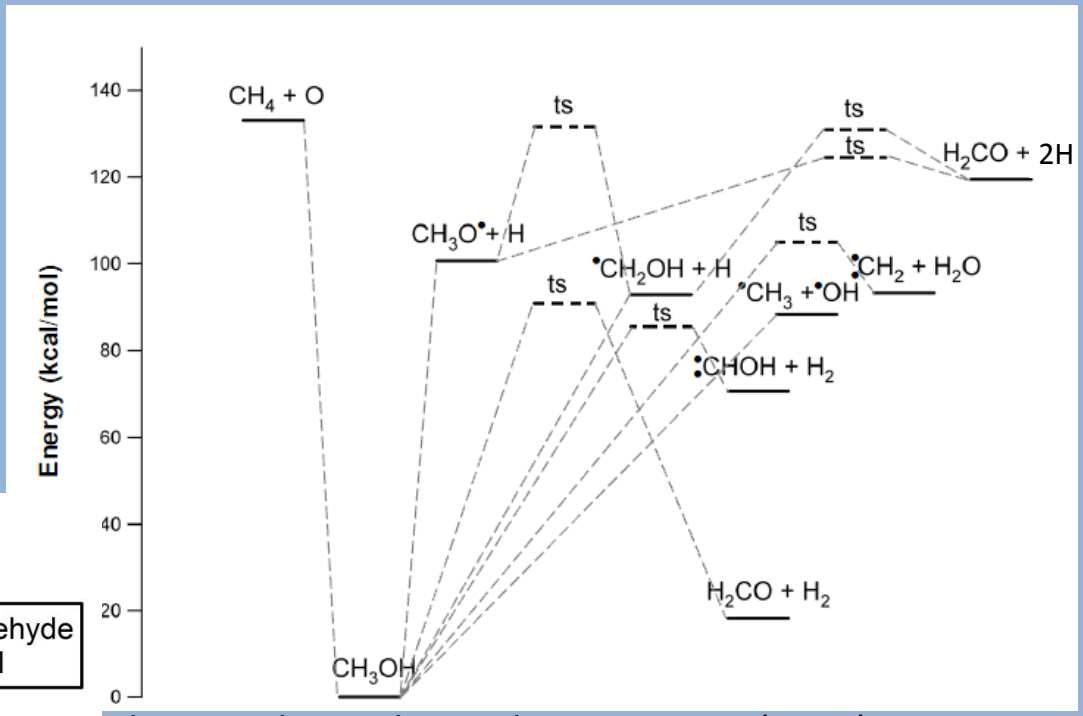
- $O(^1D) + CH_4 \rightarrow CH_3OH^*$
- $CH_3OH^* \rightarrow CH_3 + OH$
  $\rightarrow CH_2OH + H$
  $\rightarrow CH_3O + H$
- $O(^3P) + CH_4 \rightarrow CH_3 + OH$
- $OH + CH_3O \rightarrow H_2O + H_2CO$



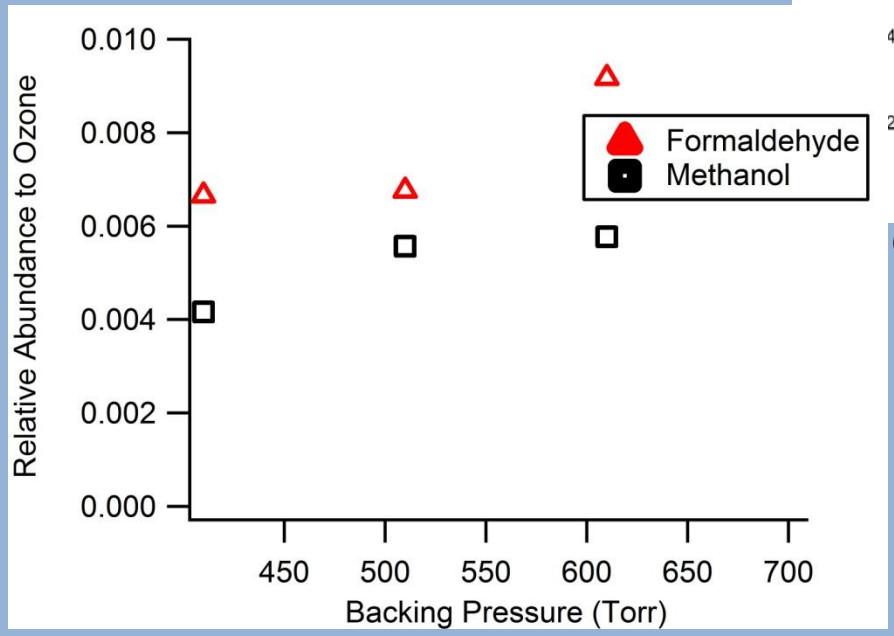


Chang and Lin, *Chem. Phys. Lett.* **363** (2002) 175-181

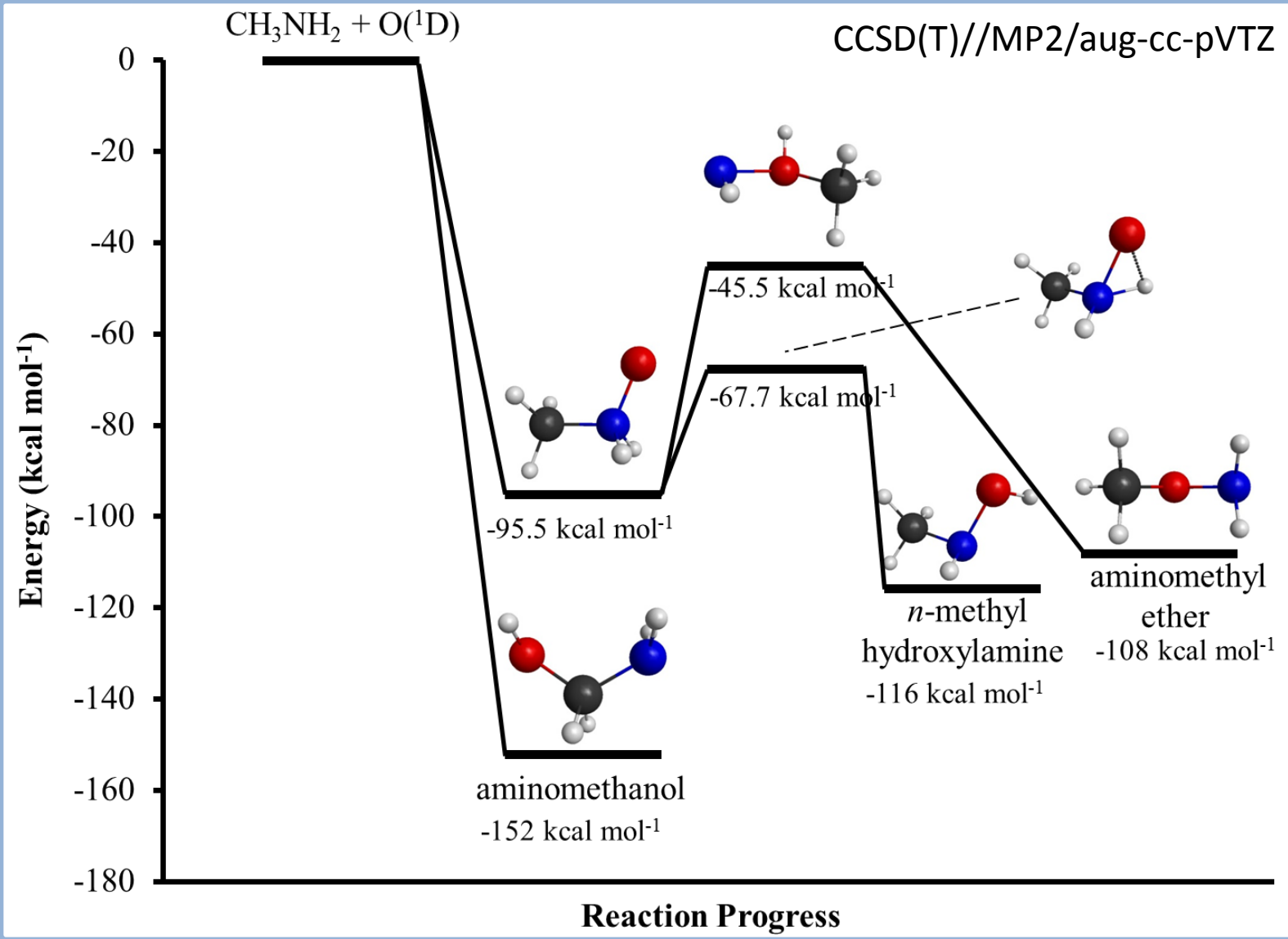
Formaldehyde Formation



Chang and Lin, *Chem. Phys. Lett.* **363** (2002) 175-181



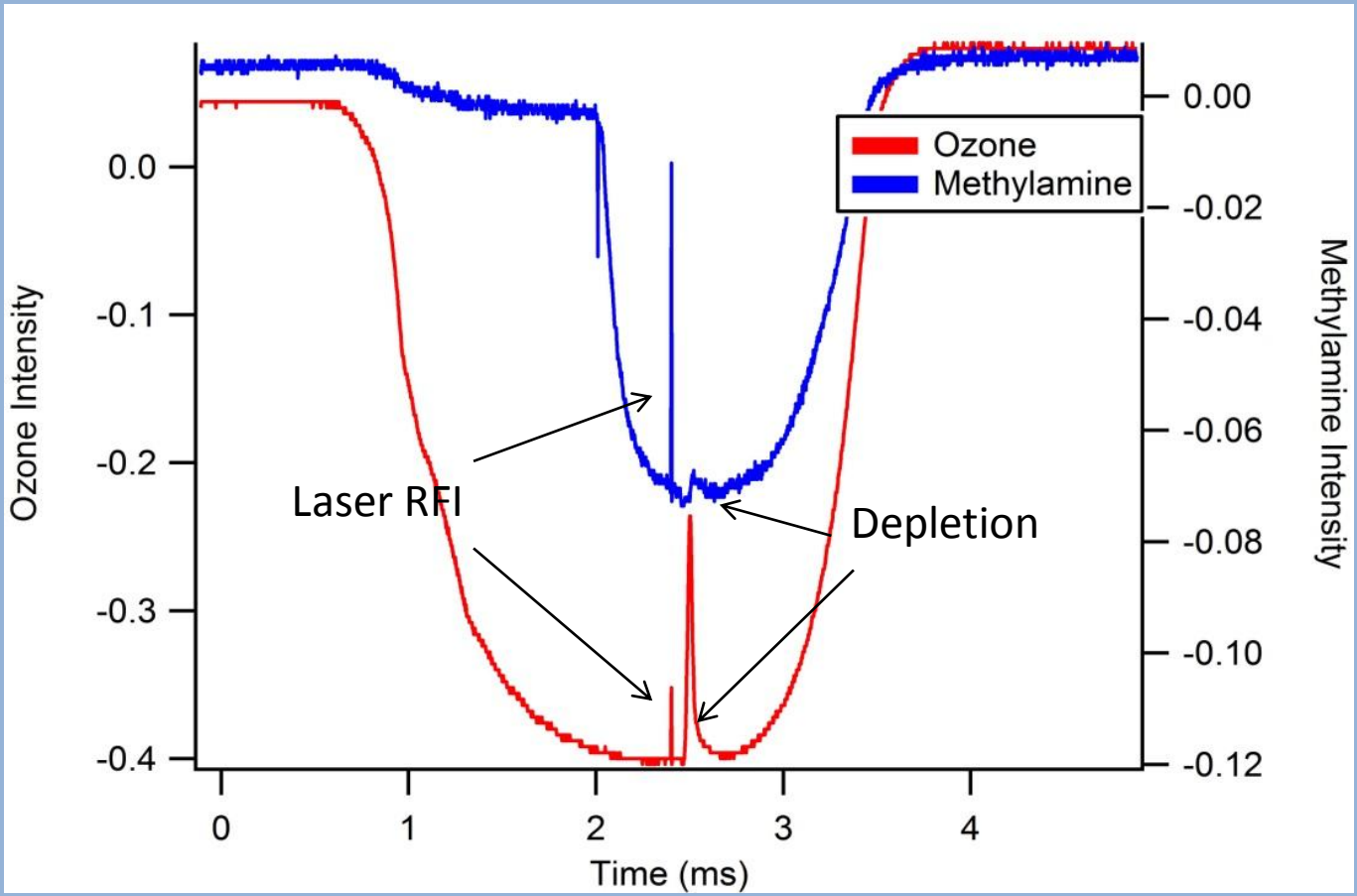
Methylamine Reaction



Hays and Widicus Weaver, JPCA 2013, online

Methylamine Reaction

$O(^1D) + CH_3NH_2 \rightarrow$ products



Methylenimine and Formaldehyde

$CH_3NH_2 + O(^1D) \rightarrow H_2NCH_2OH$

$\rightarrow CH_2OH + NH_2$

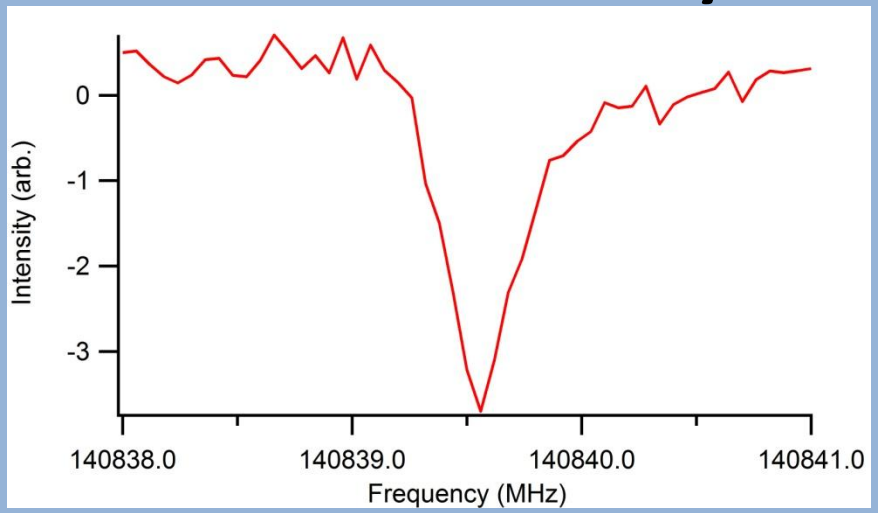
$\rightarrow CH_2NH_2 + OH$

$CH_2NH_2 + OH \rightarrow$

$H_2O + \boldsymbol{H_2CO}$

$CH_2OH + OH \rightarrow$

$H_2O + \boldsymbol{H_2CNH}$



Methylenimine

1(1,0) – 1(0,1)

F= 0 - 1

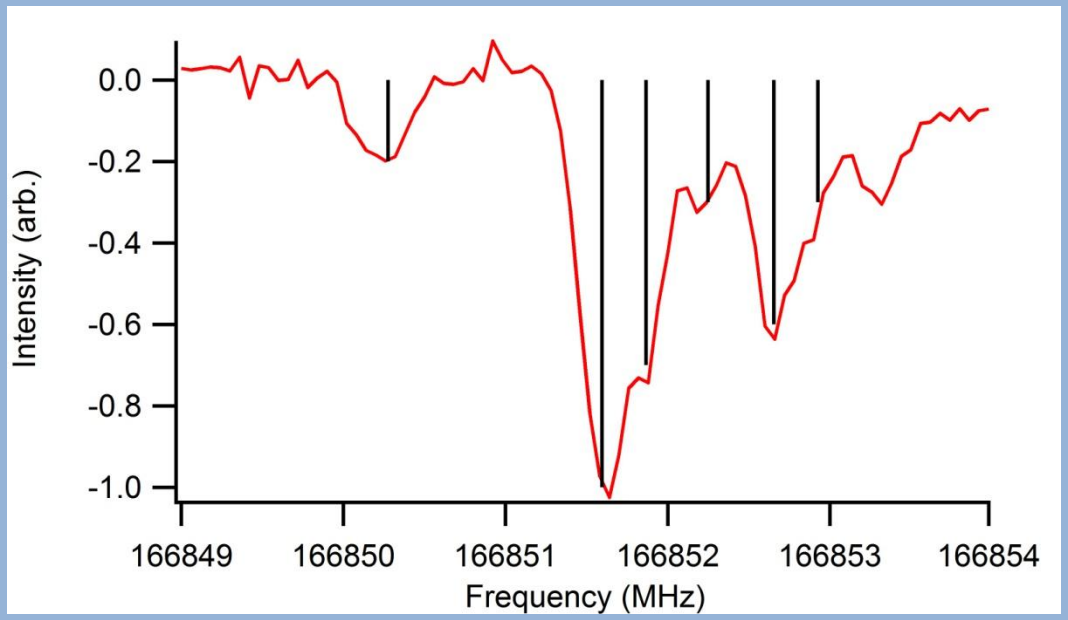
F= 2 - 2

F= 2 - 1

F= 1 - 0

F= 1 - 2

F= 1 - 1



Conclusions and Future Work

- A new spectrometer that can probe laser induced chemistry
- Investigate production mechanism
- Search for aminomethanol and other molecular transitions
- Compare laboratory spectra to observational studies

Acknowledgements

- The Widicus Weaver group
- Michael Heaven for loan of laser and ozone generator
- Kyle Mascaritolo for helpful discussion
- Cherry L Logan Computing Center
- NASA APRA (NNX11AI07G)

EMORY UNIVERSITY

NASA