SAND2007-4721C

The CN + O_2 Reaction: Measuring the Branching Ratio and Reactant/Product State Distributions by TR-FTIR

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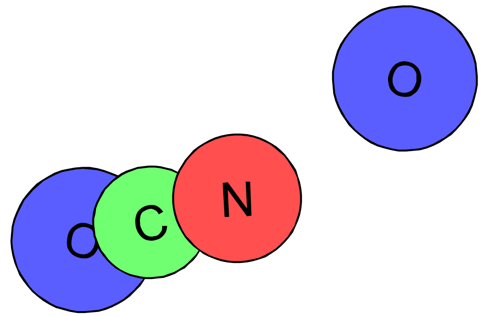
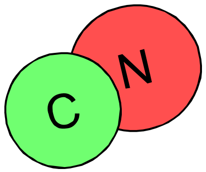
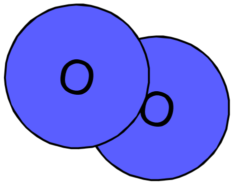
08353 Combustion Chemistry

Introduction

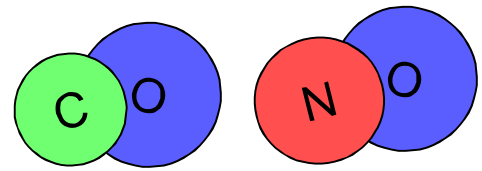
$CN + O_2 \rightarrow NCO + O$



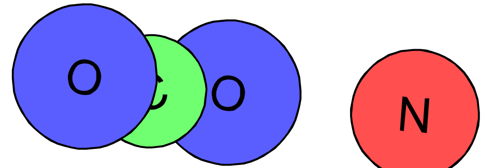




$\rightarrow CO + NO$

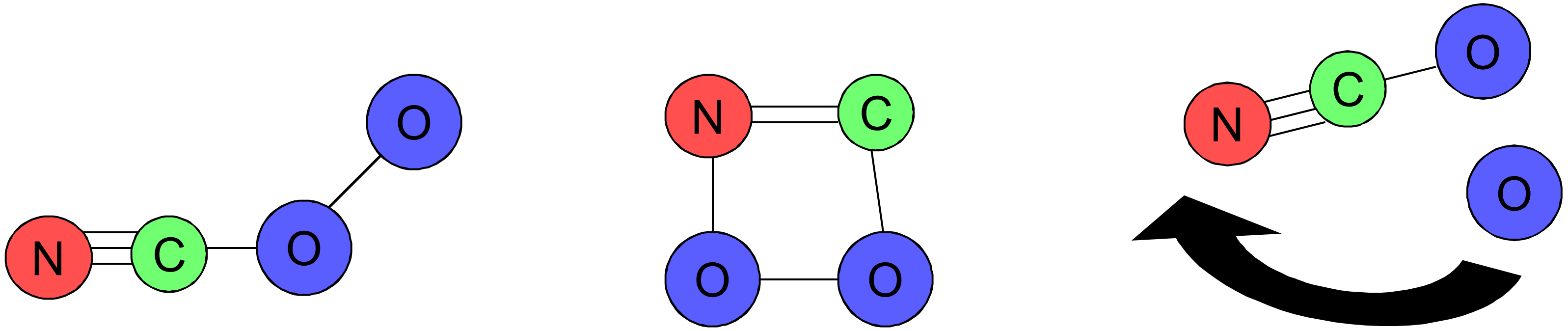


$\rightarrow CO_2 + N$



Why Study CN + O_2?

- Reaction mechanism uncertain



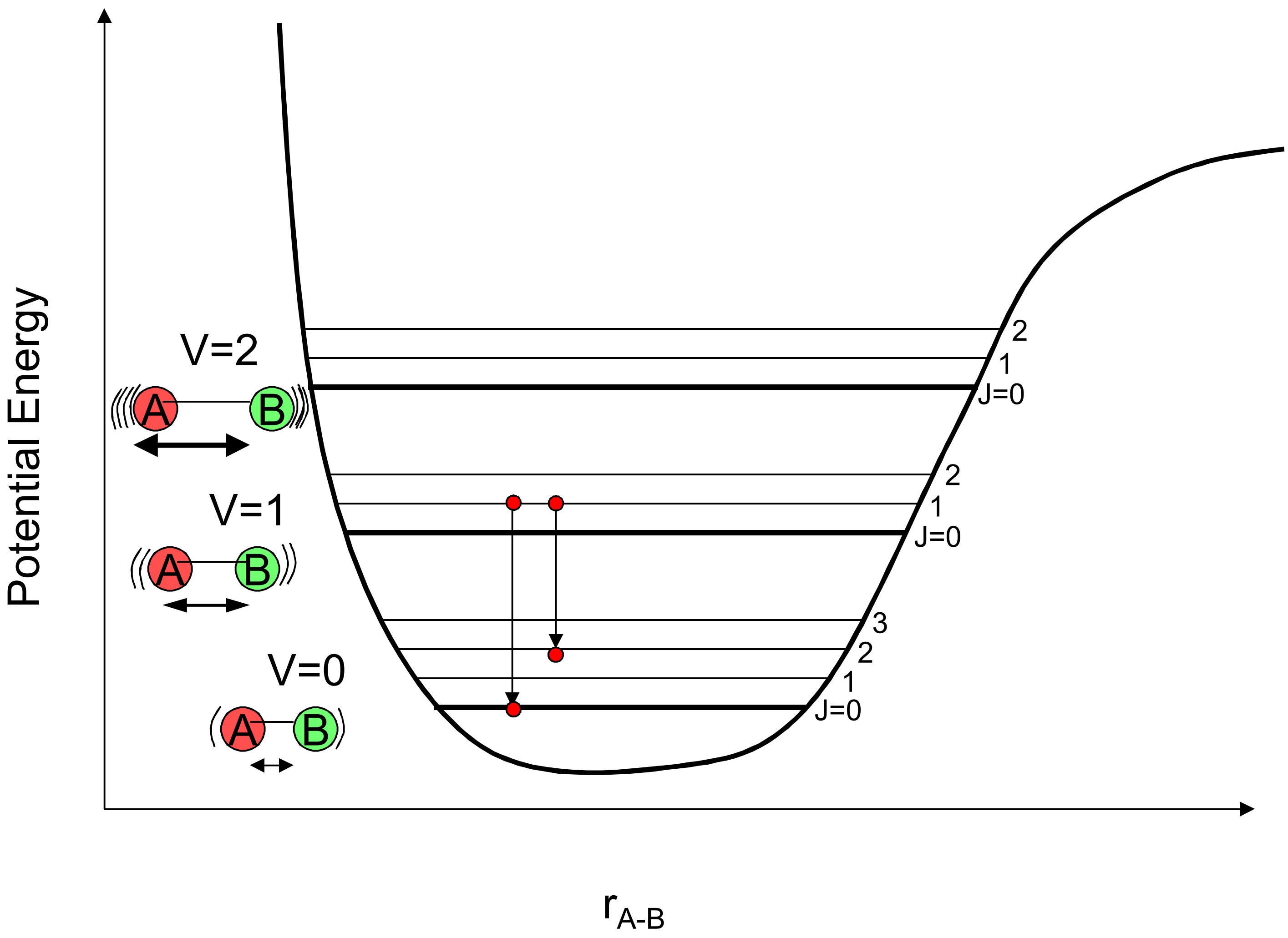
NCOO peroxy radical? Four-center transition state? Roaming atom?

- Important in N_2-rich fuel combustion
- Modeling
- Prototypical radical-radical reaction

Procedure

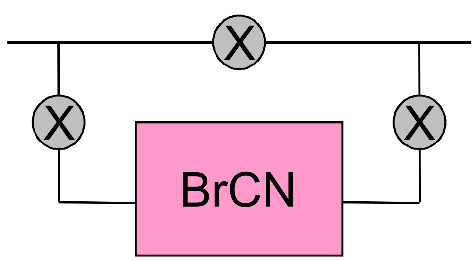
- Photodissociation: BrCN → CN
- Use TR-FTIR (**T**ime **R**esolved **F**ourier **T**ransform **I**nfra**r**ed Spectroscopy) to probe CN
- React CN with O_2
- Use TR-FTIR to probe reactants/products

Time Resolved Fourier Transform Infrared Spectroscopy

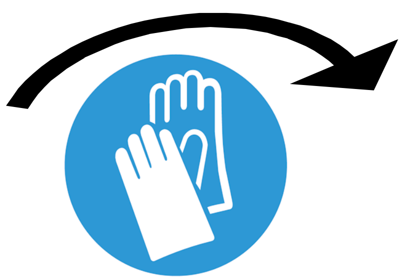


Safety

- BrCN highly toxic
- Precautions:

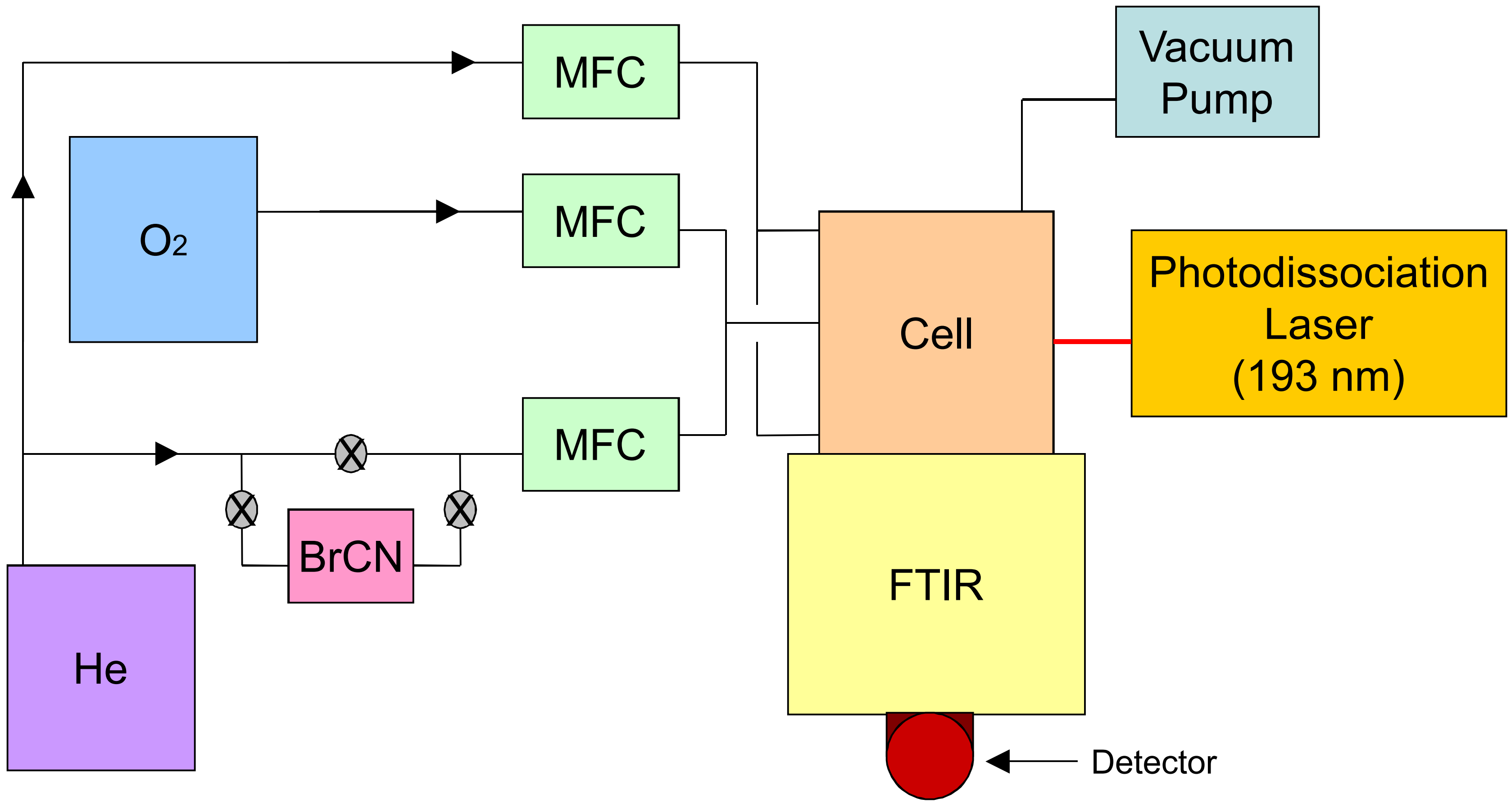


Sealed container

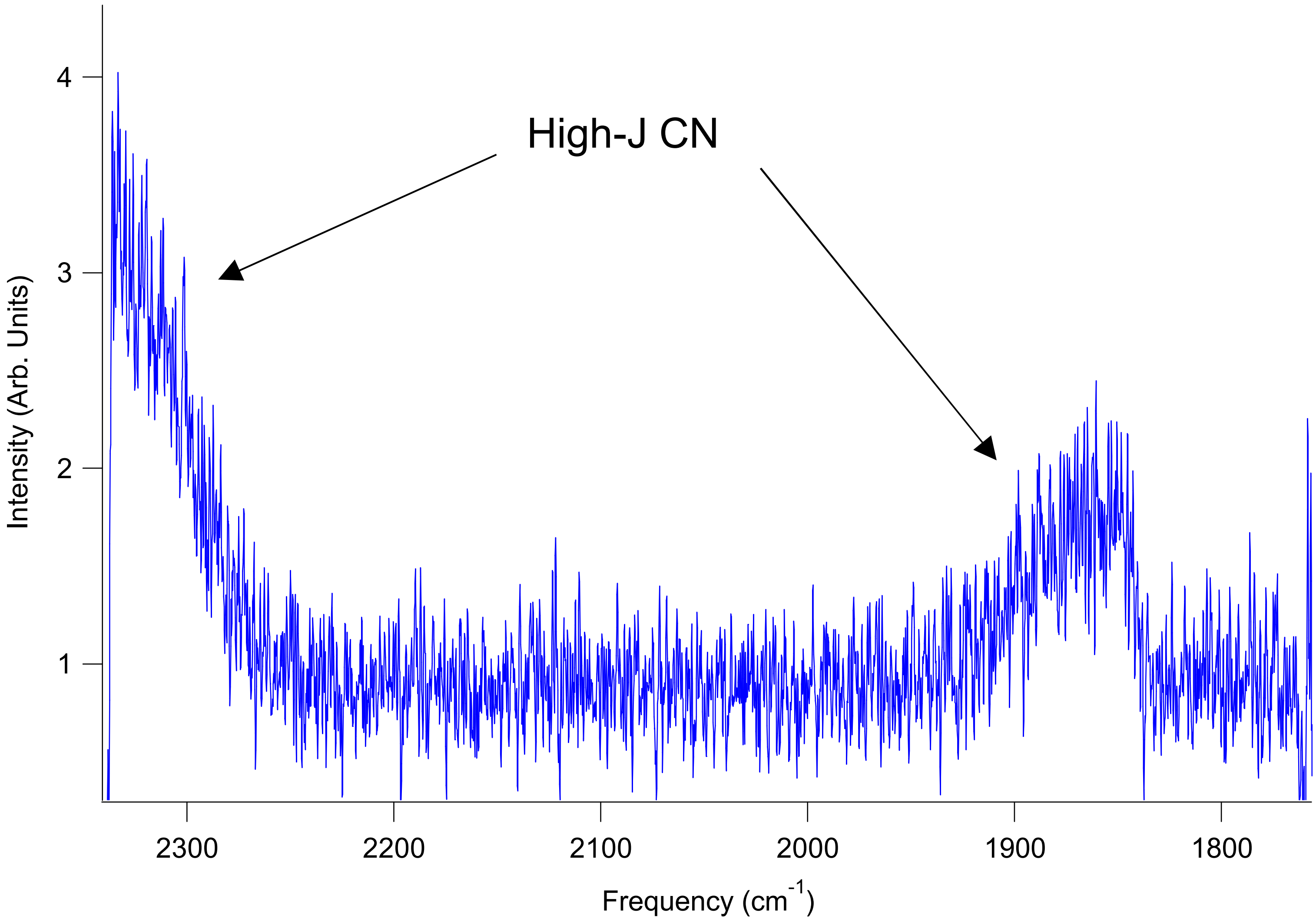


Fume hood

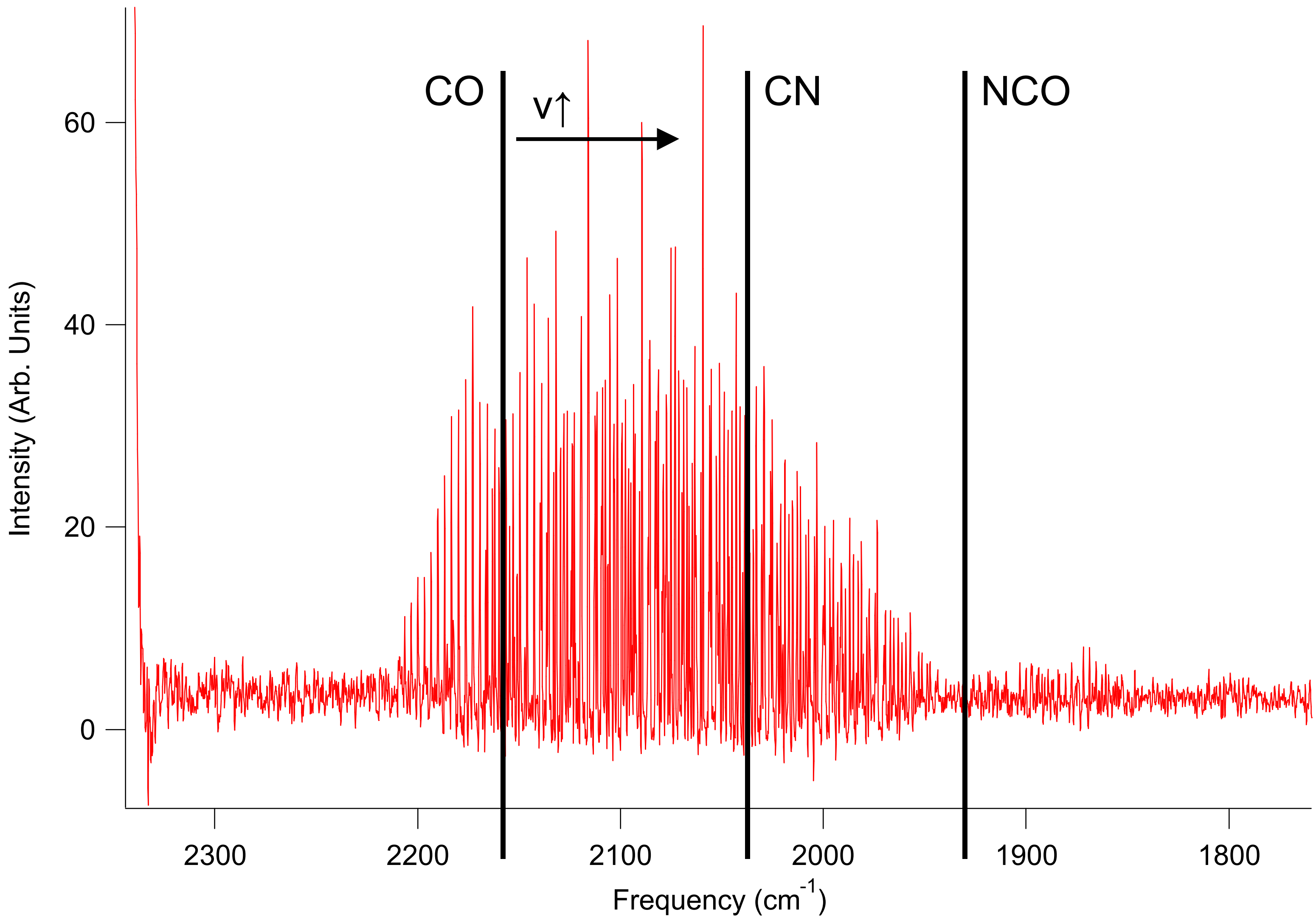
Experimental Setup



Preliminary Data: Before O_2 Added



Preliminary Data: After O_2 Added



Conclusions

- Reaction occurring
- BrCN → Rotationally excited CN
- CN + O_2 → Vibrationally excited CO (?)

Recommendations

- Increase S/N
  - Potentially use other precursors
  - Time-resolved spectra
  - Nascent distributions
- More fitting
  - Fit for NO
  - State distributions
  - Species populations → Branching ratio

Acknowledgements

- Eilene Cross + Lisa Gray
- David Osborn
- Talitha Selby
- Howard Johnsen