SOFIA/EXES Study of CH$_4$ and SO$_2$ toward Massive YSOs

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High Resolution Mid-IR Spectroscopy

1) Absorption of molecular species against strong mid-IR continuum sources: sensitive to material close to YSO

2) Mid-IR traces species with no dipole moments.

3) High resolution spectroscopy: kinematics relates to location.
GO Programs

02_0104: 3.3 hours to observe gaseous CH$_4$ in two massive YSOs (both NGC 7538 IRS1 and Mon R2 IRS3 observed)

04_0153: 4.0 hours to observe gaseous SO$_2$ in three massive YSOs (W3 IRS5 observed, GL 2136 and Mon R2 IRS3 not yet)

Different chemistries CH$_4$ and SO$_2$ offer different tracers physical conditions in massive YSOs.
Team

Matt Richter (UC Davis)
Nick Indriolo (STScI)
Curtis DeWitt (UC Davis)
David Neufeld (Johns Hopkins University)
Agata Karska (Adam Mickiewics Universit)
Ted Bergin (Univeristy of Michigan)
Rachel Smith (Appalachian State University)
Ed Montiel (UC Davis)
$\text{CH}_4$
**CH$_4$ Chemistry**

Low extinction ($A_V \sim 1$ mag):
- Gas phase CH$_4$ formation slow due to energy barriers
- C preferably in gas phase CO

High extinction ($A_V > 2$ mag):
- CH$_4$ formed on grain surfaces (C hydrogenation) as is H$_2$O (O hydrogenation)
- Low CH$_4$/H$_2$O ice ratio (few percent)

Oberg et al. (2008)
CO destruction enhances CH$_4$: at high gas phase temperature or on grain surfaces.

COM (Complex Organic Molecules) formation:

- CH$_4$ $\rightarrow$ carbon chains, e.g., “Warm Carbon Chain Chemistry Sources”
- CO $\rightarrow$ H$_2$CO, CH$_3$OH, ....

Measurements CH$_4$ important:

- Ice not possible with SOFIA... telluric CH$_4$ Q-branch, insufficient instrumentation.
- Gas phase CH$_4$ possible with EXES
Ground-based telescopes at $3.32 \, \mu m$ (C-H stretch): large Doppler shift needed to detect gas phase CH$_4$:

- $-82 \, km/s$ for NGC7538 IRS9 combination of earth motion and high source $V_{helio}$

P Cygni line profile indicates warm CH$_4$ in expanding shell.

Previous CH$_4$ Observation

- **Grain surface chemistry**
  - solid CH$_4$ formation

- **Shock chemistry**
  - $\text{CH}_4 \rightarrow \text{CO}$

- **Hot core chemistry**
  - $\text{CH}_4$ sublimation

- **CH$_4$  → complex species**

Asilomar/SOFIA: CH$_4$ with SOFIA/EXES

NGC 7538 IRS1, R=100,000

Uncorrected for atmosphere!

R(6)  R(5)  R(4)  R(3)  R(2)  R(1)  R(0)  Q-branch

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CH$_4$ with SOFIA/EXES

NGC 7538 IRS1, R=100,000

Uncorrected for atmosphere!

R(0)  Q-branch
R(6)  R(5)  R(4)  R(3)  R(2)  R(1)

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CH$_4$ with SOFIA/EXES

NGC 7538 IRS1, R=100,000

- R(0)
CH$_4$ with SOFIA/EXES

NGC 7538 IRS1, R=100,000 (3 km/s)

LTE model assumes CO parameters (Mitchell et al. 1990):

- CH$_4$/CO=1% (1.2e17 cm$^{-2}$)
- T=25 K
- FWHM=3.3 km/s

“Spectacular” non-detection of CH$_4$ in cold gas phase:
At cold temperatures it is frozen out.
CH$_4$ with SOFIA/EXES

NGC 7538 IRS1, R=100,000 (3 km/s)

LTE model (red) assumes CO parameters (Mitchell et al. 1990):

- CH$_4$/CO=1% (1.1e17 cm$^{-2}$)
- T=176 K
- FWHM=3.3 km/s

CH$_4$ in warm gas phase: consistent with sublimation off icy grains

Notice simple, narrow line profile...hot core gas, not outflow.
SO₂
Why Study SO$_2$?

Red: elements in ice
Black: element in refractory material

Location of S in dense clouds is mystery.
Why Study $\text{SO}_2$?

$\text{SO}_2$ Abundance relative to SO or $\text{H}_2\text{S}$ is hot core age indicator.

Problem: little $\text{H}_2\text{S}$ in ice. What is source of S?

Charnley et al. (1997)
**SO$_2$: Previous IR Observations**

- **ISO/SWS** detected *warm gas phase SO$_2$* toward massive YSOs

- *Factor $\sim$10 more abundant* than in sub-millimeter studies of pure rotational lines

- *What is location of this SO$_2$? Need line profile information.*

SO$_2$: Complex IR Spectrum

SO$_2$ is “asymmetric top”, just like H$_2$O. Its spectrum is complex and lines overlap.
SO$_2$ with SOFIA/EXES

portion of the observation (includes atmosphere!)

W3 IRS5, R=50,000
SO$_2$ with SOFIA/EXES

lines must be much broader than 5 km/s!

Atmosphere
SO$_2$, LTE: 450 K, 5e16 cm$^{-2}$, FWHM=5 km/s
atmosphere+LTE model
W3 IRS5, R=50,000

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SO$_2$ with SOFIA/EXES

lines must be ~30 km/s wide!

Atmosphere
SO$_2$, LTE: 450 K, $5 \times 10^{16}$ cm$^{-2}$
FWHM=33 km/s
atmosphere+LTE model

W3 IRS5, R=50,000
SO$_2$ with SOFIA/EXES

SO$_2$ line detection after Doppler shift

Atmosphere
SO$_2$, LTE: 450 K, $5 \times 10^{16}$ cm$^{-2}$, FWHM=33 km/s + Doppler shift
atmosphere + LTE model

W3 IRS5, R=50,000
SO$_2$ with SOFIA/EXES

SO$_2$ line detection after Doppler shift, but there are residuals!

Atmosphere

SO$_2$, LTE: 450 K, $5 \times 10^{16}$ cm$^{-2}$
FWHM=33 km/s+Doppler shift
atmosphere+LTE model

W3 IRS5, R=50,000

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SO$_2$ with SOFIA/EXES

Not all detected lines are due to SO$_2$

Atmosphere

SO$_2$, LTE: T=450 K, N=5e16 cm$^{-2}$
FWHM=33 km/s
atmosphere+LTE model

W3 IRS5, R=50,000
(Preliminary) Conclusions

- SO$_2$ associated with strong shocks

- SO$_2$ abundance enhanced w.r.t. large scale cloud suggests shock formation:
  - What is source of Sulfur?
    - unlikely sublimated H$_2$S.
    - S$_2$ from ice?
    - S sputtered from refractory grains?

- CH$_4$ gas only present in warm gas phase, but with relatively narrow lines: sublimation from icy grains in hot core.

- Further CH$_4$ and SO$_2$ observations needed in larger variety of sources.
EXES Posters

Montiel et al.: Science with EXES
(including line survey of oxygen-rich hypergiant VY Canis Majoris)

Rangwala et al.: SOFIA/EXES 13 µm High Spectral Resolution Observations of Orion IRc2 (ortho and para C₂H₂ temperatures and ratios, formation path C₂H₂)