Abundant $\text{SO}_2$ Gas in the Hot Core around MonR2 IRS3

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Sulfur Budget Problem

- Sulfur is the 10th most abundant element in the universe
  - From observations of HII regions, the solar photosphere, and the diffuse interstellar medium (ISM)
- Dense clouds are severely depleted
  - Abundances as low as 5% of the cosmic value
- So where does it all go?
  - Gas-phase molecules, refractory dust grains, and icy mantles
  - A wide-variety of molecules have been observed in sub-millimeter wavelengths but only in very small abundances
Fig. 1: Fraction of an Element’s cosmic abundance that is accounted for
Why do we care?

- Sulfur has an extremely rich and diverse chemistry
  - Sulfur can easily imitate oxygen in just about any molecule: e.g., ethanol (C₂H₆O) and ethanethiol (C₂H₆S)
  - Sulfur is second to only carbon in the number of allotropes it has
- Sulfuretted molecules can be used for a variety of purposes
  - Tracers of evolution in protostellar environments (i.e., chemical clocks)
  - Connect primitive solar system objects with conditions in the protosolar envelope
  - Sulfur is necessary for life as we know it
How do we chip away at this?

- We focus on SO$_2$ specifically, one of the simpler sulfuretted molecules
  - SO$_2$ is one of the three molecules thought to be useful in the “chemical clocks” approach to measuring hot core age
  - SO$_2$ measurements in the mid-infrared and sub-millimeter find differing abundances
  - SO$_2$'s formation pathway is not well understood
Invisible to the eye

- Sub-millimeter observations
  - Lower resolution only probes the colder broader gas around these objects
- Mid-infrared wavelengths enable two possibilities
  - Ice-phase observations
    - Have proven very difficult, yielding non-detections or very low abundances
  - Warm gas-phase absorption
    - Allow us to directly probe the chemistry of the hot core itself
Observations: Past...

- Sub-millimeter emission from the gas-phase SO$_2$ (van der Tak et al. 2003)
  - Yields a very low abundance (roughly 0.1% the cosmic sulfur abundance)

- Mid-infrared absorption (previously done by Infrared Space Observatory, Keane et al. 2001)
  - Indicate a much higher abundance (by over 2 orders of magnitude) SO$_2$ gas in the hot core
  - Leads us to the question, where does it come from?
Observations: ... & Present

- We use the Echelon-Cross-Echelle Spectrograph (EXES) for SO$_2$
  - Gas-phase absorption at high resolution (R of 55,000)
  - Covers a band around 7.3 $\mu$m
  - High R is the key, it allows us to resolve individual lines

- We also have Keck NIRSPEC observations for CO to determine relative abundances
  - Gas-phase absorption at medium resolution (R of 25,000)
  - M-band spectra
Hot Cores

- Envelope of warm, dense gas around a young stellar object
  - Ices have evaporated
- These conditions lead to a rich chemistry
What the Sub-mm missed

- Absorption along line of sight allows us to probe the region closest to the young stellar object (YSO)
LTE Models

- We generate model spectra through a local thermodynamic equilibrium (LTE) model
  - Three input parameters: Excitation Temperature ($T_{\text{ex}}$), Column Density ($N_{\text{col}}$), and Doppler Parameter ($b_{\text{dop}}$)
- Likelihood is computed by using a $\chi^2$ value
  - Best fit is chosen by minimization
  - Error bars are found by Monte Carlo Markov Chain sampling to determine the likelihood distributions for each input parameter
Fig. 2: Example LTE Models for SO$_2$
Best Fit

- $\text{SO}_2$ gas with a temperature of $234\pm15$ K
  - We call this the warm component, our data only allowed for upper limits on the cold foreground component
- Warm $\text{SO}_2$ abundance limit of $\text{SO}_2/\text{H} > (5.6\pm0.5)\times10^{-7}$
  - Accounts for $>4\%$ of the cosmic S abundance
  - Limit due to lower resolution of CO data
- Linewidth of $b < 3.20$ km s$^{-1}$
  - On the edge of being resolved by the instrument
Fig. 3a: Subset of \( \text{SO}_2 \) Spectrum with Best Fit
Fig. 3b: Subset of SO$_2$ Spectrum with Best Fit
Fig. 4: Line Profiles
Origin of SO2: Radiative Heating

- Gas-phase formation: sulfuretted ices sublimate before forming SO$_2$
  - Expect high temperatures due to location in hot core
  - Expect narrow linewidths due to quiescent gas
Ice-phase formation: sulfuretted ices evolve into an $\text{SO}_2$ ice before sublimating

- Expect high temperatures due to location in hot core
- Expect narrow linewidths due to quiescent gas

\[ \text{H}_2\text{S} \text{?} \quad \text{S}_2 \text{?} \quad \text{OCS} \text{?} \]

\[ \text{SO}_2 \text{?} \quad \text{SO}_2 \text{?} \]
Origin of SO2: Shock heating

- Gas-phase formation: sulfur locked in the dust is released enabling gas-phase formation
  - Expect low temperatures due to rapid post-shock cooling
  - Expect broad linewidths due to shock wave passing through gas
Best Fit

- SO$_2$ gas with a temperature of 234±15 K
  - We call this the warm component, our data only allowed for upper limits on the cold foreground component

- Warm SO$_2$ abundance limit of SO$_2$/H > (5.6±0.5)x10$^{-7}$
  - Accounts for >4% of the cosmic S abundance
  - Limit due to lower resolution of CO data

- Linewidth of b < 3.20 km s$^{-1}$
  - On the edge of being resolved by the instrument
Radiative vs Shocks

- \( \text{SO}_2 \) gas with a temperature of \( 234\pm15 \text{ K} \)
  - We call this the warm component, our data only allowed for upper limits on the cold foreground component
- Warm \( \text{SO}_2 \) abundance limit of \( \text{SO}_2/H > (5.6\pm0.5) \times 10^{-7} \)
  - Accounts for >4% of the cosmic S abundance
  - Limit due to lower resolution of CO data
- Linewidth of \( b < 3.20 \text{ km s}^{-1} \)
  - On the edge of being resolved by the instrument

Consistent with a radiative heating picture
Radiative vs Shocks

- SO\textsubscript{2} gas with a temperature of 234\pm15 K
  - We call this the warm component, our data only allowed for upper limits on the cold foreground component
- Warm SO\textsubscript{2} abundance limit of SO\textsubscript{2}/H > (5.6\pm0.5)x10\textsuperscript{-7}
  - Larger than that derived for Orion IRc 2 (2x10\textsuperscript{-7}; Blake et al. 1987)
  - Consistent with that of HH 212 (4–12x10\textsuperscript{-7}; Podio et al. 2015)
- Linewidth of b < 3.20 km s\textsuperscript{-1}
  - On the edge of being resolved by the instrument

Hot core formation of SO\textsubscript{2} is at least as efficient as shock formation
Ice-phase vs Gas-phase

- Ice-phase SO$_2$ measurements find extremely low abundances
  - The ice-phase SO$_2$/H$_2$O abundance is 0.6x10$^{-2}$*
  - The warm gas-phase SO$_2$/H$_2$O abundance is (10.0±3.0)x10$^{-2}$
- Mismatch between ice-phase and warm gas-phase abundances implies SO$_2$ can not be sublimating directly from the ice

*Calculated with values from Zasowski et al. 2009 (SO$_2$) and Gibb et al. 2004 (H$_2$O)
Then what’s in the ice?

- $\text{H}_2\text{S}$ is the chemical model’s molecule of choice
  - $\text{H}_2\text{S}$ is the dominant sulfur-bearer (roughly 60%) in comets (Calmonte et al. 2016)
  - $\text{H}_2\text{S}$ ice measurements are, at best, upper limits, and half the abundance we measure for warm $\text{SO}_2$ gas

- We believe the ice must be releasing sulfur allotropes
  - Sulfur allotropes are the next largest sulfur-bearer in comets
  - They are also highly volatile, leading to sublimation at low temperatures
  - Difficult to observe
Future work

● Higher resolution CO data with iShell
  ○ Data has been collected and reduced, awaiting analysis

● More targets
  ○ W3 IRS5, data collected and mostly reduced
    ■ Problems with standard star introduced excess noise in SO$_2$ data
Conclusions

- SO$_2$ in Mon R2 IRS 3 is consistent with a radiative heating model.
- The hot core formation of SO$_2$ is at least as efficient as the shock formation.
- SO$_2$ is unlikely to be forming in the ice.
- Sulfur allotropes may be required to explain sulfur chemistry in molecular clouds.
References

Blake et al. 1987
Calmonte et al. 2016
Gibb et al. 2004
Keane et al. 2001
Podio et al. 2015
van der Tak et al. 2003
Zasowski et al. 2009