Time-Sensitive Chemical Tracers Within Shocked Astrophysical Sources

Andrew Burkhardt
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ISMS 2017
COM Formation on Ices

- Many COMs form efficiently on IS ices
- Difficult to constrain ice abundances observationally
- How do we test it?
  - Absorption
  - Warm-up grain
  - Or...

Burke & Brown, 2010

Garrod & Herbst, 2006, Boogert et al. 2015
Shock Chemistry

- Shocks: A wave propagating faster than sound speed
- Effects:
  - Rapidly heat gas
  - Liberate species
    (Sputtering)
  - Grain shattering
- C-Shocks: non-thermal desorption → gas-phase probes of ice chem
Shock Chemistry

- Transient features may explain discrepancies (e.g. observations/models) or variations between sources
  - COMs where there shouldn’t be
  - Complex regions like Orion KL
L1157

- Class 0 protostar w/ prototypical “chemically-active” outflow

- L1157-B1 & B2: recent shock events
  - B1: warmer and younger shock
    \( T_{\text{kin}} \sim 80-100 \text{ K}, \ t_{\text{shock}} \sim 2000 \text{ yr} \)
  - B2: cooler and older shocker
    \( T_{\text{kin}} \sim 20-60 \text{ K}, \ t_{\text{shock}} \sim 4000 \text{ yr} \)

(Gueth, Guilloteau & Bachiller 1996; Tafalla & Bachiller 1995; Lefloch et al. 2012)
L1157

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Burkhardt et al. 2016
Observational Predictions

- Gas-phase CH$_3$OH globally enhanced through shocks
- Recent history of source may be important
- HNCO & other enhancement in post-shock gas

(Burkhardt et al. 2016)
More complexity in L1157!

L1157-B1, a factory of complex organic molecules in a solar-type star-forming region

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ABSTRACT

We report on a systematic search for oxygen-bearing complex organic molecules (COMs) in the solar-like protostellar shock region L1157-B1, as part of the IRAM Large Program 'Astrochemical Surveys At IRAM'. Several COMs are unambiguously detected, some for the first time, such as ketene H₂C=O, dimethyl ether (CH₃OCH₃) and glycolaldehyde (HCOCH₂OH), and others firmly confirmed, such as formic acid (HCOOH) and ethanol (C₂H₅OH). Thanks to the high sensitivity of the observations and full coverage of the 1, 2 and 3 mm wavelength bands, we detected numerous (~10-125) lines from each of the detected species. Based on a simple rotational diagram analysis, we derive the excitation conditions and the column densities of the detected COMs. Combining our new results with those previously obtained towards other protostellar objects, we found a good correlation between ethanol, methanol and glycolaldehyde. We discuss the implications of these results on the possible formation routes of ethanol and glycolaldehyde.

Key words: astrochemistry – stars: formation – ISM: abundances – ISM: jets and outflows – ISM: molecules.
Other Observational Predictions

Figure 4. Normalized line-to-continuum ratio maps (generated by computing the ratio of the PdBI zeroth-order moment maps from Fig. 3 with respect to the 1 mm continuum emission, relative to the value of the ratio at the 1 mm peak so that all figures show a comparable scale). The star symbol marks the position of the 1.4 mm peak from Cesaroni et al. (2014), also shown in Fig. 2a) and the red ellipse indicates the H$_2$ knot tracing the outflow cavity (Cesaroni et al. 2013, marked also in Fig. 3a). See Table 3 for further details about the physical conditions (abundance/temperature) that each line-to-continuum ratio map is probably tracing.

We define a factor $F$ that includes the dependence of the normalized line-to-continuum ratio on $T_{\text{ex}}$, $T_{\text{dust}}$ and $E_u$:

$$F \equiv \frac{Q_{T_{\text{ex}}, \text{disc}}}{Q_{T_{\text{ex}}, \text{outf}}},$$

(2)

Taking into account that the dependence of the partition function with $T_{\text{ex}}$ for symmetric and asymmetric top molecules is proportional to $T_{\text{ex}}^3/2$, and assuming that $T_{\text{ex}} \sim T_{\text{dust}}$, $F$ can be finally written as

$$F = \left(\frac{T_{\text{disc}}}{T_{\text{outf}}}\right)^{5/2} e^{E_u/k} \left(\frac{1}{T_{\text{disc}}} - \frac{1}{T_{\text{outf}}}\right).$$

(3)

We note that the assumption $T_{\text{ex}} \sim T_{\text{dust}}$ should be valid as a first approach because what is relevant to estimate $F$ is the ratio of those temperatures at the disc and outflows positions, and it is likely that both temperatures decrease in a similar way from one position to the other. We further discuss this assumption in Section 5.1.

Thus, if $F \sim 1$, the normalized line-to-continuum ratio will trace the abundance variation between the disc and outflow positions. But if $F$ is of the order of the normalized line-to-continuum ratio, this ratio will be a temperature tracer rather than an abundance tracer.

Since we have modelled the emission of the detected molecules at the disc and outflow positions using XCLASS, we can have a first estimate of $F$ for the transitions for which we have imaged the line-to-continuum ratio. The values of $F$ for these transitions are reported in Table 3, along with the observed normalized line-to-continuum ratio.

Table 3 shows that the observed normalized line-to-continuum ratio is very similar to the $F$ factor for HNCO, CH$_2$CO, HCOOH and CH$_3$COCH$_3$, indicating that the variations in the line-to-continuum map might be due to different temperatures in these cases. On the contrary, for the case of H$_2$^{13}CO, CH$_3$OCH$_3$ and, to a less extent, HCOOCH$_3$, the observed ratio is still larger by more than a factor 9.

Strictly speaking, also CH$_3$CN presents a large difference between the observed normalized line-to-continuum ratio and the $F$ factor, but we avoid its discussion here because the modelling of CH$_3$CN required two components, making its interpretation more difficult.
NAUTILUS Models

- Study chemical evolution after shock passage (10-10^6 year)
- Test predictions made in L1157 Observational Paper
- Make predictions of the chemical evolution of tracers in post-shock gas

Goals:
- Incorporate Physical Conditions of Shocks ($T_{\text{gas}}, T_{\text{dust}}, n_{\text{H}_2}, A_V$)
- Incorporate High temperature Network
- Incorporate Non-thermal desorption (e.g. Sputtering)
Regime 1:
Standard dark cloud conditions, build chemical complexity on ice
- $T = 10$ K
- $n = 5 \times 10^4$ cm$^{-3}$
- $t = 10^6$ yrs

Regime 2:
Shock occurs, liberating species, shock-chemistry
- See next slide

Regime 3:
Shock passes, with density increased temporarily
- $T = 10$ K
- $n = 5 \times 10^5$ cm$^{-3}$
- $t > 10^5$ yrs
Goals:

- Incorporate Physical Conditions of Shocks
- Parametric treatment approx structure over chemically-relevant timescales
- Matched to robust MHD simulations
- \( n_{H_2} \) & \( A_v \) scale w/ standard jump conditions
- Radiative/collisional dust heating
- Incorporate High temperature Network
- Incorporate Non-thermal desorption (Sputtering)

Jimenez-Serra et al. 2008
NAUTILUS Models - High T Network

Goals:

- Incorporate Physical Conditions of Shocks
- Incorporate High temperature Network
- High-temp reactions added by Harada et al. (2010) (contributions by Furuya, Acharyya, Hincelin, & others)
- Adopted most recent NAUTILUS, including 3-phase model
- Incorporate Non-thermal desorption (Sputtering)
NAUTILUS Models - High T Network

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NAUTILUS Models - Sputtering

Goals:

- Incorporate Physical Conditions of Shocks
- Incorporate High temperature Network
- Incorporate Non-thermal desorption (Sputtering)
  - Adopted methods by JS08
  - Sputtering rate a function of:
    - gas particle collisional rate to strike dust
    - sputtering yield of target by projectile with velocity large enough for desorption
- VS Warm up:
  - Faster desorption, Short timescale heating
  - No loss of complexity

\[
\left[ \frac{dn(\text{CH}_3\text{OH})}{dt} \right]_{\text{tot}}^m = n_g r_m \left[ \frac{dn(\text{CH}_3\text{OH})}{dt} \right]_{\text{grain}}^m
\]

\[
\left[ \frac{dn(m)}{dt} \right]_{\text{grain}} = \pi a^2 n_p \left( \frac{8kT_n}{\pi m_p} \right)^{1/2}
\]

\[
x \frac{1}{s} \int_{x_{\text{th}}}^{\infty} dx x^2 \frac{1}{2} \left[ e^{-(x-s)^2} - e^{-(x+s)^2} \right] (Y(E))_\theta
\]

\[
Y(E, \theta = 0) = A \frac{(\varepsilon - \varepsilon_0)^2}{1 + (\varepsilon/30)^{4/3}}, \quad \varepsilon > \varepsilon_0,
\]

Jiménez-Serra et al. 2008
Results - Dark Cloud

- Gas-phase
- Ice-Mantle
- Ice-Surface

Abundance vs. Time [years]

- H2O
- JH2O
- KH2O
Results - Dark Cloud

Graph showing the abundance of different phases over time (years):
- Ice-Mantle
- Ice-Surface
- Gas-phase

Abundance scale from $10^{-22}$ to $10^{-4}$.

Time [years] from 1 to $10^7$.

Legend:
- H2O
- JH2O
- KH2O
Results - Shock

![Graph showing the abundance of Gas-phase, Ice-Surface, and Ice-Mantle over time. The graph plots abundance on a logarithmic scale against time in years.]

- **Gas-phase**
- **Ice-Surface**
- **Ice-Mantle**

**Legend:**
- H2O (blue)
- JH2O (green)
- KH2O (red)
Results - CH$_3$OH

[Graph showing the abundance of CH$_3$OH in gas-phase, ice-surface, and ice-mantle over time.

- Gas-phase: CH$_3$OH abundance decreases rapidly and stabilizes at around $10^{-8}$.
- Ice-surface: CH$_3$OH abundance increases significantly over time.
- Ice-mantle: CH$_3$OH abundance remains relatively constant.

Time [years]: 10, 100, 1e+3, 1e+4, 1e+5, 1e+6
Abundance: $10^{-6}$, $10^{-8}$, $10^{-10}$, $10^{-12}$, $10^{-14}$, $10^{-16}$, $10^{-18}$, $10^{-20}$, $10^{-22}$, $10^{-24}$, $10^{-26}$]
Results - Test Burkhardt et al. 2016
Results - HNCO

The graph shows the abundance of HNCO in different phases over time. The x-axis represents time in years, ranging from 10 to 1e+06. The y-axis represents abundance, ranging from 10^-26 to 10^-6.

- **Gas-phase**
- **Ice-Surface**
- **Ice-Mantle**

The graph includes three different curves:
- **HNCO** represented by a blue line.
- **JHNCO** represented by a green line.
- **KHNCO** represented by a red line.
Results - Subregimes
Results - Subregimes

- Sputtering
- Hot gas

Abundance vs. Time [years]

- HNCO
- JHNCO
- KNCO
Results - Subregimes

![Graph showing subregimes of sputtering, hot gas, and redeposition over time.](image)
Results - Subregimes

![Graph showing the abundance of molecules over time in different subregimes: Sputtering, Hot gas, Redeposition, and Dense Gas. The graph includes different molecular species such as HNCO, JHNCO, and KHNCO.](image)
Results - HNCO

<table>
<thead>
<tr>
<th></th>
<th>CH$_3$OH</th>
<th></th>
<th>HNCO</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N$</td>
<td>$N_{H_2}$</td>
<td>$N$</td>
</tr>
<tr>
<td></td>
<td>($10^{15}$ cm$^{-2}$)</td>
<td>($10^{-6}$)</td>
<td>($10^{13}$ cm$^{-2}$)</td>
</tr>
<tr>
<td>B0d</td>
<td>1.5</td>
<td>1.5</td>
<td>2.5</td>
</tr>
<tr>
<td>B1a</td>
<td>1.9</td>
<td>1.9</td>
<td>3.2</td>
</tr>
<tr>
<td>B1b</td>
<td>2.1</td>
<td>2.1</td>
<td>3.8</td>
</tr>
<tr>
<td>B2a</td>
<td>2.7</td>
<td>2.7</td>
<td>8.0</td>
</tr>
<tr>
<td>B2b</td>
<td>1.6</td>
<td>1.6</td>
<td>5.5</td>
</tr>
<tr>
<td>B2d</td>
<td>2.1</td>
<td>2.0</td>
<td>7.5</td>
</tr>
</tbody>
</table>

Adapted from Burkhardt et al. 2016
Results - HNCO

Adapted from Burkhardt et al. 2016

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<th>HNCO</th>
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<tr>
<td></td>
<td>( \frac{N}{N_{\text{H}_2}} )</td>
<td>( \frac{N_{\text{CH}<em>3\text{OH}}}{N</em>{\text{H}_2}} )</td>
</tr>
<tr>
<td></td>
<td>( 10^{15} \text{ cm}^{-2} )</td>
<td>( 10^{-6} )</td>
</tr>
<tr>
<td>B0d</td>
<td>1.5</td>
<td>1.5</td>
</tr>
<tr>
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<td>1.9</td>
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<tr>
<td>B2b</td>
<td>1.6</td>
<td>1.6</td>
</tr>
<tr>
<td>B2d</td>
<td>2.1</td>
<td>2.0</td>
</tr>
</tbody>
</table>
Results - HNCO vs OCN
Results - S Chemistry

![Graph showing abundance over time](image)
Results - S Chemistry

![Graph showing the abundance of S chemistry products over time](image-url)
Results - COMs
Results - COMs

![Graph showing abundances of various molecules over time.](image)

- H$_2$CO
- H$_2$CCO
- CH$_3$CHO
- CH$_3$CN
- NH$_2$CHO
- HCOOH
- HCOOCH$_3$
- CH$_3$OCH$_3$
- CH$_3$COCH$_3$
Going Forward

- Surveys of shocked outflows
  - Constrain time-dependence (radial/source age)
  - Test whether distributions are “physical” or “chemical”
- Robustly constraining time-sensitive tracers
  - Inclusion of more detailed networks to study
- Multiple shock-events (recent history)
- Shocks within classic “warm up model”

(Burkhardt et al. 2016)
Thanks

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- Remijanistan: Brett McGuire, Brandon Carroll, Joanna Corby, Chris Shingledecker, Ceci Xue, Ryan Loomis, Klaus Dollhopf, Tom Booth
- Herbst Group: Chris Shingledecker, Romane Le Gal, Ilsa Cooke, Ceci Xue, Niko Maffucci, Sean Shulte
- Funding:
  - Grote Reber Doctoral Fellowship
  - Virginia Space Grant Consortium
  - NASA Exobiology and Evolutionary Biology program
Observations

- Supplementary CARMA data toward L1157B from search for NH2OH (McGuire et al. 2015)

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>( \nu ) (GHz)</th>
<th>( E_u ) (K)</th>
<th>Beam (arcsec)</th>
<th>RMS (( \sigma )) (mJy beam(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH(_3)OH</td>
<td>( 2_{1,2} - 1_{1,1} )</td>
<td>96.73936(5)</td>
<td>12.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(methanol)</td>
<td>( 2_{0,2} - 1_{0,1} + + )</td>
<td>96.74138(5)</td>
<td>6.9</td>
<td>6''03 ( \times ) 5''53</td>
<td>8.5</td>
</tr>
<tr>
<td></td>
<td>( 2_{0,2} - 1_{0,1} )</td>
<td>96.74455(5)</td>
<td>20.1</td>
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<tr>
<td></td>
<td>( 2_{1,1} - 1_{1,0} )</td>
<td>96.75551(5)</td>
<td>28.0</td>
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<tr>
<td>HCN</td>
<td>( J = 1 - 0, F = 1 - 1 )</td>
<td>88.63042(2)</td>
<td>4.25</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(hydrogen cyanide)</td>
<td>( J = 1 - 0, F = 2 - 1 )</td>
<td>88.63185(3)</td>
<td>4.25</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( J = 1 - 0, F = 0 - 1 )</td>
<td>88.63394(3)</td>
<td>4.25</td>
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<td></td>
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<tr>
<td>HCO(^+)</td>
<td>( J = 1 - 0 )</td>
<td>89.18853(4)</td>
<td>4.28</td>
<td></td>
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<tr>
<td>(formylum)</td>
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<tr>
<td>HNCO</td>
<td>( J = 4_{0,4} - 3_{0,3} )</td>
<td>87.92524(8)</td>
<td>10.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\( \sim 90 \text{ hr in C, D, \& E config.} \)

\( \text{Spec. Res: \sim 0.7 \text{ km s}^{-1} } \)

Transitions and parameters accessible at www.splatalogue.net (Remijan et al. 2007)
Spectra – CH$_3$OH

Relatively consistent enhancement toward shocks

Primarily produced by grain liberation

Can compare shock enhancements of other species relative to CH$_3$OH
E/W Differentiation in C2

- Previously reported in literature with for most species (Benedettini et al. 2007)

- W wall = liberation of grain species

- E wall = Destruction of complex species, Core sputtering (SiO)
E/W Differentiation in C2

- Proposed scenario for C2:
  - Western wall is shocking cold, pristine material
  - CH$_3$OH, HNCO liberated off grains
  - Eastern wall is interacting with pre-shocked material within C1
  - HCN, HCO$^+$ produced from destruction of complex species in gas-phase
  - SiO enhanced as bare grains shocked
B2 Enhancement

- Enhancements observed for HCN, CH$_3$OH, and HNCO toward B2
- Largest HNCO enhancement in galaxy (Rodríguez-Fernández et al. 2010; Mendoza et al. 2014)
- B2 = older  ➔ time-sensitive tracer?
- post-shock, gas-phase reactions
- Chemistry from enhanced O$_2$ from ice (Bergin et al. 1998; Gusdorf et al. 2008)

- HNCO, proposed dominant pathways:
  a) initial grain erosion, then
  b) high-temp gas phase rxs
  CN + O$_2$/H$_2$O ➔ ...OCN... ➔ HNCO (Rodríguez-Fernández et al. 2010)
Maps

- Global CH$_3$OH enhancement
- E/W Chemical Differentiation
- Enhancement of HNCO in B2
Spectra

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### Derived N & N/N$_{H_2}$ for CH$_3$OH, HCN, HNCO with RADEX
(Van der Tak et al. 2007)

- Physical constraints from CH$_3$OH CSO observations (McGuire et al. 2015)
- Compared enhancement relative to CH$_3$OH and H$_2$
- HCN, strong enhancement in East C2 and B2b
- HNCO displays strongest enhancements in galaxy in B2
-15 -> -4 km s\(^{-1}\) wings of HCN, HCO\(^+\) exclusively on East C2

Also, ~4 km s\(^{-1}\) wing seen for CH\(_3\)OH, HNCO on West C2

Supports E/W differentiation scenario

Pre-shocked material -> Less drag on shock
HCN 4\textsuperscript{th} Feature

- 4\textsuperscript{th} feature seen in HCN spectra
- Possibilities:
  - Velocity shifted component?
  - Hyperfine line ratios
  - Different species?
  - None as strong as HCN (1-0)
  - Self-absorption?
  - Significant underestimation of shock enhancements
HCN 4th Feature

- 4th feature
- Possibilities
  - Velocity
  - Hyperfine line ratios
  - Different species?
  - Self-absorption?
  - Significant underestimation of shock enhancements

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