From Molecules to Dust (and back)

Jan Cami

Image Credit: Rogelio Bernal Andreo
Important chemically (molecules $\Leftrightarrow$ dust).

Tremendous potential diagnostic value (figure out the physical conditions).

Pathways to dust often go through molecules.

Like dust, complicated interplay between physics and chemistry.

→ Better understanding of life cycle of molecular gas will lead to improved understanding of life cycle of dust.
Chemistry is just like cooking (but don’t lick the spoon).
High mass loss rates: Silicates

Dust Diversity: \(\rightarrow\) physical conditions and/or chemical inventory must be sufficiently different to change the outcome of the dust formation process (but molecular inventory very similar).

Low mass-loss rates: Oxides
How do the species form & evolve, are they linked? Matsuura et al. (2007; 2014), Sloan et al. (2014), Bernard-Salas et al. (2012)

What's their dust composition and production over cosmic time?

What is the origin of this diversity?

We don’t really understand the carbon chemistry leading to large aromatics and carbonaceous dust in evolved star environments.
Wavelengths, widths & relative strengths match measured (lab) values.

Buckyballs In A Young Planetary Nebula
NASA / JPL-Caltech / J. Cami (Univ. of Western Ontario/SETI Institute)

Spitzer Space Telescope • IRS
ssc2010-06a

Cami et al. (2010)
The discovery of $C_{60}$ and $C_{70}$

Graphite vaporization.

Survival of the fittest discovery of $C_{60}$ and $C_{70}$.

Widespread and abundant in space?

Time of flight mass spectra.

High He pressure

Low He pressure

Graphite vaporization.
Kinetic, bottom-up, C-rich

$T \lesssim 1,700 \, K$

PAHs

Very H-poor
(Wang et al., 1995)

$T \gtrsim 3,000 \, K$

C$_{60}$

Closed Network Growth (CNG)
(Dunk et al. 2012, 2013)

(Jäger et al., 2009)
**C_{60} to carbon dust.**

Dunk et al., 2013, PNAS.
Metallofullerenes: form as easily as fullerenes in “dirty” atmospheres.

Source of anomalous $^{22}\text{Ne}$ in meteorites, originating from SN?
11 Galactic C\textsubscript{60}-PNe:

- No (or very weak) PAHs.
- 6—9 μm plateau.
- 11—13 μm plateau. SiC?
- Strong 30 μm feature.

Strength of C\textsubscript{60} bands relative to continuum is variable.

*Conditions that favor fullerene formation or survival also result in other dust components!*

Otsuka et al., 2014
Tc1: Lord of the Fullering

PAHs?
Red: Dust Continuum
Green: Fullerenes
Blue: Ionized Gas
PAHs $\rightarrow$ Fullerenes?

Berné & Tielens (2011)
Meanwhile at the lab (II)

266 nm

Zhen et al (2014)
**Kinetic, bottom-up, C-rich**

\[ T \lesssim 1,700 \, K \]

PAHs

**Very H-poor**

(Wang et al., 1995)

\[ T \gtrsim 3,000 \, K \]

C\(_{60}\)

**Photochemistry, top-down**

PAHs

\[ T \gtrsim 3,000 \, K \]

Closed Network Growth (CNG)

(Dunk et al., 2012, 2013)

Zhen et al., 2015

C\(_{60}\)
Fullerenes appear in low-excitation (low-T$_{\text{eff}}$) objects.

Fullerene and Mixed
Big-11

PNe with normal PAHs

PNe with no dust features

Sloan et al. (2014)
Fullerenes’ true colors

Sloan et al. (2014)
Kinetic, bottom-up, C-rich

$T \leq 1,700 \text{ K}$

(Jäger et al., 2009)

Very H-poor

(Wang et al., 1995)

Photochemistry, top-down

Carbon Dust or PAHs, XL

$T \geq 3,000 \text{ K}$

(Zhen et al., 2015)

$C_{60}$

$C_{60}$

PAHs

Closed Network Growth (CNG) (Dunk et al. 2012, 2013)
Start with material that is C-rich and either H-poor, or hotter than usual for some reason (unusual evolutionary status?)

- Condensation: fullerenic dust.
- Onset of PN phase: much of the dust is destroyed (Radiation? Shocks?), but fullerenes survive.
- Special geometry: does the torus play a role?

If dust destruction is key, this is relevant to ISM as well!
Hundreds of interstellar absorption features, from near-UV to near-IR. Some very strong, most are rather weak. Some broad, most are fairly narrow.
1919: Mary Lea Heger detects first 2 DIBs; their carrier unidentified.
2018: Many hundreds of unidentified DIB carriers.
DIB carriers are stable, widespread

DIBs in Antennae Galaxy
Monreal-Ibero et al., 2018
DIB carriers are stable, widespread and abundant \( \rightarrow \) carbonaceous carriers that lock up \( \sim 0.5\% \) of the cosmic carbon.
Profiles point to molecular carriers.
Ro-vibrational lines: Peak separation scales with BT

\[ \Rightarrow 8\text{–}15 \text{ C atom molecule.} \]

Line Profile Variations of 6614 DIB Cami et al., 2004
DIB behavior points to family of DIB carriers (one DIB, one carrier).

Distance Indicator Bands

Friedman et al., 2010
Jan Cami

Molecules to dust

Carbon Chains
...and their cousins

PAHs
...and their cousins

Fullerenes
...and their cousins
Laboratory confirmation of $C_{60}^+$ as DIB carriers
Campbell et al., 2015
The DIBs point to a voluminous chapter of interstellar physics and chemistry that we have yet to discover and understand.

- What are the DIB carriers?
- How are these species formed, excited, destroyed?
- What can these features tell us about the physical conditions of the environments in which they reside, and what about the chemical evolution of the ISM?
DIBs and their tool potential

A Principal Component Analysis of the DIBs
Ensor et al., 2017

Single-cloud sightlines
Medium / strong DIBs require:

- High Abundance and/or
- Small(er) size and/or
- Large Oscillator strength: can we find species (or mechanisms) with much stronger transitions?
M-C_{60} complexes

C_{60}  Na^+
DIBs ...due to charge transfer bands of $C_{60} \cdot M^+$?

(Kroto and Jura 1992)
We can turn the DIBs into powerful probes of physical conditions in the Universe near and far even without knowing the identity of their carriers!

- Carry out a **sensitive** and **systematic** study of the DIBs in order to:
  - Characterize the observational properties of a large number of DIBs in great detail.
  - Establish **quantitative** relationships between the DIB properties and other line of sight parameters.
  - Map in detail how the DIBs depend on environmental parameters – both physical and chemical.
The ESO Diffuse Interstellar Band Large Exploration Survey (EDIBLES)


Image Credit: Miguel Claro
EDIBLES is a Large Program on VLT/UVES (P.I. N.L.J. Cox; Acting P.I. J. Cami)

- 286 h; ~80% complete to date
- 114 targets (mostly O and B stars) with wide range in interstellar parameters (dust & gas).
- Large spectral range: 304.2 nm – 1042.0 nm; allows to include many known atomic and molecular lines.
- Sensitive: S/N ~1000 per target in the red.
- Detailed: Resolving power R~80,000 across range.
EDIBLES target distribution

Range in $E(B-V)$, $A_V$, $R_V$, $N(H)$, $f_{H_2}$, elemental depletion

Fig. 1. Galactic distribution of EDIBLES targets. The symbol size reflects the value of $R_V$, while the interior colour represents the line-of-sight reddening, $E(B-V)$. Symbols with green edges represent the observed targets, while blue edges correspond to the targets to be observed by the end of the programme.
Access to diagnostic lines that could yield important clues. Example: \( \text{OH}^+ \rightarrow \) cosmic ray ionization rate from ground-based observations!

Cosmic ray ionization rate from \( \text{OH}^+ \)

Bacalla et al., under review.
All (weak) $C_2$-DIBs show substructure in their profiles!

→ Size distribution of DIB carriers.

C$_2$-DIBs and their profiles
Elyajouri et al., in press
Supporting the identification of the $C_{60}^+$ DIBs

The profiles of the $C_{60}^+$ -DIBs. Lallement et al., in prep.
- Cosmic Fullerenes may form from bottom-up dust formation followed by dust destruction – but the fullerenes survive.
- Top-down processes are important to include in astrochemistry.
- DIBs can reveal much about interplay between atomic gas, (large) molecules and dust in the ISM. Identification not required – stay tuned!