Astrochemistry and Spectroscopy using SOFIA

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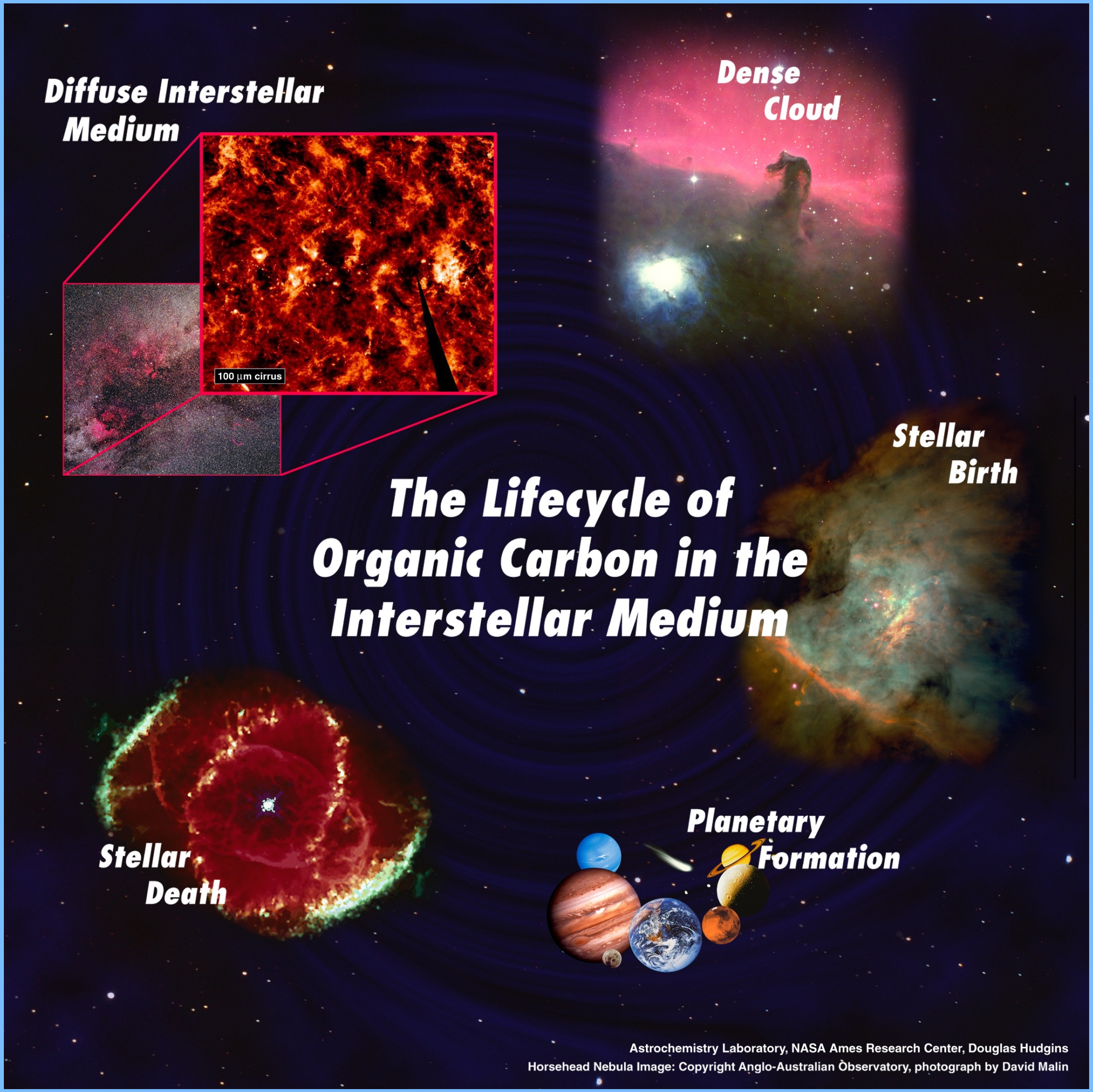
Astrochemistry - A middling difficult enterprise

"Physicists love the early universe -- because it is EASY. You've got protons, electrons, light, and that's it. Once atoms come together, you get chemistry, then biology, then economics… it pretty much goes to hell."

-Andrew Lange (5/3/2000)

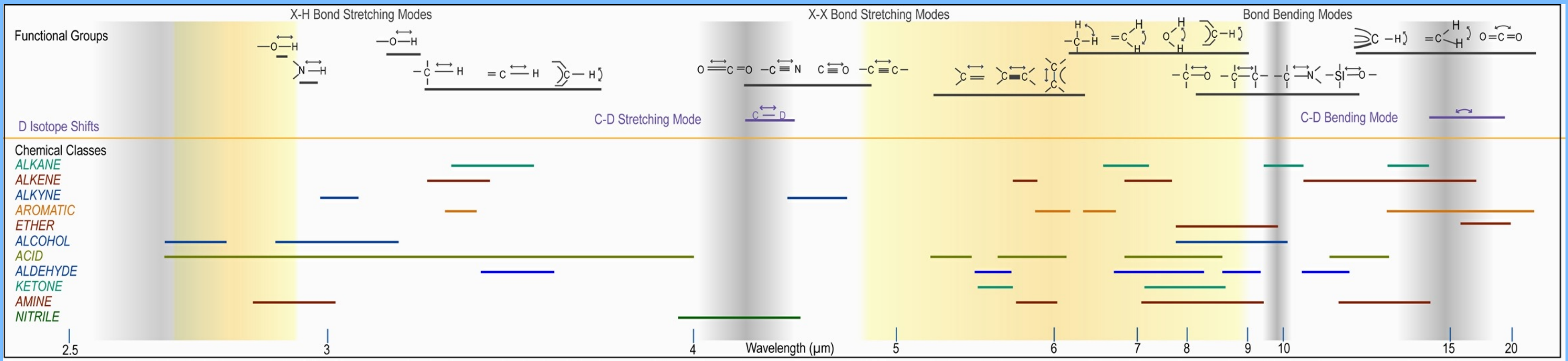
Galaxies are not static - materials in them cycle between a number of different environments which can create new chemical compounds, and destroy or modify old ones

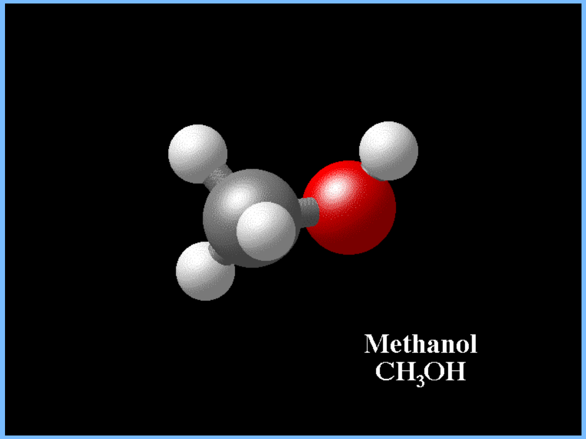


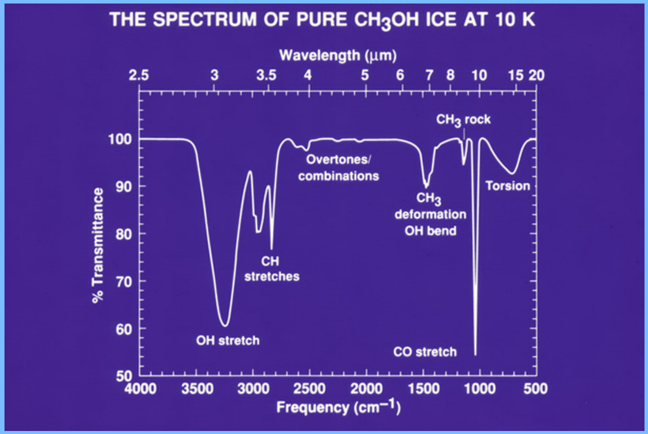
Organic compounds are particularly interesting because they:

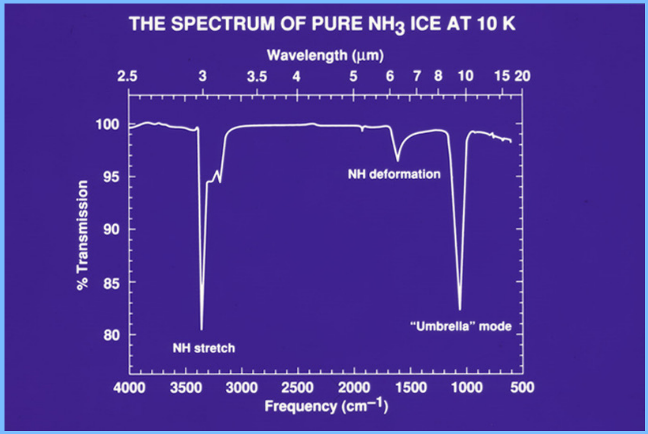
- Are abundant in space
- Are seen in a wide variety of astrophysical environments
- Show variations that provide insights into astronomical processes
- They provide a direct link between presolar and solar system materials
- Their delivery may have played an important role in the origin of life on Earth and elsewhere

IR spectroscopy, particularly in the 2-40 µm range, provides an ideal way to detect and identify many molecular species since different molecules have different IR spectral "fingerprints"

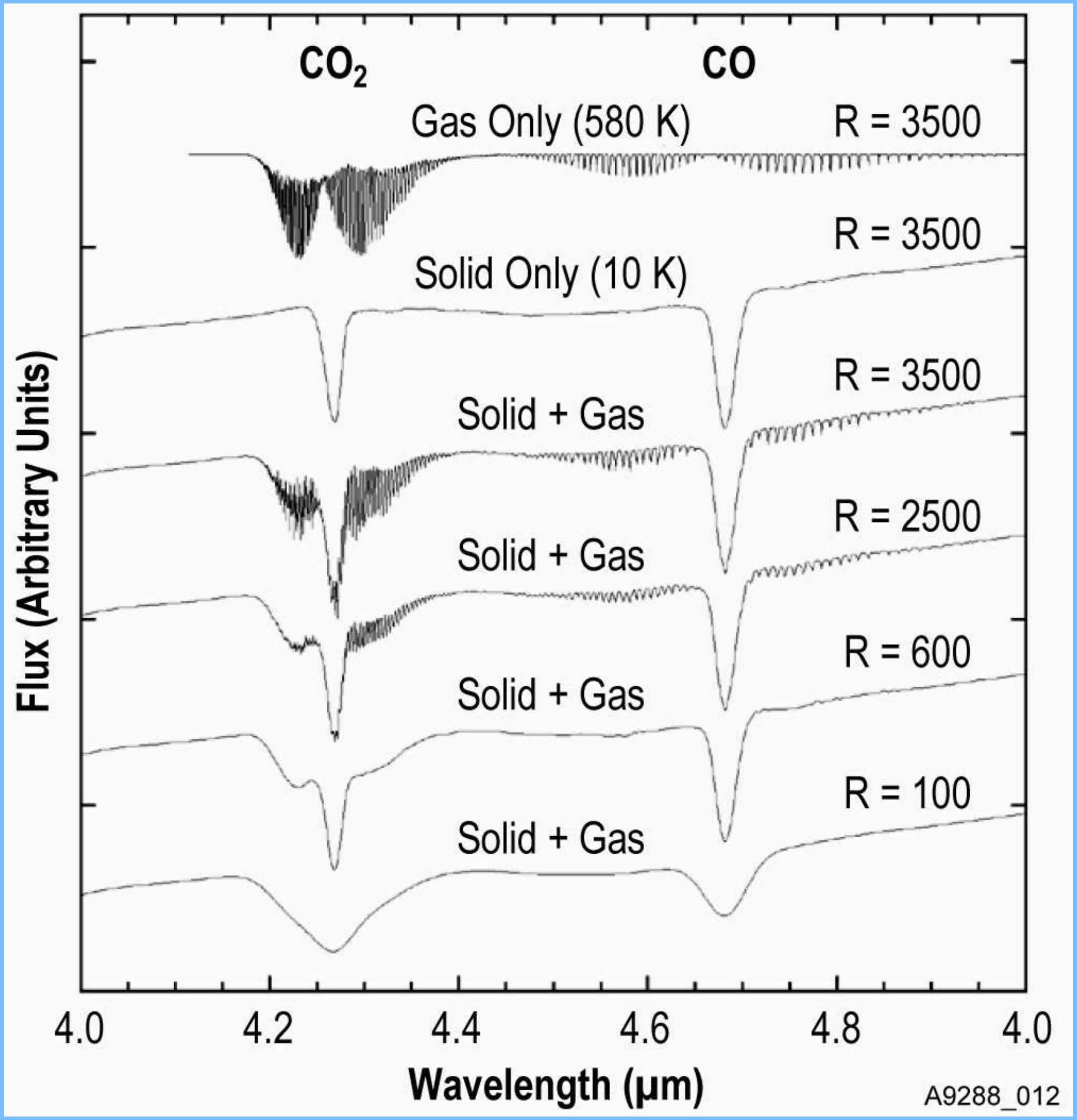




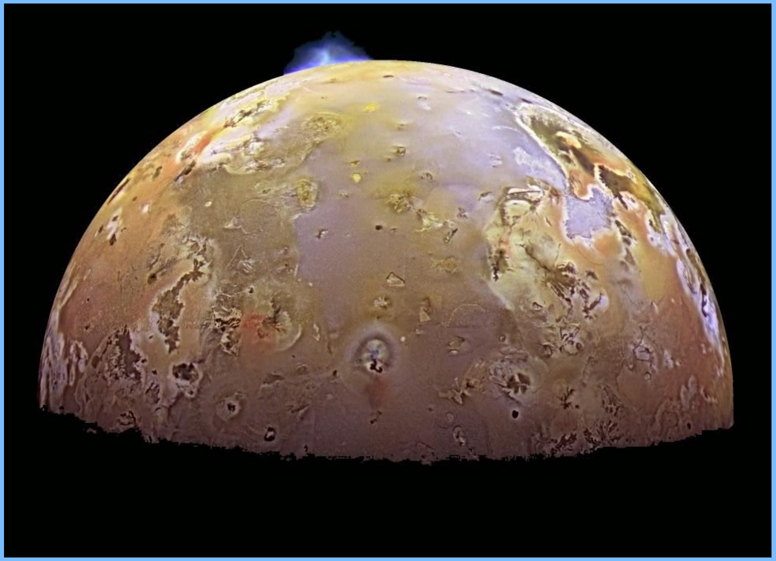


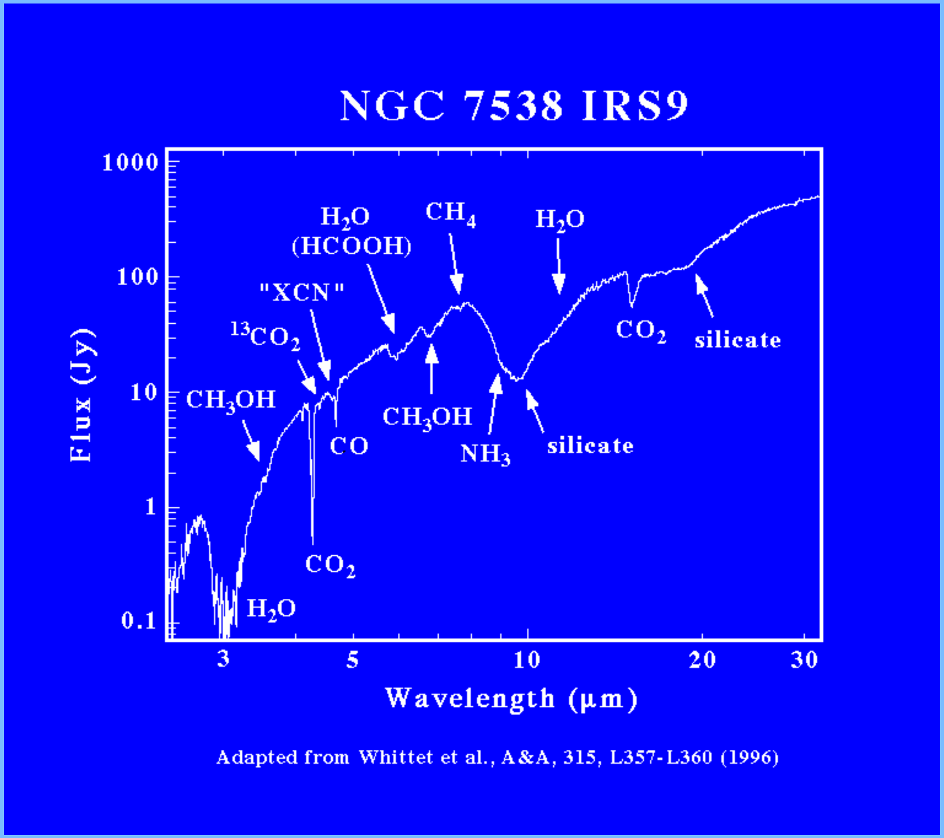


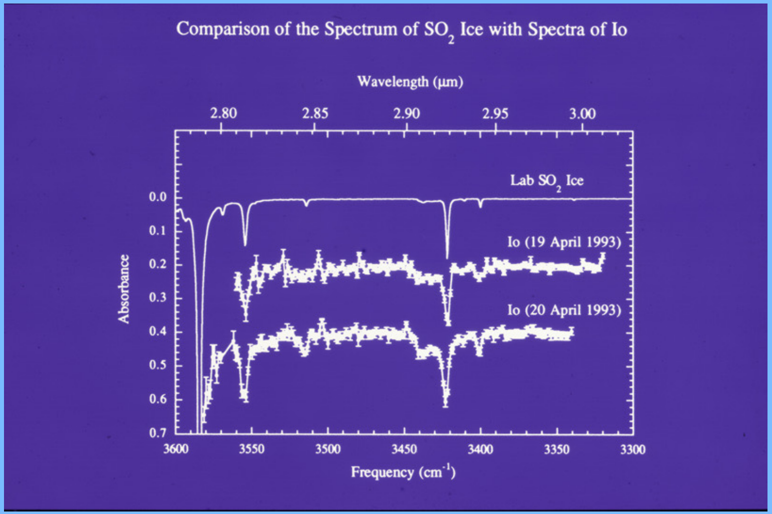
Armed with the appropriate spectral resolutions, one can also distinguish between solids and gases



Comparisons of Astronomical Spectra and Laboratory spectra can be used to identify molecules and even constrain their physical states and past histories



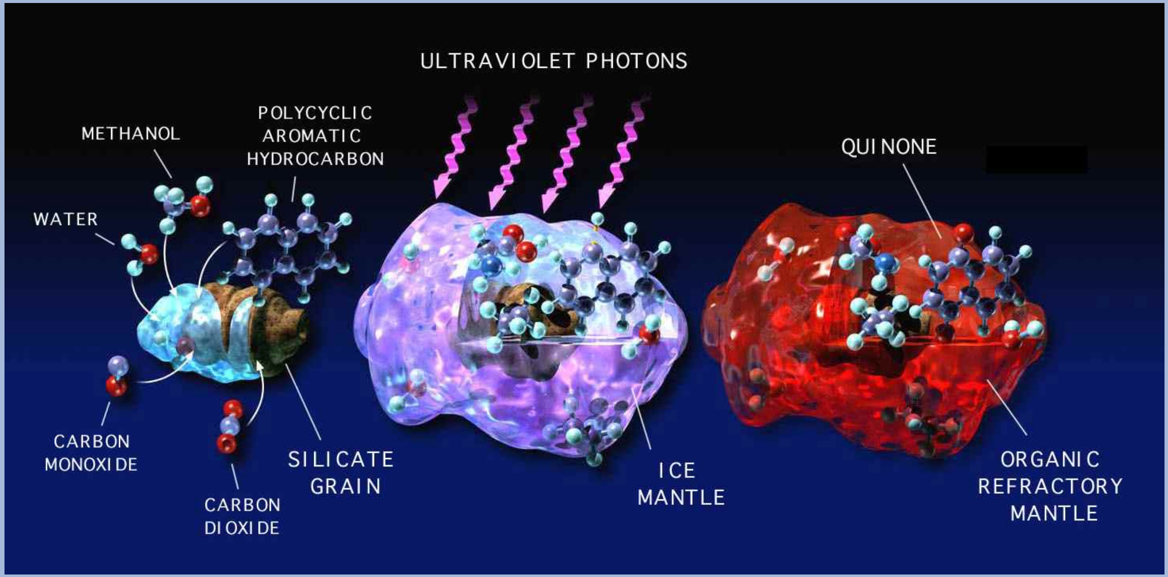




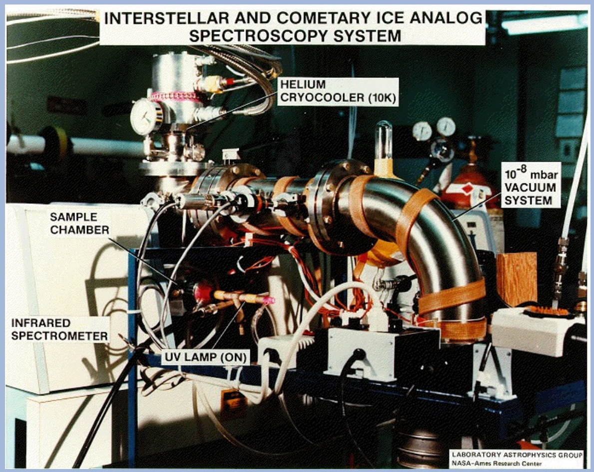
The identification of even simple molecules can have implications that extend well beyond their mere existence. Their presence can:

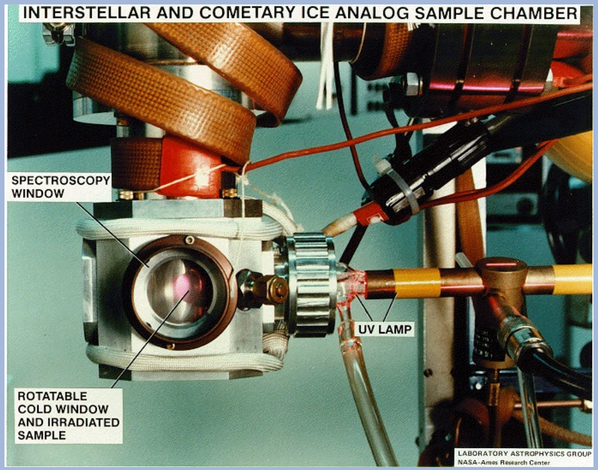
- place constraints on their environment's past history
- place constraints on environmental conditions
- imply the presence of other, low abundance materials

For example, at the low temperatures found in interstellar dense molecular clouds, most molecules are expected to freeze out onto the dust grains. Here, they may be exposed to ionizing radiation in the form of cosmic rays and UV photons, resulting in the production of new molecular compounds.

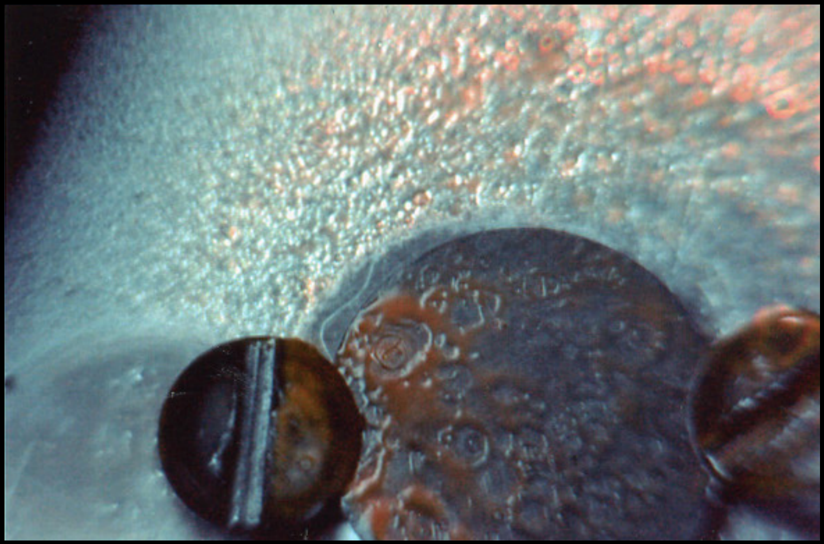


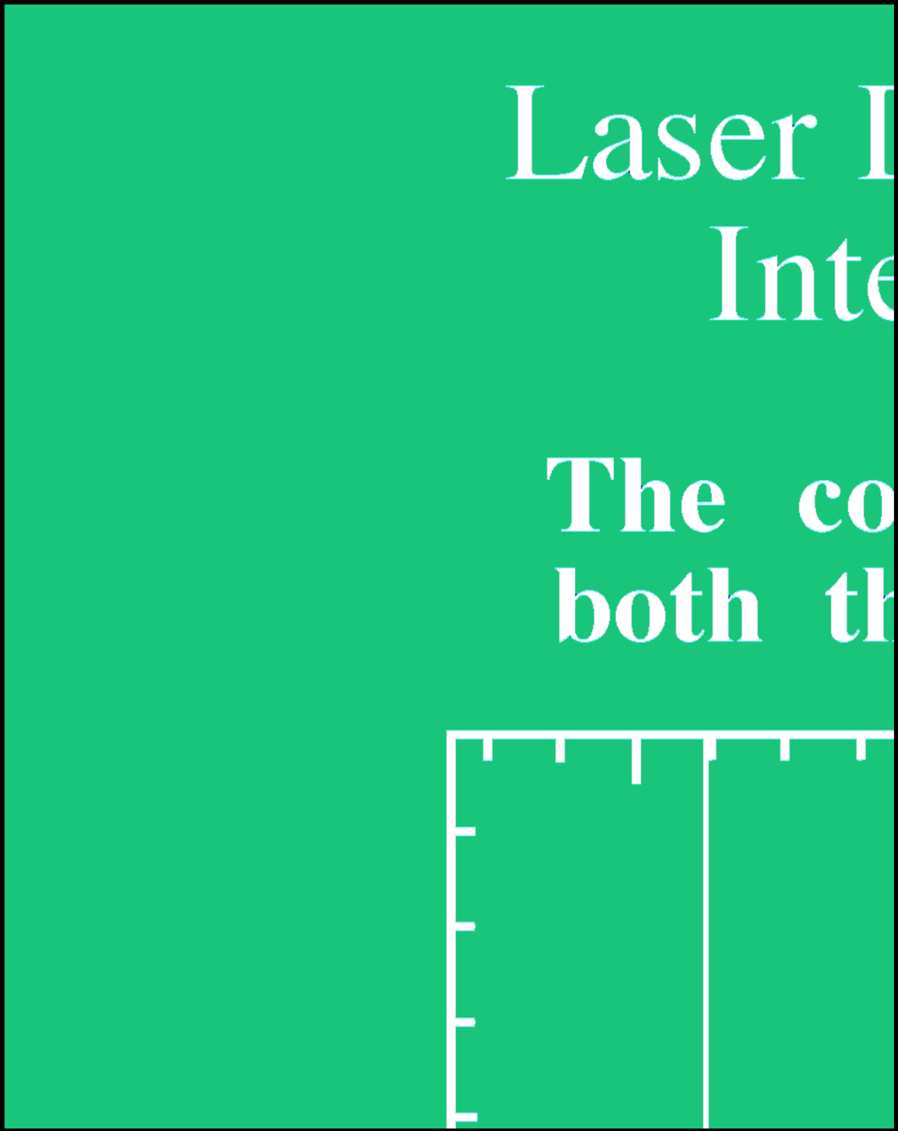
These processes can be simulated in the laboratory under astrophysically-relevant conditions using realistic ice analogs





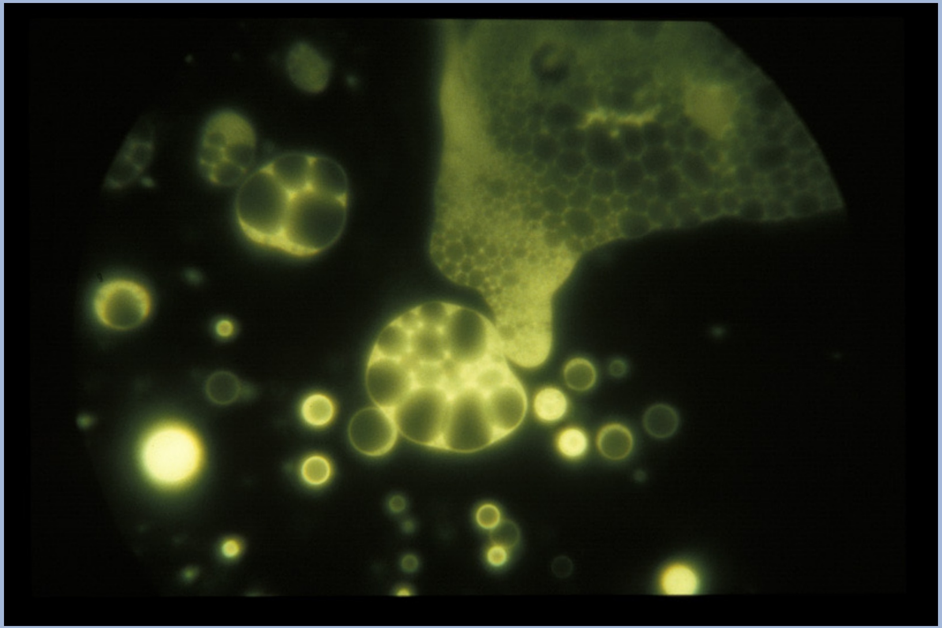
The irradiation of even simple ices results in the *robust* production of complex organic materials





Products of this sort of processing include:

- Species of astrobiological importance
  - Amino acids & related compounds
  - Amphiphiles
- Species seen in meteorites

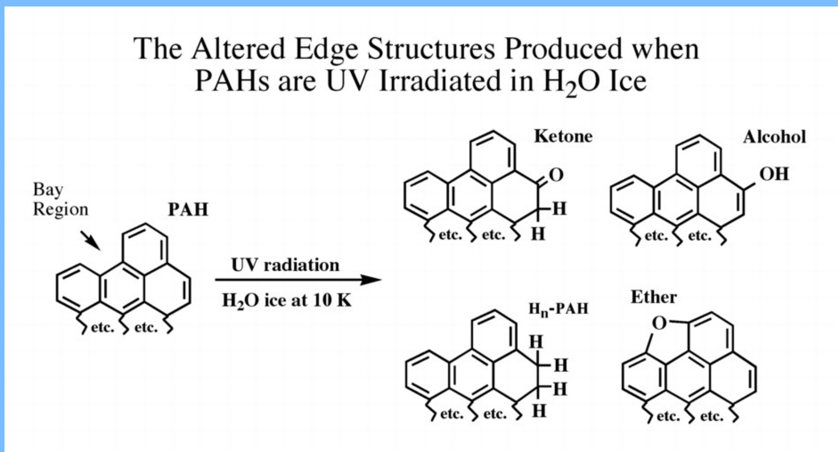


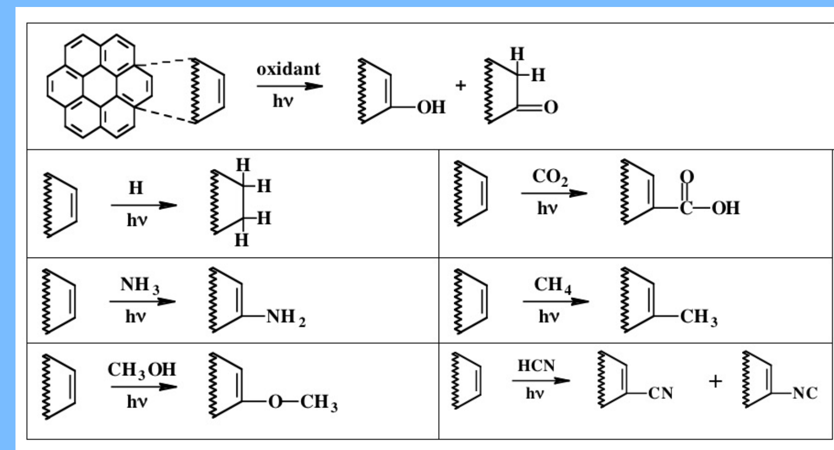
Ice composition:
$H_2O:CH_3OH:HCN:NH_3 = 20:2:1:1$

If aromatic molecules are present in the ices, you can also make:

- Quinones
- Nucleobases

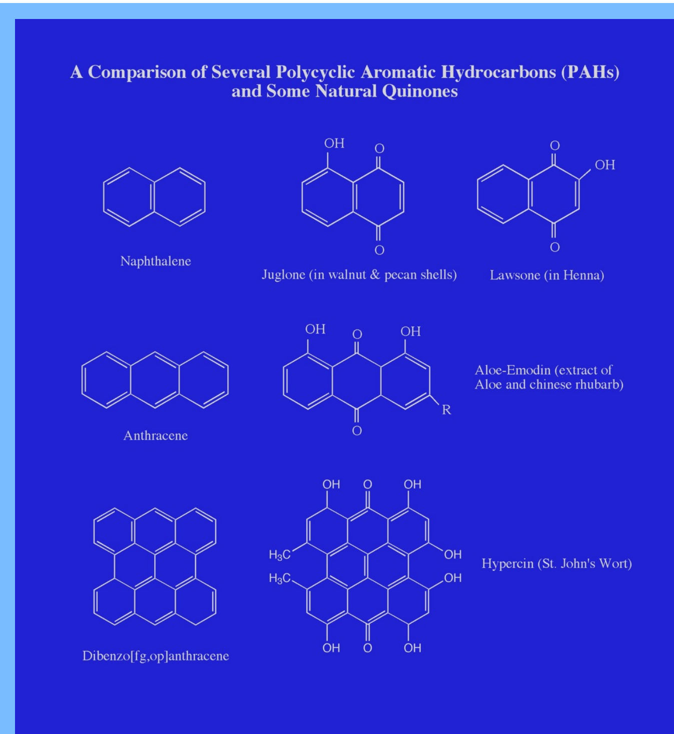
PAHs irradiated in H_2O-rich ices show various forms of O and H addition. PAHs irradiated in more complex ices add all kinds of functional groups to the main PAH structure.





Aromatic Ketones are called *Quinones* and their production has significant astrobiological implications.

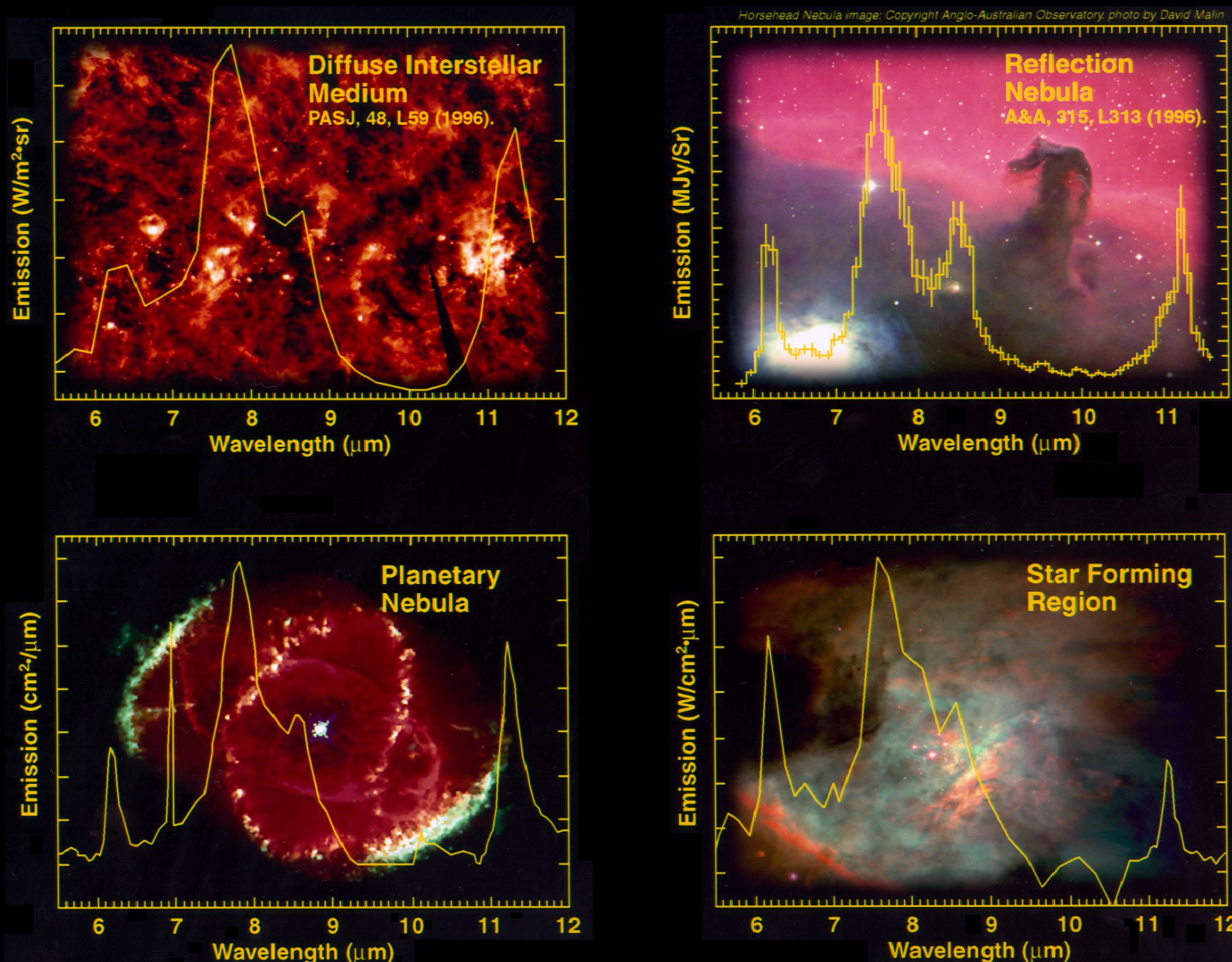
We see this class of compounds facilitating some of the most basic chemical reactions in 'primitive' organisms, implying these molecules are 'ancient'

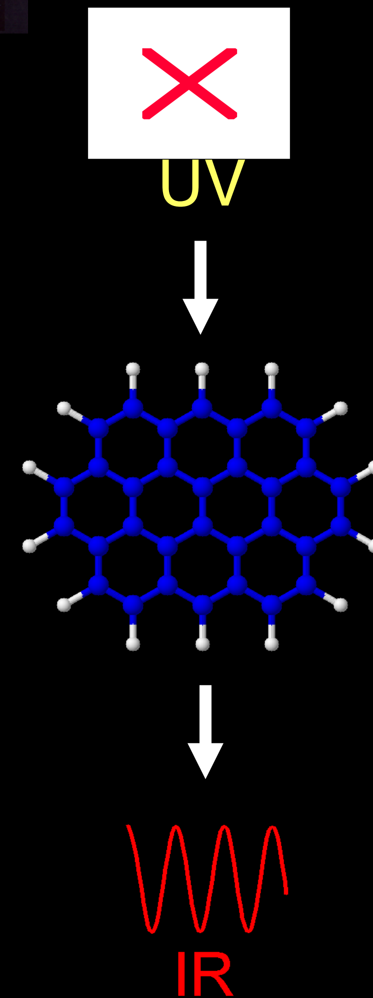


Some examples of SOFIA investigations relevant to astrochemistry involving Polycyclic Aromatic Hydrocarbons (PAHs)

- Variations in PAH emission spectra
- Longer wavelength PAH “drumhead modes”
- PAHs and PAH ions in absorption

A host of very different kinds of objects in space show similar infrared emission spectra due to PAHs and related materials

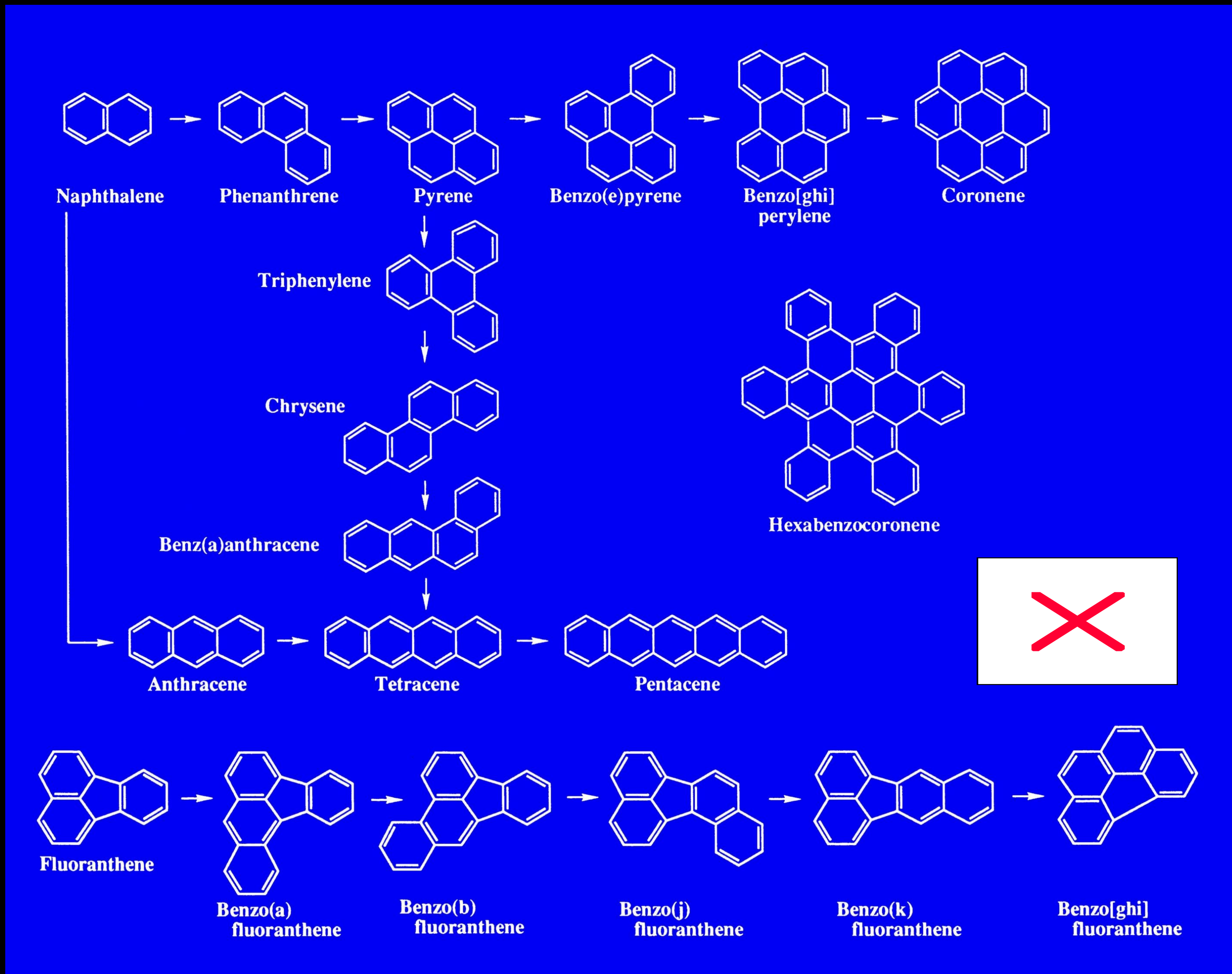




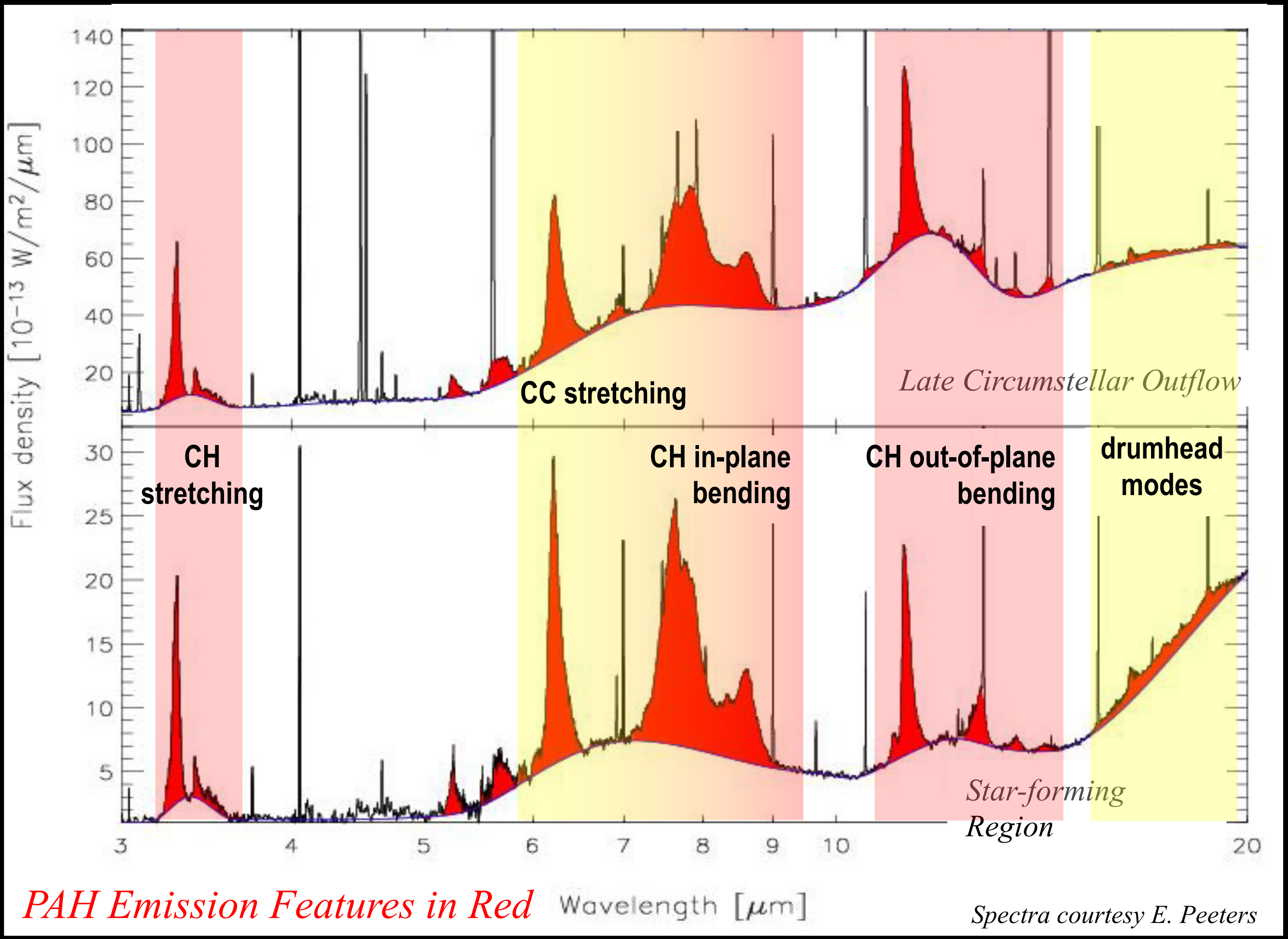
CC_{str}

CH_{ip}

Emission spectra can vary because different regions can have different populations of PAHs, different excitation conditions, and PAHs in different charge states



The interstellar emission spectra represent the composite emission of a complex mixture of aromatic compounds.
The features are not resolvable, but show subtle variations.



Much of the next generation science in this area will require high S/N data to detect and interpret these small variations

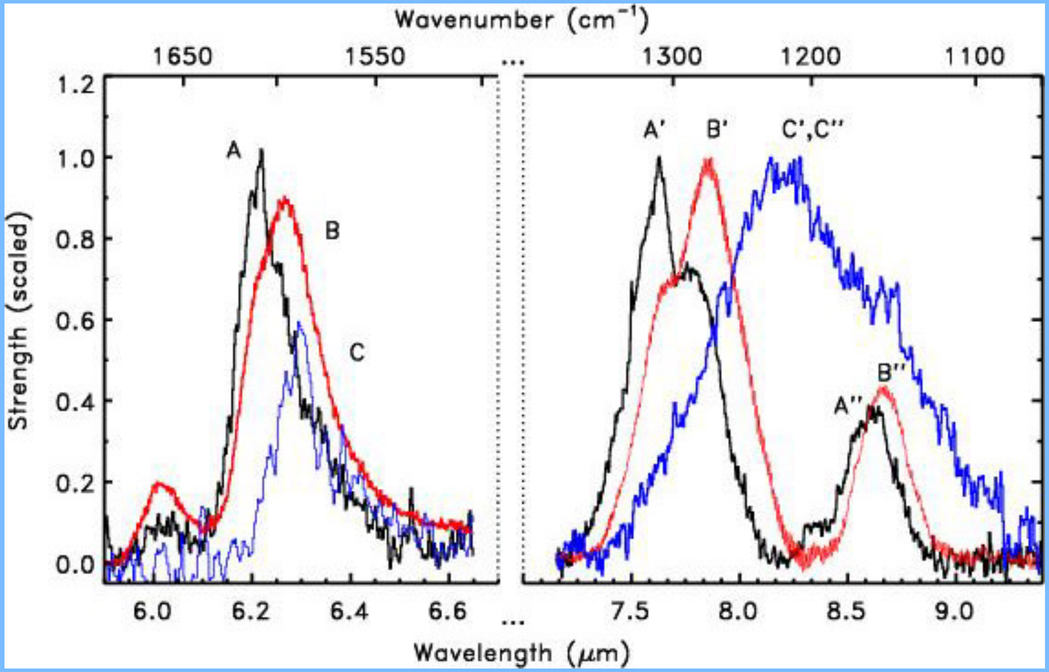
"Endoskeletal" Polycyclic Aromatic Nitrogen Heterocycles (PANHs) provide an example of how small variations can help us constrain the PAH population

N substitution within the carbon skeleton of a PAH produces a depth-dependant blue shift in the position of the dominant CC stretching feature near 6.2 μm.

Hudgins, IAU Symposium 231, 9/2005

Based on an analysis of ISO/SWS data, Peeters et al. found:

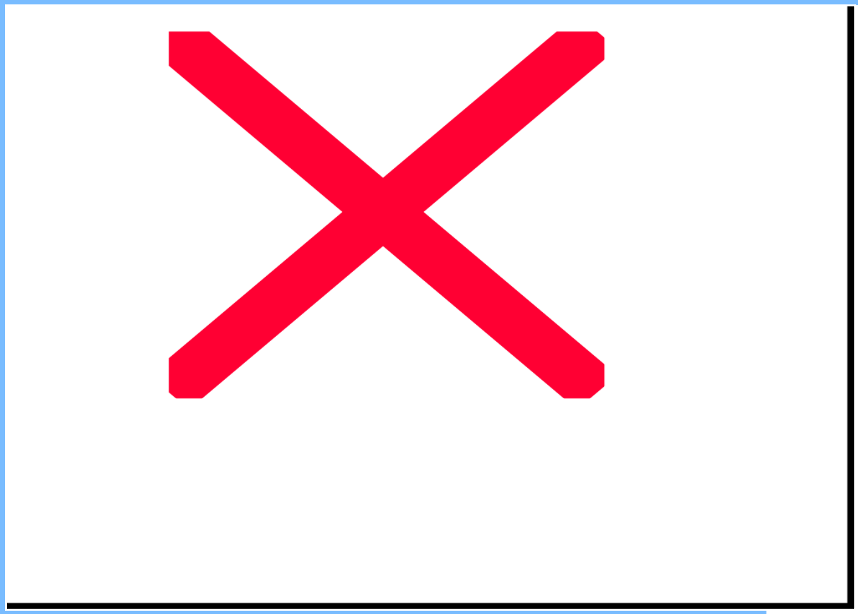
- Bands in the 6.2 µm region are variable
- The “6.2” µm band is a composite of 2 bands
- 6.2 µm band variations correlate with those of the 7.7/8.6 µm bands

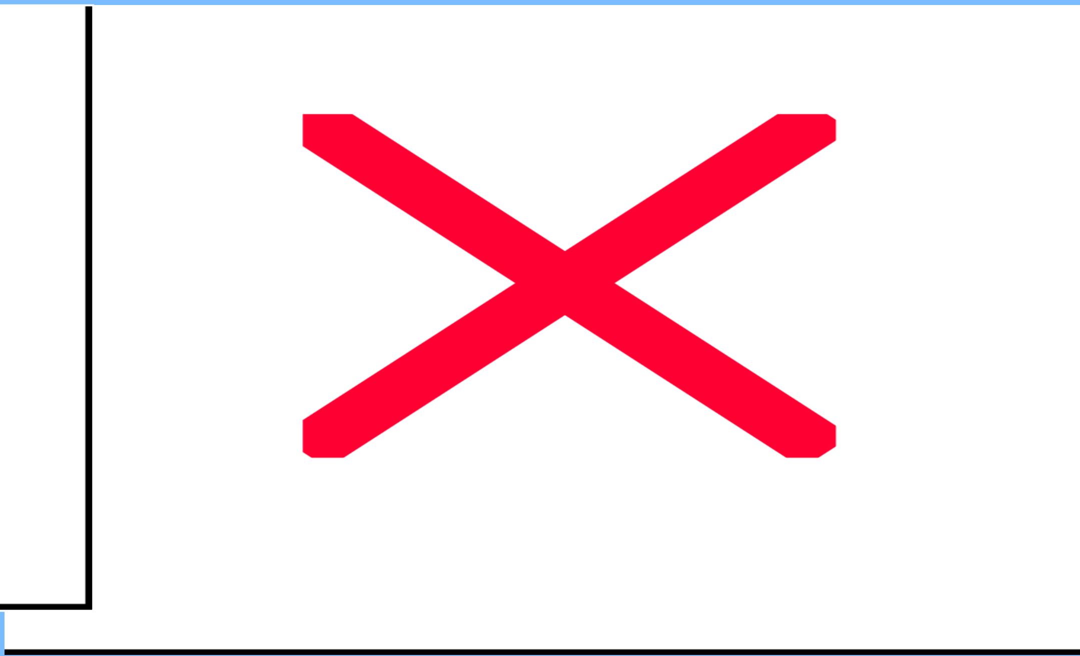


Peeters et al., A&A, 390, 1089 (2002)

- **To date, Endoskeletal PANH cations are the only PAH-related species known that can reproduce the position of the interstellar 6.2 µm emission band.**
- **The shift from 6.2 to 6.3 µm in going from circumstellar ejecta to the interstellar medium suggests that large, compact, nitrogen-containing PAHs evolve into open and uneven structures as they are ‘aged’ in the ISM**

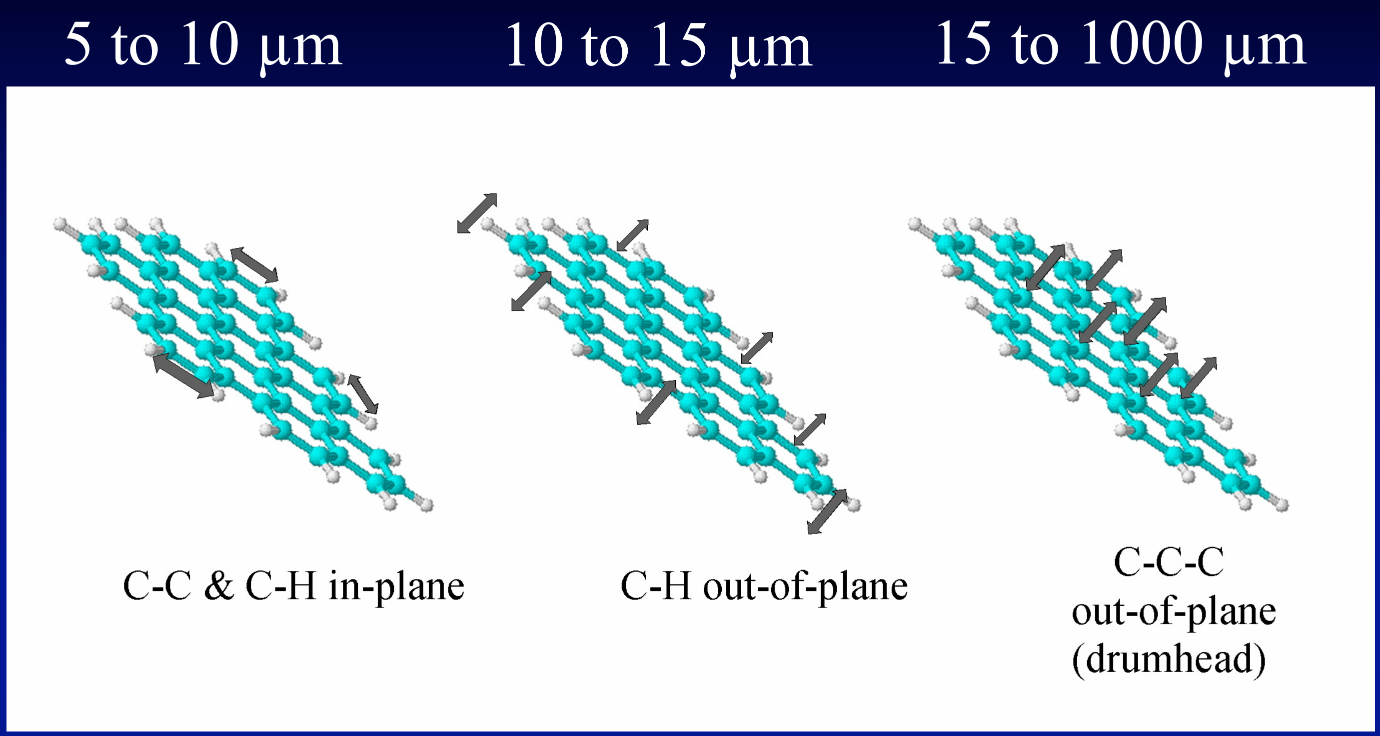
The ultimate goal is to be able to obtain astronomical spectra that show these subtle variations, use extensive laboratory databases to determine the composition of the PAH population present, and use this as a tool to constrain environmental history and conditions.





(These fits are circa 1996-1998. Expanding laboratory databases and new software tools are becoming available that will soon make these sorts of matches look a little ‘shabby.’)

PAH "Drumhead" Vibrations



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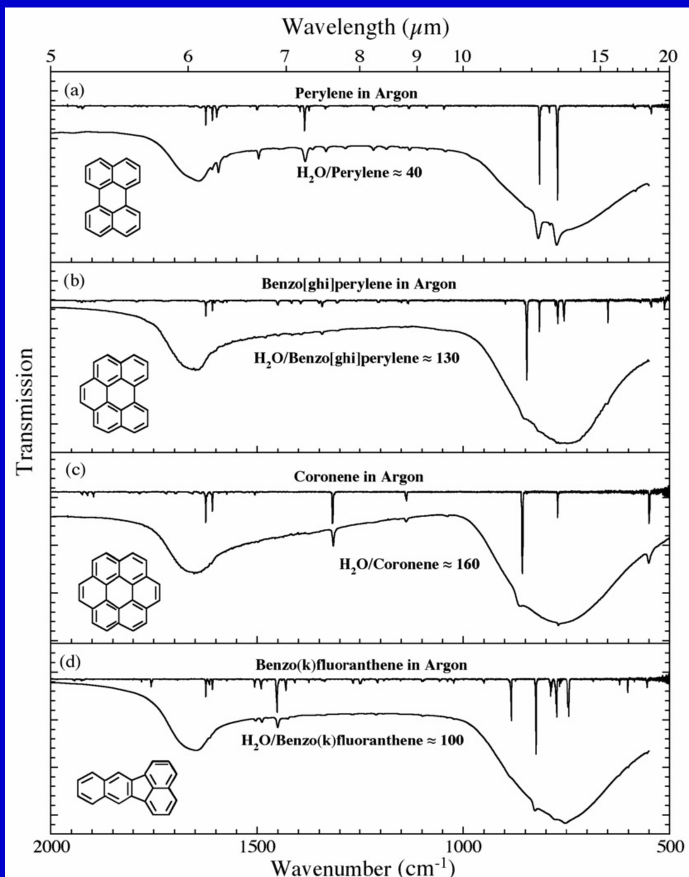
- These vibrations fall in the far-IR.
- They are a direct function of PAH size and shape.
- They are unique and will allow the identification of specific PAHs.
- They are wholly unexplored and should be particularly important in regions with low energy radiation fields where the fluorescent PAH emission process overwhelms thermal emission. SOFIA and Herschel should pioneer observations in this region.

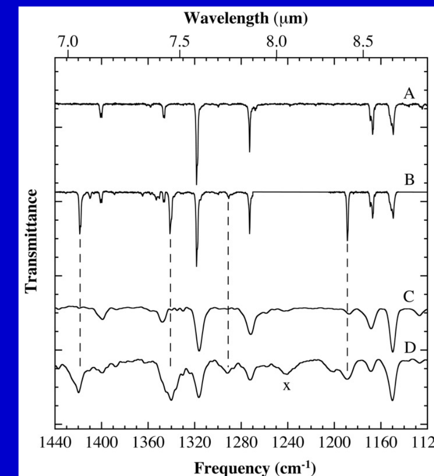
The spectra of PAHs and PAH ions in absorption

PAHs are most easily seen in emission in the gas phase. However, they should also be weakly detectible in absorption in the solid phase, for example, in dense clouds where these molecules should freeze onto grain mantles.

PAHs ionize easily in ices and they are highly reactive. This drives additional ice phase chemistry.

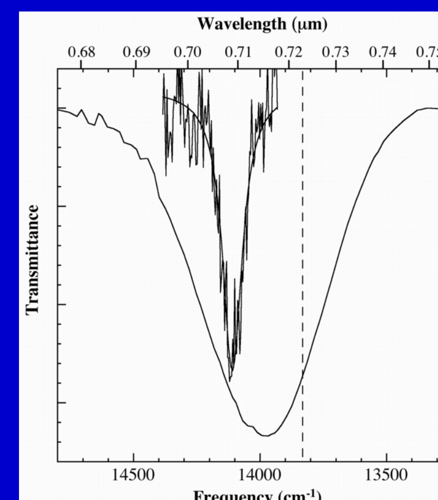


Neutral PAHs produce weak absorption bands in ices and other solids in the same spectral regions where emission bands are seen.



Ionized PAHs produce absorption bands in ices in the mid-IR and can produce strong absorption bands in the near-IR.

This particular example is the PAH anthracene.



Conclusions

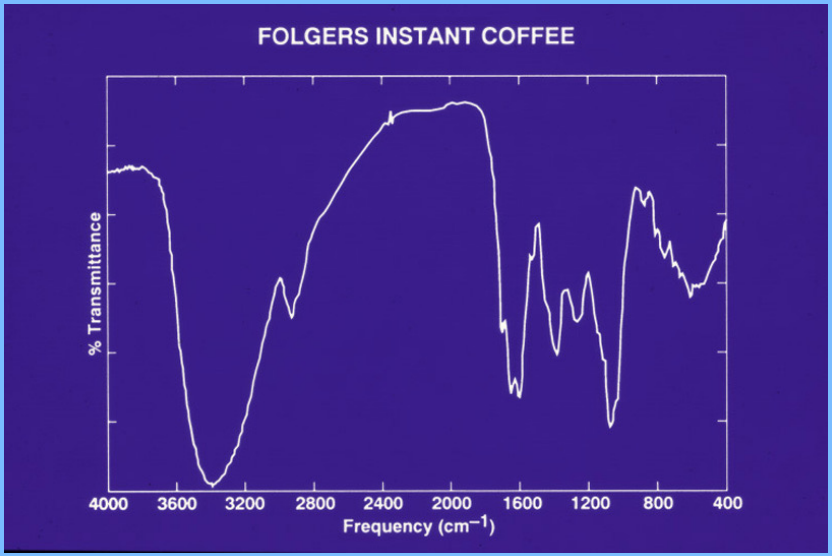
- SOFIA will be able to obtain IR spectra at wavelengths and resolutions that are ideal for pursuing investigations associated with understanding astrochemistry in a wide variety of astrophysical environments.

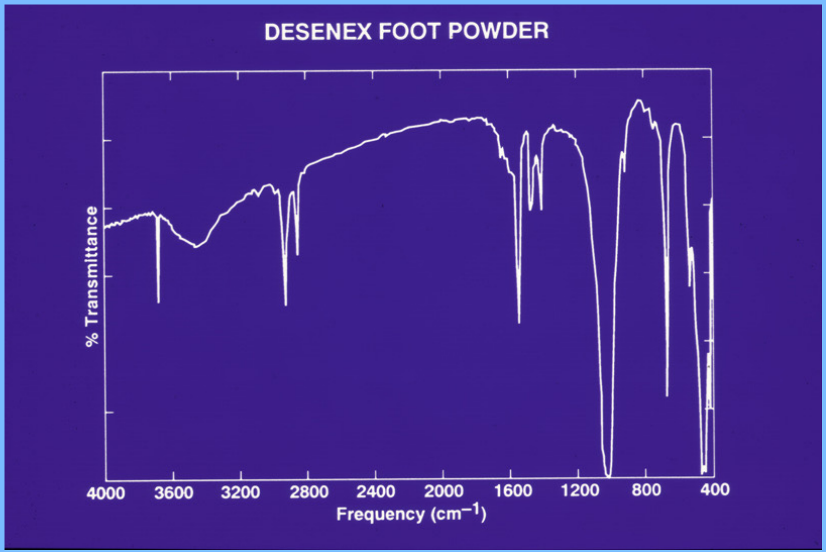
- Results from such investigations will have implications for astrophysics, astrochemistry, and astrobiology.

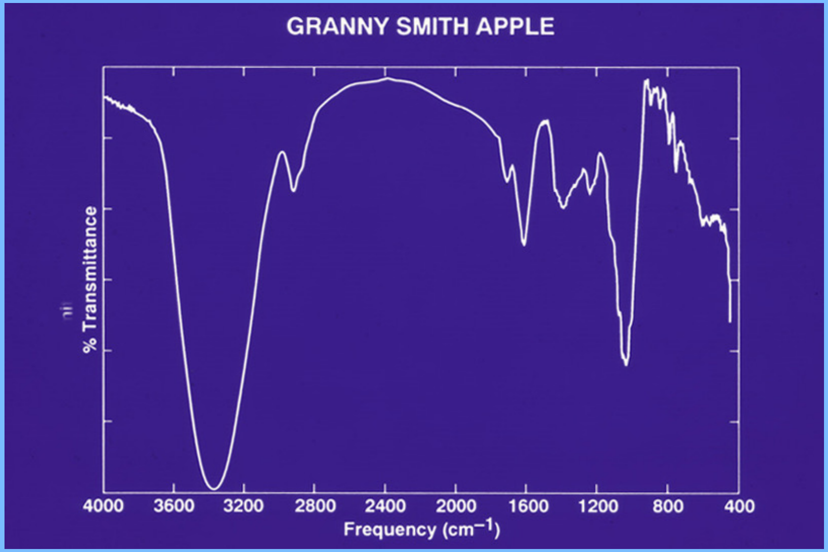
You will certainly be able to count on members of the Ames Astrochemistry Laboratory applying for time on SOFIA to pursue a host of scientific programs!

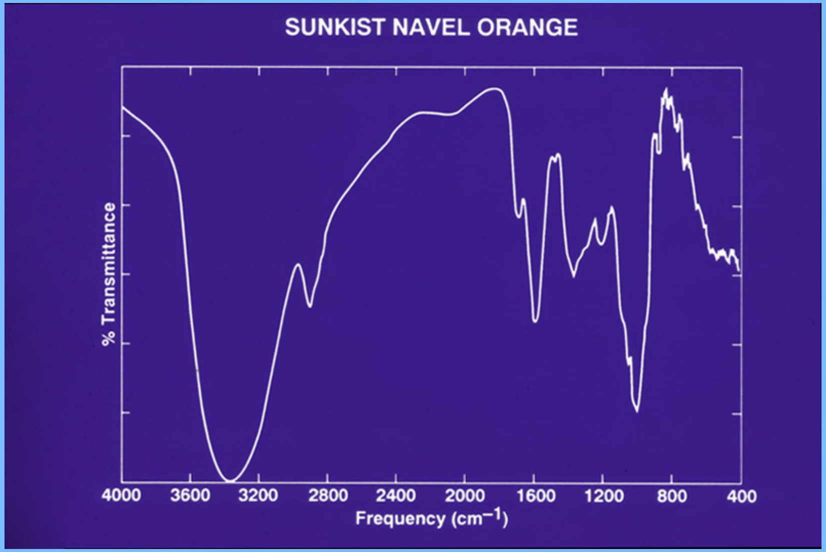
Backup Slides

Most materials show infrared features









Comparing Apples and Oranges!