CRLS Astrophysics Lecture Series: Molecules in Space

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Week 1: Introduction to Astrochemistry

Goals

Next week, we will explore how astronomers detect and characterize molecules in space. You will even get a chance to identify and 'discover' new molecules for yourselves. To get prepared, this week we will first learn about the fundamentals of chemistry in space. We will then learn about the abundance of molecular species that have been discovered so far as well as the methods and telescopes astronomers use to make these exciting discoveries. Finally, we will learn how the identification of biologically-important molecules is informing our understanding of the origins of life and the potential for discovering alien life.

Outline

The following sections outline some questions to guide your exploration of the listed resources. Please take note of any questions that arise and we can discuss them next week. If you are especially interested in any of these topics, additional reading materials are suggested below.

1. **Molecules in Space:**
   Guiding questions: How many molecules have been detected in space so far? Where are they typically found? Are smaller or larger molecules more likely to be observed? Have there been any extragalactic - outside of the Milky Way - molecular detections?

   Important Terms:
   `1) ISM`: The Interstellar Medium, which is the gas and dust that is located between stars.
   `2) IR`: Infrared, longer wavelengths than those of visible light and is invisible to the human eye; most thermal radiation emitted by objects near room temperature is infrared.
   `3) Isotopologue`: Molecules differing in isotopic composition, e.g. ^{13}CO instead of ^{12}CO.

   Resources:
   "Molecules in Space" – A clickable database from the University of Cologne with all molecules so far identified. https://www.astro.uni-koeln.de/cdms/molecules
   "Interstellar and Circumstellar Molecules" – Up-to-date historical overview of important molecular discoveries. http://www.astrochymist.org/astrochymist_ism.html
   "The Interstellar Medium" – A brief introduction to the interstellar medium or ISM. http://www-ssg.sr.unh.edu/ism/what1.html

Want to learn more? – Look through the "Astromolecule of the Month" at http://www.astrochymist.org/AMOTM/ and choose your favorite one. Share a new molecular fact that you learned with each other.

2. **Molecules in Space:**
Guiding questions: What is spectroscopy? In what part(s) of the electromagnetic spectrum are most molecules identified? How do molecules emit radiation? How is this different than electronic transitions? Be able to name three ways that a molecule can emit energy.

Important Terms:
1) `Molecular Cloud:` Interstellar clouds with sufficient density and size to form molecules and stars; mostly comprised of molecular hydrogen (H_2).
2) `Nebula:` An interstellar cloud of dust, hydrogen, helium, and other ionized gases.

Resources:
"The Electromagnetic Spectrum" – A quick introduction to the EM spectrum and spectroscopy. https://chem.libretexts.org/Textbook_Maps/Organic_Chemistry_Textbook_Maps/Map%3A_Organic_Chemistry_with_a_Biological_Emphasis_(Soderberg)/Chapter_04%3A_Structure_Determination_I/4.1%3A_Introduction_to_molecular_spectroscopy
"The Hunt for Alien Molecules" – A nice article about the process of discovering a new molecule. https://www.scientificamerican.com/article/the-hunt-for-alien-molecules/

Want to learn more? – Look over these articles on molecular rotation and vibration: https://en.wikipedia.org/wiki/Rotational_spectroscopy and https://en.wikipedia.org/wiki/Molecular_vibration. Please feel free to ignore the complicated math and just skim these articles. There's certainly no expectation that you have to understand most of the details presented here.

3. **Telescopes, Origins of Life, and Molecules in Exotic Places:**
Guiding questions: What are some of the telescopes primarily used by astronomers for detecting molecular emission? What are prebiotic molecules? How has astrochemistry impacted origins of life studies?

Important Terms:
1) `Supernova:` Star that suddenly increases greatly in brightness because of a catastrophic explosion that ejects most of its mass.
2) `Chirality:` An object or a system that is distinguishable from its mirror image; that is, it cannot be superposed onto it.
3) `Protostar:` Contracting mass of gas that represents an early stage in the formation of a star (before nucleosynthesis has begun).

Resources:
"Radio Telescopes" – A photo gallery of 10 prominent radio telescopes around the world. http://www.kuriositas.com/2012/03/10-spectacular-radio-telescopes-around.html
"NASA's Super 747 SOFIA" – An article about a flying telescope. https://www.cnn.com/travel/article/worlds-biggest-flying-observatory-747-nasa-sofia/index.html
"Heart of an Exploded Star Observed in 3-D" – A 3D reconstruction of molecules around a recent supernova. https://public.nrao.edu/news/2017-alma-dust-sn1987a/
"Astrochemists Detect Chiral Molecules in Interstellar Space for the First Time" – An article about a biologically-important molecule in space. https://www.scientificamerican.com/article/astrochemists-detect-chiral-molecules-in-interstellar-space-for-the-first-time

Want to learn more? If you have extra time / are more ambitious, take a look at a recent CfA colloquium on astrochemistry https://www.youtube.com/watch?v=wGpq-yl5HtU. The video is quite long (1 hr) so feel free to skim it or just watch the first few minutes.

Week 2: Exploring Molecular Spectra and Detecting your own Molecules

Goals

Last week, we learned what molecules have been detected in space and what techniques astronomers use to make these discoveries. This week, you will get a chance to discover and identify your own molecules in a real astrophysical dataset.

Outline

Below I have included a suggested outline with additional references for future consultation. However, the activity this week will be open-ended and hands-on, so feel free to ask any questions that come up!

1. **Recap from last week:**
   How many molecules have been detected in space? Where are they typically found and what can we learn from them? What's the most interesting thing you learned last week? Are there any questions you had during the meeting last week?

2. **Experimenting with Molecular Emission:**
   We will briefly explore molecular rotations and vibrations using Chemtube3d, developed by the University of Liverpool. For rotations: `http://www.chemtube3d.com/spectrorotcd0-CE-TEST-ROTATE-ALL.html`. Read over the first two paragraphs and then scroll down to the molecule selection. Play around with the animation, selecting different molecules and different energy levels - what do you notice? Are molecules allowed to rotate with any energy at all? If there's time/interest, there's also one for vibrations: `http://www.chemtube3d.com/spectrovibhcl1-CE-final.html#models`.

3. **Discovering your own Molecules**
   Now you get a chance to discover molecules in a real astronomical spectra of an intermediate-mass protostar[1]. Let's split up into groups and work together to identify 10 molecules in this spectrum. We will be working with the spectrum at end of this document. Here are some basic instructions to get you started:

   - Go to the Splatalogue webpage: `https://www.cv.nrao.edu/php/splat/advanced.php`. This is a searchable molecular spectroscopy database that complies data from several independent sources.
   - Enter a plausible frequency range in GHz as well as an upper E_U value of 250 K (this just tells the database how hot we expect the source to be). We can also select for only the stronger lines by going to "Line Intensity Lower Limits" and then choosing CDMS/JPL (log) and entering -5. Note that less negative implies a stronger line! Next, for clarity, uncheck every box in "Line List Display" except for CDMS, which just means that we are only using data from one external database. When you are done, it should look something like this:

[1] called NGC 7129 FIRS 2; it's $\sim$500$\times$ brighter than our Sun and is located 2.4×10^{16} miles away (or 1250 pc); see http://adsabs.harvard.edu/abs/2014A%26A...568A..65F

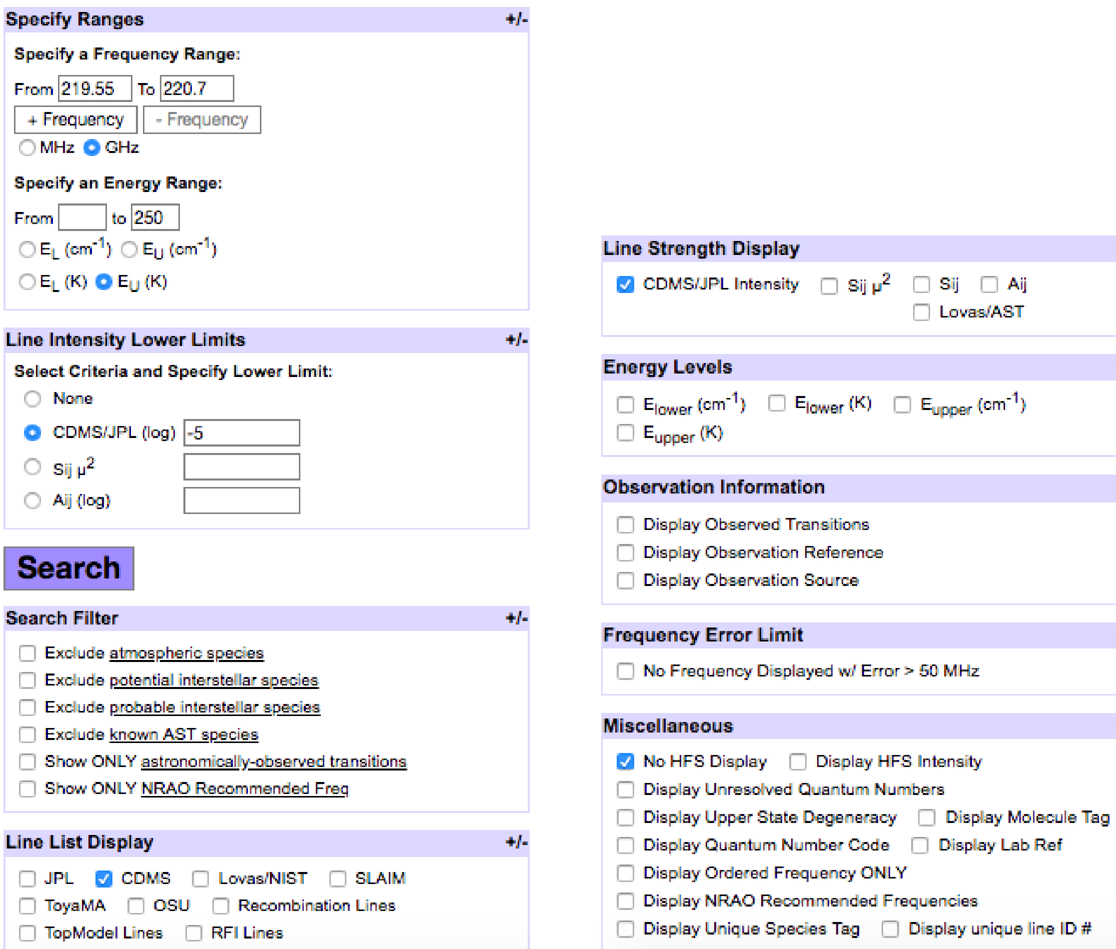

Figure 1: Splatalogue Settings

- To help you out, here's a list of molecules to choose from (some will appear more than once; why could that be the case?): $C^{18}O$, HNCO, ^{13}CO, CH_3CN, $H_2^{13}CO$, CH_3OH. However, you are on your own for **Molecule 3** and we will see how many groups can correctly identify it. Also, don't worry about which transition it (i.e., the quantum numbers listed in the database), we only care about molecular identifications.
- After $\sim$20 minutes, you will share your findings and we can compare against the correct identifications.

Spectrum for Line Identification