

Frozen Chemistry and Fantastic Origins: Molecular Reactions and the Chemical Tapestry of Planet-Building Disks

INTERVIEW WITH: DR. JENNIFER BERGNER

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Jennifer Bergner is an assistant professor in the Department of Chemistry at the University of California, Berkeley. She is also the Chevron Chair in Chemistry and winner of the 2024 Annie Jump Cannon Award for her innovations in astrochemistry exploring exotic chemical pathways. In this interview, we discuss Dr. Berger's work using the James Webb Space Telescope to analyze mixed ice compositions, her focus on the role of organic molecules in planetary formation and its implications on the origins of life.



BSJ: What drew you to astrochemistry, and was there a specific challenge or scientific question that motivated you to explore astronomical ices and complex organic molecules in the context of celestial body formations?

JB: I first learned about astrochemistry right before I was about to graduate college. I had just done a standard chemistry degree up until I saw a talk by someone in the department who did astrochemistry. I had never heard of him before, but I went to a lecture by him, and it blew my mind. I felt like I had spent three and a half years learning chemistry, and then he was showing all these crazy molecules, I was wondering how does that even exist? So I was initially just intrigued by the weirdness of thinking about how you could have the same chemical rules, but under extreme conditions in space, the outcomes can be really different. Then, as I learned more about the field, I became especially drawn to the application of astrochemistry to regions of space where solar systems are forming. I was interested in thinking about how this unusual chemistry that is happening alongside the formation of planets really influences what types of planets you make, what their compositions look like, and whether they might be habitable.

BSJ: Within investigating those regions of space, why did you specifically choose to focus on the oxygen atom reactions with the hydrocarbon? And what about the success of these reactions at low temperatures is astronomically significant?

JB: In the field of astrochemistry, we know that relatively large organic molecules are forming in space, which is surprising because space is really hostile. So the fact that we form mid-sized

organics, similar to ingredients that participate in prebiotic chemistry, is this really tantalizing connection. Perhaps the synthesis of organic building blocks in space can provide the ingredients needed to jump-start prebiotic chemistry on young planets. The explanatory challenge then is to figure out how you actually make these mid-sized organics under extreme environments. A lot of astrochemical processes are happening within what is called the ice phase. Since it is so cold, molecules that exist as gases here on earth, freeze and form these icy mantles on the surfaces of small dust grains. As a result, most of the volatile, reactive material is present in this condensed icy phase and it

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is within these ices that we think the organic molecules are forming.

In ices, it is relatively easy to stick hydrogens onto things. Forming larger molecules, such as incorporating an oxygen or nitrogen atom into a carbon-based molecule, is challenging given the chemical constraints present at extremely low temperatures. At 10 Kelvin, there is not a lot of thermal energy around, so any reactions that have an energy barrier are basically prevented. The motivation for studying the behavior of electronically excited oxygen atoms is that they can insert with no energy barrier into other molecules and build up chemical complexity in a unique way. This process has been studied in the gas phase a lot here on Earth, as these excited oxygen atoms play a big role

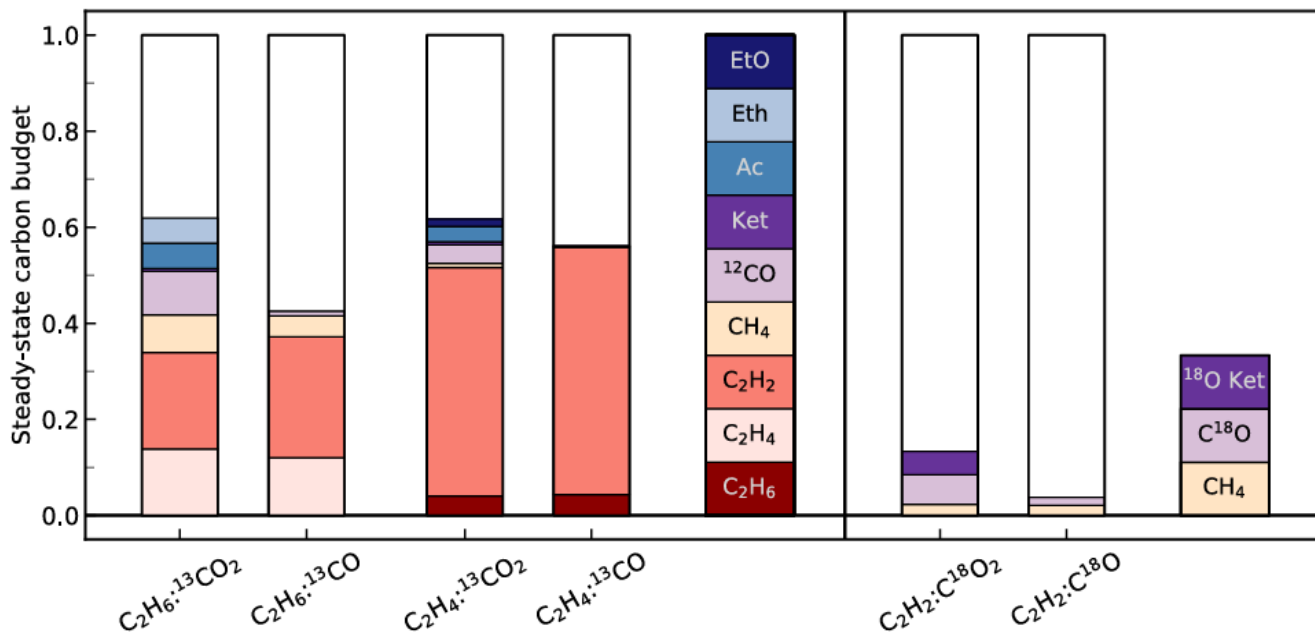


Figure 1: Graph of steady state of carbon budget for 9 Kelvin irradiations. Each bar represents the fraction of carbon atoms in a specific product relative to the total number of carbon atoms lost from the initial hydrocarbon reactant. Shows how much carbon is incorporated into each product.

in Earth's atmosphere.

However, no one had previously looked at how it might play out in the ice phase. We found that we could indeed build up the complexity present in the ices through these insertion reactions. This mechanism is attractive because it operates at 10 Kelvin and only requires some photons, which we expect to be present in interstellar environments. So this is a new possible pathway to generate chemical complexity in very cold interstellar environments (Figure 1).

BSJ: How do the experimental results from artificially replicating these reactions using photolysis and the VUV¹ in a lab differ from the natural reaction in space? If there are distinct differences, how do you account for them in your interpretations?

JB: In the lab, we do our best to simulate what we expect the conditions are like in interstellar regions. For example, we can achieve some of the lowest pressures that are possible on Earth by working in an ultra high vacuum. In terms of temperature, we can cool our ice samples down to 5-10 Kelvin. So in terms of the temperature and pressure conditions, we are doing a pretty good job of mimicking those environments.

The real variable that we will never get right is the time scales because we run an experiment in an afternoon and we might deposit a dose of energy that a molecule would experience over 100,000 years and that is an insurmountable challenge. Therefore we would never look at the outcomes of an experiment and say that is exactly what is happening in space, instead what we are interested in is measuring fundamental parameters. These parameters include reaction rates and

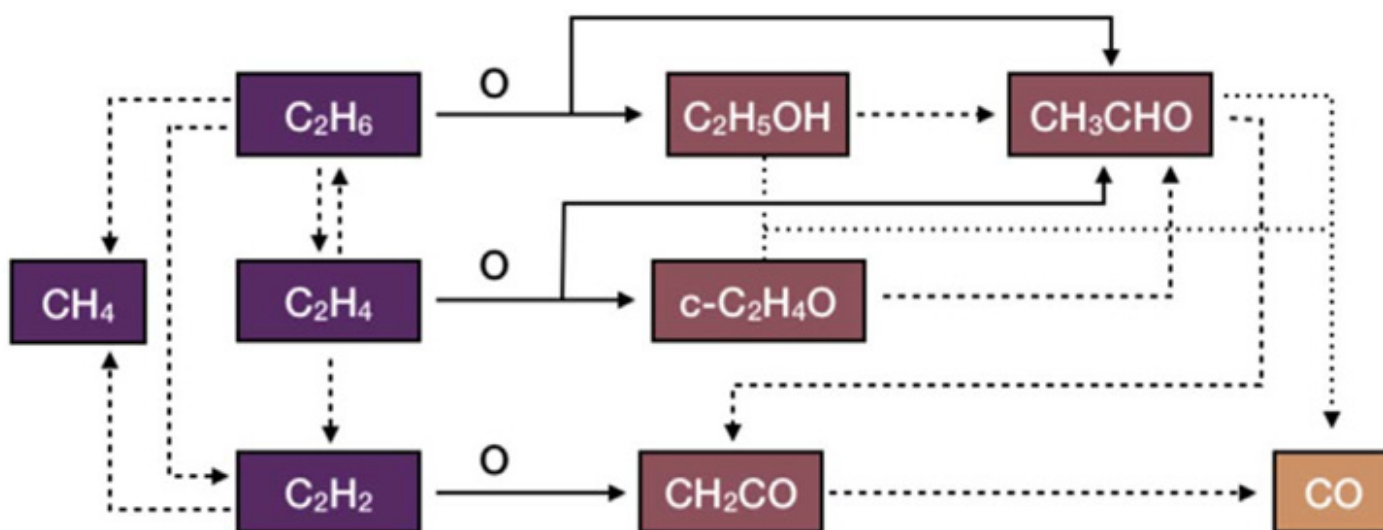


Figure 2: Reaction network which illustrates oxygen atom interactions with C₂H₆, C₂H₄, and C₂H₂ molecules. Solid lines represent primary reaction pathways, the dashed lines show the secondary pathway of hydrocarbon and organic photolysis, and the dotted lines are the tertiary pathways of organic photolysis which form CO.

energy barriers. These and other parameters can be translated and are invariant between the lab and space. And then people can plug those into chemical models and simulate how it will play out on 100,000 year time scales.

BSJ: What specifically about the oxygen atom reactions and the implied chemical complexity possibly contributes to the possibility of origin of life?

JB: The mid-sized organic molecules that are produced seem pretty small from a terrestrial chemist's point of view, but are quite complex in the context of space. People who study origins of life chemistry are using molecules like this as building blocks for prebiotic systems. The idea is that these molecules formed in interstellar ices could be delivered to young planets and participate in prebiotic chemistry on planetary surfaces. This is probably not happening for material that is directly incorporated during the formation of a planet, because making a planet is a really energetic process in which you basically reset the chemistry. What is more likely is that we have impacts of planetesimals, like we know happen all the time in our own solar system, and more pristine icy material could be delivered to planets that have already formed through these planetesimal impact events.

BSJ: Can you provide some background on the role of volatiles in planetary disks and their significance to planet formation?

JB: When we talk about volatile molecules, we are talking about things like water, carbon monoxide, carbon dioxide, methane, small molecules. Many of these small molecules would exist as liquid or gasses here on Earth. But in planet forming contexts, a lot of them are in this icy form.

The reasons that we care about where these volatiles are in the context of planet formation are, first of all, we are interested in how they are incorporated into planets. So beyond delivering chemically complex material to planets and on a much more basic level, the amount of carbon, oxygen and nitrogen that's incorporated into a planet is really

important for its habitability. Whether you have temperate conditions, whether you have carbon building blocks to proceed to biochemistry are relevant to a planet's habitability. So from a bulk composition standpoint, we are very interested in where the volatiles are and how

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they make their way into planets.

The other aspect is that the volatiles can actually influence the process of planet formation itself. As an extreme example, consider the solar system, where we have rocky planets close to the sun and we have giant planets far away from the sun. The transition between those is actually the point where water goes from an ice to a gas. So the building blocks that you have in the solid materials that are forming your planetary cores can dramatically affect the outcomes of planet formation, whether you form an Earth or a Jupiter type of planet.

BSJ: Could you explain how your radiative framework improves the retrieval of disk ice composition and mixing status using their band profiles? What challenges did you face applying it to the HH 48 NE disk's ice bands, and what did you learn?

JB: The way that we can observe ices in protoplanetary disks is not so different from how a spectrometer works here on Earth. You need a source of infrared light, you have some material that the light is passing through and being absorbed by, and then you have a detector, which in our case is a telescope. We can make these measurements of protoplanetary disks that are viewed with a certain geometry, so that

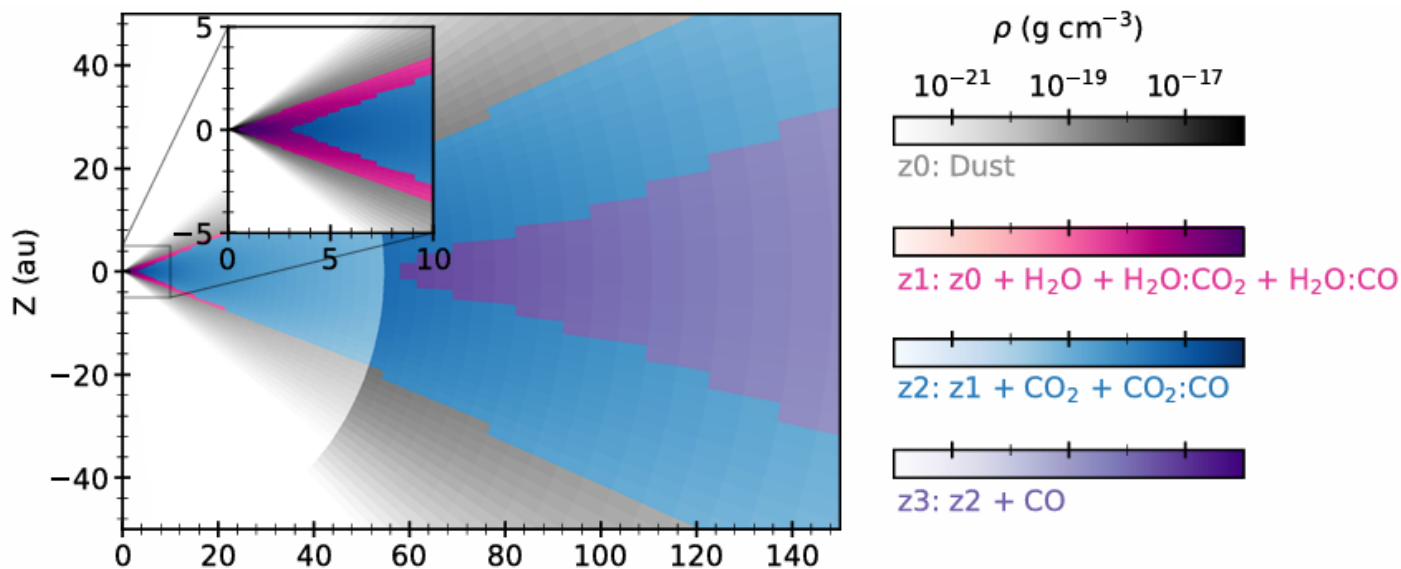


Figure 3: Zoning and Ice Composition in Protoplanetary Disks. Representation of solid materials of dust and ice and how they are distributed in the protoplanetary disk. Distribution shown in astronomical units (au) from the star of the disk. Each zone contains newly formed ices in addition to the solid materials found in all zones closer to the star (zone 1 includes water-rich ices along with the refractory dust from zone 0).



Figure 4: Early image from James Webb Space Telescope of Carina Nebula. Using such images scientists have found energetic jets and outflows from young stars like this one that were previously hidden due to dust clouds.

the disc itself is in front of the star. Then we are basically using the star like a natural spectrometer.

James Webb is the first instrument that is sensitive and powerful enough for us to actually make these measurements. So we are really doing this for the first time. Part of the challenge is the fact that we have never seen this kind of data before, and we are just developing the tools that we need to interpret it. One of the main challenges with interpreting this kind of data is that the path light takes through a protoplanetary disc is actually a lot more complex than just a simple beam of light passing through the material. It turns out that there are other effects that we call radiative transfer effects, that have to do with how the light is interacting with the material. For instance, the light can be scattered and can also saturate in some places. So, it turns out you cannot just look at a protoplanetary disk spectrum measured by James Webb and directly read off meaningful physical quantities.

Instead we have to simulate the path that the light takes in order to back out useful information. To do that we use what is called radiative transfer modeling, where we build a model of the physical structure of the protoplanetary disk, including the density of grains in the disk, the optical properties of the ices that are present, and the abundances of the ices. Then the radiative transfer framework allows us to propagate synthetic photons through the disk and make synthetic observations. By comparing the synthetic observations to what the telescope actually observed, we can tune the model and learn something about the underlying physics and chemistry of the protoplanetary disk.

BSJ: Your work in deciphering the compositions of ice bands on the HH 48 NE disk heavily relies on the James Webb Space Telescope's (JWST) observations. Could you elaborate on JWST's unique capabilities, and how do you see the future of resolution technology for your field?

JB: Fortunately, we expect to have about 20 years of James Webb operations, and there is a lot left to be done using JWST. We

are really just starting to get an initial sense of the data collected from JWST and are building the tools that we need to interpret the data properly. Beyond JWST, one exciting potential upcoming mission is a space-based far-infrared spectrometer. James Webb gives us access to certain parts of the light spectrum in the near and mid infrared range, and we can learn a lot about the volatile landscape of disks from these wavelengths. However, there is a missing piece of the spectrum that contains a lot of other information about where the water is in protoplanetary disks, and other things about the volatile reservoir available for planet formation. So, long term, a far infrared facility is what I am most looking forward to.

BSJ: The findings of ice mixing and entrapment in protoplanetary disks provide insight into how scientists understand the composition of these disks. How might these insights contribute to or change our understanding of planet formation?

JB: One of the things that we found by doing this analysis is that different molecules in the ice seem to be mixed. In our work, we focused on the most abundant ice molecules: water, CO, and CO₂. Our spectroscopic analysis provided evidence that they are mixed together and not in isolated pockets. More interestingly, some of the molecules seem trapped in one another. We talked about the water snow line and the importance that it has on the types of planets you can form, but there are also snow lines for other volatiles. Further from a star, there exists a CO₂ snow line beyond which CO₂ is in the ice, while interior to this CO₂ is in the gas phase. Moving out even farther out to colder regions, a similar transition occurs at the CO snow line. These snow lines regulate the distribution of volatiles between the gas and ice phases, ultimately influencing the types and properties of planets forming at different distances from the star. So the fact that we are seeing the trapping of CO in CO₂, means that there is a lot more carbon close to the star in the building blocks of planets than there would be if these molecules were not interacting. This makes us reevaluate the

budget of carbon, oxygen, and other volatiles that are available in the solids for forming planets throughout a protoplanetary disk. So in addition to chemistry, we can also learn about the ice microphysics and the processes governing how molecules adhere to solids versus desorb into the gas phase.

BSJ: How do you envision further research into astrochemistry, and the continued search for life beyond our planet?

JB: Telescopes obviously play a big role in giving us ground-truth information about what planet-forming environments are like. Lab experiments also play an important role in informing our

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understanding of the types of reactions that can take place as well as the microphysical processes at play. There are also people who try to put a lot of these pieces together by building really complex models of planet formation, including all of the physics of how you bring solids together, and all of the chemistry. I think we are a long way from having a unified modeling framework for describing all these processes at once, but it is a really interesting and important avenue of research.

One thing I would like to emphasize is the excitement of doing interdisciplinary science. Many fields today, not just astrochemistry, are evolving at the intersections of traditional disciplines, and I see a lot of exciting work emerging in these areas. I just want to express my enthusiasm for this kind of work and for those who are curious, willing to cross boundaries, and open to learning from different perspectives to tackle new questions.

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IMAGE REFERENCES

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