

I never thought I would study a shark tooth in my research. Nevertheless, it was there, arching upward gradually from its base before almost leveling off. Then, it dropped sharply, forming a pointy peak. The shark tooth, at over a thousand years old, contained clues about chemistry of the distant past. However, this “shark tooth” didn’t belong to a great white. Rather, it belonged to the Great Orion Nebula.

I am an astrochemist. Throughout my Ph.D., I carried out observational work using radio telescopes to understand some of the most fundamental chemical reactions in the galaxy. Much of my work thus far has focused on a region called the Orion Kleinmann-Low nebula, or Orion KL, at heart of the Great Orion Nebula. From Orion KL, chemical fingerprints of so-called complex molecules (i.e., molecules with six or more atoms in astronomical jargon) travel about 1,300 lightyears to be captured by radio telescopes on Earth. Using one of the most powerful telescopes—the Atacama Large Millimeter/submillimeter Array (ALMA)—I converted these signals into maps in which each pixel contained a rotational spectrum. From these spectra, I mapped the temperature, abundance, and velocity of different flavors of gas-phase methanol at extraordinarily high spatial resolution.

As an undergraduate, I never gave methanol much thought. It was a chemical used to make *actual* complex compounds in organic chemistry lab. In the extreme environment that is interstellar space, however, the existence of methanol is remarkable. We know from experiments and computational modeling that the bulk of interstellar methanol forms on the surfaces of icy dust grains through successive hydrogenation of CO. But what happens to methanol after it forms on the surfaces of dust grains largely remains a mystery.

In my Ph.D. thesis work, I investigated how methanol comes off of the interstellar dust grains and is injected into the gas where it observed by radio telescopes. From my data, thermal desorption, in which methanol sublimates as the dust grains are warmed by infant stars, seems to be the primary driver of methanol injection into the gas phase (at least in Orion KL). I also investigated why the relative abundance of CH₃OD is three times greater than that expected in comparison to CH₂DOH. Statistically, the CH₂DOH:CH₃OD ratio is expected to be about 3, since there are three hydrogen sites on the methyl carbon versus the one on the hydroxyl group; however, the ratio is closer to 1 in Orion KL and other massive star-forming regions. This is where the shark tooth comes in.

It has been shown that molecular abundance and temperature have a power-law relationship in star-forming regions. Thus, I expected that plotting the CH₃OD abundance against temperature would produce a gentle upward slope but certainly not something reminiscent of a great white’s dental records (Figure 1). This suggested that there was some unexpected, temperature-dependent chemistry affecting the observed CH₃OD abundances in Orion KL.

Even more curious were the temperatures where the CH₃OD abundances increased and decreased unexpectedly. The gas and dust that constitute infant stars start off extremely cold at temperatures of 10-30 Kelvin. As a protostar evolves, it becomes a “hot” 100 Kelvin and churns out an entire stock room of complex organics. Thus, most of the astrochemical models of the CH₃OD chemistry in these hot regions look at temperatures of 100 K. However, I was interested in temperatures between 110 and 120 Kelvin and 180 and 200 K where the shark tooth emerged and fell.

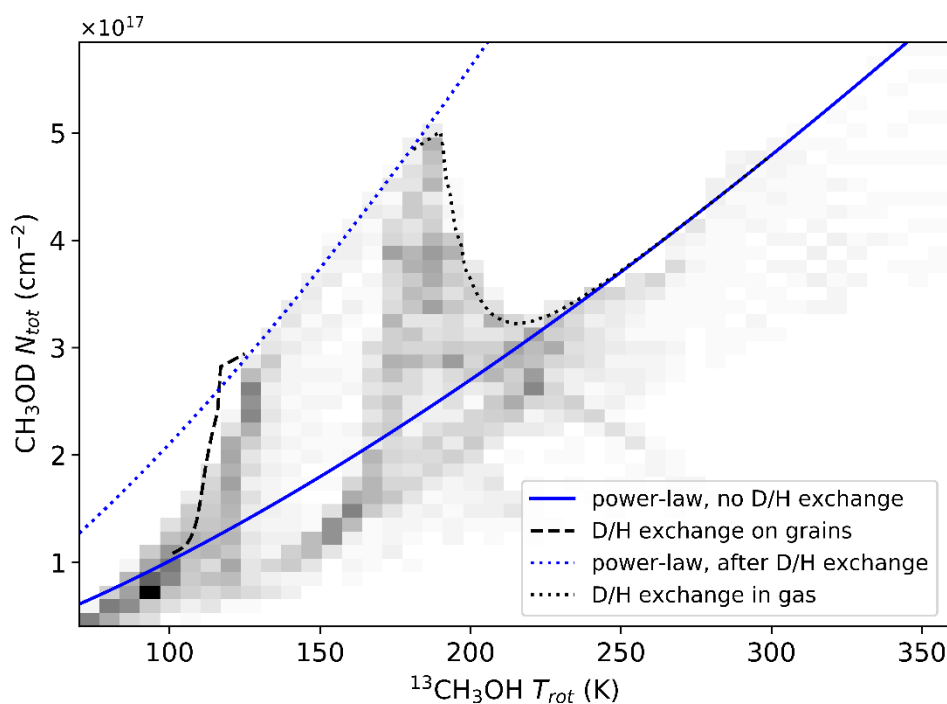


Figure 1 CH₃OD abundance (y-axis) plotted against temperature (x-axis, assumed to be the same as the ¹³C-methanol isotopologue) in Orion KL. The solid blue line shows the expected power-law relationship between the two parameters. The black lines show the results of chemical models in which D/H exchange takes place with heavy water on dust grains (dashed) and with other compounds in the gas phase (dotted).

In exceptionally interdisciplinary fields such as astrochemistry, CAS SciFinder and other information solutions (e.g., NIST Chemistry WebBook) are critical for finding gaps in the fields' existing literature. In my thesis work, I found that CH₃OD chemistry at temperatures above 100 Kelvin is mostly absent from astrochemical publications. However, consulting reaction databases pointed me to relevant work in other fields. Combining experimental and theoretical work from other subfields of chemistry, I was able to produce models suggesting that the shark-tooth feature in my data is the result of rapid D/H exchange between CH₃OH and D₂O (Figure 1, dashed black line) at 110-120 Kelvin and temperature-dependent D/H exchange between CH₃OD and H₃O⁺ (Figure 1, dotted black line). While I am still working to understand the more intimate details of this chemistry, it is abundantly clear that chemistry information databases were imperative in connecting my astronomical observations with the chemistry that could explain them.

Now, I am preparing to start a NASA Postdoctoral Program (NPP) Fellowship at NASA Goddard Space Flight Center where I anticipate bringing the open questions from my observational work into the lab. At Goddard, I will work on the Sublimation Laboratory Ice Millimeter/submillimeter Experiment (SubLIME) to better understand interstellar surface chemistry through ice analogue experiments. I hope to use the experiment to study the chemical reactions (found through chemistry information solutions) that seem to explain CH₃OD chemistry in Orion KL but under conditions more relevant to interstellar space. I also hope to take existing experimental work that shows what products are formed upon irradiating

interstellar ice analogues and apply rotational spectroscopy to derive branching ratios and desorption rates, which can then be applied to observational data. In such experiments, tools like CAS SciFinder are critical for finding relevant reactions, especially ones not typically considered in the astrochemical literature, to ensure all mechanisms are considered to formulate more robust astrochemical models.

Ultimately, I aspire for a career in which I continue combining observational astronomy with laboratory astrophysics to understand the intricacies of interstellar chemistry. Doing this effectively requires making connections with scientists across different fields. I was struck by how many Future Leaders alumni testimonials mentioned the powerful connections made during this program, and I am hopeful that I will have the opportunity to forge a network beyond my field. Furthermore, I am passionate about science communication, including inreach (Figure 2) and outreach, and I am eager for professional development opportunities to enhance my leadership and communication skills through connections with industry leaders and peer early-career scientists.

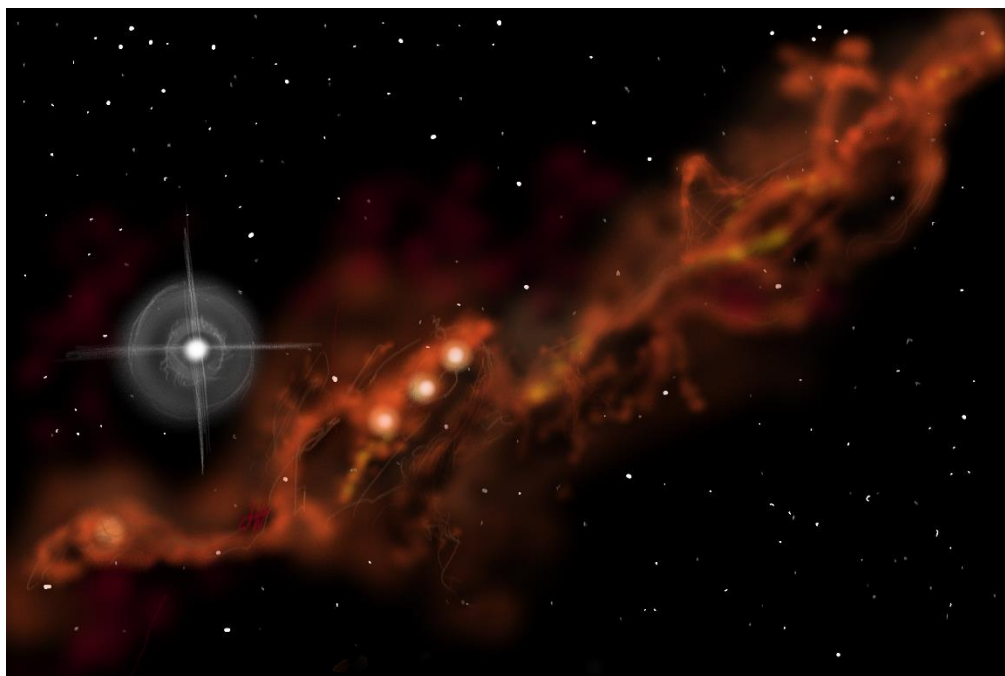


Figure 2 Illustration of the Taurus Molecular Cloud, an interstellar laboratory teeming with different molecules. I illustrated this image (digitally, using Microsoft Paint) for the ACS In Focus e-book I wrote about *Astrochemistry* (Wilkins & Blake, 2021). I enjoy using the intersection of science and art to communicate about my lesser-known field of astrochemistry, especially to undergraduate chemists who are only just beginning to see how expansive the chemistry discipline is.