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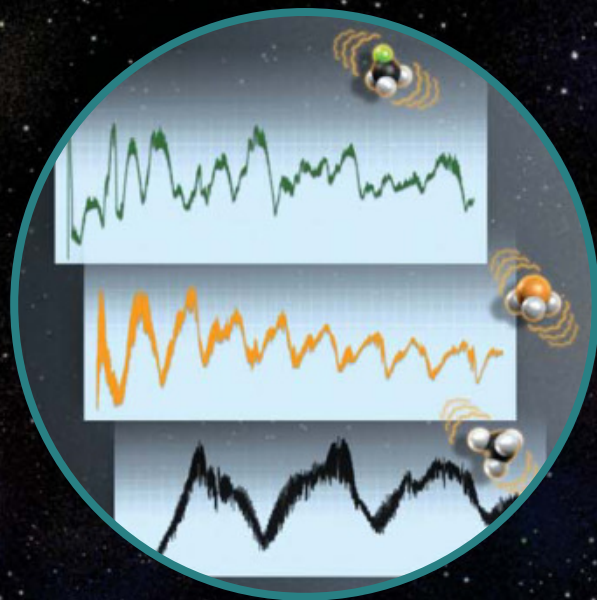
Building a Better Biosignature

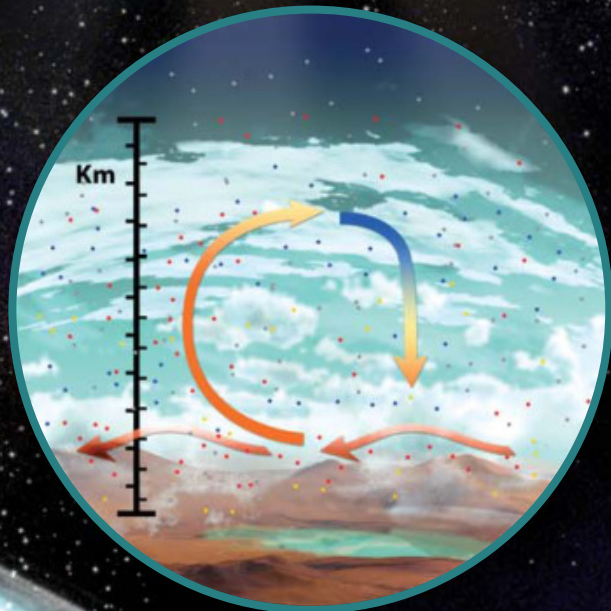
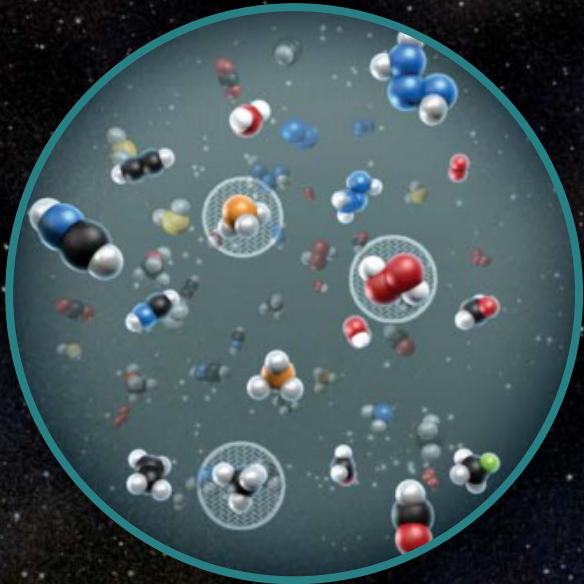
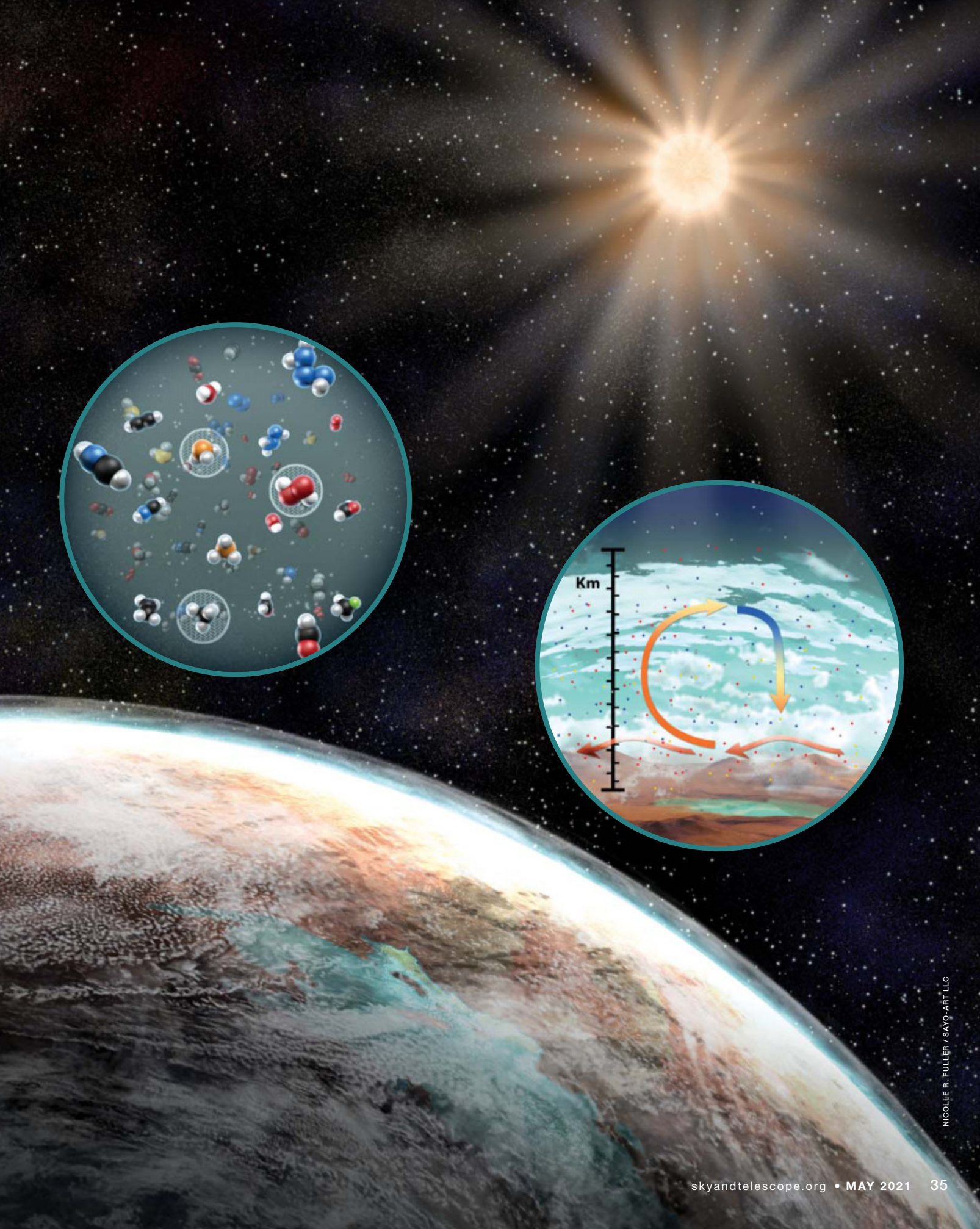
Finding signs of alien life requires more prep work than you might think.

Every genre has its tropes, and science fiction is no exception. Stories set in space often center around the discovery of strange new worlds, and the narrative tradition in these situations usually demands that someone “scan for signs of life.” It’s quite simple, really: An order is given, a touch-screen touched, and an answer promptly received.

If you’ve ever wondered at this fictive sleight-of-hand, and whether such remote sensing is even possible, you’re in good company. Astrobiologists all across the world are laboring to transform this pretend practice into a real science. We are a long way from, “Alexa, check for life signs on Kepler-186f.” But someday, we may know enough about the clues life creates to estimate what portion of our galaxy’s terrestrial worlds, if any, are life-bearing.

The key for remote sensing is *biosignatures*. A biosignature is something — whether a substance, a pattern, or even an object — that (probably) had to be made by life in order to exist. It is not life itself, but something made by life, a kind of fingerprint.





In looking for biosignatures on distant worlds, astrobiologists are mostly focusing at the moment on chemical compounds in a planet's atmosphere. Find the right molecules in the proper context, and it could be circumstantial evidence for life.

But to get to this point, astrobiologists must first construct a methodology for identifying reliable, resilient, and detectable biosignatures. That might sound boring, but it's crucial: We can't find life's fingerprints if we don't know what to look for or how to interpret it once we find it. Hints of methane on Mars (*S&T*: Jul. 2019, p. 9) and the recent tentative detection of phosphine in the clouds of Venus (*S&T*: Mar. 2021, p. 9) remain contentious in part because we don't fully understand what could create these signals. As exciting as it is to reach out into the solar system and the galaxy, the work of understanding what we find begins back here on Earth, with fundamental research in three fields: quantum chemistry, molecular biology, and atmospheric science.

A Work in Progress

There are probably plenty of exo-Earth candidates in our line of sight. And the next generation of instruments will give us unprecedented views of these worlds' atmospheres. But before we get too excited about any potential biosignatures, we need a better understanding of the basic nature and behavior of molecules under a wide range of temperatures. This is the purview of quantum chemistry, the first pillar of the biosignature framework. Scientists do this work both in the lab and computationally.

Biology is the next pillar. Specifically, we need to know all the gases that all the various lifeforms on Earth produce. There are a few groups tackling this monumental task, utilizing both analog methods (graduate students) and machine learning to scroll through a vast agglomeration of scientific literature and compile useful databases.

Then comes atmospheric science, which takes a litany of chemical information from the above-mentioned efforts and

Key Constituents of Earth's Atmosphere, Relative Abundances

Molecule	Ground-truth Earth	Galileo Value	Thermodynamic Equilibrium
N ₂	0.78	--	0.78
O ₂	0.21	0.19 +/- 0.05	0.21 (ignoring the crust's under-oxidized state)
H ₂ O	0.03-0.001	0.01-0.001	0.03-0.001
CH ₄	1.6 × 10 ⁻⁶	3 +/- 1.5 × 10 ⁻⁶	<10 ⁻³⁵

▲ **TOO MUCH METHANE** These data from a 1993 paper by Carl Sagan and others highlight the disparity between the methane level expected in a steady-state atmosphere and that found in Earth's atmosphere. Methane should not survive more than a decade or so in our oxygen-rich atmosphere without being replaced, they noted.



EXO-EARTHS

Based on Kepler data, astronomers estimate that there should be four rocky planets in the habitable zones around G and K dwarfs within 30 light-years of the Sun.

plugs it into a computer code that simulates how everything would behave in a planetary context. This allows scientists to model gases' abiotic production, abundances, lifetimes, movements, and altitudes.

The first time these specialties were brought together to look for signs of life from space, the effort was a stunning success. The year was 1990, the spacecraft was NASA's Galileo, and the planet, Earth. (We'd stacked the deck.) At a distance of about 1,000 kilometers (600 miles), Galileo detected an unstable combination of methane and oxygen in our atmosphere, which researchers interpret as one of Earth's particular life signs. A similar chemical cocktail on another world might also be a biomarker.

But 30 years later, astronomers are still trying to understand the total context and composition of Earth's biosphere, both in the present and throughout geologic time — and then use that to aid in the search for life elsewhere.

"It's not just about finding liquid water, or oxygen, or even methane and oxygen together," Sarah Rugheimer (Oxford University, UK) says. "There's the whole planet to consider, and with that comes so much potential for false positives. On top of all this is the fact that we don't really understand exotic chemistry very well, which I think is what Venus is showing us."

Venus has taken center stage in the biosignatures hunt thanks to the 2020 announcement by Jane Greaves (Cardiff University, UK) and others that there's phosphine in the cool cloud deck of our sister planet. On Earth, phosphorus and hydrogen don't tend to get together to make phosphine unless life forces their hand. On Jupiter and Saturn, the chemical forms thanks to the extremely hot, high-pressure environments deep below. But the conditions on our planet's evil twin are nothing like those distant cousins, the gas giants. So, could phosphine form on Venus abiotically? We don't know yet because, until recently, we had no reason to find out.

Quantum Chemistry, Lab Edition

There is a bias in exoplanet data towards very hot worlds — worlds like WASP-79b, a gas giant where the clouds are 1500°C (2700°F). This is because both of the most successful detection techniques used by astronomers (radial velocity and transit) tend to find planets very close to their stars.

The transit method allows us to observe the way the starlight changes when the planet passes in front of its host. The specific wavelengths that the planet's atmosphere absorbs give us information about the chemicals therein. But interpreting these data has proven difficult.

“Historically, almost all the databases for absorption spectroscopy are confined to room temperatures and pressures,” says engineer Christopher Strand (Stanford). “This is because the main driver of previous research was atmospheric studies of Earth.”

Stanford’s High Temperature Gasdynamics Laboratory hopes to rectify this gap in our knowledge. Typically, it does research for the aerospace industry. But the group’s facilities turned out to be perfect for replicating and studying high-temperature exoplanet atmospheres, Strand says.

One important piece of equipment is *shock tubes*. A shock tube is a long steel pipe — between about 8 and 61 meters (25 and 200 feet), depending on the facility — that is divided into sections and capped at both ends. A thin diaphragm separates the sections. One side is pressurized to the point that the diaphragm ruptures. When that happens, a shock wave forms and travels down the tube to the low-pressure gas at the other end, compressing and heating it. Lasers then shoot through the compressed gas, and the gas molecules absorb some of the light. How strongly the gas absorbs photons of different wavelengths depends first on the molecules’ structures and second on the gas’s temperature, pressure, and composition.

Such experiments provide ground-truth tests for theoretical predictions of spectra, derived from complex adaptive algorithms. “There are groups that are simulating billions upon billions of [spectral] lines ab initio,” Strand says. “And this is very useful. But are these calculations correct? I know from experience that low-temperature models do not accurately reflect what actually happens at high temperatures.”

LAB: CHRISTOPHER STRAND

Astronomers are still trying to understand the total context and composition of Earth’s biosphere.

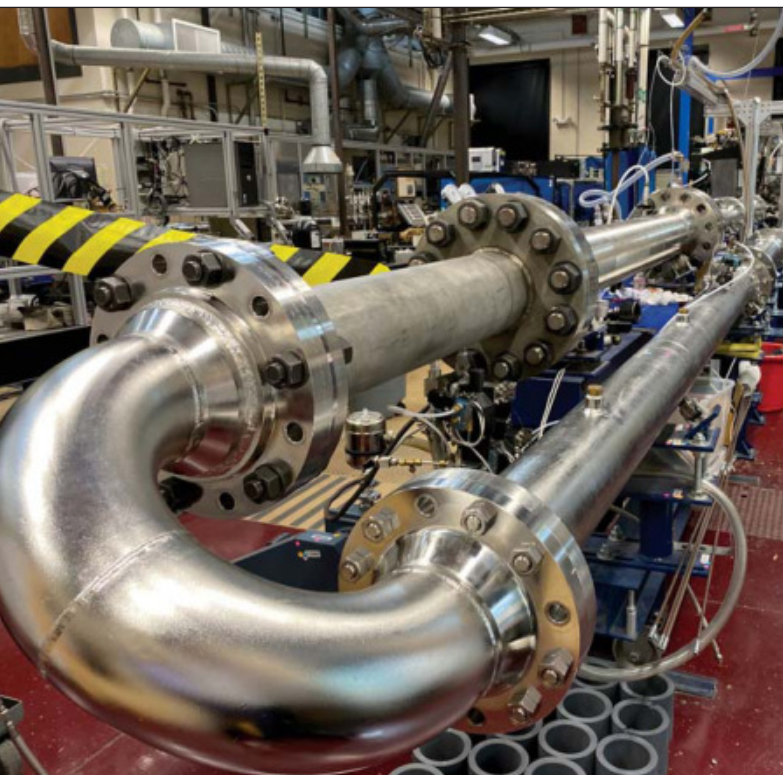
Still, although lab experiments are a common-sense way to discover where our assumptions fail, charting the vast number of possible reactions between all the molecules in existence at every temperature and pressure is impossible. Safety is one problem. Phosphine, for example, is highly toxic and dangerous to work with. Funding is another problem. This is why the majority of our spectral information is predicted with machine learning instead.

Quantum Chemistry, Office Edition

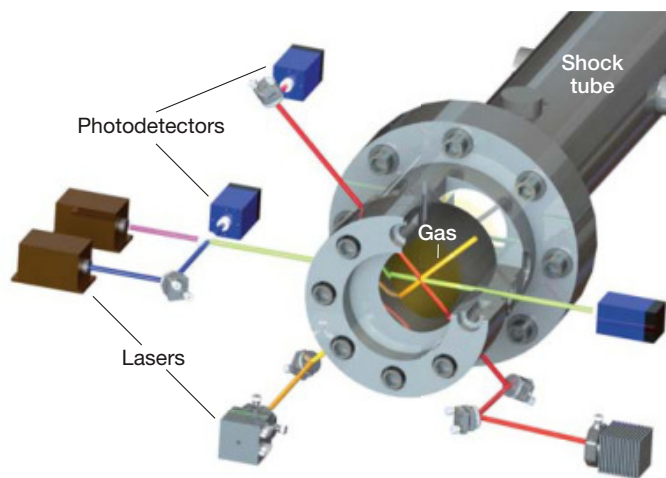
One such project, ExoMol at University College London, has produced data on more than 80 simple molecules since 2011. Headed up by Jonathan Tennyson and Sergey Yurchenko, the group’s aim is to create highly descriptive, open-source listings of all the important molecules and their spectra that astronomers might see on extrasolar planets and cool stars.

“We use existing experimental data to compute from what we call first principles,” Yurchenko says. “We try to describe a molecule’s motion, and then eventually, conclusions can be drawn about spectroscopy.”

The best understood molecules, the ones with the most accurate and trustworthy data, are those that are simple and common on Earth — things like water, oxygen, carbon diox-



▼ **SHOCK TUBE** *Left:* The longest shock tube in Stanford’s High Temperature Gasdynamics Lab curls around itself to fit its 23.2-meter (75.6-ft) length into the lab. Near the camera is the high-pressure section. At the far end is the optical table with lasers that pass through the gas. *Below:* This schematic by Stanford graduate student Nico Pinkowski shows the laser setup. Semiconductor lasers (gray and brown boxes) each send a beam of a specific infrared wavelength through optical ports in the shock tube. High-speed infrared photodetectors (blue boxes) determine how much of each beam the gas absorbs. From these measurements, researchers infer the gas’s absorption properties.



ide, and methane. They have the longest, most comprehensive experimental record, and their biosignature potentials are relatively well understood.

When it comes to expanding beyond these molecules, most astrobiology research leans on *extremophiles* as aliens-by-proxy. Extremophiles are microorganisms that live in conditions deadly to “normal” lifeforms — environments with extreme temperatures, chemical concentrations, or pH levels. One example is anaerobes, which either don’t need oxygen or would die if it’s present. Venus’s atmosphere has very little free oxygen, so any life there would be anaerobic. Phosphine is a byproduct of anaerobic bacteria here on Earth. And as scientists know of no abiotic production method for phosphine on rocky worlds, it is potentially a very good biosignature.

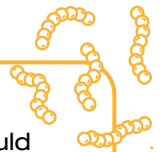
Clara Sousa-Silva (now Center for Astrophysics, Harvard & Smithsonian), one of the researchers on the phosphine study, completed her PhD at UCL. While working for ExoMol, she built a template of more than 16 billion different spectral permutations for phosphine, each of which could be a signal a telescope might pick up, depending on the planet’s conditions. The uncertainties about our neighbor’s atmosphere are huge, however. If you shift the gas content, mixing, and altitude of the models just a tiny bit, one chemical fingerprint starts to look very much like another. This is one of the reasons other researchers suspect the group actually detected something else in Venus’s clouds, perhaps sulfur dioxide.

It’s All About the Gas

The All Small Molecules project (ASM) at MIT is a database of more than 16,000 molecules meant to guide research on biosignature gases. Sara Seager started it in the early 2010s with William Bains and Janusz Petkowski, and they published the list in 2015. The project was a tacit admission that until we have full workups on all the small molecules produced by life, we do not have even the most basic foundational knowledge with which to gauge whether a particular detection is a biosignature or not. So they set out to organize what is known

ANAEROBES

Organisms that don’t need oxygen or would die in its presence might sound alien, but these anaerobic organisms are more common on Earth than you might think. Examples include *E. coli* and *Vibrio cholerae* (which causes cholera). They’re also widespread in your mouth and lower gastrointestinal tract.



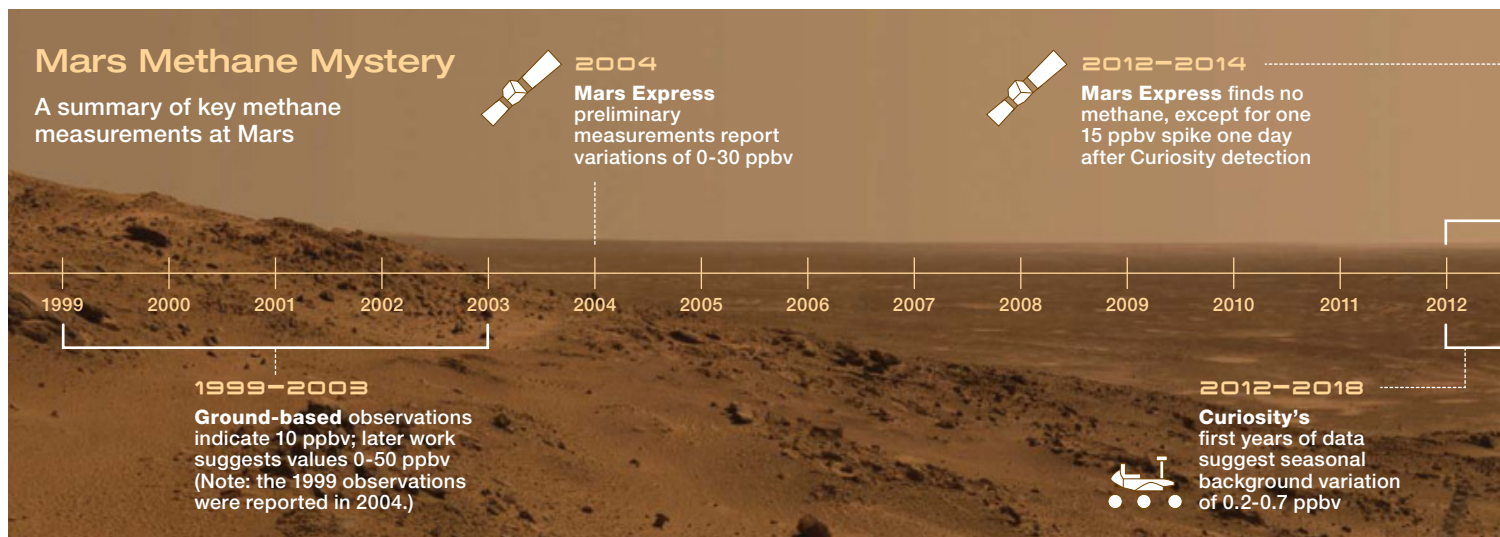
into a kind of Webster’s Dictionary for astrobiologists.

“Life on Earth produces thousands upon thousands of different volatile gases,” Petkowski says. “So, what we tried to do with ASM is to come up with an exhaustive list of all these gases, which then could be assessed in terms of their biosignature potential.”

Unlike ExoMol, which produces spectral information that is generally useful to astronomy, the ASM database was built explicitly to aid in the search for extraterrestrial life. Most of the information it contains was not created by the team but collected by trawling existing literature. Certain large gaps in our knowledge have emerged, such as microbial byproducts. It turns out that biologists don’t do a lot of fundamental research into trace gases produced by microbes unless they pose a threat to human life. This is how we know about the bacteria that produce phosphine: The toxic gas was popping up in water treatment and sewage plants, and people wanted to know why.

An offshoot project called RASCALL (Rapid Approximate Spectral Calculations for All) aims to take this work a step further and obtain spectra for all of the ASM molecules. This contribution will still not be as good as a laboratory measurement, like what Stanford’s Gasdynamics Lab does, or a full ab initio quantum chemical calculation, like what ExoMol does. But that’s okay. RASCALL and ASM are not trying to create knowledge, but rather to collect what is already known into a

ANAEROBES: OLEKSANDR PANASOVSKY / THE NOUN PROJECT; TIMELINE: TERRI DUBE / S&T; SOURCE: ESA; MARS LANDSCAPE: NASA / JPL / CORNELL



useful reference for the community.

“Our database is a tool for modeling planetary atmospheres,” Petkowski says. “Volatile gases react with other atmospheric components. Some will not be detectable, because they will be destroyed by atmospheric radicals and UV. Our goal was to find if there are groups of gases that are better candidates to be remotely detected than others. The creation of this database is just the first step on that road.”

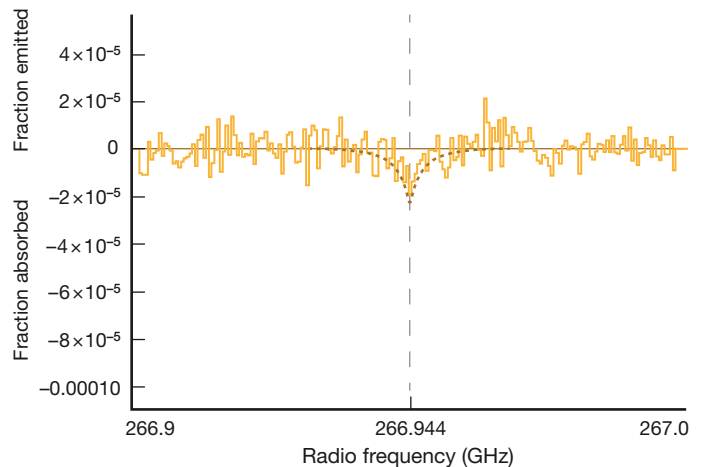
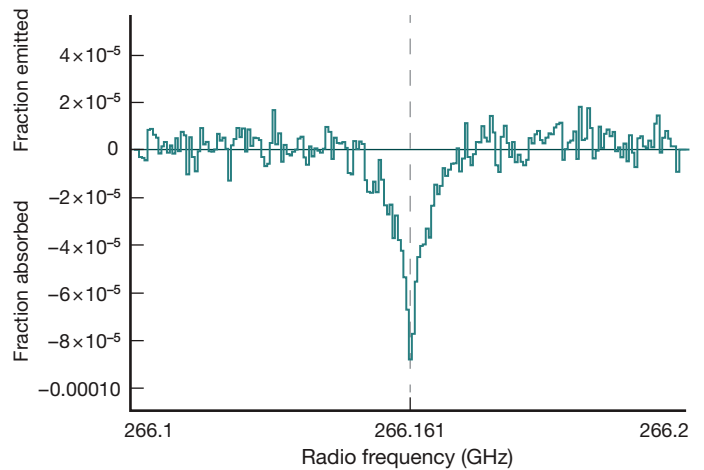
Cloudy with a Chance of Phosphine

The third pillar of the biosignature framework is atmospheric science, a broad and highly computational specialty that looks at the physics, chemistry, and dynamics of planetary atmospheres. Scientists build environmental simulations starting with physical and chemical rules, then input observations and other facts about the world in question. Then they “press go” and watch what happens to their toy planet. Do the results align with the real world, or does everything fall apart?

Through a process of trial and error, these simulations help us to understand both local phenomena like weather and even global phenomena, such as the lifetime of methane and oxygen in Earth’s atmosphere. Models that focus on chemistry allow scientists to make predictions about what might be causing unexpected gas emissions. But even a detection of methane and oxygen in thermodynamic disequilibrium on a rocky world in a star’s habitable zone wouldn’t necessarily “prove” anything. After all, there might be completely abiotic ways to produce this that we are unaware of.

Sukrit Ranjan (now at Northwestern University) had the task of figuring out how well phosphine could survive in Venus’s hot and acidic atmosphere. First, he took everything known about Venus’s surface, subsurface, and atmospheric composition (which is far from complete). He then introduced disruptive simulations of things like volcanic eruptions and meteorite impacts to the model. In theory, these events could create phosphine. But they didn’t make enough.

GREGG DINDERMAN / S&T. SOURCE: J. GREAVES ET AL. / ARXIV 2011.08176

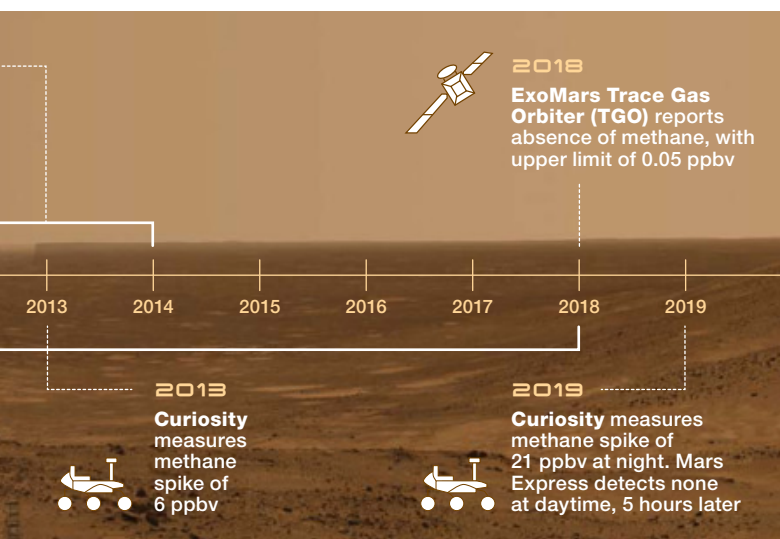


▲ A SIGN OF PHOSPHINE? These plots are two narrow slices of Venus’s spectrum, taken by ALMA and fixed from an earlier version. Jane Greaves and her team took targeted observations of Venus at multiple frequencies, one centered where they would expect to see absorption from phosphine (*bottom*), and another where they should see the more familiar signal of the water isotope HDO (*top*). The observed bands were too narrow to include many other molecules, but the absorption features (dips at centers of plots) appeared right where expected for both molecules. Finding HDO’s absorption line where they expected it gives the researchers confidence that they’re correctly identifying PH₃. The PH₃ line also matched the predicted phosphine spectrum (dotted line), calculated from lab measurements and scaled to the conditions in Venus’s atmosphere. The V-shape for both absorption features is spreading caused by the molecules’ motion in the planet’s atmosphere.

“We tried to see if abiotic mechanisms could explain the presence of phosphine at the inferred abundances,” Ranjan says. “But we couldn’t account for it.”

The phosphine detection itself is tentative, and a recent fix of the primary data out of ALMA has reduced astronomers’ confidence in the observation. But even if future in situ observations verify the sighting, this doesn’t mean we’ve discovered alien life.

The phosphine debate may have a similarly drawn-out fate as methane on Mars. Methane is easily destroyed by sunlight and should be fairly short-lived on the Red Planet. Astrono-



mers reported in the early 2000s they'd detected the molecule there, and the Curiosity rover has caught seasonal whiffs on the surface. But more than a decade after the first detection, the highly sensitive ExoMars Trace Gas Orbiter found nothing in the upper atmosphere, inciting intense debate.

The uncertain fate of biosignatures discovered right next door doesn't bode well for finding clear-cut biosignatures on exoplanets, which will suffer from much poorer and more ambiguous data and have no possibility for validation by a spacecraft visit.

A Footprint Doesn't Look Like a Boot

There are two main criticisms of remote biosignature detection research. The first criticism concerns the prevailing method. Simple molecules are easy to make. Even if we are building a framework for detection, wherein all the context of a world and multiple gases are laid out in inexplicable disequilibrium, a certain disconnect remains. Life is ultimately distinguished by its processes, not its products. So the question arises: Mightn't we focus on ways of detecting *complexity*, whether in essence or in action? Lee Cronin (University of Glasgow, UK) thinks so.

"Simple molecules can be good hints if they can be linked with a life-like process," Cronin said. "But we need a way to detect, just for example, complex molecules remotely that could not have formed on their own. Only when we can detect molecules that have high information content can we say that we have detected life unambiguously."

The remote observation of more concrete biomarkers such as complex molecules, cellular structures, stable isotope patterns, and surface evidence, is beyond our current technical abilities. These may very well be the way alien life is ultimately found. In the meantime, we are left to infer life from small molecules.

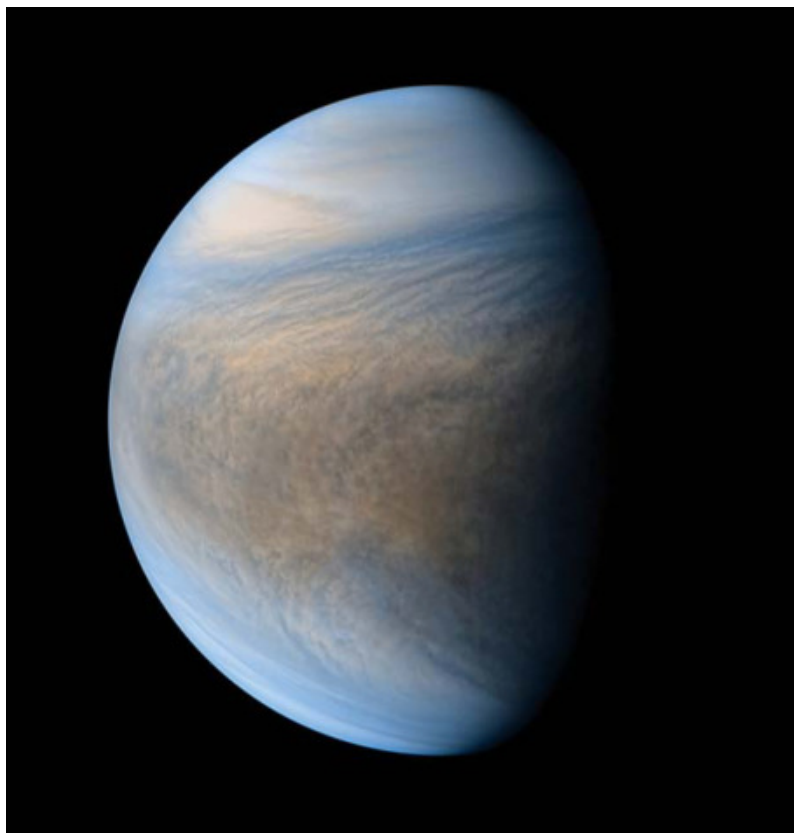
But there is reason to hope for answers from this method. Eventually. Assuming all the next-gen telescopes work, and the community cracks on with building a good framework for remote detections, a new field will soon arise: comparative exoplanet science.

"For now, we are only capable of detecting atmospheric features of various gases, like, for example, water on gas giants," Petkowski says. "If we can get enough data on rocky planets, then maybe we will be able to actually see a trend! Like, for example, how many contain carbon dioxide in their atmospheres? How many of them actually contain oxygen?"

The second criticism of remote-sensing efforts is a more

ACID CLOUDS

Venus's clouds are approximately 85% sulfuric acid and only 15% water. Droplets there are 100 billion times more acidic than the most acidic environment on Earth.



▲ **VENUS IN UV** This composite image combines two images from the Japanese Akatsuki orbiter and reveals motions in Venus's atmosphere. Venus is particularly interesting in ultraviolet: A mysterious "UV absorber" in the planet's cloudtops soaks up a wide swath of ultraviolet and visible wavelengths and may even influence wind speeds. Since the UV absorber's discovery several decades ago, some scientists have speculated that it might be an unknown lifeform. Others think it's likely a sulfur-oxygen compound.

philosophical one: All these wonderful worlds are out of reach. Even if we did detect oxygen on an Earth-twin in the liquid-water zone of a main-sequence star, we may never be able to know for certain whether it harbors life. So what is the point, then, of finding an exo-Earth if we can never go there? What is the point of having statistical evidence of alien life that we can never be certain of?

This critique gets to the heart of human nature. We want to *know*. One of the big mysteries in astronomy is whether Earth is unique, ordinary, or somewhere in between. Chances are, this question won't be answered in a "Eureka!" moment. Instead, as biosignature science matures, we will slowly inch towards enlightenment, rocky planet by rocky planet. We will learn how common certain atmospheric compositions are for terrestrial worlds in the habitable zone. And this, not a weird whiff of gas, will probably be the first true hint as to how common life is in the universe.

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