**Guido W. Fuchs**

# Chemistry of Outer Space
# An Approach with Telescope and Experiment

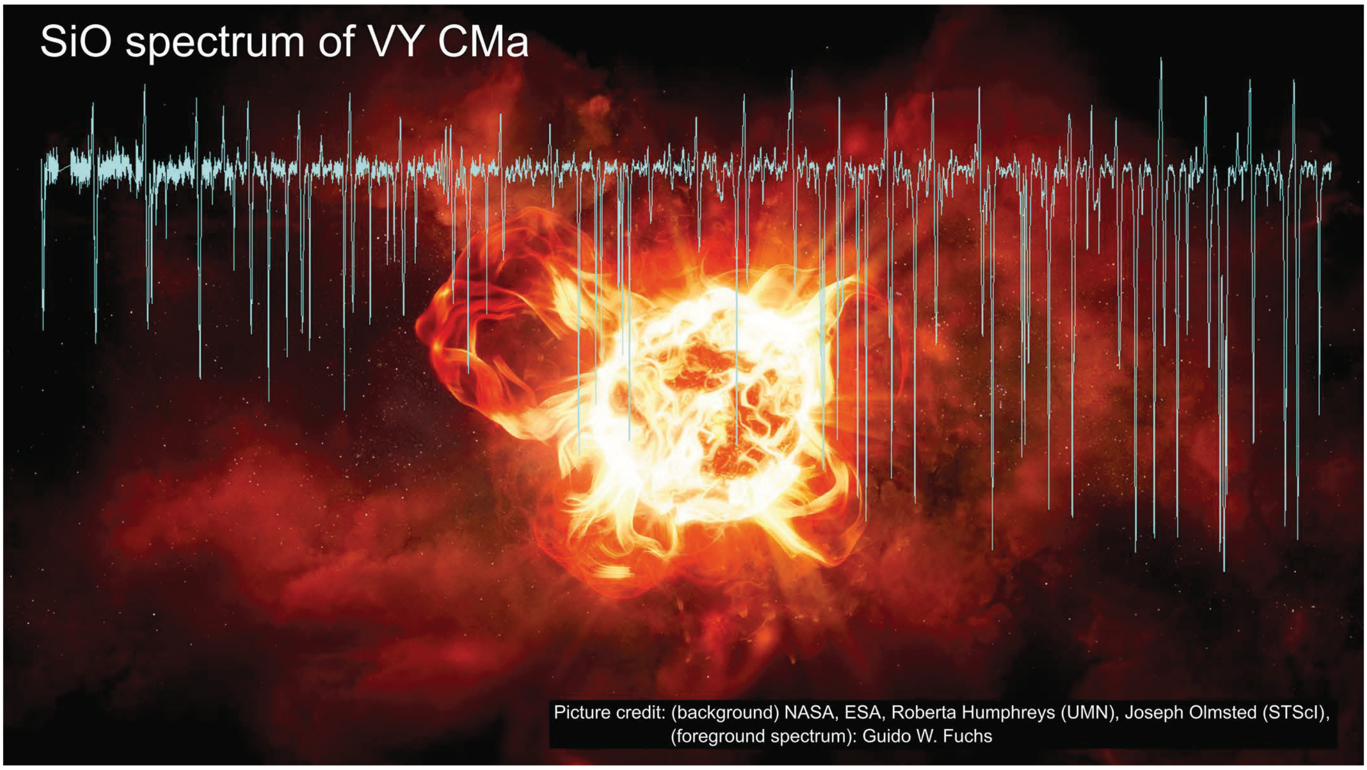

**Fig. 1**: High-resolution mid Infrared (8.3 µm) spectrum of SiO taken with the EXES instrument onboard the Stratospheric Observatory For Infrared Astronomy (SOFIA) airborne observatory. Picture credit (background): NASA, ESA, Roberta Humphreys (UMN), Joseph Olmsted (STScI), (foreground spectrum): Guido W. Fuchs

For astronomers, chemistry is not something to be taken for granted. Shortly after the hot Big Bang there was only hydrogen, deuterium, helium, and traces of lithium – nothing molecular. It took around 200 million years for the first stars to form and to produce heavier elements in their interior [1]. This marks the beginning of the Stelliferous Era in which we live, and the beginning of chemistry [2]. For a long time, molecules were expected to be non-detectable in outer space because they are fragile, and the cosmic radiation field can be very harsh and destructive [3]. To survive, the molecules must therefore either be very stable or seek shelter in less harsh regions of space. Today, more than two hundred fifty different molecular species have been identified in cosmic environments [4]. Most discoveries take place in our Milky Way, but some species can also be seen in extra galactical environments [5]. There are sources that are particularly rich in chemistry, like the dark molecular cloud TMC-1 [6], the star formation region Orion-KL [7], circumstellar envelopes of dying stars like VY Canis Majoris [8]. These sources are associated with the cosmic matter cycle, which consists of the collapse of a molecular cloud, star formation, a main sequence phase, a phase of mass loss in which the star extinguishes, and the outflow of matter into interstellar space. In this scheme, matter is partly recycled and partly converted to heavier elements. Some of the material will remain locked in stellar remnants like white dwarfs, neutron stars, or even vanish in black holes, but others will form the basis for new star and planet generations.

For the overall evolution of galaxies and their stellar composition, it is of great importance whether the building material is present in atomic, molecular, or solid form. Molecules are the seed for dust formation, and dust itself influences star formation and cosmic chemistry in many ways. For example, the presence of molecules and dust in a primordial cloud favors the formation of

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low-mass stars instead of high-mass stars. Low-mass stars produce less heavier elements than high-mass stars. Thus, chemistry also makes a difference on a large scale. Molecules can also be used as probes to measure the physical conditions like temperature and density in interstellar environments. Spectrally high-resolution observations at radio and infrared wavelengths have been the main technique to identify and investigate molecules in space. At radio wavelengths, the rotation of molecules can be observed whereas in the infrared their vibrations can be detected. For this, powerful radio telescopes such as the IRAM 30m, the ALMA telescope array, the Yebes observatory are used and infrared telescopes such as the IRTF and SOFIA (see figure 1) also made important contributions. Currently the space telescope JWST shows its power with new molecule detections [9].

## Laboratory-based research

Laboratory data is key to understanding molecular discoveries. Without the availability of molecular spectra, astrophysical observations cannot be interpreted. The chemical processes in space are surprisingly different to what we are used to here on earth. Terrestrial chemistry is often ‘wet’ chemistry, but in space the liquid phase is non-existent (if we ignore exo-planets). Only gas-phase and surface reactions on grains can occur. Understanding these processes is an important aspect of astrochemistry. How are molecules formed and destroyed in space? Since space has a lot of volume to offer but is mostly a low-density environment, even transient molecules can survive for long periods of time. For example, in the circumstellar shells around dying carbon stars many unsaturated and open-shell carbon chains can be found [10]. Also, many processes in space do not happen under thermodynamic equilibrium conditions. For example, late-type stars show mass-losses in the form of an expanding molecular and dust shell in which the temperature and density drop rapidly. It is often quite a challenge to produce the types of molecules seen in these astronomical environments in sufficient quantities in the laboratory so that they can be studied.

The first molecular species that form in the vicinity of late-type stars often consist of refractory materials such as metals, carbon, or silicates. Advanced production techniques like the laser-ablation method with a subsequent adiabatic expansion into a vacuum [11] combined with sensitive spectroscopic instruments, e.g., multi-pass optics or cavity-ringdown techniques [12], are required. Using this method, small molecules like FeO, TiO, AlO, $Si_2C$ and others have been investigated at radio and infrared wavelengths in our laboratory [13]. These molecules are believed to play a key role in the initial chemistry of circumstellar shells around old giant red stars. Some of these molecules are thought to act as seeds for dust formation. In astrophysics, dust is something tremendously important. It acts as coolant in star formation processes, but it also has a significant chemical function. Prior and during star formation dust enables surface reactions between atoms and molecules and thus enables the formation of more complex molecular species. For example, the formation of formaldehyde and methanol via carbon monoxide hydrogenation on a cryogenic surface (used as dust analog in a cold cosmic cloud) could be tested in the laboratory [14] and confirms astrochemical models and observations. Subsequent gas-phase reactions in warmed-up regions enable the formation of more complex organic molecules (COMs) which can be observed via radio telescopes [5]. It appears that COMs are found in star-forming regions around our galaxy and beyond, suggesting that carbon-based chemistry is a universal feature of our universe. The implication is that if life exists elsewhere in space, it is most likely also based on carbon chemistry.

This leads to another important question: where does our water, which we consider vital, come from and how does it form? Observations show that water is omnipresent in our universe. There are three main pathways to water formation, see figure 2. It is assumed that most of our water is formed on interstellar grain surfaces before and during the formation of stellar systems (e.g., our own solar system). Using ultra-high vacuum apparatus, it could be shown that under conditions similar to those in dense clouds or accretion disks of young stellar objects, hydrogenation processes of oxygen on dust grain analogs result in the formation of water [15]. Interestingly, the surface reactions produce an intermediate product, hydrogen peroxide (HOOH), which is not present in the gas phase scheme. Hydrogen peroxide, although initially bound to the dust particle, can detach from the surface in warmer regions in space and be detected as a free molecule in the radio wave range using its rotational spectrum. A first HOOH detection towards the star birth region ρ Ophiuchus A [16] suggested that surface reactions are indeed at play. However, further observations of other objects, including young stellar objects, could not provide any further evidence [17]. The situation remains ambiguous, i.e., it is not yet clear whether surface reactions or gas-phase mechanisms dominate.

Future experiments and observations will continue to elaborate on the chemical complexity and aspects of habitability of our universe with ever challenging questions. Here one interesting aspect is molecular chirality. Chirality is deeply rooted in organic processes and associated with life. For example: Has terrestrial homochirality its origin in cosmic processes? A few years ago, the first chiral molecular species (propylene oxide) was detected towards our galactic center (SgrB2) [19]. The observations did not provide any information about a possible enantiomeric excess. If anything, the enantiomeric excesses in

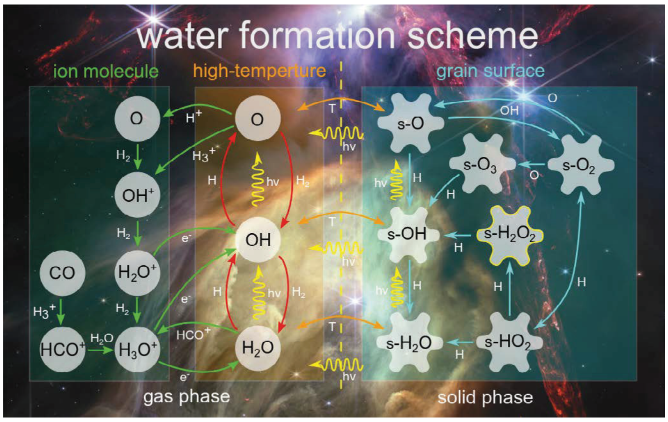

**Fig. 2**: Scheme of water formation in space [18]. Picture credit (background) Rho Ophiuchi cloud complex, the closest star-forming region to Earth by NASA/ESA/CSA James Webb Space Telescope, (foreground chemical scheme): Guido W. Fuchs

space are likely to be very small, and remote detection is an enormous technical challenge. But how wonderful would it be to know whether chiral symmetry is universal or not? We are working on it [20, 21]!

## Summary

The chemistry of outer space is different to what we are used to. Advances in the understanding of chemical processes in space not only require powerful telescopes but also dedicated laboratory experiments. Molecular species are valuable probes of physical conditions in space. Important questions such as where the chemical complexity in space comes from and whether we can find signs of chemistry that may lead to life are driving motives for modern research.

## Acknowledgements

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Guido Fuchs works at the University of Kassel as astrophysicist, molecular spectroscopist and experimental physicist. He leads a group working with laboratory apparatus to produce high-resolution spectra of astrophysically relevant molecules and that provides data for observational astronomers. He also performs own astrophysical observations using international telescope facilities. Fuchs did his PhD in Cologne, Germany in 2003 and worked at the Harvard-Smithsonian Institution, Cambridge, at the University of California, Berkeley (USA) and at the Observatory in Leiden, The Netherlands. He was editor-in-chief of Annalen der Physik and Laser Photonics Reviews.

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