Exploring the Surface Chemistry of Interstellar Dust

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Interstellar space may seem like the last place you would look for the chemical origins of life. However, many complex molecules are synthesised on interstellar dust grains. The unique structures of dust grain surfaces are believed to act as catalytic sites – allowing chemical reactions to occur.

The story of this process begins when a dying star ejects gas and dust – forming a cloud that cools and contracts over time. Hydrogen molecules, which are abundant at this stage, react with oxygen and carbon on dust grain surfaces to form simple molecules such as methanol and water – coating the grains with a layer of so-called 'dirty ice'.

As the cloud continues to collapse, its dense core may heat up, and begin to form a new star. This heat releases the frozen molecules on nearby dust grains, triggering the formation of organic molecules – including alcohols and aldehydes. The dust cloud then collapses into a disk encircling the star – which over time, coalesces to form asteroids, comets and planets.

In the coldest regions of such 'protoplanetary' disks, organic molecules become re-frozen on grain surfaces. This introduces further chemical complexity – potentially producing biological molecules such as amino acids, sugars, and nucleobases.

Our knowledge of these processes has been shaped by a combination of strategies – including theoretical models, lab experiments, and astronomical observations.

However, each of these approaches comes with limitations, preventing astrochemists from gaining a full understanding of how complex molecules form in interstellar space.

To overcome these limitations, Dr Albert Rimola at the Autonomous University of Barcelona turns to computational chemistry. This approach uses computer simulations to represent the steps of complex chemical reactions. Such steps include molecules binding onto dust grains, reacting with other molecules, and the chemical products being released from the grain surfaces.

In a recent study, Dr Rimola's team explored techniques that can simulate the surfaces of interstellar dust grains and the chemical processes they catalyse.

The first technique is 'quantum chemistry', which uses calculations to determine how individual electrons and atomic nuclei interact with each other. Quantum chemistry allows for incredibly precise simulations – but these models are limited to systems of hundreds of atoms or less.

This approach can be combined with lab experiments and astronomical observations. This is quicker and less costly, allowing researchers to simulate larger chemical systems – but comes with lower accuracy.

The second approach is molecular dynamics simulations. These ignore electrons and their interactions, and instead describe chemical systems using 'ball and spring' models – where atoms are the 'balls' and bonds are 'springs'. This approach is less accurate, but its reduced complexity allows researchers to simulate systems containing thousands of atoms. This enables them to recreate complex molecular systems, but not chemical reactions.

By drawing these approaches together, and assessing their capabilities, Dr Rimola's team hopes that their study could spark a wave of research into the computational chemistry of interstellar dust grains. Their research may also expand to consider the surface chemistry of comets and asteroids – which may have delivered biological molecules to Earth.

The team believes that computational chemistry could offer clues about the emergence of life on Earth, and even planets beyond our solar system.

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