

Key to carbon-free cars? Look to the stars

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Credit: AI-generated image ([disclaimer](#))

For nearly half a century, astrophysicists and organic chemists have been on the hunt for the origins of C_6H_6 , the benzene ring—an elegant, hexagonal molecule comprised of 6 carbon and 6 hydrogen atoms.

Astrophysicists say that the benzene ring could be the fundamental building block of polycyclic aromatic hydrocarbons or PAHs, the most basic materials formed from the explosion of dying, carbon-rich stars.

That swirling mass of matter would eventually give shape to the earliest forms of carbon—precursors to molecules some scientists say are connected to the synthesis of the earliest forms of life on Earth.

Paradoxically, PAHs have a dark side, too. The [industrial processes](#) behind crude oil refineries and the inner-workings of gas-powered combustion engines can emit PAHs, which can snowball into toxic air pollutants like soot.

Exactly how the first benzene ring formed from stars in the early universe—and how combustion engines trigger the chemical reaction that alters the benzene ring into soot particle pollutants—have long mystified scientists.

But now, researchers at Lawrence Berkeley National Laboratory (Berkeley Lab), the University of Hawaii at Manoa, and Florida International University have demonstrated the first real-time measurement, using lab-based methods, of unstable particles called [free radicals](#) reacting under cosmic conditions, prompting elementary carbon and hydrogen atoms to coalesce into primal benzene rings.

The researchers say that their findings, recently published in the journal *Science Advances*, are key to understanding how the universe evolved with the growth of carbon compounds. That insight could also help the car industry make cleaner combustion engines.

A type of free radical called the propargyl radical (C_3H_3) is extremely reactive due to its propensity for losing an electron, and has been implicated in soot formation for decades. Researchers believed that the recombination of two free propargyl radicals, $C_3H_3\cdot + C_3H_3\cdot$, gave rise to the first aromatic ring, benzene.

The current study is the first demonstration of the so-called "radical

propargyl self-reaction" under astrochemical and combustion conditions. Using a high-temperature, coin-sized [chemical reactor](#) called the "hot nozzle," the researchers simulated the high-pressure, high-temperature environment inside a combustion engine as well as the hydrocarbon-rich atmosphere of Saturn's moon Titan, and observed the formation of isomers—molecules with the same chemical formula but different atomic structures—from two propargyl radicals leading up to the [benzene ring](#).

The hot-nozzle technique, which co-senior author Musahid Ahmed, senior staff scientist in Berkeley Lab's Chemical Sciences Division, adapted 10 years ago at Berkeley Lab's Advanced Light Source (ALS) for synchrotron experiments, relies on vacuum ultraviolet (VUV) spectroscopy to detect individual isomers. The ALS is a type of particle accelerator known as a synchrotron that generates extremely bright beams of light ranging from infrared through X-rays.

The researchers steered the technique to arrest the propargyl radical self-reaction—which unfolds within microseconds—just before larger PAHs and subsequent soot form. The compelling result supports predictions from experiments led by co-senior author Ralf Kaiser, professor of chemistry at the University of Hawaii at Manoa, and quantum chemistry simulations formulated by co-senior author Alexander Mebel, professor of chemistry at Florida International University.

They believe that the finding could one day lead to cleaner combustion engines. Having more efficient gas engines, some analysts say, is still important, because it may take another 25 years before we can replace the entire fleet of gas cars with electric vehicles (EVs). Furthermore, equipping airplanes and the gas-powered component of hybrid plug-in EVs with cleaner [combustion engines](#) could help reduce CO₂ emissions contributing to climate change.

Ahmed said he plans to extend the methods employed to study PAH growth, and probe other systems of relevance to the DOE mission, such as water desalination and environmental science.

"We'd also like to go and catch a buckyball, C₆₀, one of nature's biggest clues to the secrets behind symmetry," Ahmed said.

Kaiser added that their research could help astronomers plot a carbon map of the universe, and zero in on the cosmic origins behind DNA's carbon frameworks.

More information: Long Zhao et al, Gas-phase synthesis of benzene via the propargyl radical self-reaction, *Science Advances* (2021). [DOI: 10.1126/sciadv.abf0360](https://doi.org/10.1126/sciadv.abf0360)

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