Surprisingly complex fingerprint of PAH molecules in space

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Astronomers searching for interstellar PAH-molecules interpret their data incorrectly. This is concluded by researchers from the University of Amsterdam (UvA), the Leiden Observatory, the Radboud University and NASA Ames Research Center. In a joint publication in the *Astrophysical Journal* they show that the infrared fingerprint of PAHs (polycyclic aromatic hydrocarbons) is far more complex than what was assumed thus far.

PAHs constitute a group of numerous organic molecules. As known to most people, they have a bad reputation as they are carcinogenic byproducts of for example combustion and grilled meat. However, PAHs are also found in many places in the Universe. For astronomers, they are important as they provide clues on how matter is formed in interstellar space and how it eventually evolves to form stars and planets.

The characteristic infrared radiation emitted by interstellar PAHs is a powerful means to identify these molecules. However, distinguishing the radiation emitted by PAHs from other radiation sources is far from trivial. Astronomical data are analyzed by comparison with databases containing a large body of PAH infrared spectra (the fingerprints). These spectra are based on theoretical calculations and laboratory experiments.

Complex fingerprint

To date, astronomers have not been able to identify individual PAH molecules. The current experiments, that were done at the UvA, may now change this. The researchers studied the molecule naphthalene, a relatively small PAH, using advanced laser spectroscopic methods under the same conditions as present in interstellar environments.

"According to textbook knowledge, we would have expected to find maybe three absorption bands in this range of the spectrum", says Jos Oomens, who works at the FELIX Laboratory of Radboud University. "Therefore, we were pretty surprised to see a spectrum with about twenty fairly strong bands. This means that the standard theoretical models we use are far too simple."

Quantum-chemical calculations

To rationalize these observations, the researchers developed a novel quantum-chemical approach to calculate and predict PAH spectra. The improved methods will provide astrochemists with considerably better fingerprints for an extensive series of PAH molecules, allowing for a much more detailed analysis of astronomical data.

A scenario which is now coming within reach is one in which astronomical observations can be translated directly into specific PAH compositions. Dr. Annemieke Petrignani, experimental astrophysicist at the Leiden Observatory, is very enthusiastic. Earlier this year she received a VIDI grant from NWO to determine the composition, sizes and shapes of interstellar PAHs, working in collaboration with researchers at the UvA and Radboud University. Petrignani: "PAHs are 'hot', there is a tremendous need for characteristic spectral fingerprints of these molecules and to understand these fingerprints at the most fundamental level."

More information: High-resolution IR absorption spectroscopy of

polycyclic aromatic hydrocarbons: the realm of anharmonicity. Elena Maltseva, Annemieke Petrignani, Alessandra Candian, Cameron J. Mackie, Xinchuan Huang, Timothy J. Lee, Alexander G. G. M. Tielens, Jos Oomens & Wybren Jan Buma. *Astrophys. J.*, 2015, DOI: 10.1088/0004-637X/814/1/