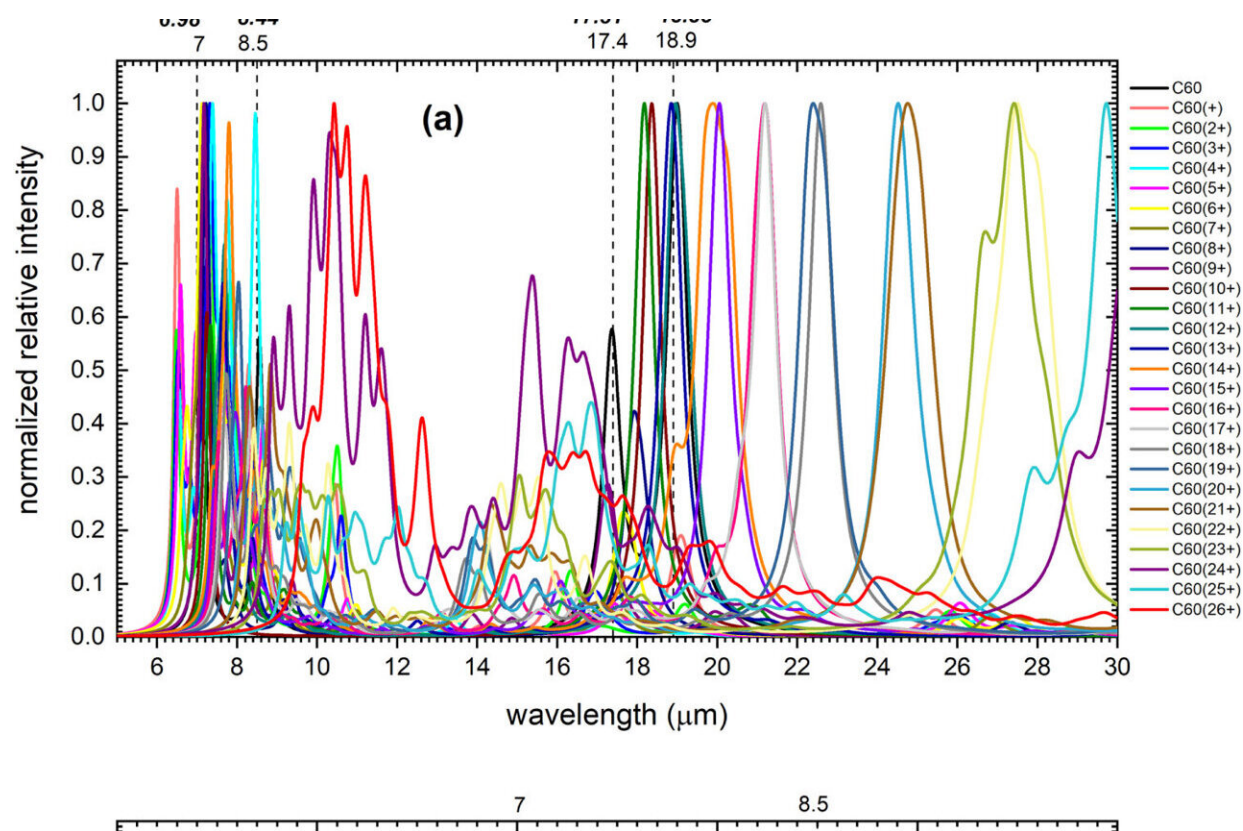


Infrared spectra of highly positively charged C60 fullerenes and their relevance to unidentified infrared emission

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Simulated infrared spectra of C60 fullerene and its 26 cationic forms. Simulation parameters: $T = 500$ K and $\text{FWHM} = 0.03$ μm . Dashed vertical lines are peak position of fullerene UIE bands. Their corresponding gas-phase experimental values from Table 2 in bold italic. a) Full range spectra at wavelength range 6–30 μm , b) 5–10 μm and c) 10–30 μm wavelength range. Credit: *The Astrophysical Journal* (2022). DOI: 10.3847/1538-4357/ac75d5

Is there now at long last some plausible theoretical basis for the molecular origins and carriers of at least some of the most prominent unidentified infrared emission (UIE) bands that have mystified astronomers for decades?

The theoretical astrophysicists and astrochemists at the Laboratory for Space Research (LSR) and the Department of Physics at the University of Hong Kong (HKU) seem to think so, at least in theory, in a peer-reviewed paper just published in *The Astrophysical Journal*.

A team led by Dr. SeyedAbdolreza Sadjadi, member of the LSR, and Professor Quentin Parker, Director of the LSR in the Department of Physics, has now placed some interesting theoretical work into the mix. It identifies highly ionized species of the famous football-shaped buckminsterfullerene C₆₀ molecule as plausible carriers of at least some of the most prominent and enigmatic UIE bands that have challenged astronomers since they were first discovered and studied over 30 years ago.

First, Dr. Sadjadi and Professor Parker proved theoretically that C₆₀ could survive in stable states from ionization up to +26 (i.e., 26 of the 60 electrons in the buckyball being removed) before the buckyball disintegrates (Sadjadi & Parker 2021). Now they have shown, by applying first principles quantum chemical calculations, what theoretical mid-infrared signatures of these ionized forms of fullerene can be expected. The results may at last provide at least a partial resolution of this enduring astrophysical mystery.

Professor Parker said, "I am extremely honored to have played a part in the astonishingly complex quantum chemistry investigations undertaken by Dr. Sadjadi that have led to these very exciting results. They concern

first the theoretical proof that fullerene carbon 60 can survive to very high levels of ionization and now this work shows the infrared emission signatures from such species are an excellent match for some of the most prominent unidentified infrared emission features known. This should help re-invigorate this area of research."

The HKU lead team found that some of these positively charged fullerenes show strong emission bands that closely match the position of key astronomical UIE emission features at 11.21, 16.40 and 20–21 micrometers (μm). This makes them key target species for identification of the currently unidentified UIE features and provides strong motivation for future astronomical observations across the mid infrared wavelength range to test these [theoretical findings](#).

They also found that the IR signatures of the group of these C_{60} cations with $q=1-6$ are well separated from the 6.2 μm bands, that are associated with free/isolated aromatic hydrocarbon molecules (so called PAHs, another potential carrier of UIE). This significantly aids in their identification from other potential carriers. This finding is particularly important for discrimination and exploration of the coexistence of complex hydrocarbon organics and fullerenes in astronomical sources.

Dr. Sadjadi said, "In our first paper we showed theoretically that highly ionized fullerenes can exist and survive the harsh and chaotic environment of space. It is like asking how much air you can push out of a football and the ball still maintains its shape. In this paper, we worked with two other leading astrophysicists and planetary scientists Professor Yong Zhang and Dr. Chih-Hao Hsia , both ex-HKU staff but still affiliated to the LSR, to determine the molecular vibrational notes of a celestial symphony, i.e., the spectral features that these ionized buckyballs would play/produce. We then hunted for them in space showing their notes/signatures are easily distinguishable from PAHs."

More information: SeyedAbdolreza Sadjadi et al, A Theoretical Study of Infrared Spectra of Highly Positively Charged C60 Fullerenes and Their Relevance to Observed UIE Features, *The Astrophysical Journal* (2022). [DOI: 10.3847/1538-4357/ac75d5](https://doi.org/10.3847/1538-4357/ac75d5)

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