Polycyclic Aromatic Hydrocarbon Molecules in Comets

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Polycyclic aromatic hydrocarbon (PAH) molecules, ubiquitously seen in the interstellar medium (ISM) of our own and external galaxies, might have been incorporated into comets if they are formed from relatively unprocessed interstellar matter. The detection of PAHs in comets would be an important link between the ISM and comets and the solar system formation. While there is yet no definite detection in comets of the infrared (IR) emission features at 3.3, 6.2, 7.7, 8.6 and 11.3 μm which are commonly attributed to PAHs, small PAHs (naphthalene $C_{10}H_8$, phenanthrene $C_{14}H_{10}$, pyrene $C_{16}H_{10}$, perylene $C_{20}H_{12}$) have been found in the *Stardust* samples collected from comet 81P/Wild 2, in the *Rosetta* samples collected from comet 67P/Churyumov-Gerasimenko, and in interplanetary dust particles possibly of cometary origin. In principle, IR spectroscopy could also provide identification of these small molecules, provided that they are sufficiently abundant and the telescope instrument is sufficiently sensitive. With the advent of the *James Webb Space Telescope* (JWST), this may become possible due to its unprecedented sensitivity. With an aim to offer spectroscopic guidance for JWST to search for these PAH molecules in comets, we model the vibrational excitation and calculate the IR emission spectra of these small PAH molecules in cometary comae, illuminated by the Sun at a range of heliocentric distances (r_h = 0.5, 0.75, 1, 1.5, 2, 3, 5 AU). By comparing the observed IR emission spectra of comets with the model spectra, one will be able to derive (in case of detection) or place an upper limit on (in case of nondetection) PAH production rates in comets.