JWST and PAHs in Protoplanetary Disks: Placing Constraints on the PAH Properties and Disk Structures

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The 3.3, 6.2, 7.7, 8.6 and 11.3 μm emission features of polycyclic aromatic hydrocarbon (PAH) molecules have been detected in protoplanetary disks (PPDs) around Herbig Ae/Be stars and T Tauri stars. PAHs are present at the disk surfaces and even in the cavity or gaps from which large grains are missing. They play an important role in the thermal budget and chemistry of the gas in PPDs, by providing photoelectrons for heating the gas and large surface areas for chemical reactions. Stochastically heated by a single UV/visible photon, PAH emission is spatially more extended than large grains and therefore, PAH emission can resolve PPDs more easily and is a powerful tracer of the disk structure.

Due to their limited sensitivities, it was not possible for ISO or Spitzer to spatially resolve PAH emission in PPDs. Indeed, so far almost all spatially-resolved observations of PAH emission were made by ground-based telescopes. Also, the low detection rate of PAH emission in T Tauri disks is probably related to their faintness. With its unprecedented sensitivity, JWST is expected to detect and spatially resolve PAH emission at all the major bands in a much larger sample of Herbig Ae/Be and T Tauri disks. This will enable far more detailed band analysis than previously possible.

To facilitate the analysis, interpretation and modeling of the incoming JWST data of PAH emission in PPDs, we develop a PAH spectral and band-ratio (i.e., $I_{6.2}/I_{7.7}$, $I_{11.3}/I_{7.7}$) library. This library will serve as a quantitative diagnostic tool for determining the PAH size and ionization fraction from the observed band ratios of the PAH emission features at 6.2, 7.7 and 11.3 μm.

We calculate the IR emission spectra of both neutral and ionized PAHs of various sizes, located at various radial distances (from the central star) in PPDs around stars of a wide range of spectral types and of several representative luminosities. We create a library of PAH model emission spectra and model band ratios and generate a series of diagrams of $I_{6.2}/I_{7.7}$ vs. $I_{11.3}/I_{7.7}$. To demonstrate the effectiveness of this diagnostic tool, we apply the model $I_{6.2}/I_{7.7}$ vs. $I_{11.3}/I_{7.7}$ diagrams to infer the PAH size and ionization fractions of a number of PPDs of representative properties (for all of which PAH emission has been detected and spatially resolved).