Polycyclic Aromatic Hydrocarbons in Protoplanetary Disks:

The 6.2/7.7 and 11.3/7.7 Band Ratios as a Diagnostic Tool

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Protoplanetary disks (PPDs) frequently emanate the so-called unidentified infrared emission (UIE) features in their infrared (IR) spectra (e.g., Seok & Li 2017). Major UIE features appear at 3.3, 6.2, 7.7, 8.6, 11.3, and 12.7 μm, commonly attributed to polycyclic aromatic hydrocarbon (PAH) molecules. PAHs play crucial roles in the evolution of PPDs physically and chemically. Exposed to ultraviolet photons from the central star, PAHs re-emit the absorbed energy through their vibrational relaxation via available internal modes at IR wavelengths. The relative strengths of the PAH emission bands prominently vary depending on the physical properties of PAHs such as their size (N_C) and charge state (ϕ_{ion}), which sensitively reflect the local conditions of PPDs.
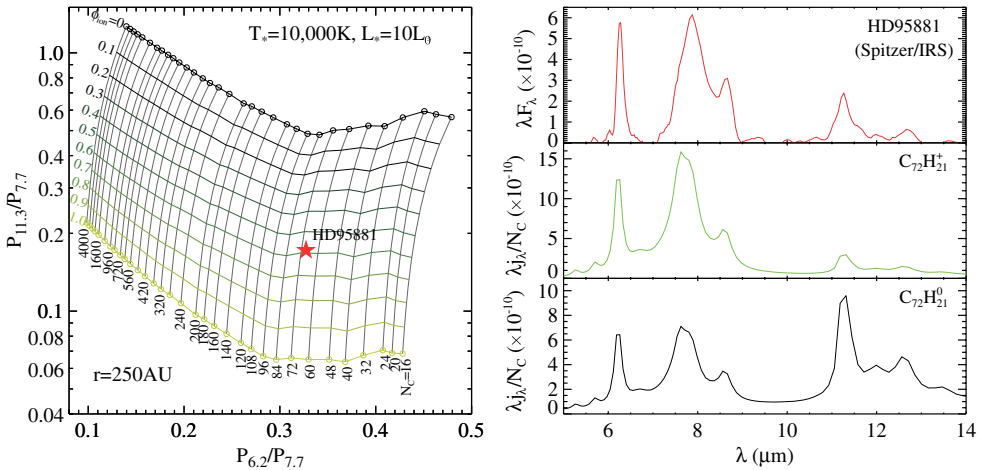

Figure 1. *Left*: A model grid of $I_{6.2}/I_{7.7}$ vs. $I_{11.3}/I_{7.7}$ for $T_{eff} = 10,000$ K, $L = 10L_\odot$ and $r = 250$ au with band ratios of HD 95881 (star symbol). *Right*: The Spitzer/IRS spectrum (top) is compared with model spectra of ionized (middle) and neutral (bottom) PAHs with $N_C = 72$.

Adopting the Astro-PAH model of Draine & Li (2007) and Li & Draine (2001), we carried out model calculations to quantitatively interpret the PAH features observed in various PPDs, taking a wide range of stellar properties such as effective temperature (T_{eff}) and luminosity (L_*) as well as PAH properties such as N_C, ϕ_{ion}, and radial distance from the central star (r) into account. For a given T_{eff}, the model emission spectra of ionized and neutral PAHs with N_C at various L_* and r are calculated. Grid diagrams of the 6.2/7.7 band ratio versus the 11.3/7.7 band ratio as a diagnostic tool allow us to

directly compare observed band ratios with the models and to easily infer N_{C}, ϕ_{ion}, and the local physical conditions where PAHs reside. As an example, a model grid for HD 95881 is shown in Fig. 1, from which we infer that PAHs in HD 95881 at $r = 250$ au are dominated by a mixture of ionized and neutral PAHs ($\phi_{\mathrm{ion}} \approx 0.6$) with a moderate size of $N_{\mathrm{C}} = 72$.

References

Draine, B. T., & Li, A. 2007, *ApJ*, 657, 810
Li, A., & Draine, B. T. 2001, *ApJ*, 554, 778
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