PAHs and 2175 Å Extinction Bump at the Cosmic Dawn

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The 2175 Å extinction bump, first detected in 1965, is the most prominent spectroscopic feature of the interstellar extinction curve. Widely seen in the interstellar medium (ISM) of the Milky Way (MW) as well as several nearby galaxies, this bump was recently detected by JWST/NIRSpec in JADES-GS-z6-0, a distant galaxy at $z \approx 6.71$ (Witstok et al. 2023). Although it is generally attributed to carbonaceous dust grains, specifically polycyclic aromatic hydrocarbons (PAHs) or nano-sized graphite, the exact carrier of the bump remains unknown. We calculate the electronic absorption spectra of a large number of PAH molecules by means of TD-DFT and meticulously examine the absorption peaks attributed to $\pi^* \leftarrow \pi$ transitions of each molecule near 220 nm in terms of central wavelength, width, and intensity (Lin et al. 2023). It shows that the absorption bumps tend to peak at slightly longer wavelengths for larger PAH molecules, while their bump widths are randomly distributed around $\gamma = 1.0 \ \mu m^{-1}$ regardless of size. By assigning proper weights for different molecules, both the Galactic 2175 Å extinction bump and that at z = 6.71 can be closely explained by mixture of PAH molecules. The derived total PAH abundance in JADES-GS-z6-0 is $\eta_{PAH} = 2.34 \times 10^{16} \text{ cm}^{-2}$, which is about ten times smaller than that of the MW. On the other hand, JADES-GS-z6-0 appears to favor larger PAHs (with a mean size of $N_{carbon} = 53$) compared to those in the MW ($N_{carbon} = 39$), indicating that active star formation at Cosmic Dawn may have preferentially destroyed smaller PAHs.