Investigating the Origins of UIR in the ISM: Theoretical Calculations of Imino-Group-Containing PAHs

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Polycyclic aromatic hydrocarbons (PAHs) and PAH-related species have been proposed as candidates for interstellar matter (ISM) responsible for unidentified infrared (UIR) emission. However, since the origin of UIR has not yet been fully identified, it remains important to explore alternative possibilities.

Previous studies have examined nitrogen-containing PAH-related species, such as amino groups and heterocyclic compounds. Given the diversity of nitrogen-containing functional groups, this study compares and analyzes the IR spectra of PAH-related species bearing various nitrogen-containing groups. In particular, this study focuses on PAH-related species containing imino groups (–C=NH), which exhibit trends similar to UIR, and performs analyses using density functional theory (DFT) calculations.

Nitrogen-substituted PAH-related species offer several advantages over PAHs in their vibrational spectra[1),2)]. These include enhanced IR intensity due to the introduction of highly electronegative nitrogen atoms, and the appearance of nitrogen-related vibrational peaks near the major UIR bands at 3.3, 6.2, 7.7, 8.6, 11.2, and 12.7 μm. On the other hand, when an N–H bond is present, as in amino groups, strong N–H stretching vibrations appear at 2.9–3.0 μm; however, such features have not been confirmed in astronomical observations[3)]. This discrepancy suggests the need for a revised model of nitrogen-containing PAHs.

We found that some imino-substituted PAH-related species exhibit spectral features consistent with observational data, particularly at 3.3, 6.2, 7.7, and 8.6 μm. Although these species contain N–H bonds, the IR intensity of the N–H stretching vibration is very weak in the neutral state. These results indicate that imino-substituted PAH-related species can retain the advantages of nitrogen incorporation while avoiding its previously identified drawbacks.

We report a theoretical investigation based on calculated IR spectra, demonstrating the potential of imino-substituted PAH-related species as candidates for UIR-emitting ISM.

References

1) Z. Peeters, et al., 2005, A&A, 432:2
2) B. A. McGuire, et al., 2018, Science, 359:6372
3)A. Vats et al.,2021,PASJ,74:1:161