Possible Molecular Origins of the Unidentified Infrared Emission Features in Planetary Nebulae

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Introduction

Proposed sources of unidentified infrared (UIE) features

- Polycyclic aromatic hydrocarbons (PAHs)
- Mixed aromatic/aliphatic organic nanoparticles (MAONs)

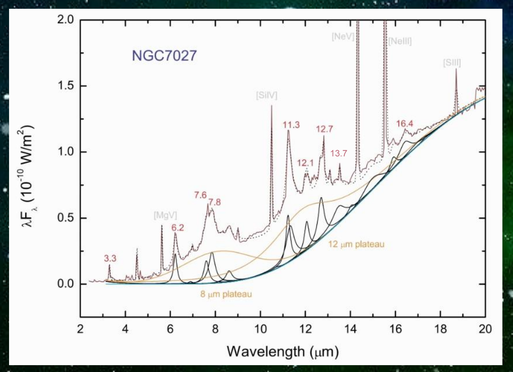

Figure 1. Infrared emission spectra of planetary nebulae NGC 7027 with UIE features in red. *Kwok, S. Astrophys Space Sci 367, 16 (2022).*

Table 1. UIE Features and Tentative Assignments

Wavelength (μm)	Wavenumber (cm^{-1})	Vibration
3.3	3030	C-H aromatic stretch[a]
3.4	2941	C-H aliphatic stretch[a]
6.2	1613	C-C stretch[a]
7.7	1299	C-C stretch[a]
8.6	1163	C-H in plane bend[a]
11.3	885	C-H out of plane bend[a]
13.3	769	C-H out of plane bend[a]

[a] *Kwok, S. Astrophys Space Sci 367, 16 (2022).*

Objectives

- Calculate IR spectra of candidate molecules
- Compare theoretical IR spectra to UIE spectra
- Find a candidate molecule that matches UIE spectra

Methodology

- Gaussview - build and visualize molecular structures
- Gaussian 09 - approximate Schrödinger equation and determine equilibrium structures
- B3LYP/6-31G** - method of density functional theory

Method Validation

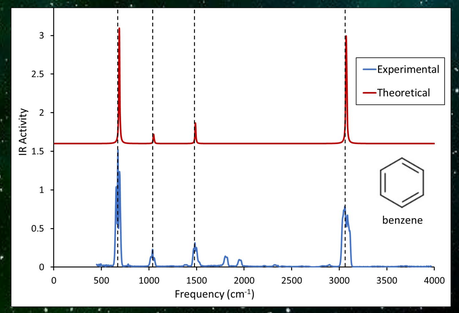

Figure 2. Method validation showing the theoretical and experimental IR spectra of benzene
Experimental Data from NIST Mass Spectrometry Data Center, William E. Wallace, director

Table 2. Peak Positions of Theoretical and Experimental Benzene Spectra

Experimental Wavenumber (cm^{-1})	Theoretical Wavenumber (cm^{-1})	Theoretical Wavelength (μm)	Difference (cm^{-1})
674	688	14.5	14
1038	1048	9.5	10
1482	1488	6.7	6
1814	-	-	-
1958	-	-	-
3058	3072	3.3	14

Results

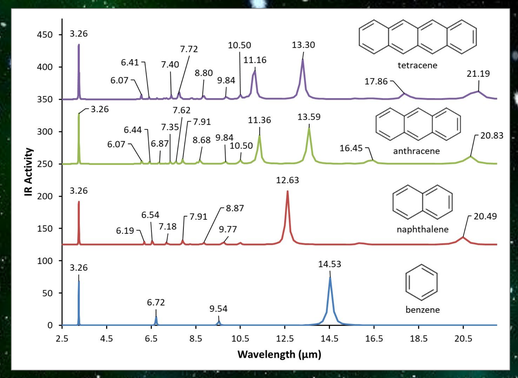

Figure 3. Calculated IR spectra of benzene and simple PAHs

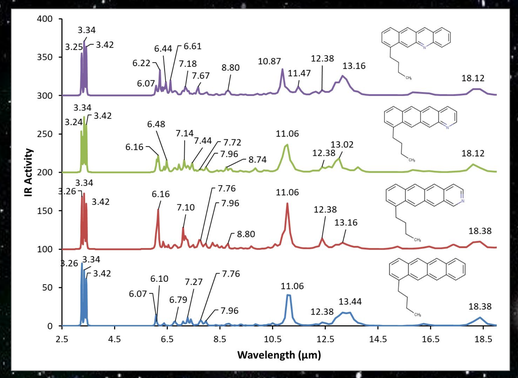

Figure 4. Calculated IR spectra of alkylated tetracene with nitrogen substitution

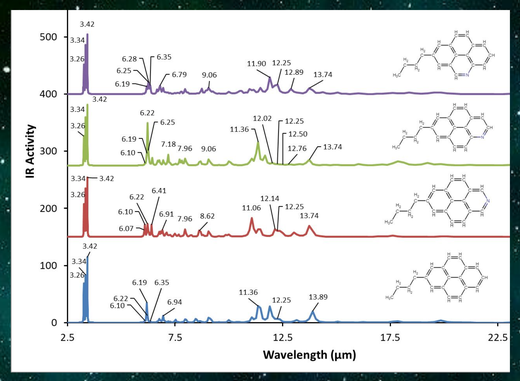

Figure 5. Calculated IR spectra of alkylated pyrene with nitrogen substitution

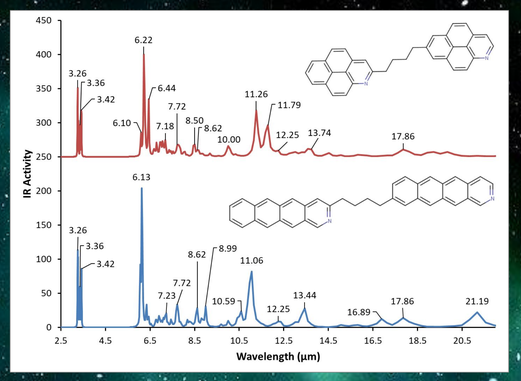

Figure 6. Calculated IR spectra of tetracene and pyrene dimers with nitrogen substitution

Dimer Molecular Structures

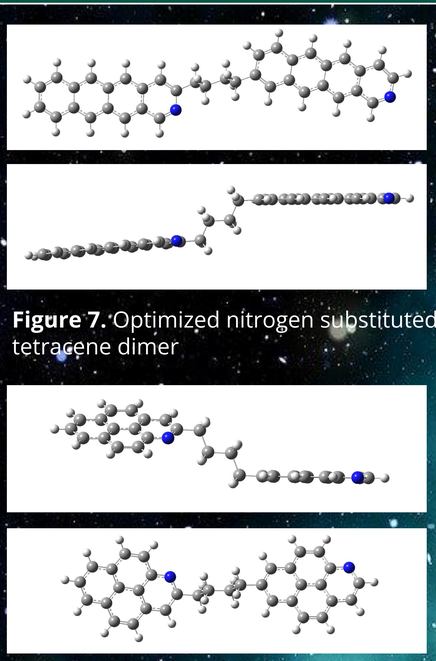

Figure 7. Optimized nitrogen substituted tetracene dimer

Figure 8. Optimized nitrogen substituted pyrene dimer

Conclusions

- Confirmed the 3.4 μm feature is from aliphatic chains
- Nitrogen substitution can enhance the intensity of the 6.2 μm feature depending on its location
- n-butyl linked nitrogen substituted pyrene and tetracene systems yield the 8.6 μm feature
- Need ≥ 3 fused rings for 11.3 μm and 13 μm features
- 12 μm feature present only after alkylating tetracene
- Pyrene's increased stability could make it a better candidate molecule

Future Work

- Construct 3D molecules containing pyrene and tetracene units
- Sulfur heteroatom substitutions
- Devise a method to make a quantitative comparison between calculated and experimental UIE spectra

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