Theoretical Study on the Complex Organic Molecules Origin of the UIE bands in Planetary Nebulae

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UIE Bands in Young PN



Despite their harsh environments, PNs can be the host of complex organic molecules Sun Kwok, Astrophys Space Sci, 319:5 (2009)



Quantum Mechanics & Quantum Chemistry

Forces define the system and the Hamiltonian \widehat{H}

 $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi \qquad \qquad \hat{H}\Psi = E\Psi$



Quantum Chemistry

BO One Many electron approximation

Guzman and Bader, Coord.Chem.Review, 249:633-662 (2005)



Applications of Quantum Chemistry

Direct modeling of the UIE bands carriers.

Understanding the vibrational origin of the UIE bands.

Search for the new species



Direct Modeling of the UIE Bands

Adding Aliphatic Groups to the PAH Core



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Direct Modeling of the UIE Bands

Mixed Aliphatic-Aromatic Organic Nanoparticles (MAONs)



We try to understand which fragments inside such a big molecule are responsible for the observed IR features. Then we can return back to the observations and track the existences of such fragments.

Sadjadi, Kwok and Zhang, Journal of Physics, Conference Series 728 (2016) 062003



Direct Modeling of the UIE Bands

Amorphous Hydrocarbon



Wavelength (µm)

Amorphous hydrocarbon shows a very complex bonding pattern, this makes the interpretation of IR spectrum very difficult. Here the advanced bonding model via quantum theory of atoms in molecules (QTAIM) is applied to reveal the nature of bonds.



The Origin of the UIE Bands

Vibrational analysis within the range of 3.3-3.4 µm



Sadjadi, Zhang and Kwok, ApJ, 845:123 (2017)

The Origin of the UIE Bands

Vibrational analysis within the range of 11-15 µm



Sadjadi, Zhang and Kwok, ApJ, 807:95 (2015)



Search for New Species

Molecules with Olefinic Functional Group



We provided an alternative new explanation that 6.0 µm feature is not due to CO but due to olefinic containing compounds (-C=C-) Hsia, Sadjadi, Zhang and Kwok, ApJ,832:213 (2016)



Search for New Species

Fulleranes



 $C_{60}H_{18}$ as one of the most kinetically and thermodynamically stable fulleranes shows unique IR feature at 15 µm. We use this feature to search for this species in space. Zhang, Sadjadi, Hsia and Kwok, ApJ,845:76 (2017)

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Babylon gate covered with the blue tiles One of the symbols of ancient chemistry (Window of the world) Shenzhen

