

Mixed Aromatic Aliphatic Organic Nanoparticles (MAON) as Carriers of Unidentified Infrared Emission Bands

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The unidentified infrared emission (UIE) phenomenon consists of a family of emission bands and broad emission plateaus superimposed on an underlying continuum. The most popular explanation for the UIE bands is the polycyclic aromatic hydrocarbon (PAH) hypothesis, but this model has a number of problems (Kwok & Zhang 2013; Zhang & Kwok 2015). While the UIE bands are likely to arise from stretching and bending modes of aromatic and aliphatic groups in a carbonaceous compound, the exact vibrational modes creating these bands and the exact chemical structure of the compound are not known.

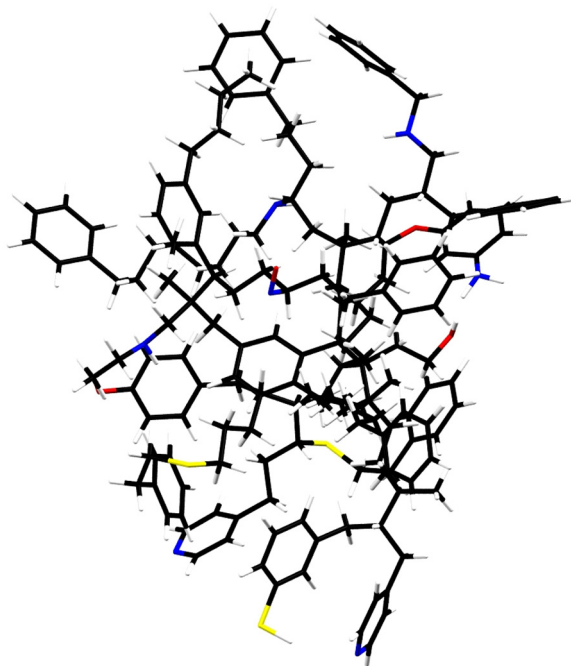


Figure 1. The MAON structure is characterized by a highly disorganized arrangement of small units of aromatic rings linked by aliphatic chains. This structure contains 169 C atoms (in black) and 225 H atoms (in white). Impurities such as O (in red), N (in blue), and S (in yellow) are also present. A typical MAON particle may consist of multiple structures similar to this one.

Some of the UIE bands are likely to be due to coupled vibrational modes and the identification of their exact nature is not trivial (Sadjadi, Zhang & Kwok 2015, 2017). We

report results of quantum chemistry calculations of large (>100 carbon atoms) molecules with mixed aromatic/aliphatic structures (MAON, Kwok & Zhang 2011, Figure 1) with the goal of identifying the origin of the UIE bands and exploring various possibilities of the chemical nature of the UIE carrier.

References

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