From Interstellar Ices to PAHs

A symposium to honor Lou Allamandola's Contributions to the Molecular Universe

Annapolis, MD, USA - September 13th to September 17th, 2015

INVITED TALK

PAH Database Fitting Techniques; A Paradigm Shift?

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It is now commonly accepted that the formerly, so-called, unidentified infrared emission bands (UIBs) are due to the relaxation of vibrationally excited polycyclic aromatic hydrocarbon (PAHs; see e.g., Rosenberg et al. 2014) and closely related species, such as PAH clusters, very small grains, HAC particles, etc. (see Omont 1983 and Tielens 2007 for very extensive and complete reviews). To further validate and examine the "PAH model", there has been a rapid increase in the number of available laboratory and density functional theory (DFT) computed PAH spectra over the past two-and-a-half decades. This has lead to the arrival of dedicated public databases, such as the Italian/French PAH database (http://astrochemistry.oa-cagliari.inaf.it/database/; Malloci et al. 2007) and the NASA Ames PAH IR Spectroscopic Database (http://www.astrochemistry.org/pahdb/; Bauschlicher et al. 2010, Boersma et al. 2014; PAHdb hereafter), that aim to provide consistent and high-quality spectroscopic data. For example, PAHdb now contains 75 experimentally measured and 700 DFT computed, critically evaluated, PAH IR spectra.

To utilize the wealth of data contained in these databases, new ways and tools have been developed to analyze astronomical PAH spectra, with the current paradigm moving towards a database fitting approach. However, before such an approach can be applied to astronomical PAH *emission* spectra, a PAH emission model is required to turn the, usually, PAH *absorption* spectra in these databases into PAH *emission* spectra. Over the past years, several approaches, incorporating different levels of detail of the PAH emission process, have been developed. A database fitting approach, in which a PAH emission model that takes the heat-capacity of different sized PAHs into account was combined with a non-negative least-square (NNLS; Lawson et al 1974) fitting technique, has now successfully reproduced the different A, B, and C Peeters et al. (2002) and van Diedenhoven et al. (2004) astronomical PAH spectral classes (Cami 2011).

The power of the database fitting approach lies in its ability to break the fitted PAH emission down into contributing PAH subclasses, i.e., charge, size, composition, and structure (hydrogen adjacency). Rosenberg et al. (2011) used this ability to confirm the nature of their principal PAH emission components (their "signals") derived from a blind signal seperation (BSS) analysis on the *Spitzer* spectral map of the northwest photon dominated region (PDR) in the reflection nebula (RN) NGC 7023. Subsequently, Boersma et al. (2013) showed that taking the database fitting approach itself as the starting point, results, when performed on the same PDR, in spectroscopic templates very similar to those determined by the BSS analysis.

Recently, Boersma et al. (2015) have been able to utilize the data and tools made available through PAHdb and exposed by the *AmesPAHdbIDLSuite* - a suite of object classes utilizing IDL's object programming capabilities - to *quantitatively* calibrate the 6.2/11.2 μm PAH band strength ratio in NGC 7023's northwest PDR as a PAH ionization fraction. Subsequently, the PAH ionization fraction could be tied to the PAH ionization parameter, which relates the strength of the exciting radiation field, the gas temperature and the electron density in the PAH emission zones to the PAH ionization fraction.

Current research focusses on extending and validating the database fitting approach and the charge calibration beyond the single RN NGC 7023. Preliminary results, which show that the spectroscopic templates derived from other RNe are consistent with that derived for NGC 7023 and that the *quantitative* calibration of the 6.2/11.2 μm PAH band strength ratio as a PAH ionization fraction is consistent across RNe, are very promising (Boersma et al. in preparation).

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