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Hydrocarbons in the ISM: Their Evolution and the Grain-to-Molecule Transition

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Abstract. The evolution of hydrocarbon grains in the ISM is determined, principally, by the effects of photo-processing (annealing) which lead to a progressive loss of hydrogen from the structure and an associated 'graphitisation' of the material. Eventually this 'graphitisation' results in a low-density, highly aromatic material that can disaggregate into its aromatic-rich molecular components. These changes are followed through the use of an extended random covalent network (RCN) model for the hydrocarbon structure. This type of 'top down' process could be a significant source of the large molecular infrared band carriers in photon dominated regions. On the basis of this simple model there should thus be a relationship between the small grain and large molecule infrared emission bands across, and within, astrophysical boundaries such as photo-dissociation regions.

Keywords. dust, extinction, ISM: general, ISM: molecules

1. Introduction

Carbon is the most abundant dust-forming element in the ISM and a large fraction of this carbon is in the form of grains comprised, principally, of hydrocarbon materials, including those where the hydrogen content is minimal. Interstellar hydrocarbon grains include: graphite, hydrogenated amorphous aliphatic and/or aromatic hydrocarbons (a-C, a-C:H) and (nano)diamond. These hydrocarbon dusts play a pivotal role in determining, amongst other things, the interstellar extinction, the dust thermal emission and the photo-electric heating of the gas in the ISM.

2. Hydrocarbon grains in the ISM

Hydrocarbon grains are formed in the circumstellar shells around C-rich evolved stars, in supernova ejecta and also in the ISM itself via accretion and solid-state chemistry. The physical and chemical properties of hydrocarbon grains are indeed complex and vary in response to the ambient conditions (density, temperature, radiation field, ...). For example they can undergo both chemical and physical processing (growth and changes in chemical composition through accretion and reaction, erosion via inertial or chemi-sputtering, photo-darkening or 'graphitisation', photo-disruption in intense radiation fields and fragmentation in interstellar shock waves).

Recently, using laboratory simulations of carbon dust analogues, Dartois, Muñoz Caro, Deboffle, *et al.* (2004,2005) have shown that hydrogen-rich (> 50 atomic % H) hydrocarbon solids can explain the observed interstellar absorption bands at 3.4, 6.85 and 7.25 μm. They also show that the thermal annealing of this material is accompanied by an increase in the aromatic component, i.e., a 'graphitisation'. Such a transformation and evolution of interstellar hydrocarbons was proposed by Duley, Jones & Williams (1989) and Jones, Duley & Wiliams (1990). This photon-driven process, acting on the hydrogen-rich hydrocarbon grains in the ISM that originate predominantly from carbon-rich evolved stars, will lead to a progressive loss of hydrogen and an associated 'graphitisation' and 'opening-up' of the structure. The end point of the 'graphitisation' process is then a low-density material that will disaggregate into its constituent aromatic molecular components and the necessarily-associated sp^3 and sp^2 carbon and hydrogen atom bridging structures, e.g., Duley (2000), Petrie, Stranger & Duley (2003).

In this work we follow the 'graphitisation' process using a random covalent network (RCN) approach that extends the work of Jones (1990). To summarise, the RCN model characterises a series of hydrocarbons based upon the sp^3/sp^2 carbon atom ratio (R) and the atomic fraction of hydrogen ($X_{\rm H}$) within the material. This model allows an essentially one-parameter determination of the a-C:H structure and a prediction of the major infrared bands. We find that the large hydrocarbon grains, with temperatures in equilibrium with the local radiation field, will be rather hydrogen-rich and that the smaller grains, which undergo stochastic heating to high temperatures, will be converted into hydrogen-poorer and more graphitic materials. The photo-fragmentation of the smaller aromatic grains can be an important source of molecular aromatic species.

The infrared spectrum of a given RCN hydrocarbon depends, principally, upon only its hydrogen content $X_{\rm H}$. The spectra predicted from this RCN model can then be compared with the interstellar absorption and emission bands in the 3–12 μm range. The compositional changes of a-C:H, and its constituent 'molecular' components, can then be mapped across a given region.

3. Conclusions

The physics and chemistry of hydrocarbon grains is complex. Interstellar hydrocarbon grains will be a mixture of many different forms arising from many different sources and modified in many different regions of the ISM. Nevertheless, we can appreciate how this complex material evolves chemically, structurally and physically as a function of the ambient conditions through the use of a rather simple, and extended, RCN model.

The transition/evolution of hydrocarbons in the ISM is, generally, from hydrogen-rich a-C:H, in the form of large grains formed around evolved stars, through to smaller, hydrogen-poor, low-density, aromatic a-C:H materials. The subsequent photo-fragmentation of the small aromatic grains could then be the origin of the aromatic emission band carriers within the ISM.

We find that the spectral and physical properties of hydrocarbons in the ISM vary in a systematic way across, and also within, astrophysical environments. However, the history of the particles, prior to their incorporation into a given region, could also play a major role in determining their physical properties in that region. Thus, the evolution of hydrocarbon grains in the ISM will be size-, time- and history-dependent. It is therefore necessary that dust models take into account this complexity in predicting the properties of hydrocarbons in the ISM.

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