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The Circle of Dust: From Nanoparticles to Macromolecules and Beyond

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There is increasing observational evidence that a non-negligible fraction of the cosmic carbon is locked up into macromolecules and nanoparticles. Carbonaceous nanoparticles and Hydrogenated Amorphous Carbon (HAC) nanoparticles represent one of the main components of interstellar dust. HAC nanoparticles have been proposed as a viable carrier for the Unidentified InfraRed (UIR) bands, which dominate the mid-infrared spectrum of almost any astronomical object. Fullerene molecules C_{60} and C_{70} have been detected in various circumstellar and interstellar environments. We present some of our recent results about the evolution of such carbonaceous structures and the possible connections between each other. We show how photo-processing of HAC nanoparticles can lead to the formation of C_{60} and C_{70} in space. There the low density of the gas precludes the formation of fullerene materials following known vaporization or combustion synthesis routes, even on astronomical timescales. We then discuss the processing of small hydrocarbon dust by energetic ions and electrons under extreme conditions, e.g., in shocked regions. Finally, we derive the astrophysical implications of such processing in terms of the observed emission.

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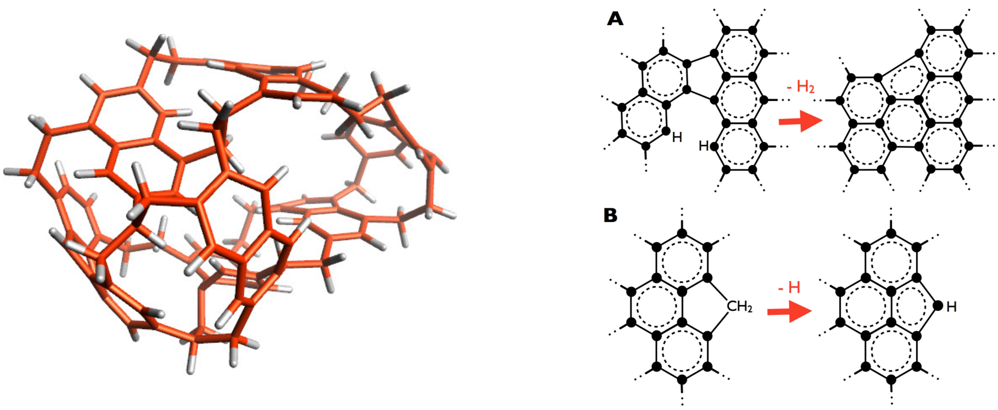

Figure 1: *Left* – A large and complex "arophatic" cluster ($C_{104}H_{80}$), precursor of cosmic fullerenes. Carbon in red, hydrogen in light gray. *Right* – Schematic view of two possible routes to aromatic pentagon formation (labeled A and B), leading to a loss of planarity, in HAC nanoparticles via aliphatic and olefinic ring system dehydrogenation. The filled circles represent carbon. *Figures adapted from [2].*

1. From HAC nanoparticles to C_{60} in space

Fullerenes C_{60} and C_{70} have been detected in space after a quest of 25 years [1]. They are made of hexagonal and pentagonal carbon rings, fused in the shape of a hollow sphere or ellipsoid (similar to a soccer and rugby ball respectively). The identification of a feasible formation mechanism for fullerenes in space has appeared immediately as not trivial. Our work [2] has shown that in space, the low density of the gas precludes the formation of fullerene materials following known vaporization or combustion synthesis routes [3, 4] even on astronomical timescales. The formation of C_{60} through dissociation-induced curvature of dehydrogenated PAHs [5] requires a specific tuning of the dissociation parameters and appears unlikely. The scheme for fullerene formation in space that we have proposed [2] is based on a top-down approach. The top of the tree is represented by Hydrogenated Amorphous Carbon (HAC) nanoparticles, i.e. materials whose presence in space has been firmly established [6, 7]. UV photolysis promotes structural transformations in the parent HAC particle with the formation of a novel entity: an "arophatic" cluster. This is a 3-D, hollow structure characterized by the presence of aromatic clusters linked by aliphatic bridging groups (Figure 1 – left panel). The crucial step is represented by the UV-induced dehydrogenation of the emerging arophatic cluster, which fulfils in a single step two essential conditions for the formation of fullerene molecules: 1) removing hydrogen atoms and 2) triggering pentagonal ring formation, and hence curvature, in the evolving structure (Figure 1 – right panel). The result is a large, vibrationally-excited fullerenic cage that shrinks down to the stable molecules C_{60} and C_{70} through emission of C_2 groups. The energy barrier for C_2 ejection from C_{60}, higher than that for the neighbours C_{58} and C_{62} [8] prevents further dissociation.

2. Collisional dissociation and excitation of HAC nanoparticles

HAC nanoparticles represent a major component of carbonaceous dust. In a hot (millions of degrees) gas, such as in the hot ionized medium of galaxies and in the intergalactic medium, they experience the effects of the bombardment by energetic ions and electrons (collisional processing)

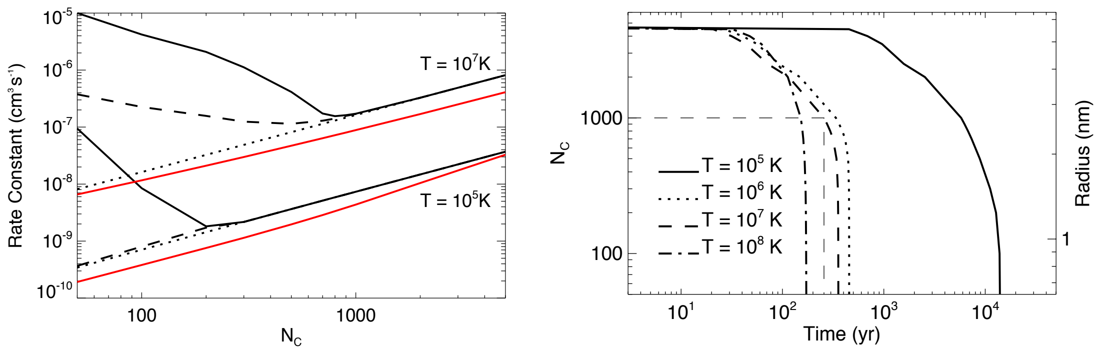

Figure 2: *Left* – Rate constant for carbon atom ejection from HAC nanoparticles (red, nuclear interaction only) and PAH molecules (black) in a gas with T = 10^5 K and T = 10^7 K. For PAHs, the dotted line shows nuclear interaction only, the dashed line the summed effects of nuclear and electronic interactions whilst the solid line includes electron collisions as well. *Right* – Time-dependent evolution of PAH molecules with N_C = 5000 carbon atoms, for a gas proton density n_H = 1 cm^{-3} and for temperatures ranging from 10^5 K to 10^8 K. *Figures reproduced from [14].*

both in terms of dissociation and excitation. To model the destruction of HAC nanoparticles via collisional processing, we compared the "molecular" approach for collisional processing, which I specifically developed for PAHs because they cannot be treated as small solid particles [9, 10, 11], with the "classical" approach developed for solid-state grains [12, 13]. We have found that the two approaches diverge for particles with less than 1000 carbon atoms (radius lower than 3 nm), but they are in very good agreement for larger grains (Figure 2 – left panel). The discrepancy arises from the fact that the classical approach only considers binary collisions between the projectiles ions and the target atoms (nuclear interaction). It does not take into account the interaction of the projectiles with the target's electrons (electronic interaction) nor collisions with electron projectiles, which are instead included in my molecular approach. Our work shows that, in order to quantify the erosion of small hydrocarbon grains a molecular approach, rather than classical sputtering, needs to be adopted [14].

Using this approach we have calculated the time-dependent evolution for a grain of a given size, shown in Figure 2 (right panel) for a hydrocarbon grain with 5000 carbon atoms in a gas with unit proton density and temperature ranging from 10^5 K to 10^8 K. The time-dependent evolution of grains with $N_C < 5000$ can be seen as a shift in time of the plot in the figure.

In terms of the excitation of HAC nanoparticles, we have evaluated the effects of collisional heating by energetic electrons on the observed emission spectrum of interstellar dust and made a comparison with the effects of photo-absorption [15]. Our results show that in a hot and tenuous medium like the halo of the galaxy NGC 891 (temperature of 10^7 K and density $n_H = 10^{-3}$ cm^{-3}) the energy absorption rate due to electron collisions is higher than the one due to photon absorption (Figure 3 – left panel). Collisional excitation increases the emission in the mid- and far-infrared regions of the spectrum (Figure 3 – right panel) and cannot be neglected.

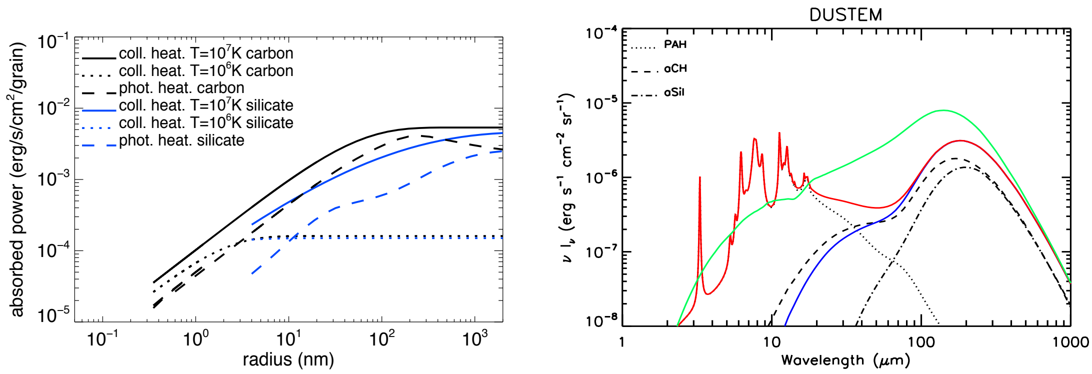

Figure 3: *Left* – Power absorbed per unit area per grain due to photon and collisional heating in the halo of the galaxy NGC 891, where $G_0 = 0.1$, according to our model. G_0 is the strength of the far-ultraviolet average interstellar radiation expressed in terms of the Habing field, this latter corresponding to about 10^8 photons cm^{-2} s^{-1} between 6 and 13.6 eV. The collisional heating has been computed for the proton density n_H = 10^{-3} cm^{-3} and the gas temperature $T_{gas} = 10^6$ and 10^7 K. The discontinuity around 1 nm in the carbon grains curves (black lines) arises from the transition between PAHs and HAC nanoparticles. *Right* – Dust SED for G_0 = 0.1 in the halo of NGC 891. The red and blue lines represent the SED due to photon heating only, with (blue line) and without (red line) imposing a minimum particle size of 2 nm. The green line represents the SED due to both photon and collisional heating with the particle size limitation of 2 nm. Black lines represent the contributors to the SED shown by the red line: PAHs, amorphous hydrocarbon particles (aCH, same as HACs) and amorphous silicates (aSil). *Figures reproduced from [15].*

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