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PAH processing in space

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Chapter 6

Conclusions and Perspectives

6.1 Key questions

As already mentioned in §1.6, the research described in this thesis aims to establish *how* the different conditions in the ISM affect PAHs, focusing on the *collisional* processing due to high velocity ions and electrons. These high velocities arise from the thermal and relative (inertial) motion induced in the gas by moderate velocity shocks, from the energy injected into the gas by very fast shocks (thermal motion), and from cosmic ray acceleration. In fact, a detailed study of the physics of the interaction between PAHs and high energy particles (ions and electrons) was lacking, although PAHs are a key component of the ISM and these processes play a crucial role in the evolution of PAHs. The first key question we addressed in this thesis is:

What happens to PAH molecules when bombarded by high energy ions and electrons? Will they be able to survive, maintaining their character, or will they be severely damaged or even completely destroyed?

From this it follows the second key question:

What are the astrophysical implications of PAH processing?

i.e.

What is the connection between the microscopic processes (ion/electron – PAH interaction) and the macroscopic effects on the interstellar PAH population?

6.2 Results

In **Chapter 2** we present a multiwavelength study of the complex environment of the supernova remnant N157B in the Large Magellanic Clouds. This chapter provides an analysis of a SNR and the different environments a PAH can find itself. The co-existence of various components, which besides the SNR include a molecular cloud, dust filaments, bubbles of hot shocked gas, an OB association and a HII region, makes this region a very good laboratory to study a variety of conditions PAHs can experience. From Spitzer photometric mapping and spectroscopy we find that there is no evidence of an infrared counterpart to the supernova remnant in the IRAC and MIPS images. The infrared emission is dominated by a cloud of dust/PAH and molecular gas adjacent to the remnant, containing the compact 2MASS source J05375027-6911071. This object has a diameter of about 3 pc, an electron-density of $100\text{--}250\text{ cm}^{-3}$, and is photo-ionized by an O8–O9 star. It is probably an open HII blister structure, seen from

the back. In spite of the projected overlap between the SNR X-ray emission and the infrared cloud, we find only weak emission from the shock-indicator [FeII], and both the excitation and the heating of the extended cloud are dominated by photo-ionization by the early O stars of LH 99. The absence of clear evidence of shocks implies that at present the molecular/dust cloud is not significantly impacted by the remnant. This suggests that the supernova progenitor was a moderately massive star of mass $M \approx 25 M_{\odot}$.

Chapter 3 and **Chapter 4** present the models we have developed and that allow for the first time a quantitative description of the collisional processing of PAH molecules by ions (H, He and C) and electrons with energies between 10 eV and 10 keV. Specific models were needed because PAHs are molecules and not small solid fragments, thus the classical approach from solid state physics cannot be applied. In a solid, the incoming energetic particle will transfer energy to a target atom. If more energy is transferred than the binding energy at the lattice site, a primary recoil atom is created. The primary recoil atom will collide with other target atoms distributing the energy via a collision cascade. In the PAH, the target atom is a single C atom, and if the energy transferred exceeds a threshold value, there will be no collision cascade but rather the atom will be ejected from the molecule. When treating a molecule then, there will be only “first” interactions, which can be conveniently described applying appropriated modifications to the binary collision approximation used for solids. The energy loss to the atomic electrons will not be distributed around the impact region, as in a solid, but spread out over the entire molecule because of the finite size of the PAH. The results in terms of PAH destruction cannot be extrapolated from the behaviour of dust grains and strongly depend on the kind of projectile and on the energies involved.

We have developed a model for the interaction of energetic ions and electrons with PAHs, taking the molecular aspects of this interaction fully into account. A schematic outline of the PAH destruction analysis is shown in Table 6.1. The interaction between PAHs and ions is described in terms of nuclear (elastic) and electronic (inelastic) energy loss, which can lead to carbon atom loss with consequent disruption and destruction of the molecules. The nuclear energy loss results from a binary collisions between the projectile and one single atom in the target. If the energy transferred exceeds a specific threshold, T_0 , a carbon atom is ejected. This is the case we are interested in, which has not been treated in previous studies. For the nuclear threshold energy we adopt $T_0 = 7.5$ eV as a reasonable value, but experimental determinations are necessary. The energy loss to the atomic electrons (electronic interaction) has been described in term of the stopping power of an electron gas with appropriate electron density (jellium approximation), adopting a geometry adequate to the shape and finite size of the PAH. For collisions with electrons having energies between 10 eV and 10 keV, we derived an analytical expression for the measured electron stopping power in graphite and applied this to the case of PAHs. The dissociation probability for a PAH excited by electronic interactions and electron collisions, has been derived using the theory of unimolecular reactions. The parameter E_0 , which governs the dissociation probability, is not well constrained. We adopt a value of 4.6 eV consistent with extrapolations to interstellar conditions but better determinations, relevant to the astrophysical situation, are needed.

Table 6.1 — Summary table for PAH collisions with ions and electrons.

Environment	Energy distrib.	Energy range (eV)	Projectiles			
			Ions		Electrons	
			Elastic (Nuclear) interaction	Inelastic (Elec.) interaction	Elastic (Nuclear) interaction	Inelastic (Elec.) interaction
Interst. Shocks ^a Chapter 3	Inertial	10 – 10 ⁴	✓ § 3.2 § 3.3.1	✓ § 3.3.2		
	Thermal	5 – 50	✓ § 3.2 § 3.3.1	✓ § 3.3.2		✓✓ ^c § 3.3.3
Hot Gas ^b Chapter 4	Thermal	10 – 10 ⁴	✓ § 4.2.2	✓ § 4.2.1		✓✓ ^c § 4.3
	CR energy distribution	5 MeV – 10 GeV		✓✓ ^c § 5.2	✓ § 5.3	
Cosmic Rays Chapter 5						

(a): Shock velocity, $v_S = 50 - 200 \text{ km s}^{-1}$.

(b): Gas temperature, $T = 10^5 - 10^8 \text{ K}$.

(c): For each environment the double check mark ✓✓ indicates the main agent for destruction of PAHs with $N_C = 50$.

In **Chapter 3** we use our models to estimate the lifetime of PAHs against collisions with ions and electrons having high velocities arising from the thermal and relative motions induced in the gas by moderate velocity interstellar shocks (v_s between 50 and 200 km s⁻¹ – cf. Table 6.1). We find that interstellar PAHs ($N_C \sim 50$) do not survive in shocks with velocities greater than 100 km s⁻¹ and larger PAHs ($N_C \sim 200$) are destroyed for shocks with velocities ≥ 125 km s⁻¹. For shocks in the $\approx 75 - 100$ km s⁻¹ range destruction is not complete and PAHs can survive, although their structure is likely to be severely denatured by the loss of an important fraction (20 – 40%) of the carbon atoms. The calculation of PAH lifetime against destruction t_{SNR} is $\sim 1.6 \times 10^8$ yr and $\sim 1.4 \times 10^8$ yr for $N_C = 50$ and 200 respectively. Small PAHs are preferentially destroyed by electrons, big PAHs by ions. These results are robust and independent of the uncertainties in the key parameters T_0 and E_0 that have yet to be well-determined experimentally. The calculated lifetimes are smaller than the values found for carbonaceous grains (6×10^8 yr) but close to that for hydrogenated amorphous carbon (2×10^8 yr), and far from the stardust injection timescale of 2.5×10^9 yr. The presence of PAHs in shocked regions therefore requires an efficient reformation mechanism and/or a protective environment.

In **Chapter 4** we adopt our models to evaluate the PAH survival time in a hot X-ray emitting gas with temperatures between 10^3 and 10^8 K (Table 6.1). In this case the high velocities of ions and electrons are due to the energy injected into the gas by very fast shocks (thermal motion). We find that the PAH destruction process is dominated by electron collisions for gas temperatures above $\sim 3 \times 10^4$ K, and by nuclear interaction with helium below this value. Small PAHs are more easily destroyed than larger ones below $\sim 10^6$ K, while the difference reduces significantly for a hotter gas. For a 1000 C-atom PAH, nuclear interactions are the dominant destruction process. In a hot and tenuous gas (e.g. M82 galactic outflows), PAHs with sizes between 50 and 200 C-atom are destroyed by electron collisions in few thousand years. In denser and colder regions (e.g. Orion), PAHs can survive for some 10^7 yr before being destroyed by nuclear interaction processes. X-ray photon absorption plays little role in PAH destruction in the hot gas associated with stellar winds and supernova explosions, with respect to electron collisions. Any PAHs observed near such regions have to be isolated from this hot gas and are presumably in a cooler PDR-type gas entrained in the stellar and galactic winds. In this sense, PAHs represent a good tracer for the presence of entrained denser material. The erosion of PAHs occurs via C₂ loss from the periphery of the molecule, thus preserving the aromatic structure. The PAH lifetime in a tenuous hot gas ($n_H \approx 0.01$ cm⁻³, $T \approx 10^7$ K), typical of the coronal gas in galactic outflows, is found to be about thousand years, orders of magnitude shorter than the typical lifetime of such objects, and also much shorter than the lifetime of an equivalent dust grain of roughly the same size ($a \approx 5$ Å). Thus, this might then imply that the destructive effects of ion and electron collisions with very small grains have previously been underestimated.

In **Chapter 5** we consider much more energetic projectiles, i.e. cosmic ray ions (H, He, CNO, Fe-Co-Ni) and electrons with energies between 5 MeV and 10 GeV (see Table 6.1). The energy loss of such high-energy particles required a specific treatment based on a different formalism with respect to the low-energy cases considered before.

Concerning the ions, the nuclear stopping is totally negligible, and the energy loss process is dominated by the electronic interaction, well described by the Bethe-Bloch equation (instead of the Lindhard & Scharff equation). The interaction of PAHs with high-energy electrons can be treated in terms of binary collisions between the incident electron and a single nucleus in the target, which is not the case at low energies. We evaluated the destructive effects of cosmic ray collisions on PAHs and estimate for how long the molecules can survive this ubiquitous cosmic ray bombardment in various environments (galactic disks, galactic halos, starburst galaxy outflows and cooling flow galaxy clusters). The cosmic ray spectra we adopt in the solar neighborhood are based on measurement near the Earth but corrected for the influence of the Heliosphere (solar modulation). To estimate the CR variation across the disk and in the galactic halo we adopt specific models based on γ -ray measurements. In external galaxies we scale the overall cosmic ray density with the star formation rate of the galaxy, and for galaxy clusters we adopt CR estimates based on γ -ray measurements.

We find that the timescale for PAH destruction by cosmic ray ions depends on the electronic excitation energy E_0 , the minimum cosmic ray energy $E_{\min}$ and the amount of energy available for dissociation. Small PAHs are destroyed faster with He and the CNO group being the more effective projectiles. The shortest survival time that we find is $\sim 10^8$ yr, which is comparable with the lifetime against destruction in interstellar shocks. Nevertheless, CRs are able to process PAHs in diffuse clouds, where the destruction due to interstellar shocks is less efficient. For electron collisions, the lifetime is independent of the PAH size and varies with $E_{\min}$ and the threshold energy T_0 , the minimum lifetime in this case is 1.2×10^{13} yr. Such a long timescale excludes cosmic ray electrons as an important agent for PAH destruction. In the halo of normal galaxies like NGC 891 and in the outflows of starburst galaxies like M82 the PAH lifetime against CR bombarding ($\gtrsim 10^8$ yr) is comparable to or longer than the circulation timescale between disk and halo and the starburst lifetime (~ 200 Myr and ~ 20 Myr respectively). In cooling flow galaxy clusters like A85 and Virgo the cosmic ray intensity is remarkably enhanced with respect to the solar neighborhoods, as a consequence the PAH lifetime is much shorter. Nevertheless, the survival time against CR bombardment is at least two orders of magnitude longer than the PAH lifetime in a hot gas ($1 - 10^3$ yr), implying that the molecules will be rapidly destroyed in the gas phase of the intracluster medium. In conclusion, PAHs dispersed in a hot gas filling galactic halos, starburst outflows and intracluster media are rapidly destroyed by collisions with thermal ions and electrons, but this mechanism is inefficient if the molecules are isolated from this gas in denser cloudlets. CRs can access the denser clouds and will set the lifetime of those protected PAHs, which can be used as an excellent ‘dye’ for tracing the presence of cold entrained material.

As a summary of this work we have evaluated the lifetime of PAHs in the interstellar medium of the Milky Way. We have adopted a 2 phase model for the ISM where matter is rapidly cycled between the Warm Intercloud and cold cloud phases. PAHs (and dust) are destroyed by supernova shocks in the intercloud phase. The timescale for supernova shock processing has been evaluated following McKee (1989) (cf. Chapter 3). Fig. 6.1 shows the timescale for cosmic rays and supernova shock waves to destroy PAHs, calculated assuming our reference values, $T_0 = 7.5$ eV and $E_0 = 4.6$ eV.

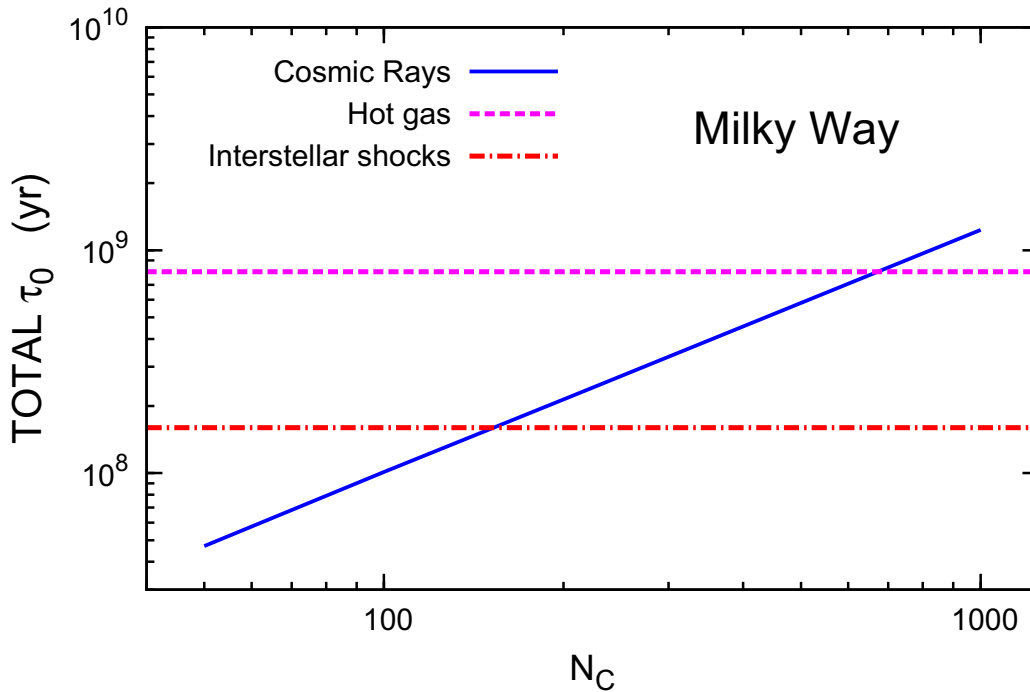


Figure 6.1 — Timescale for PAH destruction in the Milky Way by Cosmic Rays, interstellar radiative shocks ($50 \leq v_s \leq 200 \text{ km s}^{-1}$) and hot gas heated by adiabatic shocks with $v_s > 200 \text{ km s}^{-1}$, calculated assuming our reference values, $T_0 = 7.5 \text{ eV}$ and $E_0 = 4.6 \text{ eV}$.

The curve labelled cosmic rays refers to CR ion and electron in the Milky Way. The curve labelled interstellar shocks refers to low velocity shocks ($< 200 \text{ km s}^{-1}$) which cool radiatively, while the curve labelled hot gas refers to high velocity shocks ($> 200 \text{ km s}^{-1}$) when the supernova remnant cools through adiabatic expansion.

6.3 Answers to key questions

We are now able to answer the key questions listed in §6.1. Concerning the first question, we can say that the fate of PAHs when bombarded by high energy ions and electrons strongly depends on the energy range and energy distribution of the projectiles, and on the size of the target PAH molecule. PAHs with 50 carbon atoms, and more, can survive in shocks with velocities below 100 km s^{-1} , although their structure is likely to be denatured by the loss of carbon atoms due to inertial processing. Above 100 km s^{-1} they are totally destroyed by thermal collisions (**Chapter 3**), and the same happens in a million-degree gas (**Chapter 4**). In both shocks and hot gas, electrons are the main agent for destruction. When processed by high-energy (5 MeV – 10 GeV) particles from cosmic rays, destruction is due to inelastic collisions with ions (**Chapter 5**). In all considered cases big PAHs are more resistant than small PAHs.

Concerning the second key question, we first showed that, even in a region of spatially limited extent, interstellar PAHs can undergo a variety of conditions able to alter their characteristics (**Chapter 2**). Shock processing occurs predominantly in the warm intercloud phase of the ISM, while it is less efficient in diffuse clouds. On the

other hand, cosmic rays have access to all phases (except perhaps the densest molecular cloud cores) and can process all material. PAHs dispersed in a hot gas such as in galactic halos, starburst outflows and intracluster medium are rapidly destroyed by collision with electrons. This mechanism is inefficient if the molecules are isolated from this gas in denser cloudlets. However, cosmic rays can access these denser clouds and will set the lifetime of those protected PAHs, which can be used as a dye for tracing the presence of cold entrained material. This conclusion arises from combining the results from **Chapter 3**, **Chapter 4** and **Chapter 5** and highlights the connection between microscopic processing and macroscopic affects on the interstellar PAH population.

6.4 Future perspectives

The major source of uncertainty in our study resides in the choice of the two key parameters governing ion/electron collisions with PAHs: the nuclear threshold energy for PAHs T_0 which governs the elastic (nuclear) part of the ion/electron interaction with PAHs, and the fragment binding energy E_0 which governs the inelastic (electronic) part of the interaction. We explored a range of possible values and adopted $T_0 = 7.5$ eV and $E_0 = 4.6$ eV as reference. The value for T_0 is coherent with experimental determinations made on fullerene and carbon nanotubes which may be a reasonable analog for PAH molecules, but no measurement on PAHs are available. The value for E_0 is consistent with extrapolations to interstellar conditions, unfortunately the extrapolation technique is very model-dependent and the only laboratory data available refers to very small catacondensed PAHs with a very open carbon skeleton (e.g., naphthalene, anthracene, and phenanthrene), The data on astrophysically more relevant large pericondensed PAHs are missing, partly due to the difficulty in reproducing interstellar conditions on experimental timescales. The big picture resulting from our models is robust despite the large variability in the PAH lifetime induced by the uncertainties in the above parameters. Nevertheless, this variation emphasizes the importance of a better experimental determination of these quantities for PAHs under interstellar conditions.

Our models have been developed to treat ion and electron collisions with molecular targets, specifically PAH molecules with sizes between 50 and 1000 carbon atoms. Dust destruction models by Jones et al. (1994, 1996), which treat spherical dust grains using the approach for bulk particles, collect the smallest fragments (radius < 5 Å) in the smallest size bin and do not process them. We start from planar PAH molecules with a similar size (50 carbon atoms – disk radius ~ 6.4 Å), increasing progressively the number of carbon in the molecule and using an approach adequate for *molecular* target. It would be instructive to extend the PAH size up to the typical sizes for dust grains, to verify how far in size we can go with our molecular approach before getting discrepant results and to check whether and how the transition between the molecular and solid state domains takes place. In this way, the interrelationship of PAHs and small dust grains can be better understood (see § 1.2).

In this thesis we study the destructive effects on PAHs due to J-type (J for Jump) shocks, i.e. shocks where the physical conditions (density, temperature and velocity) change abruptly between the pre-shock and post-shock regions (cf. § 1.1.1). In this

case, the gas is suddenly stopped and heated to a high temperature and insignificant radiative and non-radiative relaxation can take place. A natural extension of this work would be the treatment of the other type of shock of interest in the interstellar medium, the C-type shocks, where C stands for continuous because the physical parameters vary smoothly across the shock front. Such shocks occur in a magnetized medium with a low degree of ionization (see § 1.1.1). In the diffuse ISM, the density may be 10^2 cm^{-3} with an ionization fraction of 5×10^{-4} . In molecular clouds, the density is higher, 10^4 cm^{-3} , and the ionization fraction is lower, 10^{-7} . In J-shocks the role of magnetic fields is reduced, whereas in C-shocks they can deeply modify the structure of the shock, leading to the existence of multi-fluid shocks where the neutral and charged fluids are decoupled and have to be described in term of magnetohydrodynamics. Guillet et al. (2007) studied the evolution of dust grains in C-shocks in molecular clouds, which requires a very different treatment with respect to the dust processing in J-shocks. The authors show that such shocks strongly modify the grain size distribution through erosion and vaporization processes that are modulated by the magnetic field and grain charge effects. An analogous study would be desirable for PAH in C-shocks, where they are one of the most important negative carriers, developing of course a physical model which fully takes into account the molecular nature of PAHs.

Our results indicate that PAHs do not survive the passage of shocks with velocities above $100 - 150 \text{ km s}^{-1}$ (depending on their size), while they can resist destruction in lower velocity shocks. Jones et al. (1996) proposed that PAHs can be produced in the post-shock region, by grain fragmentation in grain-grain collisions at shocked column densities of the order of $10^{17} - 10^{18} \text{ cm}^{-2}$. If the daughter PAHs are injected at velocities around 100 km s^{-1} , then they will be destroyed equally as well as the ‘primitive’ PAHs pre-existing the shock arrival. Only in low velocity shocks, or turbulent regions of the ISM, where grain-grain collisions happen at relatively low velocities (of the order of few km s^{-1}) and where there are no associated destructive processes are in operation, PAHs can form via fragmentation of big grains. Since the PAH lifetime in shocks - $\approx (2 - 4) \times 10^8 \text{ yr}$ - is much shorter than the injection timescale ($2.5 \times 10^9 \text{ yr}$), for PAHs we find the same conundrum as for dust grains, i.e. an inability to explain the observed high dust/PAH abundance because of their short lifetimes. Observations of PAHs in regions of the diffuse ISM affected by shocks faster than $100 - 150 \text{ km s}^{-1}$ would require an efficient (re-)formation route. However, because PAHs are a product of high temperature chemistry involving abundant carbon bearing precursors such as C_2H_2 and C_2H_4 , this is difficult to imagine in the low temperature diffuse ISM, which is an O-rich environment where the PAH precursors are not expected to be abundant. Further studies are required to clarify these points. Another interesting field of investigation is the *chemical* evolution of PAH after shock processing, both in terms of chemical reactions with impacting species, such as H, He, C and N, and in terms of the structural re-arrangement of the relic carbon skeleton into different species.

Our study of PAH survival in galactic halos has been stimulated by the observation of PAHs at high galactic latitudes in several normal galaxies with scale heights of $2 - 3 \text{ kpc}$ (Irwin & Madden 2006; Irwin et al. 2007; Whaley et al. 2009). Considering the specific case of NGC 891, the edge-on twin of the Milky Way, we assumed that UV photolysis is negligible in term of PAH destruction because of the decreased UV flux

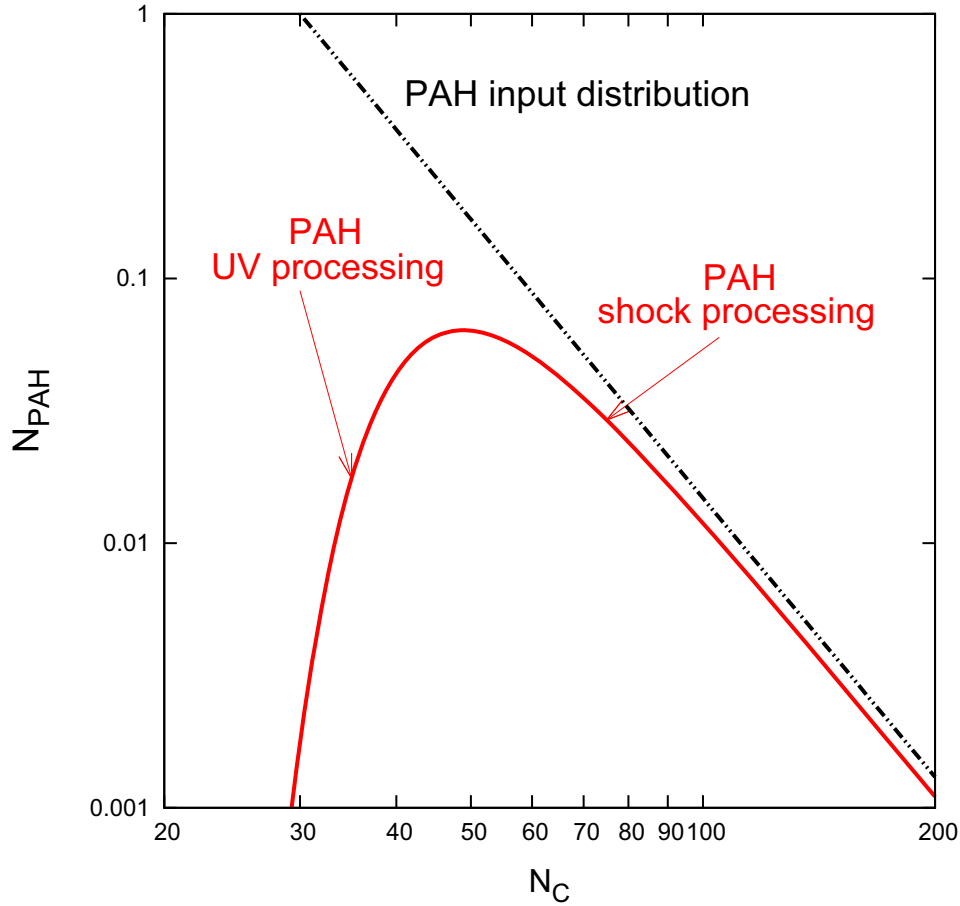


Figure 6.2 — Schematic representation of the PAH size distribution after processing (full line). The PAH input distribution (dot-dot-dashed line) and the major processes responsible for determining the size distribution are indicated.

with latitude. UV photolysis is generally considered to be the main agent for the destruction of small (< 50 C-atoms) PAHs (cf. Fig. 6.2), weeding out the less stable (eg., smallest and/or non-compact). Indeed, the minimum size in the PAH-size-distribution is thought to reflect this process. However, this process is very sensitive to size, and the minimum PAH size is not completely well established. It would be an interesting follow-up to make a more detailed study of PAH photoprocessing in the halo based on a precise modelling of the variation of the FUV field with latitude. Taking into account the possibility of local PAH production in the halo and the chemical destruction of PAHs, this study would provide a quantitative estimation of the role of PAHs as tracers of the entrainment process and the exchange between the cool and hot ISM phases on arcsecond size scales.

In this thesis we present examples of the application of our PAH processing models to specific observations, but our aim is of course to extend this application to a larger variety of objects showing the signatures of shock activity, typically supernova remnants, young stellar objects with supersonic jets, galactic outflows and regions characterized by large scale shocks and turbulence such as colliding galaxies. A very inter-

esting example of a large scale shocked region is the Stephan's Quintet (Moles et al. 1997), a compact group of galaxies where a galaxy collision produces a giant X-ray emitting shock that heats the gas to more than five million degrees (Appleton et al. 2006; Guillard et al. 2009).

Galliano et al. (2008a) and Dwek et al. (2009) considered the distinct formation and evolutionary trends for PAHs and dust in galaxies. They found that abundance of PAHs is observed to follow that of the carbon dust from AGB stars while the silicate dust follows the evolutionary trend for SN-condensed dust. The delayed injection of PAHs, from AGB stars, into the ISM provides a natural explanation for the paucity of these large molecules in low metallicity systems. The subsequent rise in the PAH-to-gas mass ratio with metallicity is then a natural consequence of the increasing contribution of AGB stars to the chemical enrichment of the gas in the ISM as they evolve off the main sequence. The success of their chemical evolution model, in reproducing the trend of PAH abundances with metallicity, strongly suggests the importance of stellar evolutionary effects in determining the abundances and composition of dust in galaxies. In particular such models can explain the presence of large amounts of dust in young dusty hyperluminous infrared galaxies in which supernovae are the only viable source of newly-condensed dust. The study of the temporal evolution of the formation and destruction processes of dust and PAHs traced back to the early universe, is also within the perspective of the new data that will be provided by the Herschel and JWST telescopes, and appears as a very promising research field for the future.