Polycyclic aromatic hydrocarbons in disks around young solar-type stars

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CHAPTER 1

Introduction

In the past decade, the topic of formation of low-mass stars comparable to our own Sun has become one of the most rapidly developing fields in modern astrophysics. The arrival of highly sensitive ground and space based telescopes at mid-infrared (IR) wavelengths has enabled us for the first time to study the faint solar-type young stars in nearby molecular clouds during their early formation phases. Many questions still remain unanswered. How many solar-type stars harbour circumstellar disks, what is the typical mass and size of those disks and how many of those remain long enough to allow planet formation to occur? What is the initial composition of the dust in the circumstellar disk and how does it evolve? How can the small grains grow to kilometer-sized planetesimals?

The aim of this thesis is to study the dust around solar-type young stars. In particular, we focus on one specific species of dust, namely the Polycyclic Aromatic Hydrocarbons (PAHs), a family of large molecules, or small grains, that have been widely observed in nearby star forming regions. We address the following questions. Are PAHs present in low-mass young star systems? Are they associated with the remnant cloud environment or located in the disks? What can we learn about their typical size, as a first step toward growth of larger grains? Can we use their presence as tracers of the structure and evolution of disks? How do they influence disk properties? What is their chemical evolution from cloud to disk?

In this introduction first a short overview of the properties and evolution of protoplanetary disks and PAHs is given, followed by a short description of our observing and modeling methods and ending with an outline of this thesis, the main questions and the main results.

1.1 PROTOPLANETARY DISKS AND THEIR EVOLUTION

A brief overview of our current understanding of intermediate and low-mass star formation, as it emerged in Shu et al. (1987), is given below. This picture is based and supported by the study of the nearest regions of isolated single-star formation.

Stars are formed within molecular clouds: cold ($T \sim 10$ K), dark, dense clouds of gas and dust at relative high density ($\sim 10^4 - 10^5$ cm^{-3}), with sizes of up to a parsec and mass between 10^2 and 10^3 $\mathrm{M}_\odot$. In terms of mass, the molecular gas dominates, with an assumed gas to dust ratio of 100 to 1. Although initially supported against gravitational collapse by magnetic fields and turbulence, random pockets of local overdensity will inevitably form. These overdense regions can develop into small cores of up to a few solar mass which can collapse, attract more mass and eventually develop into one or more stars. While the cloud matter continues to accrete inwards to the protostar, the non-zero angular momentum of the cloud will cause an accretion disk to form. At this point, the main source of energy is the release of gravitational energy by the contracting proto-star. This source is normally still completely embedded in the molecular cloud and thus unobservable at all wavelengths except at the millimeter and radio wavelengths. This phase is called the Class 0 phase, and is believed to happen relatively quickly (within 10^4 years after collapse).

As matter continues to fall onto the disk and accrete through the disk toward the star, a powerful stellar outflow can develop at both stellar poles, along the rotational axis. Evidence for these outflows has been observed in many cases. The accretion process through the disk heats up the dust and gas and, in addition to the millimeter, the source becomes also observable at infrared wavelengths. During this phase, the class 0–I stage, of about 10^5 years, the central star and hot dust in the inner disk can still be obscured by the surrounding envelope, depending on the inclination of the system and outflows toward the observer.

Inevitably the cloud material will run out and once the infall of matter onto the disk stops, the accretion rate of mass through the disk will drop off strongly, reducing the disk luminosity. Around the same time, the stellar wind from the central star will start to blow away the remaining low density cloud material above and below the disk and the entire system becomes visible at UV, optical and near-infrared wavelengths. This phase is called the Class II phase and can last from 10^6 to 10^7 years.

From 10^6 to 10^7 years, the star further contracts until hydrogen fusion starts in the center and it ends up at the zero-age-main-sequence. Gas and dust start to be removed from the disk through a variety of processes, including photo-evaporation. In the meantime, the dust in the high density regions of the disk is presumed to grow to micron and cm sized pebbles, through collision and sticking. The larger kilometer sized rocky bodies which form will start to capture more dust grains through gravitational attraction. At this point in the dust and disk evolution, these so-called planetesimals will start, through gravitational interaction, to influence the structure of the circumstellar disk and form planets, and the larger of these planets can carve out gaps at particular radii in the disk. Observationally, these gaps of warm dust in the inner parts of the disk become evident through a lack of near- and mid-infrared emission, and these disks are referred to as “cold disks” or elsewhere “transitional” disks. Throughout this phase, an increasing fraction of the small dust grains are no longer of the population that originally accreted from the cloud onto the disk, but rather produced by collisions of planetesimals. The disk is evolving into a so-called “debris” disk.

Eventually, the continued stellar wind and radiation pressure of the central star will erode the dust that has not yet been captured into larger planetesimals and planets

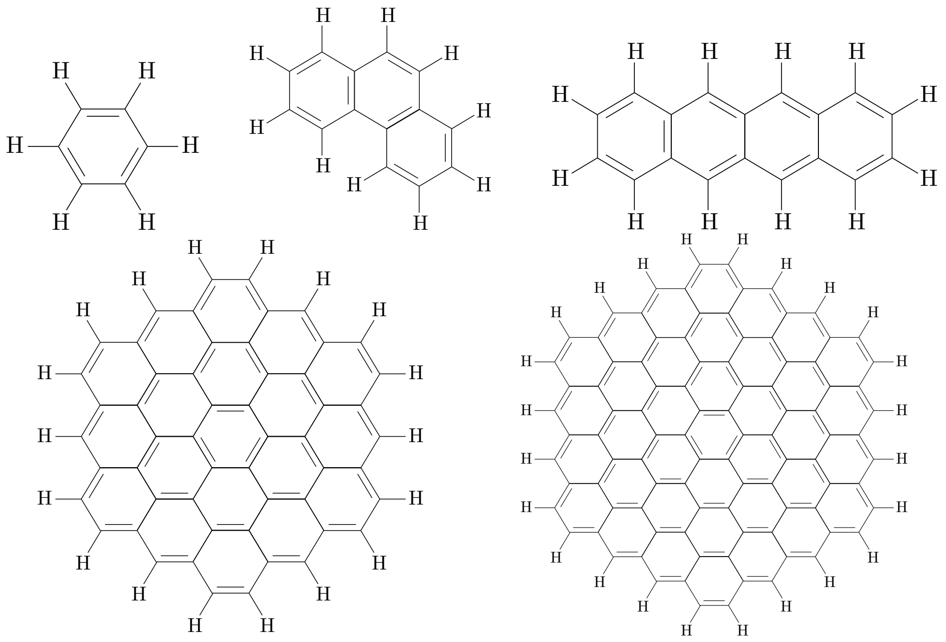

Figure 1.1: Molecule structure of benzene (C_6H_6), phenanthrene ($C_{14}H_{10}$), tetracene ($C_{18}H_{12}$), $C_{54}H_{18}$ and $C_{96}H_{24}$.

from the circumstellar disk, until only a star and planetary system remains. My thesis is concerned with the class I and II phases, up to the transition to the debris disk stage.

1.2 POLYCYCLIC AROMATIC HYDROCARBONS

From the interstellar medium (ISM) to planet-forming disks, the size, structure and composition of dust grains is known to vary significantly. In general, the dust grains are dominated by silicate and carbonaceous grains and are relatively small (0.01-1 μm) in most environments except for planet-forming disks. In molecular clouds and circumstellar disks, these grains provide the main source of opacity in the mid-infrared, and are important in the coupling of the radiation field with the temperature of the dust and gas. Second, they are believed to be an important catalyst of chemical reactions through grain surface chemistry. PAHs are another repository for one of the most abundant heavy elements, carbon, and play a similar role as small grains in terms of heating and chemistry, while at the same time their molecular structure distinguishes them from big grains, in particular their method of excitation.

1.2.1 Structure and excitation of PAHs

PAHs are hexagonal planar rings of carbon atoms, where each carbon atom is bound to 2 other carbon atoms and one hydrogen atom. The 4th electron bond of each carbon atom is shared in a delocalised bond among all neighbouring carbon atoms, which results in a so-called aromatic structure called the benzene ring. A single ring is called

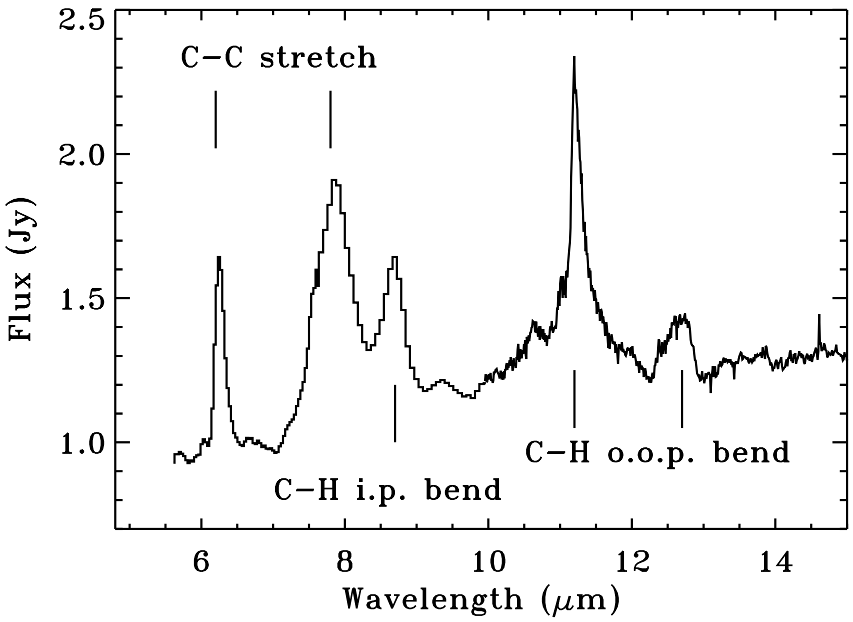

Figure 1.2: Spitzer IRS spectrum of the young star RR Tau, with 6.2, 7.7, 8.6, 11.2, 12.7 μm PAH features indicated (i.p.: in plane; o.o.p.: out of plane).

a monocyclic aromatic hydrocarbon (MAH) and forms the building blocks for larger molecules consisting of several MAHs, forming a polycyclic aromatic hydrocarbon (PAH), see Figure 1.1.

The main source of excitation of PAH molecules is through the absorption of (far-) UV photons, which causes a transition to an upper electronic state, although larger optical wavelength photons can also contribute. The molecule quickly makes radiationless transitions to the electronic ground state, converting most of the energy into vibrational energy, through the many available C-C and C-H bonds. Following this, the vibrationally excited molecule cools through vibrational transitions, resulting in radiation of mainly infrared photons. A detailed description of PAH photo-physics is given in Tielens (2005).

PAHs therefore have a very distinct emission spectrum in the mid-IR, dominated by main features at 3.3, 6.2, 7.7, 8.6, 11.2 and 12.7 μm (see Fig. 1.2). These are actually not single features, but rather emission bands, comprised of the large number of vibrational transitions of C-H and C-C bonds, which make up the general structure of the PAHs. In addition, very large PAHs are believed to cause broad emission plateaus underneath these emission bands.

The size of PAHs and the inclusion of elements heavier than hydrogen affect the available vibrational transitions in the molecule and influence the strength and shape of the PAH emission bands. To date, no single PAH emission feature from astronomical observations has been uniquely identified with a single PAH species. A further complication is that within any astrophysical environment, there will likely be a range

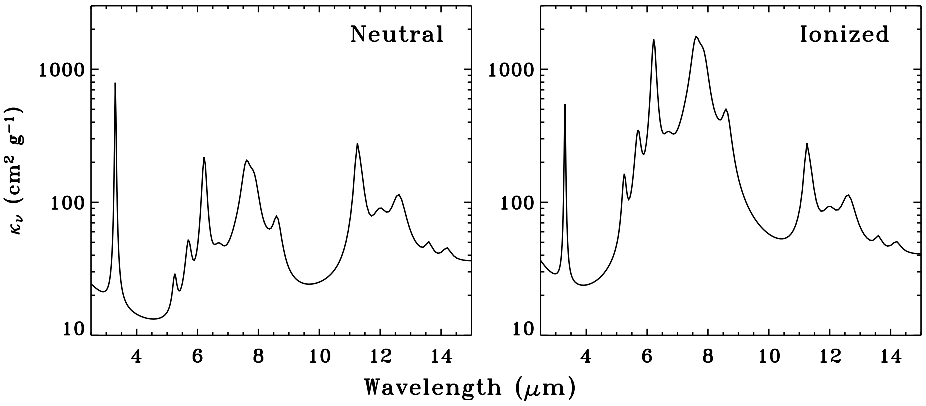

Figure 1.3: PAH opacities of neutral (left) and single ionized (right) $C_{100}H_{24}$, based on Draine & Li (2007) and Mattioda et al. (2005). Note the order of magnitude enhancement of the 6.2, 7.7 and 8.6 μm features for the ionized species.

of differently sized and shaped PAHs present, all contributing to the emission bands.

The ionization state of PAHs has a particularly strong effect on the PAH spectrum (e.g. Bauschlicher 2002). Neutral PAH molecules have relatively strong 3.3, 11.3 and 12.7 μm features, all associated with C-H bonds, while ionization will increase the relative strength of the 6.2, 7.7 and 8.6 features which are primarily caused by C-C bonds, see Figure 1.3. Thus, searches for PAHs such as those in this thesis need to cover both classes of features.

1.2.2 Evolution of PAHs in space

PAHs have been observed toward a wide range of varying astrophysical environments, ranging from evolved AGB stars, the ISM to young stars with disks, see Figure 1.4 (Hony et al. 2001; Peeters et al. 2002). PAHs are believed to be created in the outflows of carbon-rich AGB stars. The outflow wind combines high density, high temperature and high carbon abundance and thus provides the conditions for PAH formation. The growth of PAHs is believed to occur through the formation of a first monocyclic carbon ring molecule from actylene, addition of hydrogen atoms to form a MAH, and followed by growth through addition of rings by substitution of H-atoms with hydrocarbons, eventually allowing for chains of rings with typically a few tens to a few hundred carbon atoms.

The outflow of the AGB star deposits the PAH molecules in the ISM, where its evolution is similar to dust. It can still grow by coagulation and clustering, and it can accrete or be accreted onto other dust grains. Hydrogen atoms can be replaced by heavier elements, such as nitrogen. Exposure to high UV fields, cosmic rays or supernova pressure shocks in the medium can cause destruction. Observationally, however, PAHs behave very differently from large dust species. The heat capacity of these 20-100 carbon atom molecules is smaller than that of typical dust grains, which means

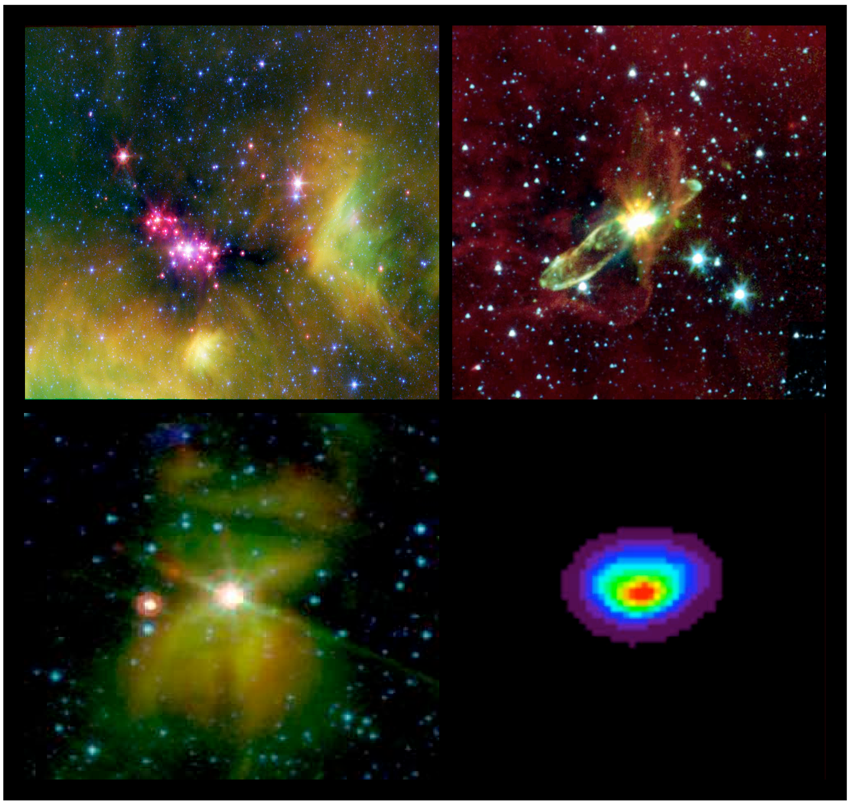

Figure 1.4: PAH emission observed toward a variety of astrophysical environments: diffuse interstellar dust in the Serpens star-forming region (PAH 8 μm indicated in green, top-left, $\sim$ 2 pc on the side), molecular cloud with embedded object HH 46 and outflows (PAH 8 μm indicated in red, top-right, 0.7 pc on the side), VV-Ser, young star with disk in remnant cloud (bottom-left, 5×10^4 AU on the side), close-up of circumstellar disk around IRS 48 at 11.25 μm (bottom-right, 600 AU on the side). Data in the first three panels all come from the c2d Spitzer Legacy program, the IRS 48 image is taken with VLT-VISIR.

Credits: top-left: Spitzer IRAC+MIPS image of Serpens cluster (courtesy NASA/JPL-Caltech/L. Cieza (UT Austin)); top-right: Spitzer IRAC image of HH46 (NASA/JPL-Caltech/A. Noriega-Crespo (SSC/Caltech), Digital Sky Survey); bottom-left: Spitzer IRAC+MIPS image VV Ser (Pontoppidan et al. 2007, ApJ, 656, 991); bottom-right: VLT-VISIR 11.2 μm image (of IRS 48, Chapter 3.

that they will be transiently heated to high temperatures. This causes PAHs to emit at mid-infrared wavelengths, even in environments where the expected dust temperature in radiative equilibrium with the (inter-)stellar radiation field is expected to be too low for significant mid-IR radiation. This observational presence of PAHs toward many lines of sight, associated not only with AGB outflows, but also with the ISM and nearby star-forming regions, suggests that PAHs are present in these environments, and that they are sufficiently large to prevent destruction. The cosmic abundance of carbon locked up in PAHs in the ISM inferred from mid-IR observations of Galactic cirrus and photo-dissociation regions is 5×10^{-5} with respect to hydrogen, which implies a typical PAH abundance of 5×10^{-7}, considering that the average PAH is estimated to be composed of about 100 carbon atoms.

In the dense environments of molecular clouds, the low temperature leads to the expectation that PAHs are (partly/completely) incorporated into the water and CO ice mantles that form on the surfaces of dust grains. In this phase, grain surface chemistry may play an important role in modifying the composition of the PAHs, most likely through replacement of hydrogen atoms at the periphery with heavier elements or small molecular groups. As will be shown in this thesis, PAH emission is not been toward YSO's in this embedded phase.

In the class I and II phase, accretion and radiation of the central source heats up the material in the disk, causing evaporation of the ice and enclosed molecules, such as the PAHs, into the gas. The radiation field of the central source is orders of magnitude higher than the interstellar radiation field, both providing more UV to excite the PAHs and make the distinct features reappear. The intense UV is also expected to destroy PAHs located in the inner few AU of the disk.

1.2.3 Why study PAHs?

PAHs play an important role in the environments where they are observed. In the ISM, PAHs can dominate the heating and cooling of the gas through photoelectric emission, infrared emission, electronic recombination and collisional cooling between dust and gas. The PAHs are a good tracer of UV, and thus indirectly of star formation in the high opacity environments of molecular clouds and even toward galaxies out to high redshifts.

In circumstellar disks, PAHs provide a tracer of the strength of the stellar radiation field. This is due to the strong dependence of PAH emission on direct excitation by UV and optical emission coupled with a weak dependence on the temperature of the surrounding matter of gas and dust. In particular, PAHs could trace the geometrical structure of localised high opacity regions, such as the geometry of circumstellar disks at larger radii.

PAHs can influence the disk structure. For example, the high opacity of PAHs could significantly reduce the stellar FUV radiation field in the inner disk. Through photoionization PAHs can produce energetic electrons, which form a major heating mechanism for the gas in the upper layers of the disk where gas and dust temperatures are not well coupled. At the same time, this process influences the charge balance in the disk, while the distinct dependence of its IR emission features on the ionization state make PAHs a good tracer of ionization level in the disk.

PAHs can play an important role in the chemistry in circumstellar disks. They are among the largest molecules detected in space, and sometimes rather considered as small grains. The large surface area of PAH molecules has been proposed to be a possible site for surface chemistry, such as for the formation of H_2 and water. In particular in circumstellar disks, where classical grains have grown to large sizes, the formation of H_2 on PAHs may be the most efficient process, thus increasing the influence of PAHs on the entire disk chemistry.

At the start of this thesis, PAHs had been observed with ISO toward about 15 young intermediate-mass Herbig Ae stars (Acke & van den Ancker 2004), but not yet toward

Table 1.1: Characteristics of the IR instruments used in this thesis.

	VLT-ISAAC	VLT-VISIR	VLT-NACO	Spitzer IRS (space)
array	1024x1024	256x256	1024 x 1024	128x128 (echelle)
coverage	2.8–4.2 μm spec	7.8–14 μm spec N-band imaging Q-band imaging	3.2–3.8 μm spec	10–35 μm 5-15 μm
spectral res. ($\lambda/\Delta\lambda$)	600	350	700	low-res: 64-128 high-res: 600
spatial res.	~0.2 ″ or seeing	~0.15 ″ or seeing	~0.1 ″	Short-Low: ~1.8″ Short-High: ~2.3″
PAH feature coverage	3.3	8.6, 11.2, 12.7	3.3	6.2, 7.7, 8.6, 11.2, 12.7

solar-mass stars.

1.3 MID-INFRARED OBSERVATIONS

Spectroscopic observations provide crucial information about the physical state and composition of the gas and dust. Many of the important dust solid-state features as well as emission lines from gas-phase atoms and molecules occur in the infrared regime.

The past decade has seen the arrival of powerful 8m class telescopes coupled with high resolution, high sensitivity infrared detectors. The results in this thesis are largely driven by the new mid-infrared capabilities available at the Paranal Observatory in Chile operated by the European Southern Observatory and through the launch of the NASA Spitzer Space Telescope. These instruments are briefly described below, their relevant characteristics are summarized in Table 1.1.

The Infrared Spectrometer and Array Camera (ISAAC) mounted on the Very Large Telescope (VLT) Antu allows full L and M-band spectra at moderate spectral resolution and high spatial resolution in a single setting, which makes ISAAC a very efficient instrument for surveys of the 3.3 μm PAH feature. A useful feature of this instrument is the ability to rotate the camera and observing slit. For example, when observing circumstellar disks for which the orientation on the sky is known from previous observations, this allows alignment of the slit parallel or perpendicular to the semi-major axis of the disk, important for studying the spatial extent of features in both directions. The spatial resolution of these observations are often dominated by seeing.

The Naos Conica (NACO) array on VLT-Yepun is a near-infrared detector instrument coupled to an adaptive optics module, which allows observations with unprecedented high spatial resolution, on or close to the diffraction limit of the 8 meter telescopes. This high resolution allows us in Chapter 4 to constrain the origin of dust and 3.3 μm PAH emission on small scales of only 10–30 AU, i.e., comparable to the size of our solar system.

The VISIR spectrometer and imager on VLT-Melipal allows for high sensitivity mid-infrared spectroscopy and imaging in two atmospheric windows, the 8–13 μm N-band and the 16.5–24.5 μm Q-band. This allowed us to study the spatial extent of small and large grains in Chapter 3, and to survey the 8.6, 11.2 and 12.7 μm PAH features in Chapter 4.

The strong shared advantages of the ground-based instruments are the combination of high spatial resolution with high spectral resolution, but the largest downside is the requirement of observing through the Earth's atmosphere. Large parts of the infrared spectrum are completely opaque due to atmospheric absorption by water, carbon-dioxide and other molecules. Even between those opaque parts, in the atmospheric windows where the transmission of the atmosphere allows infrared observations, the presence of specific atmospheric absorption lines, such as the 3.31–3.32 μm methane lines, will cause noise in the spectrum of the science object. This will lower the potential sensitivity of instruments, making it hard to observe faint sources. Several PAH features, in particular the strong 6.2 μm band, are completely obscured from Earth.

The NASA Spitzer Space Telescope, launched in August 2003, provides a very sensitive infrared observatory in space and a successor to the ESA Infrared Space Observatory (ISO). It offers imaging at 3.6, 4.5, 5.8, 8.0, 24, 70 and 160 μm and low and moderate resolution spectroscopy from 5–35 μm, which covers all major PAH features with the exception of the 3.3 μm feature. Free from observing through the atmosphere, it has a very high sensitivity. Spitzer spectroscopy obtained in context of the "Cores to Disks" Spitzer Legacy program ('c2d') (Evans et al. 2003) is used in Chapter 2 and 5 to survey the presence of PAH features around intrinsically weaker low-mass young stars with disks, sources which were too faint for ISO.

1.4 RADIATIVE TRANSFER MODELING

Radiation, recorded in spectra and images, is the only information one can acquire about the distant astronomical objects. The environments of young stellar objects embedded in envelopes or surrounded by circumstellar disks are optically thick at UV, visual and near-infrared wavelengths. Therefore the source of the radiation, the central star, is often completely obscured, its radiation being scattered by the surrounding dust particles and/or absorbed and re-emitted at longer wavelengths. This process influences the dust temperature and thus indirectly also the gas temperature in the disk, which in turn influences the structure of the disk. To properly interpret this information, models of the process of radiative transfer are needed.

In all chapters of this thesis, comparison of spectra and images with model calculations have utilized the radiative transfer model RADMC presented in Dullemond et al. (2001). This is a 3D axisymmetric radiative transfer code, which computes the absorption, scattering and emission of photons, and the dust temperature. Using a ray tracer, the results can be visualized in simulated spectra and images.

As part of this thesis, a separate module computing the PAH emission was included in the RADMC code, allowing the inclusion of excitation of non-thermal quantum-heated grains by UV and optical radiation. This module stores energy received by

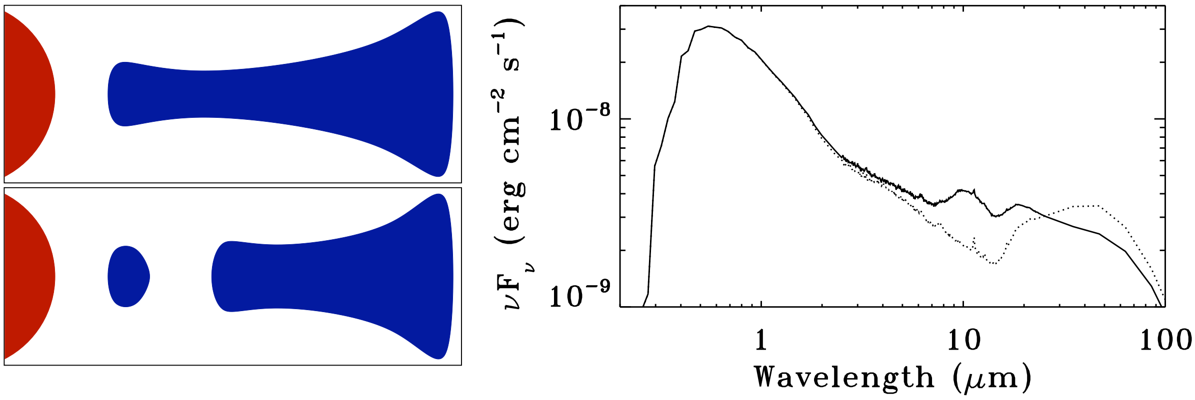

Figure 1.5: Model SED of a 6000 K star with a circumstellar disk, sketched in top-left (solid line). The SED of the same model after introducing a gap (density lowered by factor 10^{-6}) in the disk from 1–40 AU, sketched in bottom-left, is included (dotted line). In this model, the grains have grown to ~ 1 μm size, so that the silicate emission is suppressed. Note that the sketches are not to scale.

PAHs during an initial radiative transfer calculation, calculates the emission spectrum based on the discrete transitions of the PAH molecules included, following the emission model described in Visser et al. (2007), which is included in the second radiative transfer calculation. This process can be iterated if necessary. Model parameters that can be varied to fit the observations include the disk flaring, the incident radiation field and the PAH abundance. Example SEDs of disks with and without a gap are shown in Figure 1.5.

1.5 OUTLINE OF THIS THESIS

In this thesis we address the following main questions. What happens to PAHs in the embedded phase of a forming star? Are PAHs present in low-mass young star systems? Does the PAH emission originate from the envelope or from the disk? What do they tell us about disk structure and evolution and grain growth? What can we say about the evolution of PAHs during star formation and their typical size?

In Chapter 2, we present a survey with Spitzer of PAH features in a sample of intermediate and low-mass stars with disks, and compare the results with model predictions of PAH emission from flaring disks. In Chapter 3, we present VISIR images and a spectrum of IRS 48, a young M-type star with very strong PAH features, which appears to have a 60 AU radius gap in the disk as seen in large grains at 18.9 μm but with PAHs originating from inside the gap. In Chapter 4, we present an ISAAC, VISIR and NACO survey of the spatial extent of PAH features in protoplanetary disks, and compare with model predictions. In Chapter 5, we present an ISAAC and VISIR survey of PAH features toward embedded young stars, and compare the results with model predictions.

The main conclusions of this thesis can be summarized as follows:

- PAHs are shown to be present in several T Tauri disks, but at an abundance 10-100 times lower than standard interstellar values. The detection rate of only 11-14% is small compared to that toward intermediate-mass stars (~54%). At our average derived PAH abundance, PAH emission features around stars with $T_{\rm eff} \leq 4200$ K fall below the Spitzer IRS detection limit. The 11.2 μm PAH feature is most easily detected, with the 7.7 and 8.6 μm bands readily masked by silicate emission.

- High spatial resolution spectroscopy confirms that the PAH features detected toward young stars are directly associated with the circumstellar disk and not due to the presence of a tenuous envelope.

- A new class of disks with weak mid-IR continuum emission and very strong PAH features is found. This class represents a small percentage (~5%) of the total population of disks surveyed. Among disks around low-mass stars with PAH detections, it represents a large fraction. This is partially due to a detection effect, where the lower disk continuum between 5–15 μm due to absence of dust results in higher feature-to-continuum ratios for the PAH features. These disks are believed to harbour gaps and/or holes with strong PAH emission originating at, or inwards from, the outer edge of the gap. This evidence for separation of small and large grains implies that their populations evolve differently.

- PAHs are not detected toward the majority ($\geq$ 97%) of a sample of 80 embedded sources. Comparison with model calculations show that this detection rate is consistent with a PAH abundance at least 20–50x lower than in the ISM. Variability in luminosity, UV excess and/or envelope mass can change this conclusion to a typical factor of 10–20. In these cold dense environments, two possibilities for lowering the abundance of a species are recognized: coagulation or dust growth and freeze-out of the PAHs onto larger grains. Thus, PAHs likely enter the protoplanetary disks frozen out on grains.

1.6 FUTURE PROSPECTS

The sample of PAHs detected toward T Tauri disks (~5) is relatively small (Chapter 2 and 3). A larger sample is needed to draw statistically relevant conclusions on the similarities and/or differences of the kind of PAHs (size, shape, charge) in these sources. Spitzer spectra of several hundred additional sources have been obtained in other programs and can be studied using the Spitzer archive. Detailed studies of feature strength and shape can place PAHs around T Tauri disks in the context of earlier studies toward disks around intermediate mass stars and the ISM. For the small sample of T Tauri detections, high spatial resolution imaging in mid-IR and sub-mm can provide a test for the presence of gaps in small and large dust populations in the disks. Spatially resolved spectroscopy using adaptive optics and/or interferometry with, e.g., VLT-NACO, VLT-MIDI and in the future JWST-MIRI, will allow us to put much stronger constraints on the spatial extent of PAHs in disks, as shown with VLT-NACO for a few sources in Chapter 4.

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