Molecules in Space & Laboratory, Paris, 2007
J.L. Lemaire & F. Combes (eds)

PAH CHEMISTRY AND IR EMISSION FROM CIRCUMSTELLAR DISKS

R. Visser[1], V.C. Geers[1], C.P. Dullemond[2], J.-C. Augereau[3], K.M. Pontoppidan[4] and E.F. van Dishoeck[1]

Abstract. A model is presented to analyze the chemistry of, and infrared emission from, polycyclic aromatic hydrocarbons (PAHs) in disks around Herbig Ae/Be and T Tauri stars. The model calculates the equilibrium charge and hydrogenation distribution of the PAHs throughout the disk. Destruction of PAHs by ultraviolet (UV) photons, possibly in multi-photon absorption events, is taken into account. The chemistry model is coupled to a radiative transfer code to provide the physical parameters and to combine the PAH emission with the spectral energy distribution (SED) from the star+disk system. In the inner 100 AU of a Herbig disk, PAHs of 50 carbon atoms can only survive below the disk's surface layer. Larger PAHs can survive at higher altitudes at this radius. Hence, the observed emission from 50-C PAHs appears more extended than that of 100-C PAHs. A comparison with spatially resolved observations suggests that most of the observed emission comes from PAHs of at least ∼100 carbon atoms.

1 Introduction

Polycyclic aromatic hydrocarbons have been observed in a large variety of sources, including the diffuse interstellar medium, photon-dominated regions, circumstellar envelopes, planetary nebulae and external galaxies (Allamandola et al. 1989; Peeters et al. 2004). More recently, PAH features have also been detected in disks around Herbig Ae/Be and T Tauri stars (e.g. van Boekel et al. 2004; Acke & van den Ancker 2004; Geers et al. 2006). In the majority of these sources, the PAHs are electronically excited by ultraviolet (UV) photons. Following internal conversion to a high vibrational level of the electronic ground state, they cool by emission in the primary C–H and C–C stretching and bending modes at the mid-infrared (IR) wavelengths of 3.3, 6.2, 7.7, 8.6, 11.3, 12.8 and 16.4 μm. Because of the required UV pumping, PAH emission in circumstellar disks is believed to come mostly from the surface layers (Habart et al. 2004b).

[1] Leiden Observatory, Leiden University, P.O. Box 9513, 2300 RA Leiden, The Netherlands
[2] Max-Planck-Institut für Astronomie, Koenigstuhl 17, 69117 Heidelberg, Germany
[3] Laboratoire d'Astrophysique de l'Observatoire de Grenoble, B.P. 53, 38041 Grenoble Cedex 9, France
[4] Hubble Fellow; Division of GPS, Mail Code 150-21, California Institute of Technology, Pasadena, CA 91125, USA

PAHs play an important role in the physics and chemistry of a circumstellar disk and they are a useful observational tool. They are a good diagnostic of the stellar radiation field and can be used to trace small dust particles in the surface layers of disks. Photoionization of PAHs produces energetic electrons that heat up the gas (Kamp & Dullemond 2004; Jonkheid et al. 2004) and PAHs act together with the dust to shield the disk's midplane from ionizing radiation. The ionization balance in the disk is affected by charge transfer reactions between neutral PAHs and C^+ and PAHs may be a site of H_2 formation (Habart et al. 2004a; Jonkheid et al. 2006).

The chemistry of PAHs in circumstellar disks (Visser et al. 2007, hereafter V07) is an interesting topic of its own. Considered large molecules by some and small dust grains by others, PAHs exhibit a complex chemical behaviour. This behaviour has to be understood in order to use PAHs as an observational tool. In addition, PAHs are likely to survive the star formation process and end up in planetary bodies and comets (Allamandola & Hudgins 2003), as confirmed by the Deep Impact and Stardust missions (Lisse et al. 2006; Sandford et al. 2006). Understanding in what form they arrive on a planet in a habitable zone brings us a step closer to understanding how life may originate there. We recently presented the first chemistry model specifically targeted at PAHs in circumstellar disks (V07). Here, we focus on the destruction of PAHs by UV photons and the consequences for the spatial extent of the PAH emission.

2 Description of the model

Our PAH chemistry model was described in detail in V07. The model's chemical part is a combination of the models developed by Le Page et al. (2001) and Weingartner & Draine (2001), with absorption and emission cross sections from Draine & Li (2007). The main reactions are photoionization, electron recombination, and the removal and addition of hydrogen atoms. Given a gas density, electron abundance, temperature and radiation field, the model calculates the equilibrium distribution of a PAH over all of its possible charge and hydrogenation states. In addition, the rate at which the carbon skeleton is destroyed (including the effects of multi-photon absorption) is calculated as a function of UV intensity to determine where in the disk the PAHs can survive. In situ formation and growth of PAHs are assumed not to take place.

The chemistry code is coupled to the radiative transfer code RADMC (Dullemond & Dominik 2004) to obtain the temperature and radiation field throughout a circumstellar disk. After computing the PAH chemical equilibrium at every point in the disk, another code, RADICAL, is used to produce IR spectra or images. The quantized heating of PAHs in the RADMC code was first described by Pontoppidan et al. (2007). The results presented here are for the flaring Herbig Ae/Be template model from V07, which has the following parameters: $T_* = 10^4$ K, $M_* = 2.91 M_\odot$, $R_* = 2.79 R_\odot$, $M_{\rm disk} = 0.01 M_\odot$, $R_{\rm disk,in} = 0.48$ AU and $R_{\rm disk,out} = 300$ AU.

3 Results

The inner edge of the dust disk is set by the dust destruction radius. Likewise, one can define a PAH destruction radius, which depends on the UV luminosity of the central star and the size of the PAHs. Larger PAHs are better at internally redistributing the energy of an incoming UV photon than smaller PAHs, so the former can survive closer to the star. According to V07, a PAH of 50 carbon atoms can survive for more than the disk lifetime if the local UV intensity is at most 10^5 times that of the mean interstellar field. Doubling the PAH size allows it to survive in radiation fields with up to 10^7 times the mean interstellar UV intensity. By computing the UV intensity at every point in the disk, one can thus make a map of where PAHs of a given size can survive (Fig. 1). Just below the $\tau_{\rm vis} = 1$ surface, the UV field is already strongly attenuated and it can only destroy PAHs smaller than about 40 carbon atoms. At higher altitudes, the UV intensity decreases with the square of the distance, and the PAH destruction radii respond accordingly. On the $\tau_{\rm vis} = 1$ surface, PAHs of 50 carbon atoms can survive outside ∼90 AU. This analysis excludes the effects of radial and vertical mixing (Dullemond et al. 2007).

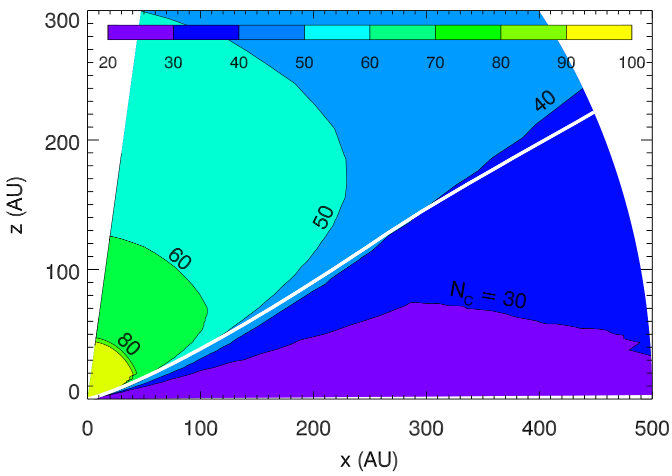

Fig. 1. PAH destruction around a Herbig Ae/Be star. The colour scale and the contours indicate the smallest PAH (in terms of its number of carbon atoms) that can survive at each point in the template 300 AU Herbig Ae/Be disk. The white line denotes the $\tau_{\rm vis} = 1$ surface.

Based on Fig. 1, one expects to find more emission close to the star from larger PAHs than from smaller ones. This is confirmed by plotting the intensity of the PAH emission as a function of radial distance from the star (Fig. 2). For all PAH features (only the 3.3 μm feature is shown), the emission from PAHs with 50 carbon atoms is more extended than that from PAHs twice that size. The thermal dust continuum at 3.3 μm is much more centrally concentrated than the PAH emission.

Geers et al. (2007) fitted Gaussian profiles to spatially resolved PAH spectra of disks and determined the full-widths at half-maximum (FWHM; 76% of the emission originates from within this radius). The FWHMs of the computed profiles are indicated in Fig. 2; they are 23 and 79 AU for $N_{\rm C} = 96$ and 50, respectively. Geers et al. were able to resolve the PAH emission in three sources, finding 3.3 μm FHWMs between 12 and 55 AU. This suggests that the PAHs observed in these sources are unlikely to be much smaller than ∼100 carbon atoms.

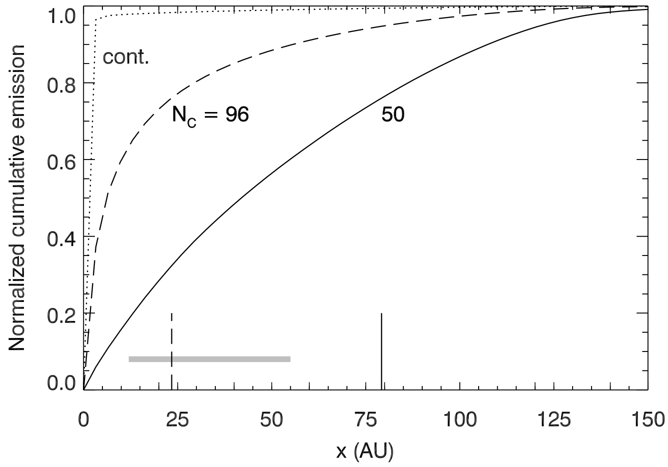

Fig. 2. The normalized cumulative intensity at 3.3 μm in the template Herbig Ae/Be disk for PAHs of 50 and 96 carbon atoms (solid and dashed lines) and the thermal dust continuum (dotted line). The vertical bars indicate the FWHM of a Gaussian fitted to the two PAH profiles. The horizontal grey bar shows the range of observed FHWMs (Geers et al. 2007).

References

Acke, B., & van den Ancker, M. E. 2004, A&A, 426, 151

Allamandola, L. J., Tielens, A. G. G. M., & Barker, J. R. 1989, ApJS, 71, 733

Allamandola, L. J., & Hudgins, D. M. 2003, in Solid State Astrochemistry, ed. V. Pirronello, J. Krelowski, & G. Manicò (Dordrecht: Kluwer), 251

Draine, B. T. & Li, A. 2007, ApJ, 657, 810

Dullemond, C. P., & Dominik, C. 2004, A&A, 417, 159

Dullemond, C. P., Henning, T., Visser, R., et al. 2007, A&A in press

Geers, V. C., Augereau, J.-C., Pontoppidan, K. M., et al. 2006, A&A, 459, 545

Geers, V. C., van Dishoeck, E. F., Visser, R., et al. 2007, A&A in press

Habart, E., Boulanger, F., Verstraete, L., Walmsley, C. M., & Pineau des Forêts, G. 2004a, A&A, 414, 531

Habart, E., Natta, A., & Krügel, E. 2004b, A&A, 427, 179

Jonkheid, B., Faas, F. G. A., van Zadelhoff, G.-J., & van Dishoeck, E. F. 2004, A&A, 428, 511

Jonkheid, B., Kamp, I., Augereau, J.-C., & van Dishoeck, E. F. 2006, A&A, 453, 163

Kamp, I., & Dullemond, C. P. 2004, ApJ, 615, 991

Le Page, V., Snow, T. P., & Bierbaum, V. M. 2001, ApJS, 132, 233

Lisse, C. M., VanCleve, J., Adams, A. C., et al. 2006, Science, 313, 635

Peeters, E., Mattioda, A. L., Hudgins, D. M., & Allamandola, L. J. 2004, ApJ, 617, L65

Pontoppidan, K. M., Dullemond, C. P., Blake, G. A., et al. 2007, ApJ, 656, 991

Sandford, S. A., Aléon, J., Alexander, C. M. O., et al. 2006, Science, 314, 1720

van Boekel, R., Waters, L. B. F. M., Dominik, C., et al. 2004, A&A, 418, 177

Visser, R., Geers, V. C., Dullemond, C. P., et al. 2007, A&A, 466, 229 (V07)

Weingartner, J. C., & Draine, B. T. 2001, ApJS, 134, 263