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The ‘soot line’: Destruction of presolar polycyclic aromatic hydrocarbons in the terrestrial planet-forming region of disks

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Abstract

Interstellar material is highly processed when subjected to the physical conditions that prevail in the inner regions of protoplanetary disks, the potential birthplace of habitable planets. Polycyclic aromatic hydrocarbons (PAHs) are abundant in the interstellar medium, and they have also been observed in the disks around young stars, with evidence for some modification in the latter. Using a chemical model developed for sooting flames, we have investigated the chemical evolution of PAHs in warm (1000–2000 K) and oxygen-rich ($C/O < 1$) conditions appropriate for the region where habitable planets may eventually form. Our study focuses on (1) delineating the conditions under which PAHs will react and (2) identifying the key reaction pathways and reaction products characterizing this chemical evolution. We find that reactions with H, OH and O are the main pathways for destroying PAHs over disk timescale at temperatures greater than about 1000 K. In the process, high abundances of C_2H_2 persist over long timescales due to the kinetic inhibition of reactions that eventually drive the carbon into CO, CO_2 and CH_4. The thermal destruction of PAHs may thus be the cause of the abundant C_2H_2 that has been observed in disks. We propose that protoplanetary disks have a ‘soot line’, within which PAHs are irreversibly destroyed via thermally-driven reactions. The soot line will play an important role, analogous to that of the ‘snow line’, in the bulk carbon content of meteorites and habitable planets.

Keywords: PAH; Protoplanetary disk; Chemical model; Presolar organics; Solar nebula

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) are extremely stable, in oxidizing or reducing conditions, at high temperatures, and in the presence of intense, high-energy UV radiation, allowing them to persist in a very wide range of astrophysical and planetary environments. In particular, PAHs have been observed in the interstellar medium, and, at much lower abundances, in the disks around young stars (e.g. Bouwman et al., 2008; Geers et al., 2007; Boersma et al., 2008).

Bright emission features at 3.3, 6.2, 7.7, 11.2, and 12.7 μm dominate the mid-IR spectra of regions of star and planet formation. These emission features are generally attributed to infrared fluorescence of PAH molecules excited by ultraviolet radiation. Observations show that large (50 C-atom) PAH molecules are an abundant – containing some 5–10% of the elemental C – and ubiquitous component of the interstellar medium of galaxies (see Tielens, 2008 for a recent review). These molecules are thought to form at high temperatures in the ejecta of carbon stars in a chemical process akin to incomplete combustion in sooting flames (Frenklach and Feigelson, 1989;

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Cherchneff et al., 1991). The ejected PAHs mix with the rest of the interstellar gas where they may survive for some 100 million years (Micelotta et al., 2009). Eventually, some of these PAHs may become part of regions of star formation and enter the protostellar disk where they contribute to the organic reservoir of the forming planets.

In our own solar system, structure in the UV spectrum of Comet Halley obtained by the Vega 2 spacecraft has been attributed to fluorescence of the small PAH, anthracene (Clairemidi et al., 2008). Reflectance spectra of some asteroids also show a feature reminiscent of PAHs (Lazzarin et al., 2009). PAHs are also present in both ordinary and carbonaceous chondrites (Clemett, 1996). Specifically, PAHs identified in the Murchison CM2 carbonaceous chondrite meteorite include pyrene, acenaphthalene, naphthalene, and phenanthrene. Much evidence points to a presolar heritage for these PAHs. Meteoritic PAHs are generally enriched in deuterium from 244‰ to 468‰ (Cronin and Chang, 1993). Messenger et al. (1998) discovered PAHs in graphitic grains extracted from carbonaceous chondrites and concluded that the isotopically anomalous PAHs are presolar and likely many of the PAHs with a solar $^{12}C/^{13}C$ ratio are presolar as well. Earlier studies (Morgan et al., 1991) concluded that PAHs can form under conditions appropriate for the protosolar nebula; however, these models started with fairly high amounts of methane and acetylene and did not include H_2O in the reaction mixture. In this study, the PAH yield decreased at very long times and lower pressures. Equilibrium models ultimately cannot explain the abundance and variety of organic compounds that have been found in protoplanetary disks, meteorites, comets, and interplanetary dust particles. However, such models can be used to address the relative stability of different species. For instance, Zolotov and Shock (2001) use thermodynamic models to address the stability of PAHs under disk conditions, and find that they are more stable than their alkylated and/or aliphatic counterparts with the same carbon number.

The spectral characteristics of PAHs in protoplanetary disks around young stellar objects differ from those in the interstellar medium from which the material originated (Sloan et al., 2007; Boersma et al., 2008). These differences have been attributed to chemical processing of the emitting PAHs in the direct environment of the newly formed star. Alternatively, these variations have been interpreted either as loss of nitrogen atoms from heterocycles (Peeters et al., 2002) or as a higher non-aromatic character of the PAH species (Sloan et al., 2007; Pino et al., 2008; Brunetto et al., 2009) in protoplanetary disks. PAHs also have a lower abundance (relative to the dust) in these disks than in the ISM, suggesting that PAH destruction is an important process in these dense environments (Visser et al., 2007; Siebenmorgen and Kruegel, 2010). Previous studies of PAH processing in circumstellar disks have exclusively focused on the role of UV and X-ray photons (Visser et al., 2007). These studies are inconclusive given that the parameters describing the photodissociation process are poorly constrained by experiments (cf., Micelotta et al., 2009), and that these PAHs survived for a long time in the far-UV field of the ISM between their formation site and the protoplanetary disk. As an alternative, in this paper, we consider the chemical evolution of PAHs in a warm (1000–2000 K), O-rich ($C/O < 1$) environment appropriate for the midplane of the inner disk surrounding young stellar objects. These conditions are conducive to a rich organic chemistry that may well have a profound influence on the chemical make-up of the interstellar PAH family present in the disk.

The goals of this study are (1) to delineate the physical conditions (density, temperature) within disk environments that induce chemical modifications of PAHs on astronomically relevant timescales and (2) to identify the dominant thermally-driven chemical pathways to destroy PAHs.

2. Modeling the kinetics of PAH chemistry

The chemistry of PAHs has been well studied under hydrocarbon-burning conditions ($P \sim 1$ atm, $T > 1000$ K). We have implemented a combustion model to investigate the reaction kinetics of PAHs within nebular timescales and temperatures to understand the chemistry that modifies PAHs in the inner disk environment. Our model is based upon studies of combustion kinetics occurring in sooting flames (Smith et al., 2000; Appel et al., 2000). The chemical model only considers thermally-driven reactions involving H, C, O and N. We will discuss the heterocycles (e.g., PAHs containing nitrogen) in future work. The model has been tailored to inner disk conditions, in which the temperature and pressure are typically lower than in sooting flames. Fig. 1 shows the chemical structures of several of the important species considered in the model. Centrally condensed, compact PAHs are, as a class, very stable because this structure allows complete electron delocalization and truly aromatic bonding between all adjacent C atoms. The largest PAH considered in our model study is pyrene ($C_{16}H_{10}$) as a representative of this class of stable PAHs. As such, pyrene is a bottleneck through which all of the larger PAH molecules must pass before they rapidly decompose into phenanthrene (3 aromatic rings), naphthalene (2 aromatic rings), etc. We therefore start the calculations with all the PAHs in the form of pyrene.

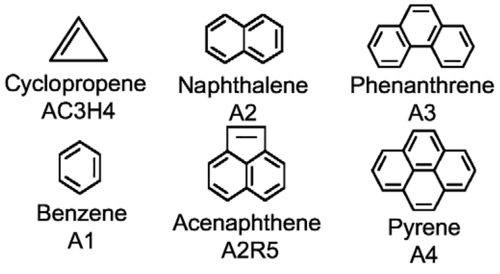

Fig. 1. A few examples of the aromatic compounds and other important hydrocarbons considered in the chemical model, followed by their labels (see time-dependent model results in Figs. 2 and 3).