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Benzene formation in the inner regions of protostellar disks

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Abstract. Benzene (c-C_6H_6) formation in the inner 3 AU of a protostellar disk can be efficient, resulting in high abundances of benzene throughout the midplane region. The formation mechanism is different to that found in interstellar clouds and in protoplanetary nebulae, and proceeds mainly through the reaction between allene (C_3H_4) and its ion. This has implications for PAH formation, in that some fraction of PAHs seen in the solar system could be native rather than inherited from the interstellar medium.

1. Introduction

Benzene is the smallest aromatic molecule, and is presumed to be a basic building block in the formation of polycyclic aromatic hydrocarbons (PAHs). PAHs have been observed in protostellar disks around both low-mass T Tauri (Geers et al. 2006) and intermediate-mass Herbig Ae/Be (HAeBe) stars (Acke & van den Ancker 2004). The number of detections in T Tauri-type disks is low, although this is to be expected since the incident UV radiation field is several orders of magnitude smaller than in HAeBe stars. Models indicate that the PAH emission comes from surface layers (Habart et al. 2004), leading to speculation as to whether PAHs form in these high UV environments or elsewhere. PAHs are similarly seen in protoplanetary nebulae (PPNe) – both in the circumstellar tori and in the bipolar outflows (Matsuura et al. 2004), and benzene has also been observed in this class of objects (Cernicharo et al. 2001). Here we consider the formation of benzene in a protostellar disk, and the implications this has for PAH formation.

2. Benzene formation in different environments

The interstellar medium (ISM)

$$C_4H_2^+ + H \longrightarrow C_4H_3^+ + h\nu \quad (1)$$
$$C_4H_3^+ + C_2H_2 \longrightarrow C_6H_5^+ + h\nu \quad (2)$$
$$C_6H_5^+ + H_2 \longrightarrow C_6H_7^+ + h\nu \quad (3)$$
$$C_6H_7^+ + e^- \longrightarrow C_6H_6 + H \quad (4)$$

In a dense ($n \sim 10^4\,\mathrm{cm^{-3}}$) interstellar cloud model, McEwan et al. (1999) calculated a fractional abundance of benzene of $\sim 10^{-9}$.

Protoplanetary nebulae

$$\mathrm{HCO^+ + C_2H_2 \longrightarrow C_2H_3^+ + CO} \quad (5)$$
$$\mathrm{C_2H_3^+ + C_2H_2 \longrightarrow C_4H_3^+ + H_2} \quad (6)$$
$$\mathrm{C_2H_2^+ + C_2H_2 \longrightarrow C_4H_3^+ + H} \quad (7)$$

followed by Eqs. (2-4). Woods et al. (2002, 2003) studied the dense ($n \sim 10^9\,\mathrm{cm^{-3}}$) torus around the protoplanetary nebula CRL618, and produced a fractional abundance of benzene of $\sim 10^{-6}$ in their chemical model – a very good match to observations (Cernicharo et al. 2001).

Jupiter, Saturn & Titan

$$\mathrm{C_3H_3 + C_3H_3 \xrightarrow{M} C_6H_6} \quad (8)$$
$$\mathrm{C_6H_5 + H \xrightarrow{M} C_6H_6} \quad (9)$$
$$\mathrm{C_4H_5 + C_2H_2 \longrightarrow C_6H_6 + H} \quad (10)$$

The dense atmospheres of planetary bodies make three-body reactions an efficient mechanism for the production of benzene and other molecules. Wong et al. (2000) calculated a mixing ratio of $\sim 10^{-9}$ for benzene in a model of the Jovian atmosphere.

3. The model

See Woods & Willacy (2007) for more detail on the protostellar disk model. Density and temperature profiles are shown in Fig. 1, and brief details are given here:

Property	Sources	Details
Density	D'Alessio et al. (2001)	α disk model $\dot{M}$=$10^{-8}\,\mathrm{M_\odot\,yr^{-1}}$
Dust temp.	D'Alessio et al. (2001)	T Tauri star $a = 0.25\,\mu$m
Gas temp.	Kamp & van Zadelhoff (2001) Gorti & Hollenbach (2004)	Heating/cooling balance, inc. X-ray irradiation
UV flux	Yorke & Bodenheimer (1999)	Ray-tracing method Includes scattering
Chemistry	Le Teuff et al. (2000)	UMIST Rate99 + freezeout, thermal desorption and grain surface reactions

The model follows the passage of a parcel of gas as it flows inwards from the outer regions of the disk (>35 AU), and as such it traces a period in the evolutionary history of the disk. At the outer edge of the disk the parcel has the composition of a million-year old molecular cloud. The parcel then accretes onto the central star over a period of approximately 200 000 years.

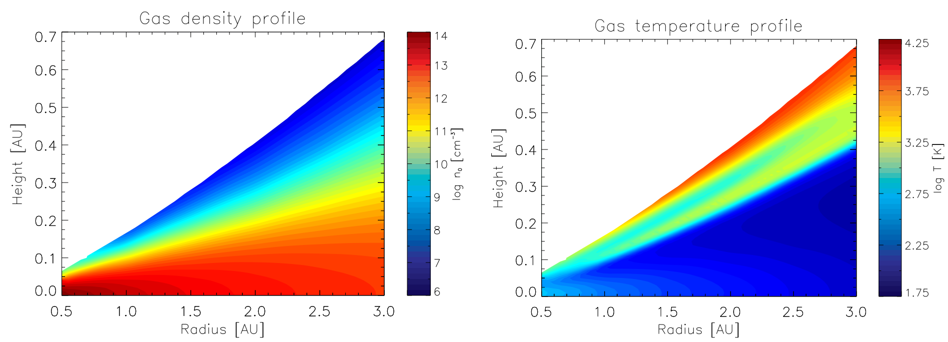

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Figure 1. Density and gas temperature profiles for the inner 3 AU of the disk model. The left panel shows gas density, whereas the right panel shows the gas temperature calculated by a heating/cooling balance.

4. Results

We find that benzene formation in a protostellar disk is efficient within 3 AU of the central star, and fractional abundances of $\sim 10^{-6}$ are achieved inside a radius of 2 AU (Fig. 2). The most efficient formation mechanism for benzene in this region is due to the reaction between C_3H_4 and its ion, $C_3H_4^+$, which has been measured in the laboratory (Anicich et al. 1984):

$$C_3H_4 + C_3H_4^+ \longrightarrow c{-}C_6H_7^+ + H \tag{11}$$

$$c{-}C_6H_7^+ + \mathrm{grain} \longrightarrow g{-}C_6H_6 + g{-}H, \tag{12}$$

where $g-$ signifies a species adsorbed onto a grain surface.

In this reaction scheme, the adsorption energy (E_{ads}) of benzene becomes an important factor in determining the amount of gaseous benzene. The value of this number varies wildly: from $\sim$4 750 K (estimated from Hasegawa & Herbst (1993); experiment by Arnett et al. (1988) using a graphite surface) to $\sim$7 580 K (estimated using the approach of Garrod & Herbst (2006); experiment by Lozovik et al. (1995) using a graphite surface). Thus we ran two models with a low E_{ads} and a high E_{ads} (Fig. 2). Results show a decrease in the extent of the gas-phase benzene distribution with the higher E_{ads}, as to be expected, with no change in the peak fractional abundance.

5. Discussion

The region in which benzene is abundant in our model (Fig. 2) is also rich in other organic molecules: high densities mean fast collision timescales with other molecules and with dust grains, and also protection from the strong stellar UV field in this region. These prime conditions for the growth of organic molecules may allow hydrocarbons to grow beyond the single aromatic ring of benzene into PAHs, either by substitution of hydrogen by acetylene in the ring, as has often been assumed (Wong et al. 2000; Moses et al. 2000), or by the dimerisation of benzene with successive phenyl rings (Cherchneff 1996). Benzene itself is unlikely to persist through to the formation of planets: calculations show that

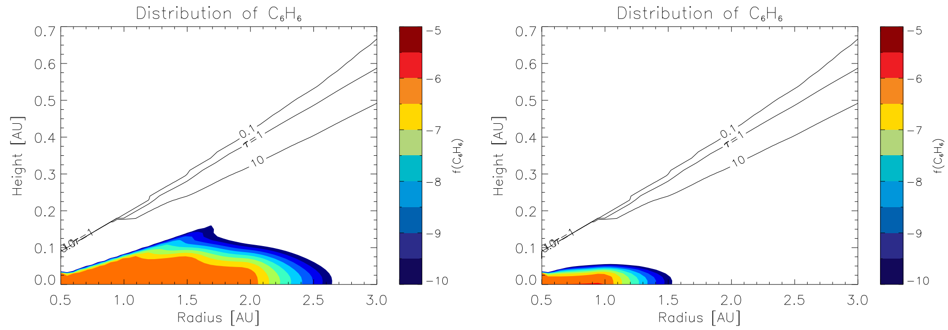

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Figure 2. The inner 3 AU of the disk, showing the distribution of (gaseous) benzene in terms of fractional abundance. The black solid lines are optical depth (τ) contours. The left panel shows a model with a low binding energy for benzene, 4 750 K. The right panel shows the effect of a higher binding energy, 7 580 K.

benzene has a timescale for UV destruction in the diffuse solar system of only hundreds of years (Allain et al. 1996; Ruiterkamp et al. 2005).

In order for PAHs to form, the constituents must be present in a region warm enough for ring closure to occur. PAHs only seem to form efficiently at temperatures in the region of 900–1 100 K (Frenklach & Feigelson 1989) and not greater. Production may be possible, too, at lower temperatures (700–900 K) given a high pressure (Helling et al. 1996). The region of benzene production is at a temperature of a few hundred degrees, and sits just below a region of sufficiently high temperature for PAH formation. Invoking vertical mixing here could raise benzene and other organics into the higher temperature region, as well as push newly-formed PAHs into the surface layers of the disk, where they are observed. Mixing timescales at a few AU are fast enough ($\sim$625 yr; Ilgner & Nelson 2006) to dredge material from the midplane to surface layers within the lifetime of a T Tauri disk ($\sim 10^6$ yr).

For PAHs to subsist in the solar system, the rate of growth of the PAH must be greater than the rate of photodissociation. However, once a PAH reaches 30-40 carbon atoms in size, it is effectively safe from photodissociation since at this size the IR radiative rate of the PAH dominates the photodissociation rate. In the ISM, a benzene molecule is destroyed (by removal of an acetylene molecule) at a rate of $1.5\times10^{-10}\,\mathrm{s}^{-1}$, giving a lifetime of around 200 yr.The growth time (accretion of an acetylene molecule) is given by $\tau_{\mathrm{gr}} = (n_0 X_{\mathrm{C_2H_2}} k_{\mathrm{C_2H_2}})^{-1}$ s (Allain et al. 1996). Inserting typical values for the abundance of acetylene in the inner part of the disk, $X_{\mathrm{C_2H_2}}$=10^{-7}, and the reaction rate for accretion of acetylene, $k_{\mathrm{C_2H_2}}$=$10^{-11}\,\mathrm{s}^{-1}$, gives a necessary density of $1.5\times10^{8}\,\mathrm{cm}^{-3}$ for PAH growth from benzene. This tallies with the low abundances of benzene in (low density) IS cloud models (see left) and the lack of benzene detection in the ISM. However, these conditions are met within the inner regions of a protostellar disk, as has been shown in our chemical model (which includes destruction of benzene by reactions with ions, as well as photons). Thus PAH production from benzene could possibly be prolific in this type of environment.

Having ascertained that benzene can survive for an amount of time long enough for PAHs to form from it, the question arises, do PAHs form in the same regions in which benzene forms? The answer to this is unclear, since the supporting observational evidence is sparse – there have been only 3 detections of PAHs in T Tauri-type disks (Geers et al. 2006); all three have inner dust holes. Thus it may just be a selection effect that PAH emission is only detected from the upper layers of disks because of the presence of these dust holes: otherwise the continuum emission swamps any possible PAH emission feature originating from deeper in the disk. Further observations are necessary to confirm the correlation between the presence of benzene and PAHs.

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