Can PAHs Support Grain-Formation in Carbon-Stars ?

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Most studies of stellar dust formation assumes (directly or indirectly) that all carbon grains, except SiC (Cadwell et al. 1994), are formed via conversion of C_2H_2 into PAHs (Polycyclic Aromatic Hydrocarbons). The agglomeration of PAHs leads to grains with crystalline or amorphous structures dependent on the temperature and gas pressure conditions in the atmosphere (Gail & Sedlmayr 1984). We show here that there exists a serious theoretical problem in producing the necessary PAH molecules.

1. The Method

We present here the first calculations of partial pressures of PAHs and other macro-molecules in realistic stellar photospheric models of carbon-rich stars. The model atmosphere code used is an updated version of the MARCS code (Jørgensen et al. 1992), improved with extended chemical equilibrium computations (Cherchneff et al. 1992), extensive cool-star opacities, spherical geometry, and opacity sampling treatment. We have included 36 different atomic species and the formation of 338 different molecules in chemical equilibrium. Our computed models have the following parameters: T_{eff}=(2800K, 2600K, 2400K), $Z=Z_\odot$, $M=M_\odot$, $\log(g) \in [-1,0.5]$, $C/O \in [1.1,7.0]$.

2. The Results

The minimum temperature reached by our hydrostatic photospheric models are about 1200K. The only aromatic ring molecules that form at such high temperatures are C_6H and C_6H_2, independent of gravity and C/O ratio. At lower temperatures, we performed a systematic chemical equilibrium exploration of the T-P_{gas} plane, $T \in [700K,1000K]$, $\log P_{gas} \in [-5,3]$ (see Fig. 1). It discloses PAHs as the type of molecules containing the largest fraction of the total amount of carbon not bound in CO. They contain more than 10% of the available carbon although they are still very low abundant. More carbon is locked up into PAHs than in CO at these temperatures for C/O>2, in contrast to the above mentioned warmer part of the photosphere. The higher the C/O ratio the larger are the occurring PAHs, although their total partial pressures do not increase significantly. At high temperatures C_2H_2 dominates the fraction of bound carbon, and at high gas pressures and low temperatures CH_4 dominates.

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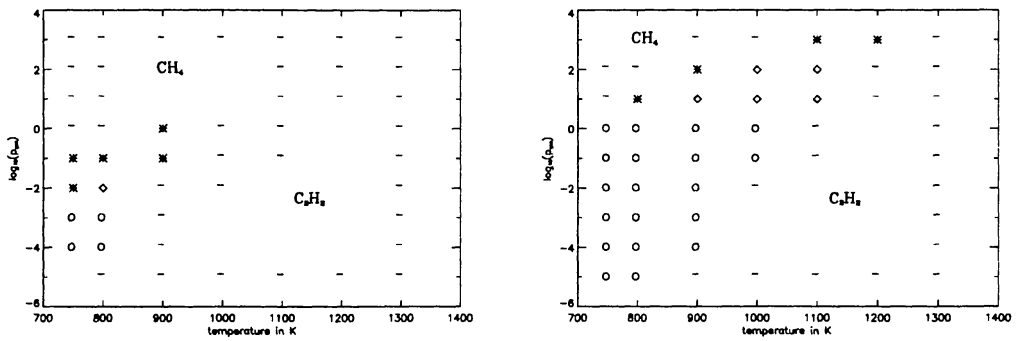[2]also Indiana University, Bloomington, IN 47405, USA

Figure 1.   Molecules accounting for the largest fraction of C not locked into CO at equilibrium in the T-P$_{gas}$ plane. In all cases the fraction is larger than 10%. Note that PAHs do also appear, even in smaller amounts, outside the region where they dominate. The symbols relate to the following PAHs at C/O=1.1(left panel) and C/O=5.0 (right penal): asterisks = $C_{10}H8$, diamond = $C_{18}H_{12}$ (triphenylen), circles = $C_{22}H_{14}$ (benzo(c)chrysene).

In contrast to our chemical equilibrium computation (where the allowed formation time is infinite) PAH formation at favourable T and P$_{gas}$ requires a residence time ($\Delta t \approx 10^{11}$s, Frenklach & Feigelson 1989) which is longer than the timescales of realistic wind models. In order to fulfil the law of mass conservation, with typical $\dot{M} \geq 10^{-7} M_{\odot}$/yr and v$_{\infty} \approx$10km/s, possible photospheric regions with T$\leq$1000K will not support strict hydrostatic equilibrium, and the residence time of the gas in this part of the photosphere will be considerably less than 10^{11}s. We therefore conclude that PAH do not have enough time to form, in the photosphere and in the wind of AGB stars. Therefore either the observed dust grains do form via other routes, or more complex stellar environments are required (e.g. with inhomogeneous hot and cool regions or combined infall-outflow).

References

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