

N91-15015

## PAH FORMATION IN CARBON-RICH CIRCUMSTELLAR ENVELOPES

Eric D. Feigelson\* and Michael Frenklach\*\*

\*Dept. of Astronomy, Penn State University,  
University Park, Pennsylvania 16802 USA

\*\*Dept. of Material Science and Engineering,  
Penn State University, University Park,  
Pennsylvania 16802 USA

### Motivation and Summary

While there is growing observational evidence that some fraction of interstellar carbon is in polycyclic aromatic hydrocarbons, the mechanisms by which these molecules might be formed have not been extensively studied. We briefly present here, and more completely elsewhere (Frenklach and Feigelson 1988), a detailed investigation of PAH production in the outflowing molecular envelopes of carbon-rich red giant stars. The gas-phase kinetics of a chemical reaction mechanism developed by Frenklach and co-workers to study soot production in hydrocarbon flames is modified to apply in circumstellar environments. We find that astrophysically significant quantities of PAHs can be formed in carbon star envelopes provided the gas is sufficiently dense and resides for a long time in the temperature range 900 to 1100 K. The precise yield of PAHs is very sensitive to astronomical parameters of the envelope (e.g. mass loss rate, outflow velocity, acetylene abundance) and certain poorly determined chemical reaction rates.

### Chemical and Astronomical Model

A chemical reaction mechanism involving >40 hydrocarbon species and >100 reactions was constructed from the models of PAH formation and growth in terrestrial pyrolytic and combustion environments (e.g. Frenklach et al. 1985, 1986). The terrestrial mechanism was shortened, revised for high temperatures and low pressures, and updated with recent rate coefficients. Four different first-ring cyclization paths are considered, including chemical activated processes. PAH growth beyond two rings is modeled with a linear lumping algorithm (Frenklach and Gardiner 1984).

Time-dependent non-equilibrium concentrations of each species was calculated for a range of density and temperature profiles characteristic of outflowing circumstellar envelopes. Most models were based on simple constant-velocity winds with density  $n \sim \dot{M}/r^2v$ ,

temperature  $T \sim r^{-\alpha}$ , and time variable  $t \sim r/v$ . The concentration of acetylene  $C_2H_2$  at the base of the wind must also be assumed. Published models of red giant molecular envelopes, particularly IRC +10216, were also examined.

## Results

Figure 1 presents the calculated PAH production in a constant-velocity model with wind parameters  $\dot{M} = 10^{-4} M_{\odot}/\text{yr}$ ,  $v = 0.01 \text{ km/s}$ ,  $[C_2H_2]/[H_2] = 10^{-4}$ ,  $\alpha = 0.5$  and stellar parameters  $R_* = 10^{14} \text{ cm}$  and  $T_* = 1500 \text{ K}$ . The top panel shows the assumed temperature and density profiles. The middle panel (right axis) shows that the calculated PAH yield increases only when  $1100 > T > 900 \text{ K}$ . Yield is defined to be the fraction of carbon initially in  $C_2H_2$  incorporated into molecules with  $>2$  aromatic rings. The mean PAH size  $\mu$  is generally  $\sim 40$  carbon atoms per molecule. The lower panel gives the standard deviation and skewness of the PAH  $A_{\text{size}}$  distribution. Our models all show a wide range of PAH sizes. This contrasts with the results of Keller (1987), who concludes that PAH growth in circumstellar envelopes proceeds rapidly until extremely large molecules are formed.

A grid of wind models similar to Figure 1 indicates PAH production is very sensitive to certain wind parameters. We find the yield depends approximately as:

$$Y \approx 1\% \left( \frac{v}{10^{-2} \text{ km s}^{-1}} \right)^{-4.0} \left( \frac{\dot{M}}{10^{-4} M_{\odot} \text{ yr}^{-1}} \right)^{2.5}$$

and scales with the cube of the acetylene abundance. Stated from a different perspective, the yield appears to depend mainly on the density and time spent in the PAH-producing temperature range  $900 < T < 1100 \text{ K}$ , approximately as:

$$Y \approx 1\% \left( \frac{n_{T=1000\text{K}}}{3 \times 10^{12} \text{ cm}^{-3}} \right)^{2.5} \left( \frac{\Delta t_{1100 > T > 900\text{K}}}{1 \times 10^{11} \text{ s}} \right)^{1.5}$$

for  $R_* = 10^{14} \text{ cm}$  and  $0.3 < \alpha < 0.8$ . Yields can exceed 90% in extreme cases. The yield for a fixed wind model can change by 1-2 orders of magnitude as certain chemical reactions rates (e.g. involving  $H_2C=C:$ ) are varied over ranges consistent with measurements. Given these strong dependencies and uncertainties, it is difficult to predict accurately the PAH production in a given star or ensemble of stars.

## Discussion

The dominant pathway we found for PAH formation in the outflowing envelopes is shown in Figure 2. The principal feature -- H abstractions followed by  $C_2H_2$  additions -- is the same as that

identified in terrestrial acetylene pyrolysis (Frenklach et al. 1985). However, important differences are seen: in circumstellar environments the high ambient H<sub>2</sub> concentration suppresses H abstraction, and thus PAH production, at the high temperatures (1400-2000 K) seen under terrestrial conditions. At temperatures around 1000 K, the irreversibility of the acetylene addition step drives PAH formation and growth. Analysis also suggests that the addition of other chemical species (e.g. CO, O<sub>2</sub>, electronically excited species) will not qualitatively affect our PAH-producing mechanism. Condensation of PAHs onto silicon carbide grains, however, should be considered.

Astronomically, our study implies that PAHs will form in carbon-rich circumstellar envelopes if their densities, [C<sub>2</sub>H<sub>2</sub>]/[H<sub>2</sub>] ratios, and residence times in the 900-1100 K temperature window are sufficiently high. Outflow velocities at these temperatures must be 10<sup>-3</sup> times typical terminal wind velocities. Such quasi-static warm regions have in fact been observed in red giant and supergiants (Tsuji 1987), and appear in the Lafont et al. (1982) model of IRC +10216. If such conditions are sufficiently common, then the concentration of PAH molecules introduced into the interstellar medium could be substantial.

#### References

- Frenklach, M., Clary, D. W., Gardiner W. C., and Stein, S. E.: 1985, in 20th Symp. Intl. Combustion, Pittsburgh:Combustion Inst., 887.
- Frenklach, M., Clary, D. W., Yuan, T., Gardiner, W. C., and Stein, S. E.: 1986, Combust. Sci. Technol. 50, 79.
- Frenklach, M. and Feigelson, E. D.: 1988, submitted to Astrophys. J.
- Frenklach, M. and Gardiner, W. C.: 1984, J. Phys. Chem. 88, 6263.
- Keller, R.: 1987, in PAHs and Astrophysics (A. Leger, L. d'Hendecourt and N. Boccarda, eds.), Dordrecht:Reidel, 387.
- Lafont, S., Lucas, R. and Omont, A.: 1982, Astron. Astrophys. 106, 201.
- Tsuji, T: 1987, in Astrochemistry (M. S. Vardya and S. P. Tarafdar, eds.), Dordrecht:Reidel, 409.

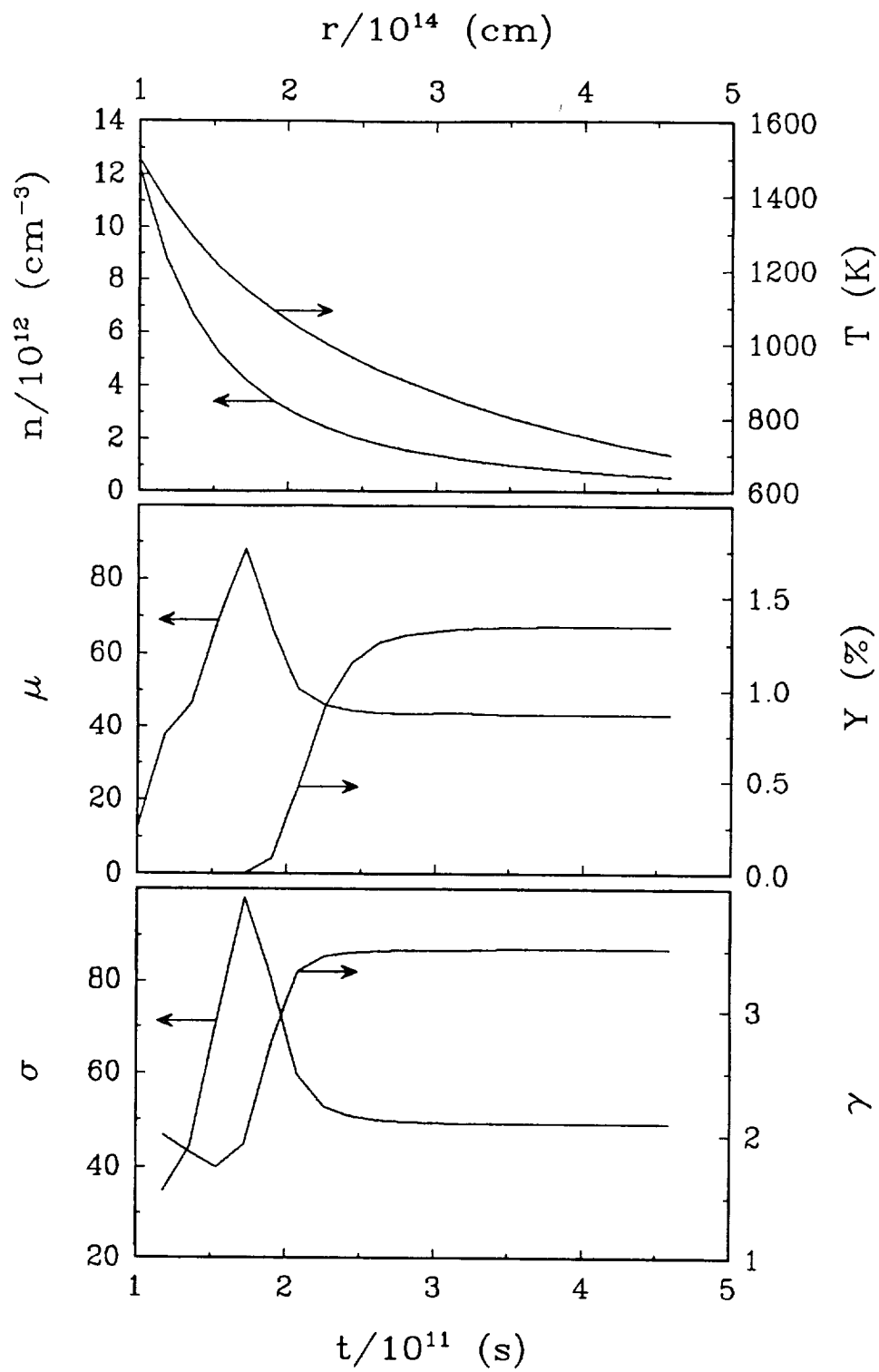


FIGURE 1

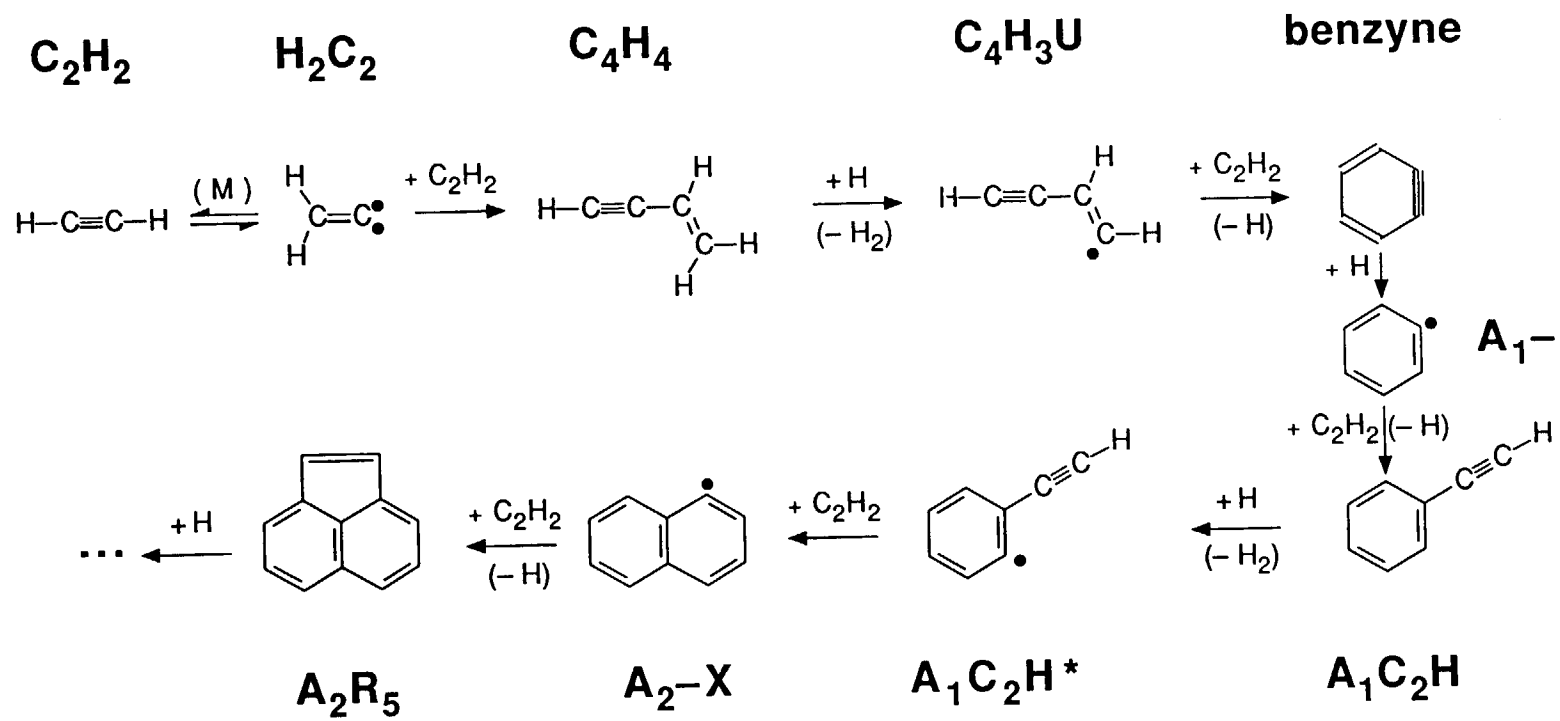


FIGURE 2

