

DUST FORMATION IN C-STAR SHELLS

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ABSTRACT. The formation of carbon grains is described by a chemical pathway from acetylene via polyaromatic hydrogens (PAHs). The proposed mechanism is in excellent agreement with the observations and provides in particular the observed low condensation temperature which cannot be explained by classical nucleation theory.

1. INTRODUCTION

The cool extended envelopes of C-stars are well known to be places of copious dust formation. The observational evidence for this fact is manifested by the broad band extinction and reddening of the star light and by the occurrence of particular spectral features attributed to transitions of special functional groups within carbon compounds like the famous 2200 Å band which is characteristic for electronic transitions of graphite-like structures or the IR transitions at 3.4, 6.2, 7.7, 8.6 and 11.3 μ which are due to particular vibrations of C-H or C-C groups of hydrogenated carbon or polyaromatic compounds, respectively, (e.g. Weast, 1976; Duley and Williams, 1979, 1981, 1983; Léger and Puget, 1984) but allow no definite conclusion about the real chemical and physical structure of the grains. Because of this rather vague observational and theoretical picture, any reliable theory on dust formation has to be based on the study of the elementary chemical processes (like soot formation in flames).

2. THE CONDENSATION TEMPERATURE AND THE BASIC NUCLEATING MOLECULE

Observations of the inner edge of dust shells confine effective dust formation to temperatures which are definitely lower than 1000 K (e.g. Rowan-Robinson and Harris, 1983). This low condensation temperature raises objections against explanation of carbon formation in the frame of classical nucleation theory which yields condensation temperatures around $T \approx 1200$ K, values which are definitely too large for being compatible with the observations (Gail and Sedlmayr, 1985).

In the relevant p-T-regime, the most abundant carbon bearing molecule able to condensate is acetylene (C_2H_2) which, therefore, has to be considered as the basic nucleating species. These two facts, the low condensation temperature and C_2H_2 as condensating molecule, provide the basis upon which any nucleation theory has to rely.

3. CARBON DUST FORMATION

A detailed study of hydrogen chemistry in order to construct a reliable pathway from acetylene to macroscopic "carbon grains" has been essentially performed in our group by R. Keller in his thesis (Keller, 1986a, b). In the following, we list the main results of our investigation:

- In the temperature-pressure regime where dust formation is observed PAHs are by far the most abundant large molecules. Therefore, the nucleation path has to proceed via a chain of PAHs.
- In order to obtain sufficiently large particle densities, i.e. a sufficient nucleation rate, the gas kinetic temperature has to be about 700...950 K.
- At this temperature the critical cluster is acephenanthrylene, a molecule containing 16 C-atoms.
- The growth of the supercritical molecules occurs by radical reactions, i.e. by a three step mechanism: i) formation of a free radical site by hydrogen abstraction, ii) attachment of an acetylene molecule as a side chain, and iii) ring closure. By the first two steps PAH growth and H_2 formation are coupled by a fixed proportion.
- In order to obtain sufficiently large growth rates, the H/H_2 -ratio has to depart strongly from chemical equilibrium.

4. CONCLUSION

Along these guiding lines, a pathway to carbon grains can be constructed which is compatible both with fundamental chemistry and astrophysical observations.

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