Growth and destruction of PAHs in reactions with C atoms

Serge A. Krasnokutski

Friedrich Schiller University of Jena, 07740 Jena, Germany

MPI for Astronomy, Königstuhl 17, 69117 Heidelberg, Germany
Dust in the ISM

\[
\Downarrow
\]

Lifetime issue

\[
\Downarrow
\]

Formation in the ISM
The Boomerang Nebula $T = 1 \text{ K}$
Motivation

1) Most of the dust-destruction processes produce single atoms in the gas phase. Different estimations show that 30% and even up to 80% of all carbon exists in the form of atomic gas (Snow & Witt 1995; Sofia et al. 2011).

2) The dust growth proceeds by accretion of gaseous species on the surface of survived grains.

3) Low-temperature reactions of carbon atoms on the grain surface is responsible for the reformation of carbonaceous dust grains.

4) PAHs are believed to be an important component of the carbonaceous ISM dust.

5) In order to study the reactions on the surface of dust grains in laboratories, the energy absorption ability of the dust has to be reproduced.

6) This can be achieved by placing the reactants inside liquid helium.
PAHs + C, background

Dust surface / He droplet
290 kJ/mol

Gas phase
35 kJ/mol
The He droplet experimental setup
Differential mass spectra for the reactions of carbon atoms with benzene and naphthalene.
Reactions inside He droplets

1. $n > 30000$

$$E = (n_1 - n_2) \times 5 \text{ cm}^{-1}$$

2. $n < 10000$
The intensity of the He droplet beam, measured via the He vapor pressure in the detector chamber.
Molecular structures of possible products of the C + C$_{10}$H$_8$ reaction

b3lyp/6-311+g(d p)
Energy level diagram for the C + C\textsubscript{10}H\textsubscript{8} reaction
Differential mass spectra for the reactions of carbon atoms with anthracene and coronene.
Partial pressure of helium in the detector chamber as a function of time

372.1 kJ/mol
Molecular structures of the initial associative complexes of C with C\textsubscript{24}H\textsubscript{12}

15.5 kJ/mol

23.9 kJ/mol

65.2 kJ/mol

134.5 kJ/mol
Summary

- Small PAH molecules barrierlessly react with atomic carbon.
- This reaction leads to the formation of seven membered carbon rings and expecting to provide a broad variety of non-classical small PAHs.
- With increasing the molecular size, PAH molecules are getting more inert toward reaction with atomic carbon.
- Large graphene sheets cannot be produced by condensation of atomic carbon. Instead, at larger scales, the condensation of carbon atoms would likely lead to the formation of aliphatic or sp$^3$ hybridized carbon.