

PAH notes

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In this network, the PAHs are only considered as small grains (neutral or negatively charged). The reactions included are: electron attachment to neutral PAHs, electron photodetachment and reactions between positive ions and negative PAHs. Any details can be found in Wakelam & Herbst (2007). The format of the column is the same as for osu.

For reactions between positive ions and negative PAHs, ITYPE=14. Column A gives the branching ratio of the reaction in case there are two products. The second column is the mass of the reactant in amu. The rate coefficient is computed as a function of the PAH radius (a) :

$$k = \pi a^2 \sqrt{\frac{8k_B T}{\pi \mu}} \left(1 + \frac{e^2}{a k_B T} \right)$$

k_B is the boltzmann constant = 1.38×10^{-16} erg/kelvin

a is the PAH radius in cm

T is the gas temperature

e is the electronic charge = 4.803×10^{-10} esu

μ is the reduced mass ~ mass of the reactant in gram

This expression assumes that Coulomb attraction between the two reactants. If this process is not efficient (for large grains for instance), remove the second term of the parenthesis.

For the electron attachment reaction, ITYPE=15. We use the formula given by Omont (1986):

$$k = 10^{-7} (N_C)^{3/4} \text{ cm}^3 \text{ s}^{-1}$$

with N_C the number of carbons in the PAH.

For the photodetachment reaction, ITYPE=13. The rate coefficient is computed as a function of A_ν the normal way (see the osu database).