Calculation of rate coefficients for ion-polar systems

V. Wakelam Sept. 2015

In the KIDA database, two formula have been introduced for ion-polar systems : ionpol1 and ionpol2. This document aims at explaining these formula and how they are used in the database and models. Rate coefficients for unmeasured reactions between ions and neutral species with a dipole moment are computed using the Su-Chesnavich capture approach. This approach is discussed in Woon & Herbst (2009), Wakelam et al. (2010) and Wakelam et al. (2012).

The rate coefficient for these type of reactions is expressed in terms of the temperature-independent Langevin rate coefficient k_L using two formulas, one for lower and one for higher temperatures. The temperature ranges will depend on a unitless parameter x, defined by the relation :

$$x = \frac{\mu_D}{\sqrt{2\alpha k_B T}}$$

with μ_D the dipole moment in units of Debye, α the scalar polarizability in cubic angstroms, T the temperature and k_B the Boltzmann constant. The temperature ranges are divided by that temperature for which the parameter x is equal to 2.

The Langevin rate coefficient (the approximation for ion-polar reactions where the neutral is non-polar) is given by the expression :

$$k_L = 2\pi e\sqrt{\frac{\alpha}{\mu}}$$

where k_L is in units of cm^3s^{-1}, μ is the reduced mass in amu ($\frac{1}{\mu} = \frac{1}{m_{ion}} + \frac{1}{m_{neutral}}$) and e is the electronic charge in units of cgs-esu.

In terms of the parameters x and k_L, the rate coefficient for an ion-dipole collision is as follows :

$$\frac{k}{k_L} = 0.4767x + 0.62 \text{ if } x \geq 2$$

$$\frac{k}{k_L} = \frac{(x+0.5090)^2}{10.526} + 0.9754 \text{ if } x \leq 2$$

Those are totale rate coefficients. If there is more than one production channel, then the rate coefficient has to be multiplied by the branching ratio. In KIDA, the partial rate coefficients are stored and the two formula to compute the temperature rate coefficients defined for the two temperature ranges are :

$$k = \alpha\beta\left(0.62 + 0.4767\gamma\left(\frac{300}{T}\right)^{1/2}\right) \quad \text{ionpol1}$$

$$k = \alpha\beta\left(1 + 0.0967\gamma\left(\frac{300}{T}\right)^{1/2} + \frac{\gamma^2}{10.526}\frac{300}{T}\right) \quad \text{ionpol2}$$

Here α, β and γ are the three parameters stored in the database. α represents the branching ratio of the reaction, β is the Langevin rate while γ represents the value of x at 300 K.