The way to calculate the ionization rate and the KROME datafile

Based on Latif+ (2015).

$$\zeta_x^i = \zeta_p^i + \sum_{j=H,He} \frac{n_j}{n_i} \zeta_p^j \langle \phi^j \rangle$$

where n_j is the number density.

$$\zeta_p^i = \frac{4\pi}{h} \int_{E_{min}}^{E_{max}} \frac{J(E)}{E} e^{-\tau(E)} \sigma^i(E) \mathrm{d}E$$

$$J(E) = J_{X,21} \left(\frac{E}{1\mathrm{keV}} \right)^{-1.5} \times 10^{-21} \text{ erg cm}^{-2} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1}$$

where $J_{X,21} = 1$

$$\tau(E) = \sum_{i=H,He} N_i \sigma^i = \frac{\lambda_J}{2} \sum_{i=H,He} n_i \sigma^i$$

Jeans length:

$$\lambda_J = \sqrt{\frac{\pi k T}{G \rho \mu m_p}}$$

$$\mu = \frac{1.00794 n_H + 4.0026022 n_{He}}{n_H + n_{He}}$$

σ^i comes from Verner & Ferland (1996)

$\langle \phi^j \rangle$ is much more complex. For $E > 100$eV and H, He mixture

$$\phi^H(E, x_e) = \left(\frac{E}{13.6\mathrm{eV}} - 1 \right) 0.3908 (1 - x_e^{0.4092})^{1.7592}$$

$$\phi^H e(E, x_e) = \left(\frac{E}{24.6\mathrm{eV}} - 1 \right) 0.0554 (1 - x_e^{0.4614})^{1.666}$$

where x_e is the electron fraction

$$\langle \phi^i \rangle = \frac{\int J(E) \phi^i(E, x_e) \mathrm{d}E}{\int J(E) \mathrm{d}E}$$

In the datafile that KROME offers:

$$E_{min} = 2 \text{ keV} \qquad E_{max} = 10 \text{ keV}$$

$$T = 160 \text{ K}$$

$$J_{X,21} = 1$$

The datafile is a 30 table which shows log(N_H), log(N_H)-log(N_{He}), N is the column density. The size of the cloud is estimated by its Jeans length and the number density n

$$n^i = \frac{N^i}{\lambda_J/2}$$

To get the certain X-ray ionization rate, the KROME package first turns the number densities(H, He) into column densities. Notice that the Jeans length now does not only depend on H/He but other atoms. then it reads the datafile rateH.dat/rateHe.dat and does 2-Dimension linear interpolation to find the ionization rate. This is how these 'auto' rates in the network are calculated.