1. CX fit model

Let ψ_i denote the projectile state i, and χ_{nlj} denote the charge exchange capture orbital. The final state after the capture can be expressed as a linear mixing of the product of the two functions:

$$\Psi_k = \sum_{i,nlj} b^k_{i,nlj} |\psi_i \chi_{nlj}; \gamma \pi J > \tag{1}$$

where π and J are the parity and total angular momentum of the product state, and γ represents all other quantum numbers required to fully describe the state. Therefore, final state index k represent a collection of quantum numbers i, nlj, γ, π, and J. $b_{i,nlj}$ are the mixing coefficients, which can be determined solving the atomic structure problem of the recombined ion. Ignoring the interference terms, the charge exchange cross section from the projectile state ψ_i to the recombined state Ψ_k can be approximated as:

$$\sigma_k = \sum_{nlj} |b^k_{i,nlj}|^2 a_{i,nlj,\gamma \pi J} \sigma_{\alpha,nlj} \tag{2}$$

where $a_{i,nlj,\gamma \pi J}$ are the angular momentum decoupling factors, and $\sigma_{\alpha,nlj}$ is the charge exchange cross section to a one electron orbital χ_{nlj}, which may depend on a subset of the quantum numbers describing the product state. For typical EBIT measurements on highly charged ions, the only important initial state is the ground state ψ_0. Due to configuration interaction mixing, the capture to core excited final state k may have non-vanishing cross sections. However, the free parameters in our model are the one-electron capture cross sections from the ground state, the coefficients $b^k_{0,nlj}$ and $a_{0,nlj,\gamma \pi J}$ can all be calculated from atomic structure codes.

In the most simple model, $\sigma_{\alpha,nlj}$ only depends on the non-relativistic quantum numbers of the one-electron orbital nl, such that:

$$\sigma_{\alpha,nlj} = \frac{2j+1}{4l+2} \sigma_{nl} \tag{3}$$

For complex ions, this represent a huge reduction of number of free parameters required to describe the detailed final state resolved capture cross sections. For low energy charge exchange collisions, it is well known that the capture is dominated by a few n values around its maximum n_{max}. One can further simplify the parametrization as

$$\sigma_{nl} = \sigma_t \beta_n f_l \qquad (4)$$

where σ_t is the total capture cross section, β_n and f_l are the n and l distribution, respectively, where we assume f_l is the same for the few neighboring n values that dominate the charge exchange process. The complete factorization of the n and l distributions further reduces the number of free parameters in the model. This procedure of reducing the parameter space is very important to obtaining a physically meaningful solution from the measured cascade spectra.

It is possible that the n and l distribution functions may have some dependence on certain quantum numbers of the projectile or product state, such as total spin and total angular momenta. Therefore our spectral basis set is comprised of a set of lines, where the intensity of the m-th line can be written as:

$$I_m = A_{m,k}\sigma_k = B_{m,nl}^{\gamma\pi J}\beta_n^\alpha f_l^\alpha \qquad (5)$$

The matrix A, and therefore B can be obtained by the radiative cascade calculation.

In practice, I found that for CX of H-like ion, a set of β_n amd f_l parameters are enough to adqequately fit the measured spectra. for He-like ions, choosing $\alpha = S$ as the total spin of the product state is appropriate. To fit the Ne-like Ni spectra, it is required to choose α to the the combination of S and J.