Charge exchange cross sections in nitrogen ions and hydrogen collisions

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Injected Impurities CRP - First Research Coordination Meeting (Virtual) – March 2023

OUTLINE

- Motivation
- Workplan
- The impact parameter approach
- Our implementation

Summary Report of a Consultancy Meeting in preparation of a Coordinated Research Project on Atomic Data for Injected Impurities in Fusion Plasmas

7 – 8 June 2022
IAEA Headquarters, Vienna Austria and virtual

3. Which species should (and should not) be considered within the scope of the CRP?

a. Tungsten in plasma is not in scope; in particular, W as a catalyst for NHx formation should be considered as part of the forthcoming CRP F43027: *Molecules in Edge Plasmas;*

b. The following species should be considered, in order of priority:

Ar, N, Ne, (Kr), (Xe)

(the first three in all ionisation states, the last two in those ionisation states present for T_i > 500 eV);

c. Lithium, particularly in its interactions with $H_2(v)$ and its isotopologues, and isotopes of H and H^+ may be considered, but with lower priority than the above species and may be better served by CRP F43024: *Atomic Data for Vapour Shielding in Fusion Devices*. Similarly for tin;

d. Boron and related species (BN, BC) may also be considered, with lower priority, depending on the need for modelling the effects of its ions in edge plasmas.

4. Which processes involving these species are of greatest importance?

In order of priority:

a. Charge exchange (HCX) with H^0 across the energy ranges for which the relevant ions exist;

b. Electron impact excitation (EEX), above threshold;

c. Dielectronic recombination (ERD), for Ar and Ne, and state-resolved;

d. Spectra: line strengths and wavelengths;

e. (With lower priority) collisions with He^{2+} (alpha particles), for energies > 100 keV.

1. What categories of data are needed for modelling the atomic and molecular physics of injected impurities?

Cross sections (possibly differential cross sections), and in particular for state-resolved processes

Rate coefficients (also state-resolved, where possible)

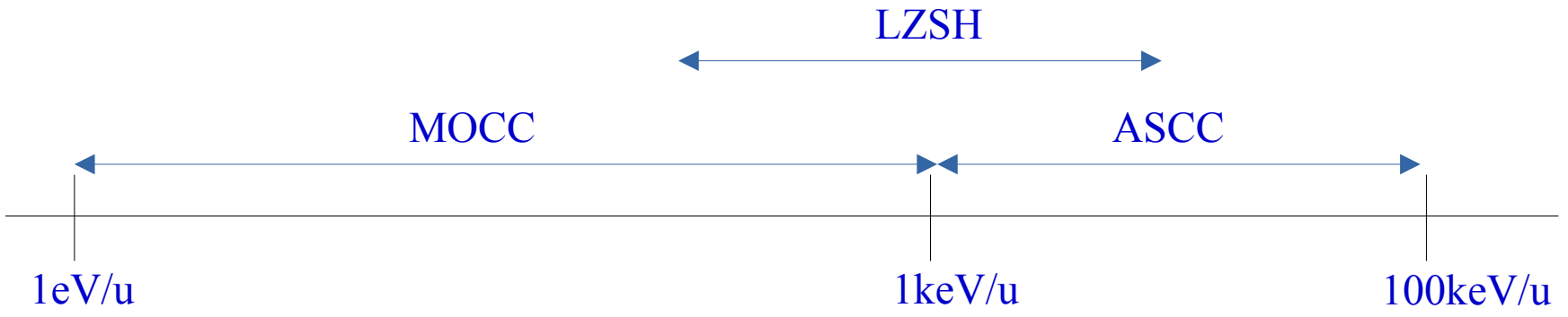
Spectral data: Line strengths / Einstein *A* coefficients; wavelengths. It was noted that no particular data are currently required by modelling codes regarding the Zeeman and Stark effects and that these are adequately parameterised from well-known physics considerations.

It was also noted that the uncertainties associated with existing data are often not well characterised and that particular effort should be expended, where possible, to promote the appropriate assessment of uncertainties in data produced or evaluated during the CRP.

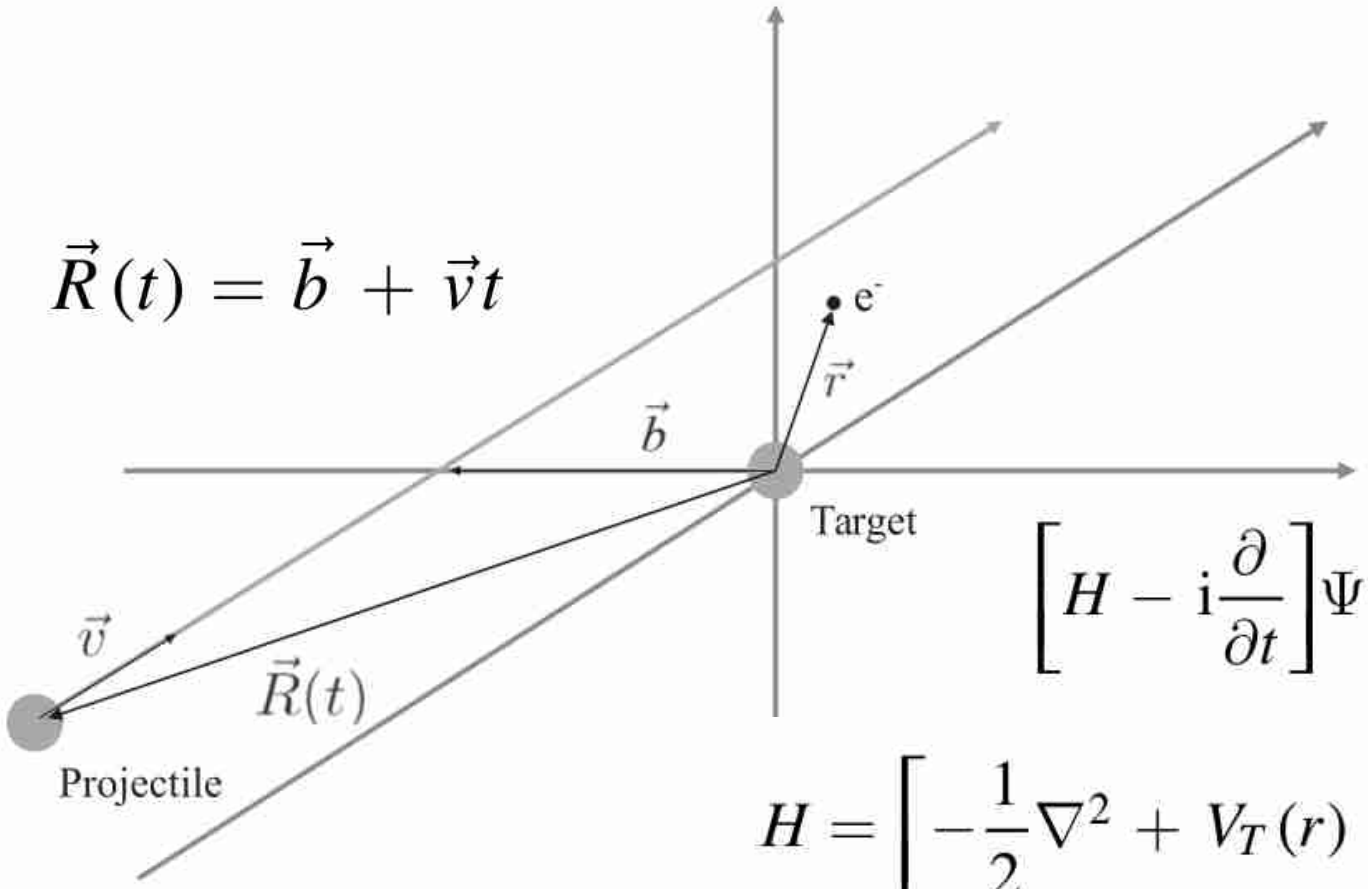
Workplan

Impact energies from 1eV/u to 100keV/u

1st year	state-resolved cross-sections for N^{2+} - H
2nd year	state-resolved cross-sections for N^{3+} - H & N^{2+*} - H
3rd year	state-resolved cross-sections for N^{3+*} - H



The impact parameter approach



$$\left[H - \mathrm{i}\frac{\partial}{\partial t}\right]\Psi(\vec{r}, \vec{R}(t)) = 0$$

$$H = \left[-\frac{1}{2}\nabla^2 + V_T(r) + V_P(|\vec{r} - \vec{R}(t)|)\right]$$

$$\sigma_f = 2\pi \int_0^{+\infty} b P_f(b)\,\mathrm{d}b$$

Close-coupling method (ASCC)

$$\left[H - \mathrm{i}\frac{\partial}{\partial t}\right]\Psi(\vec{r}, \vec{R}(t)) = 0$$

Wavefunction ansatz

$$\Psi(\vec{r}, \vec{R}(t)) = \sum_i c_i^T(t)\Psi_i^T(\vec{r})\mathrm{e}^{-\mathrm{i}\epsilon_i^T t}$$

$$+ \sum_j c_j^P(t)\Psi_j^P(\vec{r})\mathrm{e}^{-\mathrm{i}\epsilon_j^P t}\mathrm{e}^{\mathrm{i}\vec{v}\cdot\vec{r}+i\frac{1}{2}v^2 t}$$

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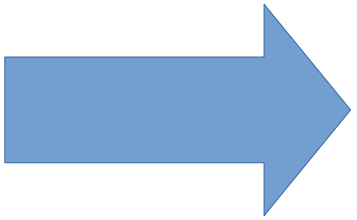

$$i\mathbf{S}(b, v, t)\frac{d}{dt}c = \mathbf{M}(b, v, t)c$$

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ETF

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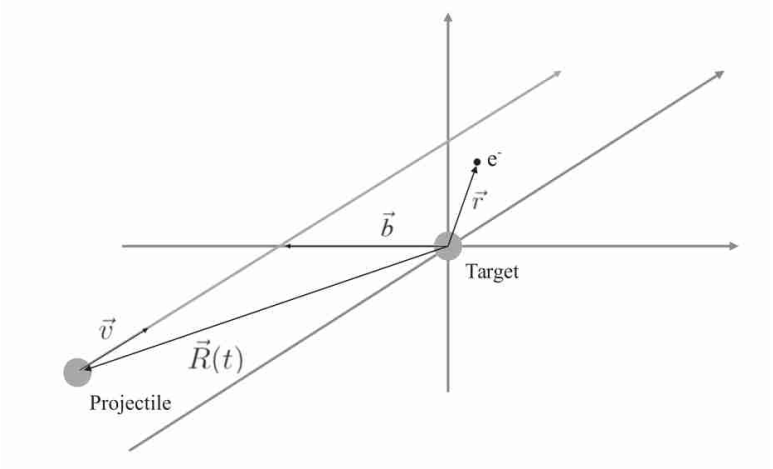
Close-coupling method (ASCC)



$$i\mathbf{S}(b,v,t)\frac{d}{dt}c = \mathbf{M}(b,v,t)c$$

$$P_f(b) = \lim_{t\to\infty} |c_f(b,t)|^2$$

$$\sigma_f = 2\pi \int_0^{+\infty} bP_f(b)\,\mathrm{d}b$$

Our implementation

Multi-center Gaussian type orbitals (GTO)

$$\Psi_i^X(\vec{r}) = \sum_k d_k \chi_k(\vec{r} - \vec{r_k})$$

$$\chi_k(\vec{r}) = N_k (x - x_k)^{u_k} (y - y_k)^{v_k} (z - z_k)^{w_k} e^{-\alpha_k (r - r_k)^2}$$

Advantages of GTO
- Gaussian product rule
- Efficient algorithms for integrals evaluation
- Extension to multi-electron systems

Advantages of multicenter expansion
- Description of ionization

Our implementation

$$i\mathbf{S}(b,v,t)\frac{d}{dt}c = \mathbf{M}(b,v,t)c$$

Adams Bashford Moulton predictor-corrector method

Full code in FORTRAN 90

Parallelization with Open-MP

Code for N-e systems

Thank you for your attention

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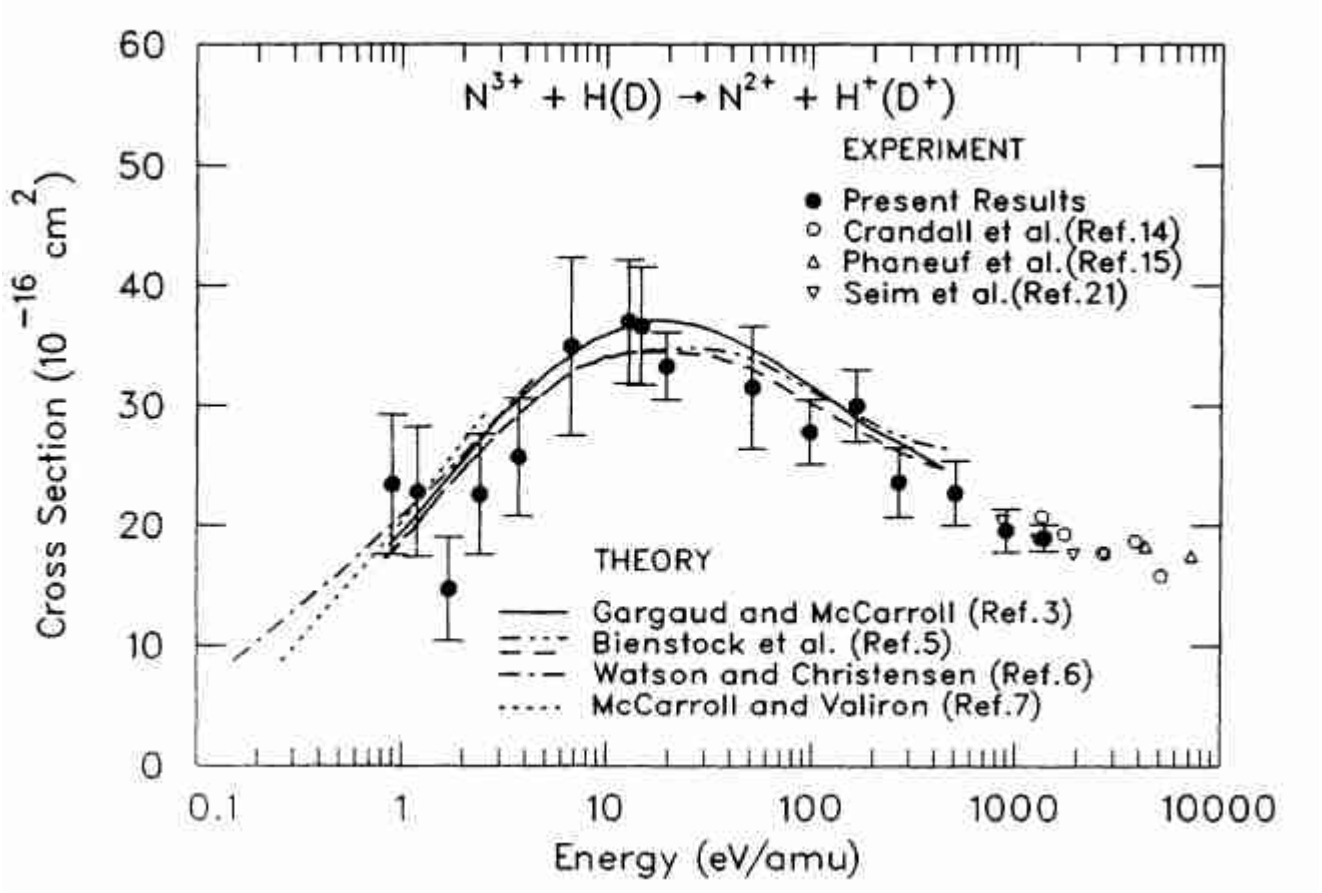
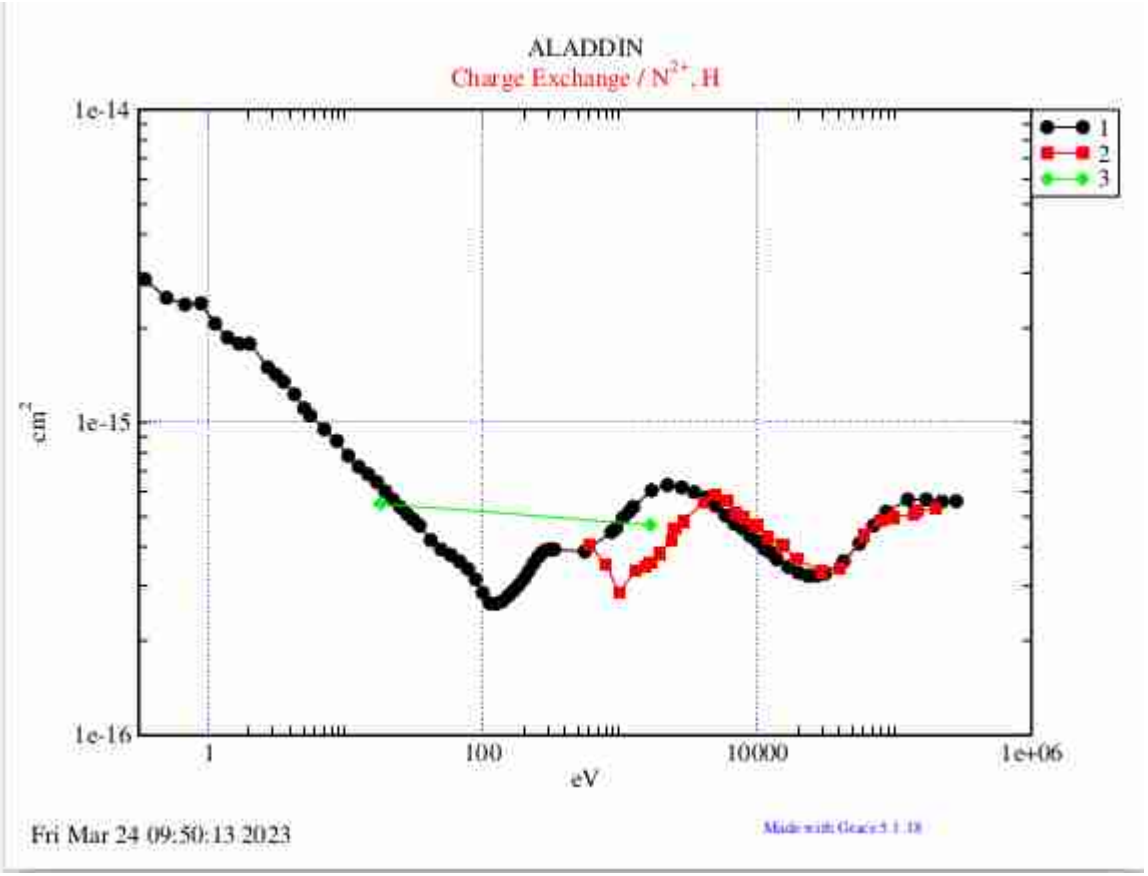
Low-energy electron capture by N^{3+}, N^{4+}, and N^{5+} from hydrogen atoms using merged beams

M. S. Huq, C. C. Havener, and R. A. Phaneuf
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6372
(Received 22 December 1988)



ID	Process	Reaction
1		N^{2+} *[2s²2p¹ ²P]*, H *[1s]* --> N^{+}, H^{+} *(P. Barragan et al)*
2		N^{2+}, H *(WILKIE F)*
3		N^{2+}, H --> N^{+}, H^{+} *(C.C. Havener et al.)*



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