atoms

MDPI

Article

Fully-Stripped Beryllium-Ion Collisions with $2\ell m$ States of Atomic Hydrogen: Target Excitation and Ionisation cross Sections

Nicholas W. Antonio [1,*], Corey T. Plowman [1], Ilkhom B. Abdurakhmanov [2], Igor Bray [1] and Alisher S. Kadyrov [1,*]

[1] Department of Physics and Astronomy and Curtin Institute for Computation, Curtin University, GPO Box U1987, Perth, WA 6845, Australia
[2] Pawsey Supercomputing Research Centre, 1 Bryce Ave., Kensington, WA 6151, Australia
* Correspondence: nick.antonio@curtin.edu.au (N.W.A.); a.kadyrov@curtin.edu.au (A.S.K.)

Abstract: The wave-packet convergent close-coupling approach is used to calculate integrated target excitation and ionisation cross sections in bare beryllium-ion collisions with the $2\ell m$ states of atomic hydrogen (where n, ℓ and m are the principal, orbital angular momentum and magnetic quantum numbers, respectively). The calculations are performed at representative projectile energies between 10 keV/u to 1 MeV/u. The calculated cross sections for collisions with H($2s$) are compared with recent theoretical results. Generally, good agreement is observed for the n-partial excitation and total ionisation cross sections. However, a significant discrepancy is found for excitation into the dominant $n = 3$ states at 100 keV/u, where the target excitation cross-section peaks. We also present the first calculations of the excitation and ionisation cross sections for Be^{4+} collisions with H($2p_0$) and H($2p_{\pm1}$).

Keywords: ion-atom collisions; fully-stripped beryllium ion; target excitation; ionisation

check for updates

Citation: Antonio, N.W.; Plowman, C.T.; Abdurakhmanov, I.B.; Bray, I.; Kadyrov, A.S. Fully-Stripped Beryllium-Ion Collisions with $2\ell m$ States of Atomic Hydrogen: Target Excitation and Ionisation cross Sections. *Atoms* **2022**, *10*, 137. https://doi.org/10.3390/atoms10040137

Academic Editors: Izumi Murakami, Daiji Kato, Hiroyuki A. Sakaue and Hajime Tanuma

Received: 7 October 2022
Accepted: 5 November 2022
Published: 10 November 2022

1. Introduction

Establishing a database of accurate cross-sections for various ion-atom collisions is important for plasma modelling and diagnostics [1]. Among the primary impurity ions expected to be present inside fusion reactors such as ITER and JET is the Be^{4+} ion. This is due to the erosion of beryllium-containing plasma-facing wall components [2,3]. The effects the Be^{4+} ions have on properties such as the density and temperature of the plasma can be measured using the charge-exchange recombination spectroscopy (CXRS) technique [4]. This is done by injecting a neutral beam of hydrogen atoms into the reactor so that collisions between Be^{4+} and H can occur. These collisions can lead to charge exchange whereby Be^{3+} ions are formed in excited states. The impurity ion densities may then be measured through the emission spectra of these hydrogen-like ions. This requires accurate total and state-selective electron-capture cross-sections. However, performing diagnostics using the CXRS technique also requires knowledge of the neutral beam densities which are obtained using beam emission spectroscopy (BES) [5,6]. For BES, target excitation and ionisation cross-sections are also needed. Therefore, a complete set of cross-sections for all possible processes taking place in Be^{4+} collisions with atomic hydrogen is essential for plasma impurity diagnostics.

The neutral beam that is injected into the reactor for diagnostics is mostly comprised of ground-state atomic hydrogen. However, it is predicted that a fraction of the H atoms become excited as they penetrate the plasma. The cross sections for impurity ions colliding with H initially in the ($2s$, $2p_0$, $2p_{\pm1}$) states are expected to be approximately an order of magnitude larger than that for collisions with H($1s$) in the low to intermediate energy range [7]. Therefore, contributions to the charge-exchange, target-excitation and ionisation processes due to scattering on H in excited states cannot be neglected.

Despite the importance of these cross-sections for plasma diagnostic studies, there exists no experimental data for Be^{4+} collisions with atomic hydrogen. However, there are theoretical calculations made for Be^{4+} collisions with H(1s) [8–14]. Given the importance of accounting for collisions with excited states of atomic hydrogen, calculations have also been performed for Be^{4+}-H($2\ell m$) collisions [11,15–19]. The theoretical methods that were used to calculate the cross sections of interest include the first-order Born approximation with corrected boundary conditions (B1B) [8], the two-centre atomic-orbital close-coupling (AOCC) method [9,11,13], the molecular-orbital close-coupling (MOCC) method [10,15,17], the classical trajectory Monte Carlo [12,14,18,19] method, and lattice-based numerical approaches [12,13,19]. However, all these works, except one, were focused on obtaining the total and state-selective electron-capture cross sections. Calculations of the target excitation and ionisation cross sections for collisions with H($2\ell m$) are limited to the recent results by Jorge et al. [19], obtained by grid-numerical solution of the time-dependent Schrödinger equation (GTDSE) and a CTMC approach with hydrogenic initial distribution (h-CTMC).

In this study, we use the two-centre wave-packet convergent close-coupling (WP-CCC) approach to investigate collisions of bare beryllium ions with all the $2\ell m$ states of atomic hydrogen. This approach accounts for the strong coupling effects between all possible reaction channels, including ionisation. The method has been applied to collisions of multiply charged ions with atomic hydrogen [20–22] and proton collisions with multielectron targets [23–26]. Recently, we have also studied Be^{4+} collisions with the ground and $2\ell m$ states of atomic hydrogen [27,28]. Specifically, we have calculated the total, n- and $n\ell$-resolved electron-capture (EC) cross sections. The total cross section for ionisation in collisions with H(1s) has also been presented in [27]. In this work, we extend the aforementioned studies to the target-excitation and ionisation processes in fully-stripped beryllium ion scattering on hydrogen initially in the $2\ell m$ states.

2. Details of Calculations

The formalism of the wave-packet convergent close-coupling approach to fully stripped ion collisions with atomic hydrogen is outlined in [21,29,30]. In short, the motion of the projectile is treated with a classical straight-line trajectory while the electron dynamics is treated fully quantum mechanically. We solve the full three-body Schrödinger equation by expanding the scattering wavefunction using a basis comprised of negative-energy eigenstates and positive-energy wave-packet pseudostates on both the projectile and target centres. The use of the wave-packet pseudostates allows one to discretise the continuum of the electron with a required density which is advantageous for calculations of the ionisation cross-section. Through substitution of the scattering wavefunction into the three-body Schrödinger equation, we obtain a set of coupled-channel first-order differential equations for time-dependent expansion coefficients in impact-parameter representation. In the asymptotic region, these expansion coefficients represent the transition probability amplitudes for all the channels included in the expansion of the scattering wave function. By solving for these transition probability amplitudes over a fine impact-parameter grid, we obtain the weighted probability (which is the probability, $P(b)$, times the impact parameter, b) distributions for all scattering processes. The corresponding cross sections can then be calculated by integrating over these weighted probabilities with respect to b.

To calculate accurate cross sections, we ensure the maximum impact parameter, $b_{\max}$, used is sufficiently large so that the corresponding probability distributions fall off at least three orders of magnitude from the maximum. We find that at all projectile energies considered in this work, $b_{\max}$ required for the excitation and direct ionisation processes is considerably larger than that needed for both EC and the electron-capture into the continuum (ECC) component to ionisation. Accordingly, at sufficiently large impact parameters, where the total EC and ECC probabilities become sufficiently small, coupling to the capture channels becomes negligible. Therefore, in this work, we take a new approach to calculating excitation and ionisation cross-sections. Here, we employ two-centre (2c) calculations up to some $b^{2c}_{\max}$, where both the EC and ECC probabilities have fallen off at least three orders of magnitude. We then extend these calculations by using single-centre (1c) calculations up to some final b^{1c}_{max} and integrate over the entire combined weighted probability distributions to obtain the target-excitation and ionisation cross sections. Figure 1 illustrates this approach by showing the weighted probabilities for total EC, target excitation into the $n = 3$ states and ionisation as functions of impact parameter for Be^{4+}-H(2s) collisions at 100 keV/u. The lines given in red represent two-centre calculations whereas black lines indicate single-centre calculations. At this projectile energy, we set $b^{2c}_{max} = 21$ a.u., whereas $b^{1c}_{max} = 100$ a.u. One can see that the single-centre and two-centre calculations for the ionisation and excitation probabilities join seamlessly. Therefore, this procedure allows one to extend the weighted probability distributions to sufficiently large b to obtain the excitation and ionisation cross sections without requiring extensive two-centre calculations where coupling to the capture channels has negligible effect.

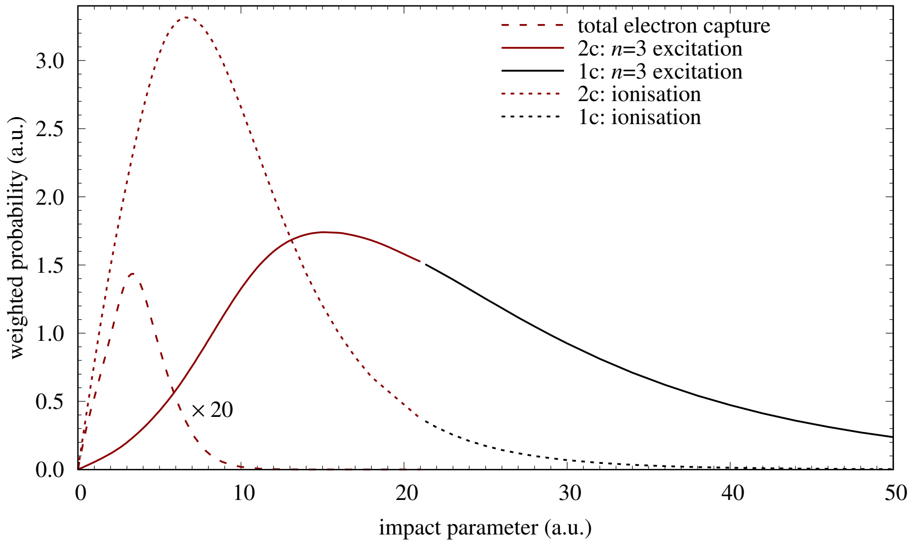

Figure 1. The weighted probability distributions for total electron capture, target excitation into the $n = 3$ states and ionisation in Be^{4+} collisions with H(2s) at the projectile energy of 100 keV/u. Only half of the impact-parameter range used in the cross-section calculations is shown.

Obtaining accurate cross-sections within the WP-CCC framework depends on the level of convergence reached with respect to the number of basis states included in the expansion of the scattering wave function. All two-centre calculations presented in this work use the same basis and numerical parameters that were reported in [28]. Briefly, as the projectile energy is increased, we find that the minimum necessary size of the symmetric two-centre basis can be reduced. With reference to three key impact energies (low, intermediate and high), the required two-centre basis size at 20 keV/u is 4770 states, whereas at 100 keV/u and 500 keV/u the minimum necessary size reduces to 3480 and 2198 states, respectively. Single-centre calculations generally require a larger maximum angular momentum quantum number, ℓ_{max}, to converge in comparison to two-centre calculations [21]. To this end, ℓ_{max} required in the present single-centre calculations varies from 8 to 11. With the basis parameters discussed here and in [28], we find that all cross sections presented below have converged to within a few percent.

3. Results and Discussion

In this section, we present our calculations for the n-partial excitation and total ionisation cross sections for Be^{4+} scattering on the $2\ell m$ states of atomic hydrogen. It is worth noting that the results obtained for collisions with H(2p_1) are the same for H(2p_{-1}) as our calculations do not depend on the sign of the magnetic quantum number.

Figure 2 presents cross sections for target excitation into the $n = 3$, 4 and 5 states as functions of projectile energy. The left, middle and right panels correspond to the results for Be^{4+} collisions with H(2s), H(2p_0) and H(2p_1), respectively. The two-centre WP-CCC results extended in the impact parameter range using single-centre calculations are labelled as 2c. Alongside these results are completely single-centre calculations (denoted by 1c). This is done to establish the internal consistency of both calculations. For all overlapping projectile energies, excellent agreement between the two sets of the WP-CCC results is found. This suggests that at least starting from 20 keV/u, the target excitation cross sections for Be^{4+}-H(2ℓm) collisions can be obtained through purely single-centre calculations. Figure 2 also shows that the $n = 3$ states represent dominant excitation channels across the entire projectile energy range. Furthermore, we see the excitation cross sections decrease significantly with increasing n.

Also shown in Figure 2 are the GTDSE and h-CTMC results for collisions with H(2s) by Jorge et al. [19], available at 20 and 100 keV/u. The WP-CCC cross-sections are in excellent agreement with the GTDSE ones at 20 keV/u. This level of agreement is also found at 100 keV/u with the exception of the dominant excitation cross-section into the $n = 3$ states. Here, we find the WP-CCC results to be approximately 25% smaller than the GTDSE ones. The reason for this disagreement is undetermined. We also find the WP-CCC results to be in excellent agreement with the h-CTMC ones for excitations into the $n = 4$ and $n = 5$ states. However, the h-CTMC results for the $n = 3$ target excitation cross section [19] (not shown) are significantly larger than the present ones.

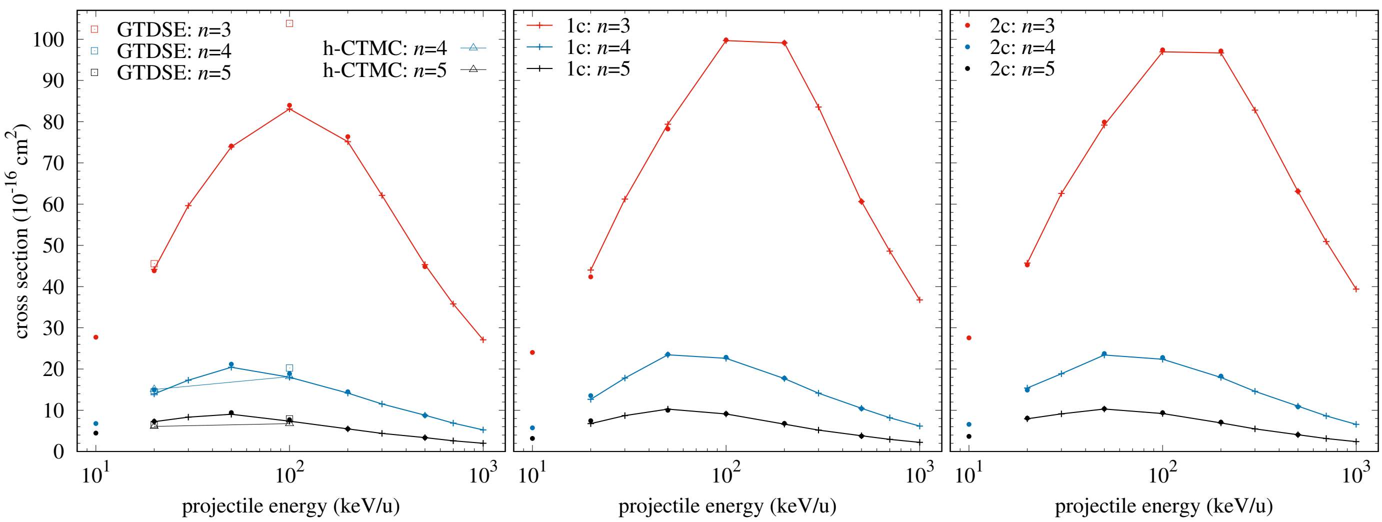

Figure 2. The WP–CCC cross sections for target excitation into the $n = 3$, 4 and 5 states in Be^{4+} collisions with H(2s) (**left** panel), H(2p_0) (**middle** panel) and H(2p_1) (**right** panel). The left panel also shows the GTDSE and h-CTMC results for H(2s) by Jorge et al. [19]. The keys shown in the middle and right panels apply to all three panels.

Figure 3 displays the energy dependence of the total ionisation cross section obtained using the two-centre WP-CCC method extended by single-centre calculations as described above. The left, middle and right panels correspond to the results for Be^{4+} scattering on H(2s), H(2p_0) and H(2p_1), respectively. Also shown are the electron-loss (EL) cross-sections obtained with a completely single-centre calculation. The left panel compares the present results for collisions with H(2s) with the corresponding h-CTMC ones by Jorge et al. [19]. As one-centre calculations cannot distinguish electron capture from ionisation, the EL cross-section represents these two processes together. However, for collisions with excited state H, we find that the total electron-capture cross section becomes considerably smaller than the ionisation cross section above 100 keV/u [28]. Therefore, we conclude that the EL cross-section accurately represents the total ionisation cross-section above 100 keV/u. Clearly, this is not the case at lower projectile energies, where we see considerable differences between the EL and ionisation cross-sections. Note that the WP-CCC and h-CTMC ionisation cross sections are in excellent agreement with each other at all projectile energies where the h-CTMC results are available.

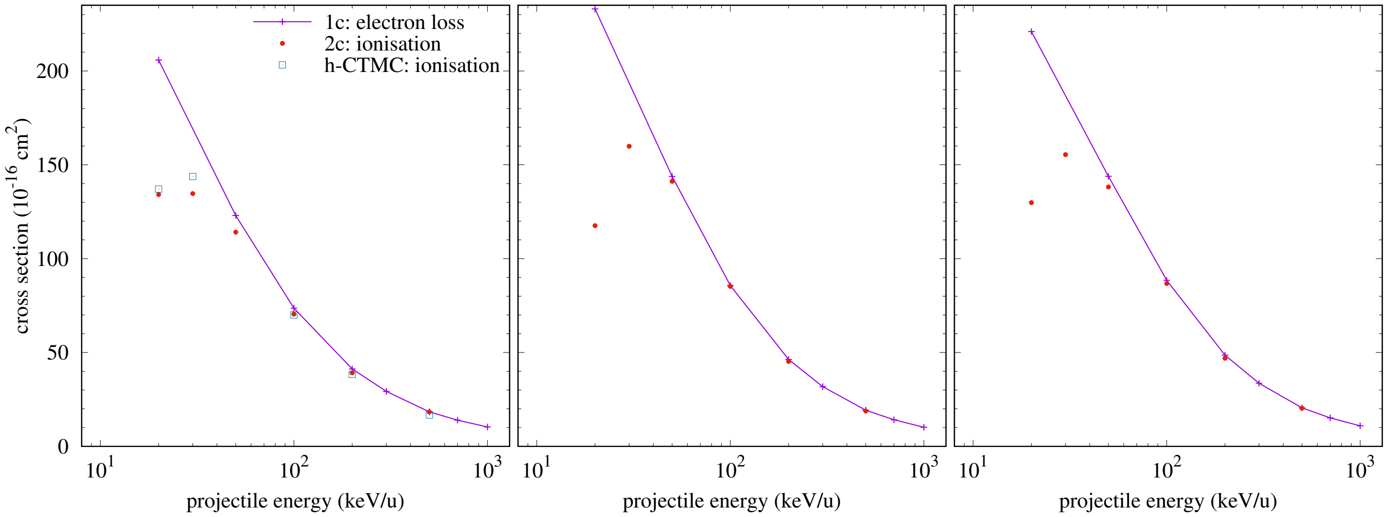

Figure 3. The WP–CCC cross sections for ionisation and electron loss in Be^{4+} collisions with H(2*s*) (**left** panel), H($2p_0$) (**middle** panel) and H($2p_1$) (**right** panel). The left panel also shows the h-CTMC results by Jorge et al. [19] for H(2*s*).

4. Conclusions

Excitation and ionisation in bare beryllium-ion collisions with the $2\ell m$ states of atomic hydrogen have been studied using the WP-CCC approach. Two-centre calculations have been performed up to a sufficiently large impact parameter, uniquely determined at each projectile energy, where the EC and ECC probabilities are considerably smaller than the target excitation and direct ionisation probabilities. We then perform single-centre calculations to extend the impact-parameter range so that accurate target-excitation and total ionisation cross-sections can be calculated. Furthermore, purely single-centre calculations have also been performed to check for internal consistency in our results. In all cases, we find excellent agreement between these two sets of calculations for all the target excitation cross sections. The present results for H(2s) are compared with the recent calculations using the GTDSE and h-CTMC approaches by Jorge et al. [19]. In general, good agreement is seen. However, at a projectile energy of 100 keV/u, where the dominant $n = 3$ excitation cross-section peaks, we see a significant difference between the WP-CCC and GTDSE results. Further calculations by alternative methods are called for to address this discrepancy. We present the first calculations of the excitation and ionisation cross sections for Be^{4+} collisions with H($2p_0$) and H($2p_1$).

This work was part of the Coordinated Research Project on Data for Atomic Processes of Neutral Beams in Fusion Plasma carried out under the sponsorship of the International Atomic Energy Agency [31]. Data obtained in this work can be used for plasma spectroscopy and plasma diagnostics where beryllium impurity ions are expected to be present.

Author Contributions: N.W.A., C.T.P., I.B.A. and A.S.K. developed the underlying theoretical techniques. N.W.A., C.T.P. and I.B.A. developed the code. N.W.A. performed the calculations and gathered data. N.W.A. and A.S.K. wrote the manuscript. A.S.K. conceptualised and supervised the project. Writing—review and editing, I.B. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: All the data reported in this work, as well as a comprehensive set of state-selective cross-sections will be available through the IAEA data repositories. In addition, these are available on reasonable request from the author.

Acknowledgments: This work was supported by the Australian Research Council, the Pawsey Supercomputer Centre, and the National Computing Infrastructure. C.T.P. acknowledges support through an Australian Government Research Training Program Scholarship. This work was part of the Coordinated Research Project carried out under the sponsorship of the International Atomic Energy Agency.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Marchuk, O. The status of atomic models for beam emission spectroscopy in fusion plasmas. *Phys. Scr.* **2014**, *89*, 114010. [CrossRef]
2. Pitts, R.; Carpentier, S.; Escourbiac, F.; Hirai, T.; Komarov, V.; Kukushkin, A.; Lisgo, S.; Loarte, A.; Merola, M.; Mitteau, R.; et al. Physics basis and design of the ITER plasma-facing components. *J. Nucl. Mater.* **2011**, *415*, S957–S964. [CrossRef]
3. Summers, H.P.; Dickson, W.J.; Boileau, A.; Burke, P.G.; Denne-Hinnov, B.; Fritsch, W.; Giannella, R.; Hawkes, N.C.; von Hellerman, M.; Mandl, W.; et al. Spectral emission from beryllium in plasmas. *Plasma Phys. Control. Fusion* **1992**, *34*, 325–352. [CrossRef]
4. Isler, R.C. An overview of charge-exchange spectroscopy as a plasma diagnostic. *Plasma Phys. Control. Fusion* **1994**, *36*, 171–208. [CrossRef]
5. Delabie, E.; Brix, M.; Giroud, C.; Jaspers, R.J.E.; Marchuk, O.; O'Mullane, M.G.; Ralchenko, Y.; Surrey, E.; von Hellermann, M.G.; and, K.D.Z. Consistency of atomic data for the interpretation of beam emission spectra. *Plasma Phys. Control. Fusion* **2010**, *52*, 125008. [CrossRef]
6. Suarez, J.; Guzman, F.; Pons, B.; Errea, L.F. Excitation cross sections for Li^{3+}, Ne^{10+} and Ar^{18+} + H(1s) collisions of interest in fusion plasma diagnostics. *J. Phys. B* **2013**, *46*, 095701. [CrossRef]
7. Isler, R.C.; Olson, R.E. Contribution of excited hydrogen atoms to charge-exchange excitation of impurities in fusion plasmas. *Phys. Rev. A* **1988**, *37*, 3399–3402. [CrossRef]
8. Belkić, D.; Saini, S.; Taylor, H.S. Critical test of first-order theories for electron transfer in collisions between multicharged ions and atomic hydrogen: The boundary condition problem. *Phys. Rev. A* **1987**, *36*, 1601–1617. [CrossRef]
9. Toshima, N. Ionization and charge transfer of atomic hydrogen in collision with multiply charged ions. *Phys. Rev. A* **1994**, *50*, 3940–3947. [CrossRef]
10. Harel, C.; Jouin, H.; Pons, B. Cross sections for electron capture from atomic hydrogen by fully stripped ions in the 0.05–1.00 a.u. impact velocity range. *At. Data Nucl. Data Tables* **1998**, *68*, 279–302. [CrossRef]
11. Igenbergs, K.; Schweinzer, J.; Aumayr, F. Charge exchange in Be4+–H(n= 1, 2) collisions studied systematically by atomic-orbital close-coupling calculations. *J. Phys. B* **2009**, *42*, 235206. [CrossRef]
12. Jorge, A.; Suárez, J.; Illescas, C.; Errea, L.F.; Méndez, L. Application of a grid numerical method to calculate state-selective cross sections for electron capture in $Be^{4+} + H(1s)$ collisions. *Phys. Rev. A* **2016**, *94*, 032707. [CrossRef]
13. Minami, T.; Pindzola, M.S.; Lee, T.G.; Schultz, D.R. Lattice, time-dependent Schrödinger equation approach for charge transfer in collisions of Be4+with atomic hydrogen. *J. Phys. B At. Mol. Opt. Phys.* **2006**, *39*, 2877–2891. [CrossRef]
14. Ziaeian, I.; Tökési, K. Interaction of Be4+ and Ground State Hydrogen Atom—Classical Treatment of the Collision. *Atoms* **2020**, *8*, 27. [CrossRef]
15. Errea, L.F.; Harel, C.; Jouin, H.; Méndez, L.; Pons, B.; Riera, A. Quantal and semiclassical calculations of charge transfer cross sections in + H collisions for impact energies of. *J. Phys. B* **1998**, *31*, 3527–3545. [CrossRef]
16. Hoekstra, R.; Anderson, H.; Bliek, F.W.; von Hellermann, M.; Maggi, C.F.; Olson, R.E.; Summers, H.P. Charge exchange from D(n= 2) atoms to low-Zreceiver ions. *Plasma Phys. Control. Fusion* **1998**, *40*, 1541–1550. [CrossRef]
17. Shimakura, N.; Kobayashi, N.; Honma, M.; Nakano, T.; Kubo, H. Electron capture from excited hydrogen atoms by highly charged beryllium and carbon ions. *J. Phys. Conf. Ser.* **2009**, *163*, 012045. [CrossRef]
18. Ziaeian, I.; Tökési, K. State-selective charge exchange cross sections in Be^{4+} – H(2lm) collision based on the classical trajectory Monte Carlo method. *Eur. Phys. J. D* **2021**, *75*, 138. [CrossRef]
19. Jorge, A.; Illescas, C.; Méndez, L. Classical and semiclassical calculations of state-selective cross sections for electron capture and excitation in $Be^{4+} + H(2s)$ collisions. *Phys. Rev. A* **2022**, *105*, 012811. [CrossRef]
20. Faulkner, J.; Abdurakhmanov, I.; Alladustov, S.U.; Kadyrov, A.; Bray, I. Electron capture, excitation and ionization in He2+–H and H+–He+ collisions. *Plasma Phys. Control. Fusion* **2019**, *61*, 095005. [CrossRef]
21. Abdurakhmanov, I.B.; Massen-Hane, K.; Alladustov, S.U.; Bailey, J.J.; Kadyrov, A.S.; Bray, I. Ionization and electron capture in collisions of bare carbon ions with hydrogen. *Phys. Rev. A* **2018**, *98*, 062710. [CrossRef]
22. Kotian, A.M.; Plowman, C.T.; Abdurakhmanov, I.B.; Bray, I.; Kadyrov, A.S. State-selective electron capture in collisions of fully stripped neon ions with ground-state hydrogen. *J. Phys. B* **2022**, *55*, 115201. [CrossRef]
23. Spicer, K.H.; Plowman, C.T.; Abdurakhmanov, I.B.; Kadyrov, A.S.; Bray, I.; Alladustov, S.U. Differential study of proton-helium collisions at intermediate energies: Elastic scattering, excitation, and electron capture. *Phys. Rev. A* **2021**, *104*, 032818. [CrossRef]

24. Spicer, K.H.; Plowman, C.T.; Abdurakhmanov, I.B.; Alladustov, S.U.; Bray, I.; Kadyrov, A.S. Proton-helium collisions at intermediate energies: Singly differential ionization cross sections. *Phys. Rev. A* **2021**, *104*, 052815. [CrossRef]
25. Plowman, C.T.; Abdurakhmanov, I.B.; Bray, I.; Kadyrov, A.S. Effective one-electron approach to proton collisions with molecular hydrogen. *Eur. Phys. J. D* **2022**, *76*, 31. [CrossRef]
26. Plowman, C.T.; Abdurakhmanov, I.B.; Bray, I.; Kadyrov, A.S. Differential scattering in proton collisions with molecular hydrogen. *Eur. Phys. J. D* **2022**, *76*, 129. [CrossRef]
27. Antonio, N.W.; Plowman, C.T.; Abdurakhmanov, I.B.; Bray, I.; Kadyrov, A.S. Integrated total and state-selective cross sections for bare beryllium ion collisions with atomic hydrogen. *J. Phys. B* **2021**, *54*, 175201. [CrossRef]
28. Antonio, N.W.; Plowman, C.T.; Abdurakhmanov, I.B.; Bray, I.; Kadyrov, A.S. Fully-stripped-beryllium-ion collisions with $2\ell m$ states of atomic hydrogen: Total and state-selective electron-capture cross sections. *Phys. Rev. A* **2022**, *106*, 012822. [CrossRef]
29. Abdurakhmanov, I.B.; Kadyrov, A.S.; Bray, I. Wave-packet continuum-discretization approach to ion-atom collisions: Nonrearrangement scattering. *Phys. Rev. A* **2016**, *94*, 022703. [CrossRef]
30. Abdurakhmanov, I.B.; Bailey, J.J.; Kadyrov, A.S.; Bray, I. Wave-packet continuum-discretization approach to ion-atom collisions including rearrangement: Application to differential ionization in proton-hydrogen scattering. *Phys. Rev. A* **2018**, *97*, 032707. [CrossRef]
31. IAEA Coordinated Research Project: Data for Atomic Processes of Neutral Beams in Fusion Plasma. Available online: https://amdis.iaea.org/CRP/neutral-beams (accessed on 1 October 2022).