Appendix A.

1.0 Review of the fundamental ion-atom collision database

The ion-atom collision database is utilised by ADAS310 to replace the cross-sections which have been calculated internally using approximate methods. The database, which is of the ADAS ADF02 type format, contains fundamental cross sections for ion impact ionisation and excitation of neutral H with impurity species up to the first period. Charge exchange data from neutral H is also included. The cross sections are tabluated as a function of collision energy per atomic mass unit and can also be used to describe the behaviour of the atomic processes associated with neutral deuterium and tritium. The main species of interest in this work being deuterium. The database was originally constructed in 1989 by Summers[54] and was later reviewed in 1991 and partially updated in 1993. Where possible, theoretical and experimental values were combined to give a composite data set for each individual atomic process. This database is referred to as the JET 1989 data. To update the present database involved reviewing the literature for both theoretical and experimental cross sections. The aim being to either create a new composite data set for each individual process or to simply supplement an existing data set with improved data. The ion-atom data assessment presented here represents the best available data up until March 1997.

1.1 Review of Ion impact ionisation data

The existing database contains fundamental data for ion impact ionisation of neutral $H(1s)_{beam}$ as described in equation 1.1 , where Z0 is the nuclear charge of the impurity and ranges from 1 to 10.

$$X^{+Z0} + H(1s)_{beam} \rightarrow X^{+Z0} + H^{+}_{beam} + e^{-} \qquad 1.1$$

The data used for the case when Z0 = 1, i.e. ion impact ionisation of neutral $H(1s)_{beam}$ with H^{+} , was a composite data set compiled from the experimental work of Shah & Gilbody[87], Shah, Elliot & Gilbody[88] and the theoretical calculations of Ryufuku

[89]. This was compared with the data reported by Janev & Smith[90], see figure 1.0. There is excellent agreement. The data reported by Janev & Smith[90] is a composite data set constructed from the experimental and theoretical data reported by eight independent sources. We decided to combine the data reported by Janev & Smith[90] with the existing data to construct a new data set. This was achieved by modifying the peak value of the existing data set to agree with the value reported by Janev & Smith[90]. The new data set is the preferred data for this process and is referred to as the comparative data set.

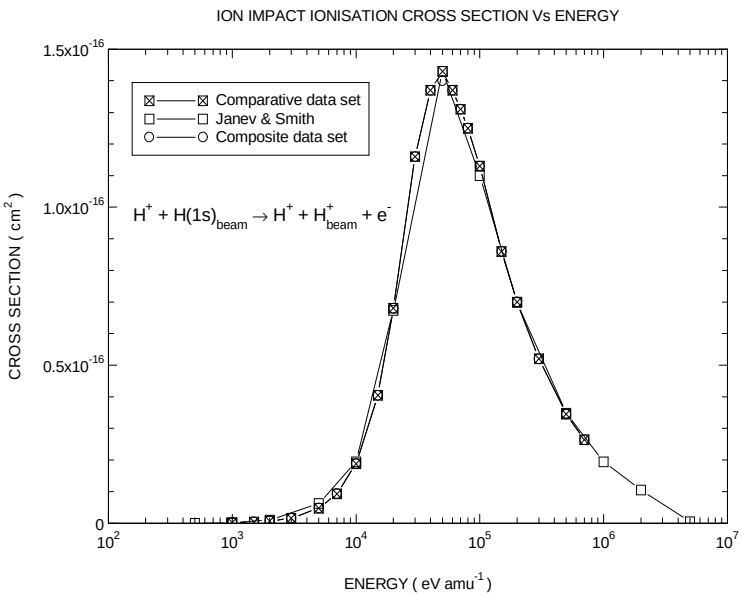

Figure 1.0 A plot of the ion impact ionisation cross section Vs energy. A comparative data set was constructed by modifying the peak value of the existing composite data set to agree with the results reported by Janev & Smith [90]. The comparative data set is taken as the preferred data.

The data employed for Z0 = 2, was a composite data set compiled by Hugh Summers, this data set was based on the experimental work of Shah & Gilbody[87] and Shah, Elliot & Gilbody[88]. A comparison was made between this data set and the theoretical work of Toshima & Tawara[91]. The results can be seen in figure 2.0 . Below 90 keV/amu both data sets agree, however above 90 keV/amu there is a slight difference. Since the composite data set is based on experimental measurements it is taken as the preferred data set for this process. For convenience of reference the new preferred composite data set is called the comparative data set, see figure 2.0

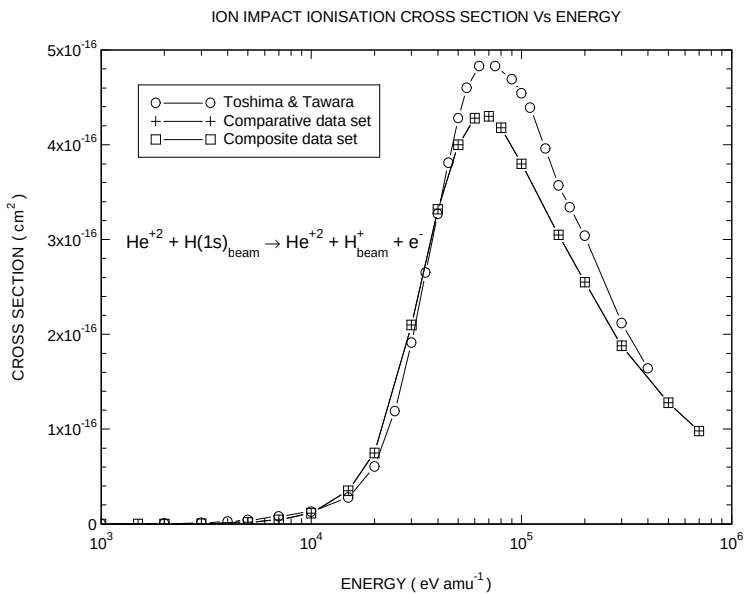

Figure 2.0 A plot of the ion impact ionisation cross section Vs energy. The composite data set is based on experimental measurements and is taken as the preferred data. For convenience the preferred data set is called the comparative data set.

For Z0 = 3, the data used was a composite data set based on the work of Shah & Gilbody[87] . A comparison was made between this data set and the data of Toshima & Tawara[91], see figure 3.0. As before, due to the influence of experimental data, the composite data set it is taken as the preferred data set. The preferred data set is called the comparative data set, see figure 3.0 . The data used for Z0 = 4, was a composite data set which was obtained by interpolating between the data of neighbouring species. This data was compared to the work of Janev & Smith[90] and Toshima & Tawara[91]. The results can be observed in figure 4.0 . The data of Janev & Smith[90], which is based on the work of three independent workers, is taken as the preferred data. When Z0 = 5, a composite data set compiled by Summers[54] was used. This was compared to the new calculations of Toshima & Tawara[91] and the data reported by Janev & Smith[90] , see figure 5.0. The data reported by Janev & Smith[90] is a composite data set based on the work of eight independent sources and is taken as the preferred data.

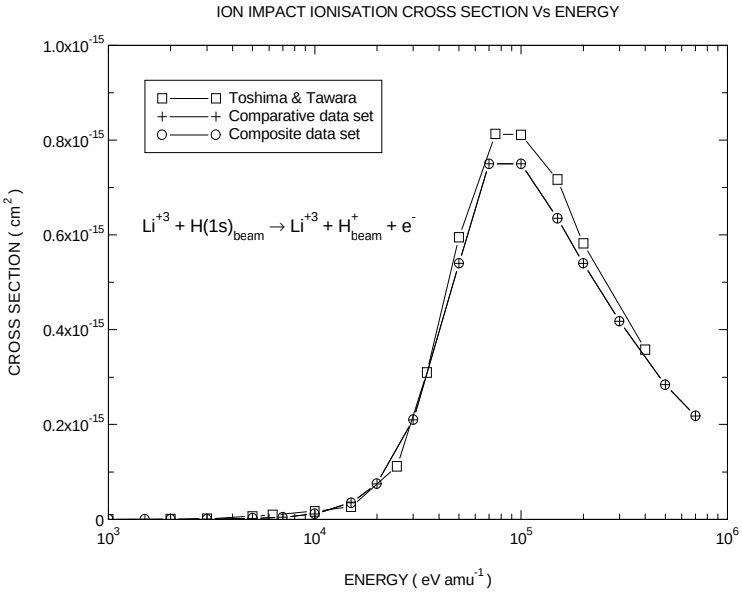

Figure 3.0 A plot of the ion impact ionisation cross section Vs energy. The composite data set is taken as the preferred data set and for convenience it is referred to as the comparative data set.

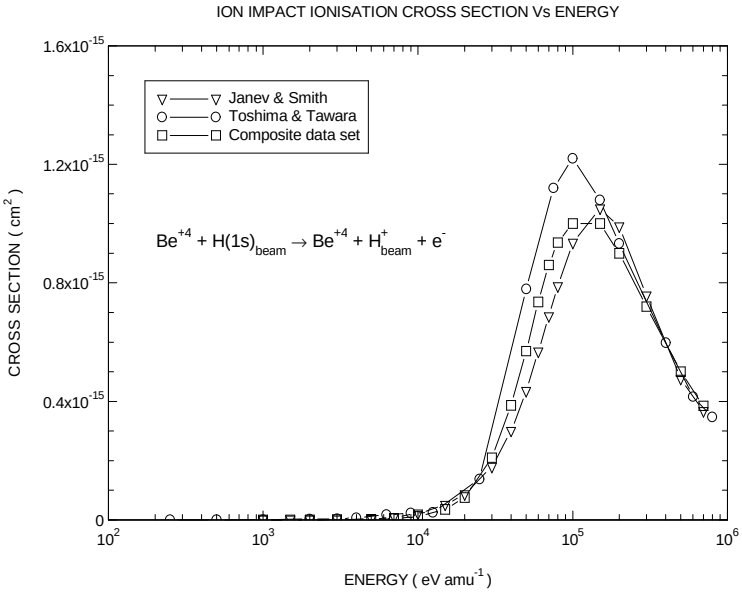

Figure 4.0 A plot of the ion impact ionisation cross section Vs energy. The data of Janev & Smith[90] which is based on the work of three independent sources is taken as the preferred data set.

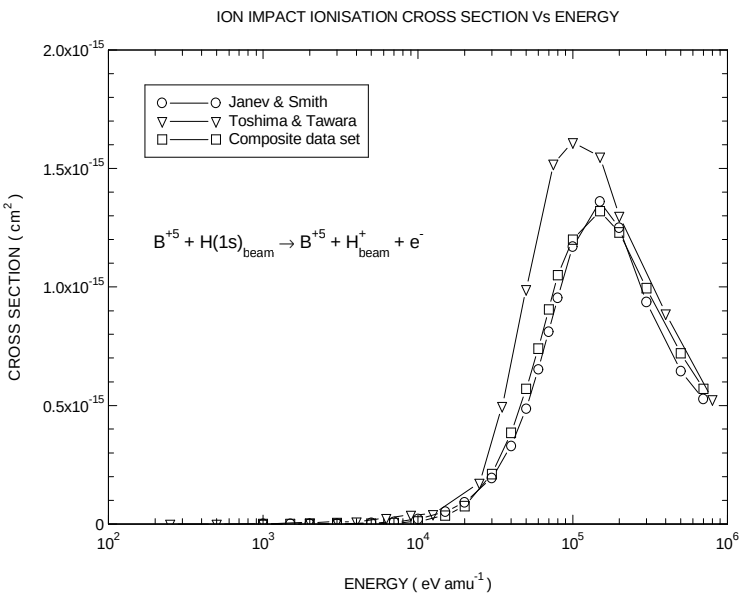

Figure 5.0 A plot of the ion impact ionisation cross section Vs energy. The data of Janev & Smith[90] is based on the work of eight independent sources and is taken as the preferred data set.

A composite data set based on the work reported in the 'red book' [92] was used for when Z0 = 6. This data set was compared to the work of Janev & Smith[90] and the theoretical calculations of Toshima & Tawara[91]. Figure 6.0 illustrates the results.

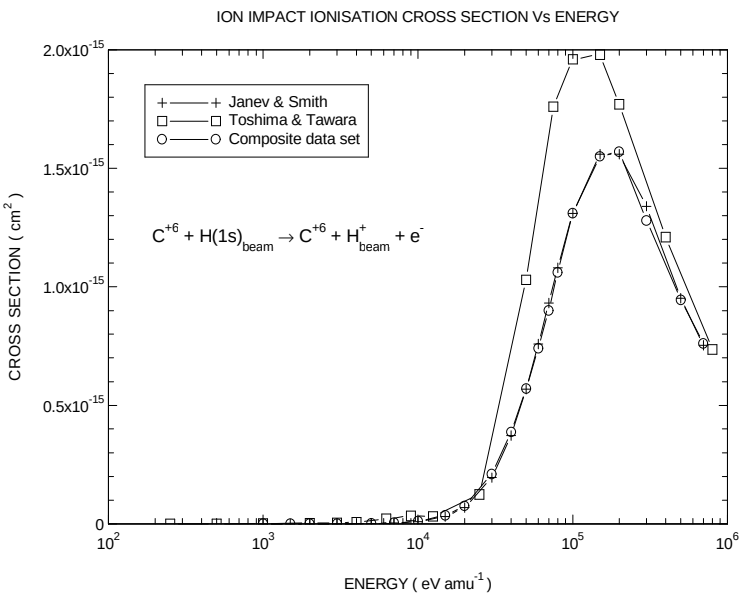

Figure 6.0 A plot of the ion impact ionisation cross section Vs energy. The data of Janev & Smith[90] is taken as the preferred data.

The data of Janev & Smith[90], which is based on the results of many workers, is considered to be the best for this particular process. For Z0 = 7, a data set which has been obtained by interpolating through the data of neighbouring species was used. This data set was compared to the work of Toshima & Tawara[91] . A comparative data set was constructed by interpolating through the data of neighbouring species using the data reported by Janev & Smith[90]. The comparative data set is chosen as the preferred data set for this process, see figure 7.0 .

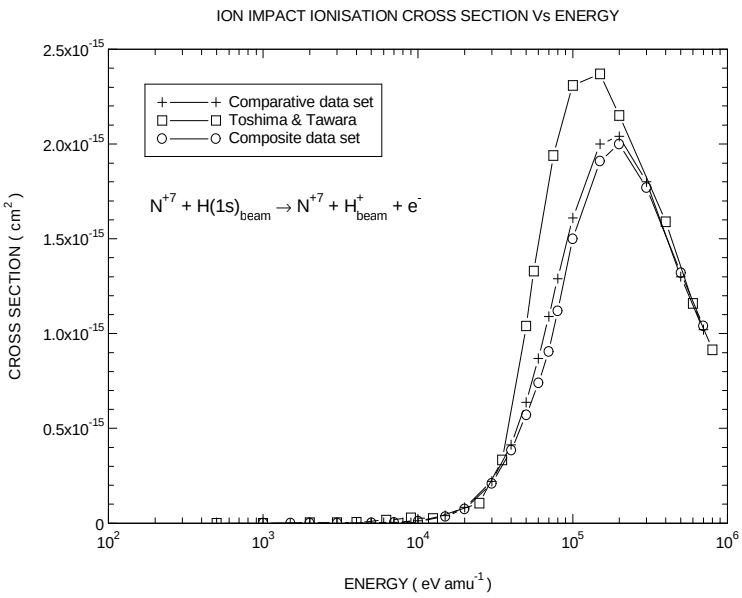

Figure 7.0 A plot of the ion impact ionisation cross section Vs energy. The comparative data set is taken as the preferred data.

When Z0 = 8, data based on the ‘red book’ [92] was used. This data was compared to the calculations of Toshima & Tawara[91] and the composite data reported by Janev & Smith[90]. The results can be seen in figure 8.0. The data of Janev & Smith[90] is based on four independent sources and is taken to be the best. The data used for Z0 = 9 was a composite data set which was obtained by interpolating between neighbouring species, see figure 9.0 . For Z0 = 10, a composite data set was used which was obtained by scaling the oxygen data, see figure 9.0. A review of the literature failed to improve the data for these species.

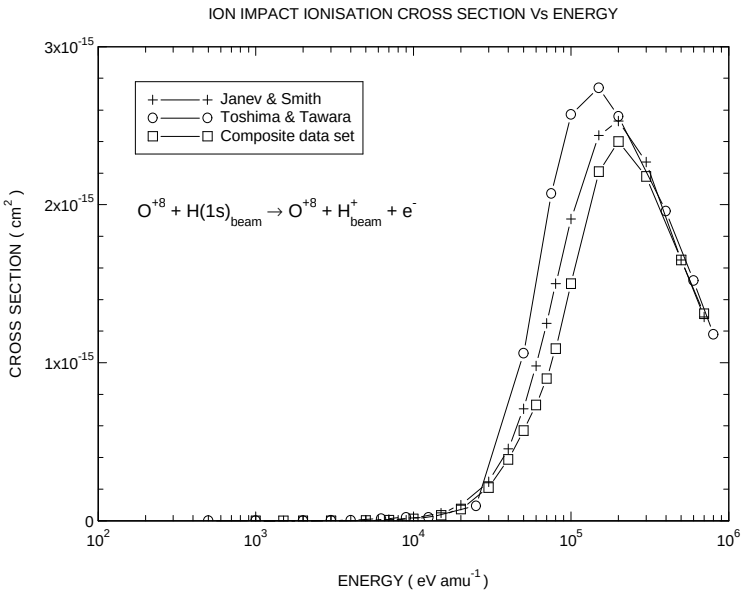

Figure 8.0 A plot of the ion impact ionisation cross section Vs energy. The data reported by Janev & Smith[90] is taken as the preferred data set.

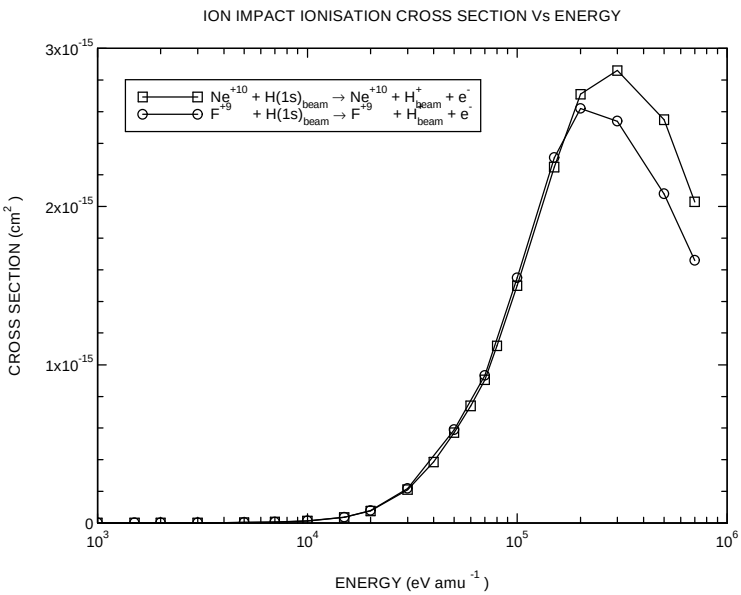

Figure 9.0 A plot of the ion impact ionisation cross section Vs energy. The data for F^{+9} both was obtained by interpolating through the data of neighbouring species. The data for Ne^{+10} was obtained from scaling the data for Oxygen . A review of the literature failed to improve the data for both species.

1.2 Review of charge exchange data

The existing database contains fundamental data for charge exchange from $H(1s)_{beam}$ as described in equation 1.2 , where Z0 is the nuclear charge of the impurity and ranges from 1 to 10.

$$X^{+Z0} + H(1s)_{beam} \rightarrow X^{+Z0-1} + H^{+}_{beam} \qquad 1.2$$

The data used for Z0 = 1, was a composite data set based on the work of Mc Clure[93] & Greenland[94]. This data was compared to the data reported by Janev & Smith[90], the results can be seen in figure 10.0 .

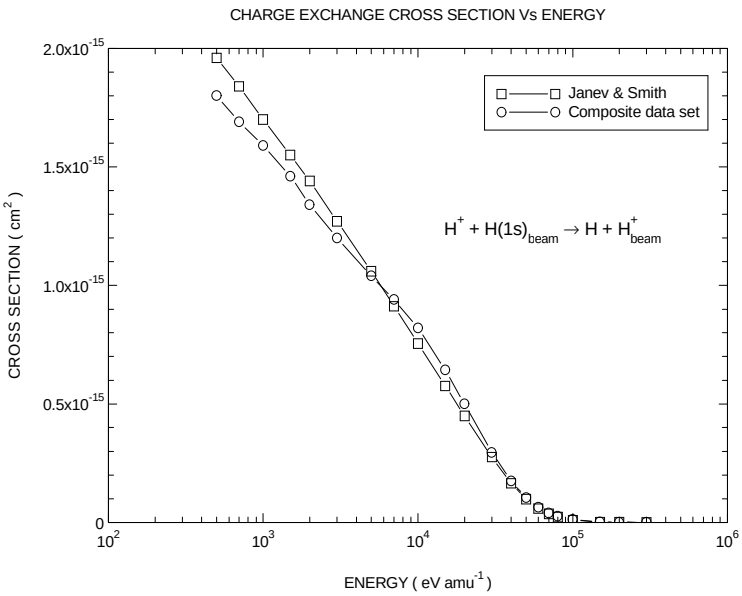

Figure 10.0 A plot of the charge exchange cross section Vs energy. The data of Janev & Smith[90] is taken as the preferred data.

The data of Janev & Smith[90], which is based on the work of twelve independent sources, is the preferred data set. When Z0 = 2, the data which was used is a composite data set based on the work of Frieling[95]. A comparison between this data set and the work of Janev & Smith[90] and Toshima & Tawara[91] can be observed in figure 11.0 .

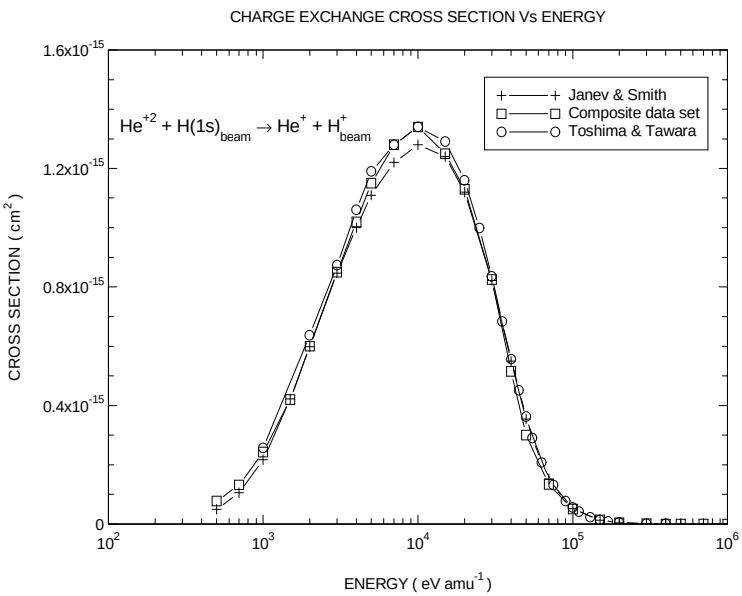

Figure 11.0 A plot of the charge exchange cross section Vs energy. The data of Janev & Smith[90], which is based on the results of many workers, is taken as the preferred data.

The difference between the work of Toshima & Tawara[91] and Frieling[95] is some what insignificant .The data reported of Janev & Smith[90], which is based on the results from many workers, is taken as the preferred data set. For Z0 = 3, the data which was used is a composite data set constructed from interpolating through the data of neighbouring species. This data set was compared to the theoretical calculations of Toshima & Tawara[91], see figure 12.0 . A comparative data set was constructed by interpolating through the data of neighbouring species using the data of Janev & Smith[90]. The new comparative data set is taken as the preferred data set.

The data set used when Z0 = 4, was a composite data set based on the work of Greenland[94] and Ryufuku[96]. This data set was compared to the work of Toshima & Tawara[91] and Busnengo et al[97], see figure 13.0. The composite data set is still considered to be the most accurate and is taken as the preferred data set. For Z0 = 5, the data which was used is a composite data set based on the work of Ryufuku[96] and influenced by the data of Z0 = 4 & 6 . A comparison between this data set and the work of Toshima & Tawara[91] and Busnengo et al[97] can be observed in figure 14.0. A comparative data set was constructed from

interpolating through the data of neighbouring species. The new comparative data set is taken as the preferred data set, see figure 14.0.

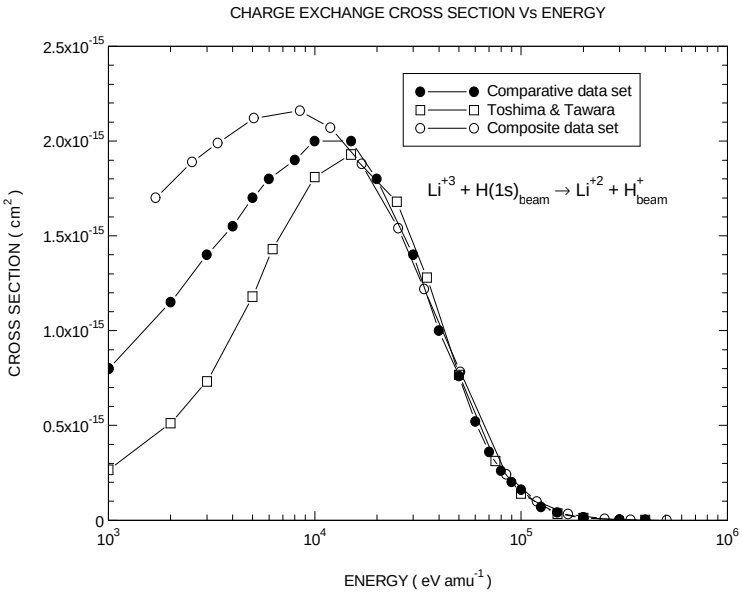

Figure 12.0 A plot of the charge exchange cross section Vs energy. The new comparative data set is the preferred data.

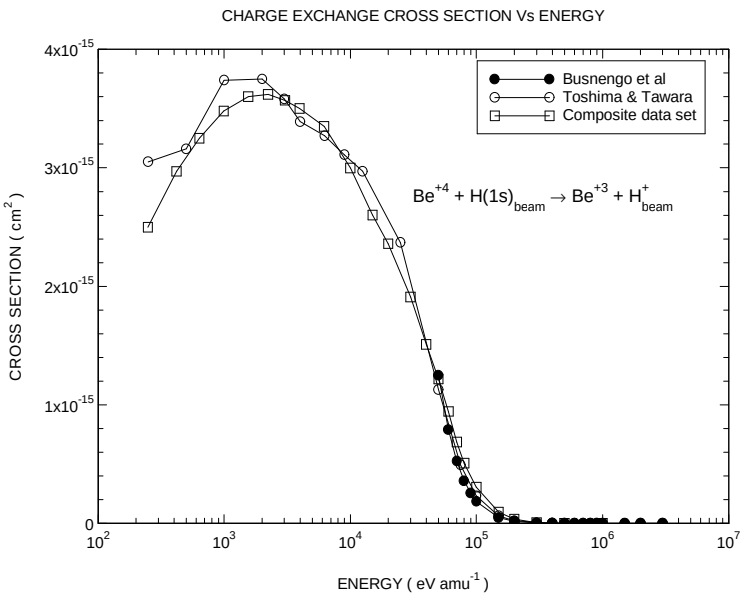

Figure 13.0 A plot of the charge exchange cross section Vs energy. The composite data set is still considered to be the most accurate and is taken as the best data for this particular process.

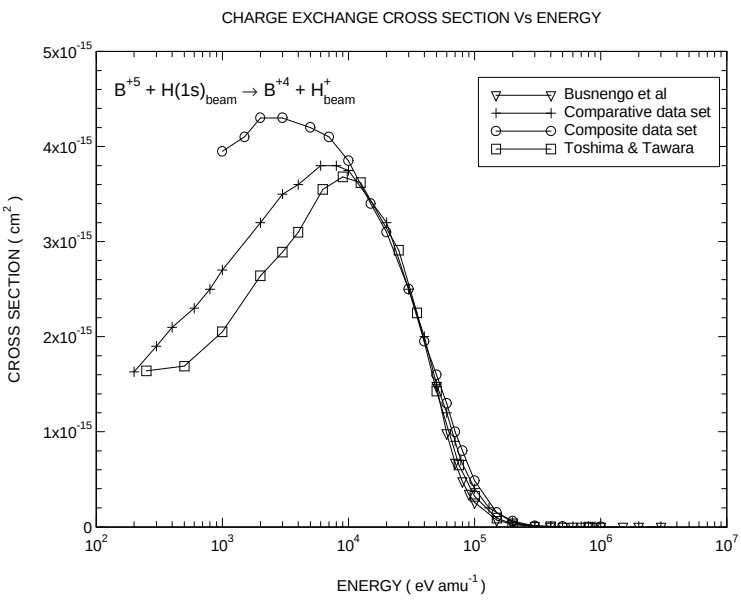

Figure 14.0 A plot of the charge exchange cross section Vs energy. The comparative data set is taken as the preferred data.

When Z0 = 6, a composite data set based on the work of Greenland[94] and Ryufuku [96] was used. A comparison was made between this data set and the work of Janev & Smith[90] and Toshima & Tawara[91]. The results can be seen in figure 15.0 .

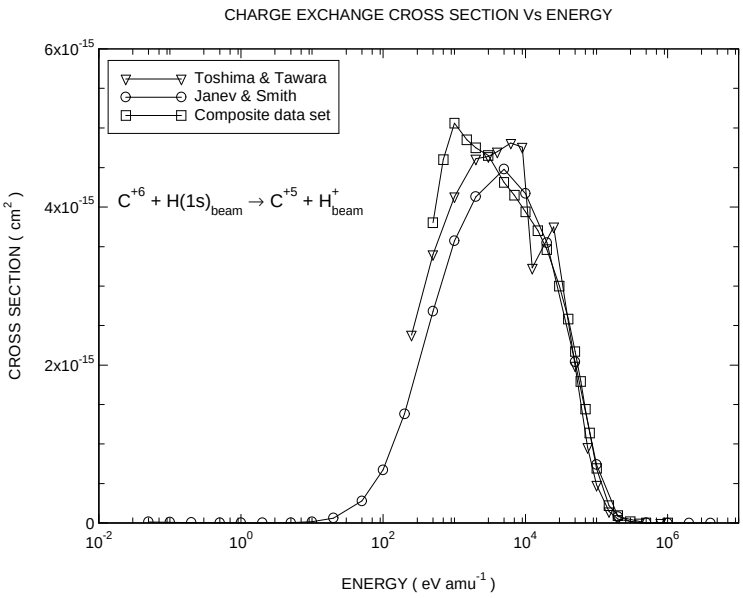

Figure 15.0 A plot of the charge exchange cross section Vs energy. The data reported by Janev & Smith[90] is taken as the preferred data.

The data of Toshima & Tawara[91] and Janev & Smith[90] above ~ 20 keV/amu agree with the existing composite data set. However, there is an anomalous point in the data set of Toshima & Tawara[91] which adds some uncertainty on the reliability of the data. The data of Janev & Smith[90] is therefore taken as the preferred data. For Z0 = 7, a composite data set based on interpolating through the data of neighbouring species was used. This data set was compared to the theoretical calculations of Toshima & Tawara[91], see figure 16.0 . A comparative data set was constructed by interpolating through the data of neighbouring species using the data reported by Janev & Smith[90]. The new comparative data set is taken as the preferred data set.

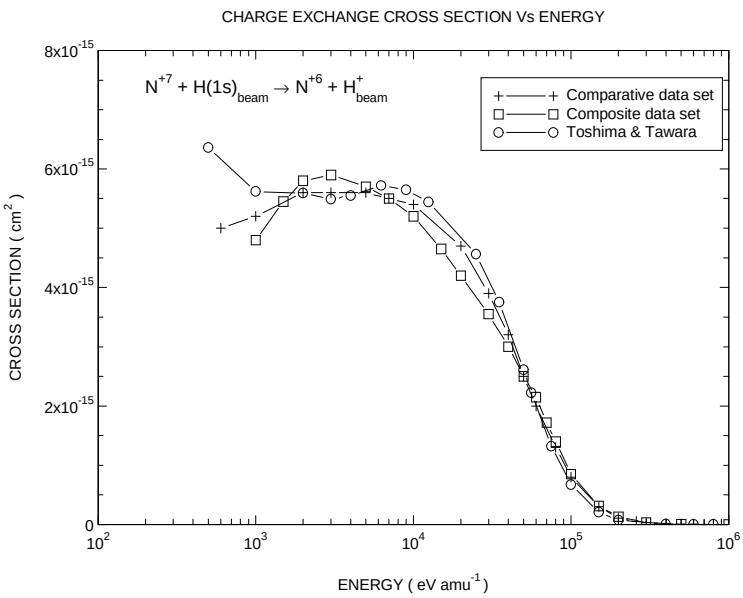

Figure 16.0 A plot of the charge exchange cross section Vs energy. The new comparative data set is taken as the best data for this process.

The data used for Z0 = 8, was a composite data set based on the work of Greenland [94] and Ryufuku[96]. This data set was compared to the data of Janev & Smith[90] and Toshima & Tawara[91].The results can be seen in figure 17.0 . The data of Janev & Smith[90] is taken as the preferred data. The data used for when Z0 = 9 was a composite data set obtained by interpolating through the data of neighbouring species, see figure 18.0. When Z0 = 10, a data set obtained by extrapolating from the oxygen data, as well as being influence by the work of Ryufuku[96], was used, the

results can be seen in figure 18.0. A review of the literature failed to improve the data for these species.

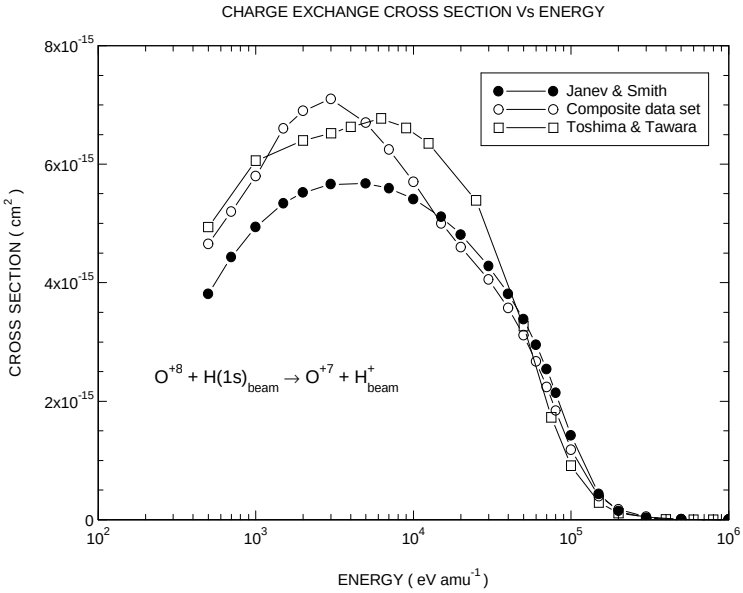

Figure 17.0 A plot of the charge exchange cross section Vs energy. The data reported by Janev & Smith[90] is taken as the preferred data.

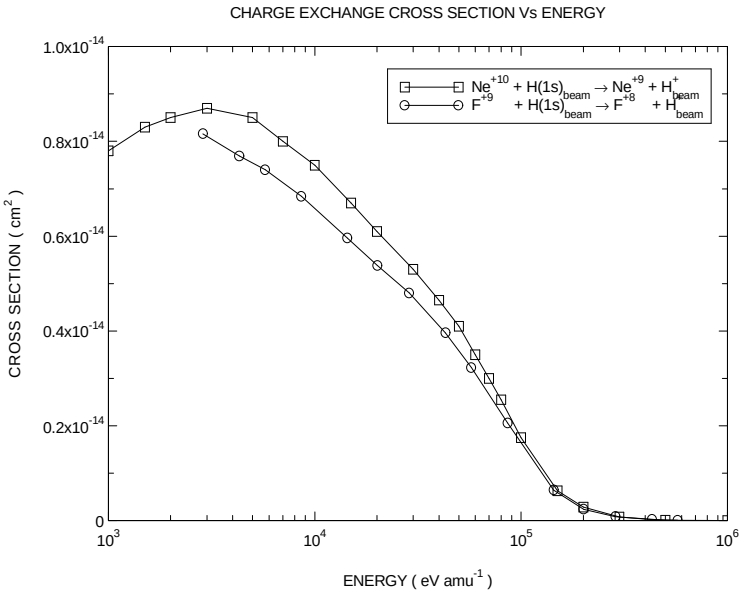

Figure 18.0 A plot of the charge exchange cross section Vs energy. The data for F^{+9} was obtained by interpolating through the data of neighbouring species. The data for Ne^{+10} was obtained from scaling the data for Oxygen . A review of the literature failed to improve the data for both species.

1.3 Review of ion impact excitation data

The existing database contains fundamental data for ion impact excitation of $H(1s)_{beam}$ as described in equation 1.3 , where Z0 is the nuclear charge of the impurity and n is the principal quantum number with values from 2 to 5 .

$$X^{+Z0} + H(1s)_{beam} \rightarrow X^{+Z0} + H(n)_{beam} \qquad 1.3$$

In the case were Z0 =1 and n =2 , the data used was a composite data set based on the work of many workers [98], [99], [100], [101] and [102]. This data set was compared to the data reported by Janev & Smith[90], the results can be seen in figure 19.0 .

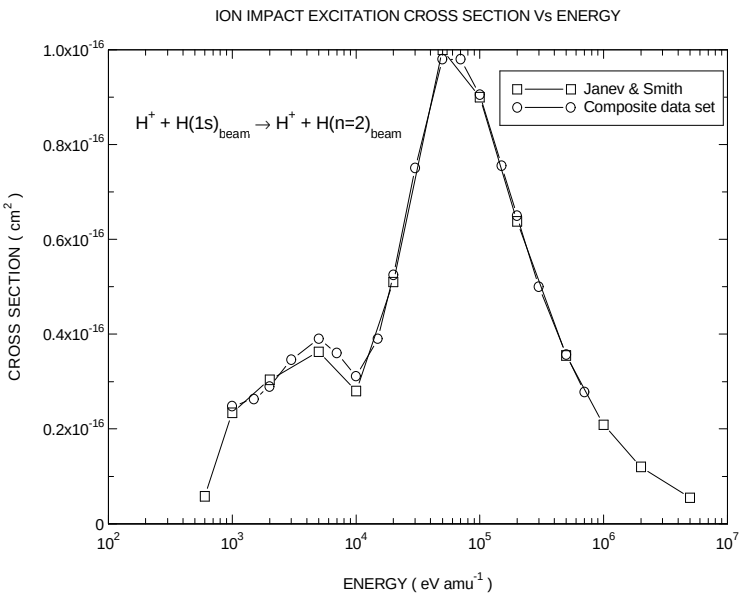

Figure 19.0 A plot of the ion impact excitation cross section Vs energy . The data of Janev & Smith[90], for convenience of reference, is taken as the preferred data for this particular process.

Both data sets agree, however for convenience of reference the data of Janev & Smith[90] is the preferred data set. When n = 3 for Z0 = 1, the data which was used is a composite data set based on the 1st Born approximation as well as the work of many others [98], [99], [100], [101], [102] and [103]. This data set was compared to the data reported by Janev & Smith [90], see figure 20.0

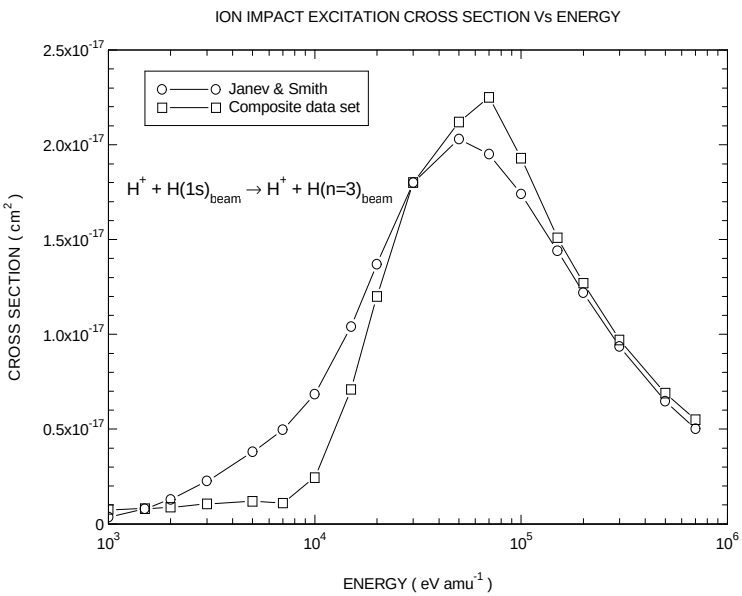

Figure 20.0 A plot of the ion impact excitation cross section Vs energy . The data reported by Janev & Smith[90] is taken as the preferred data set.

The data of Janev & Smith[90] is compiled using various sources such as [98],[99],[100] and [101], however they also include more recent work such as [104] and [105]. Therefore the data of Janev & Smith[90] is the preferred data set. For n = 4 and Z0 = 1, the data used is based on the 1st Born approximation and the work of Fritsch [106] and Theodosian[103]. This data set was compared to the data of Janev & Smith[90]. The results can be observed in figure 21.0. The data of Janev & Smith[90], which is based on the work of five independent sources, is taken as the preferred data. A composite data set based on the 1st Born approximation and the work of Theodosian[103] is used when n = 5 and Z0 = 1. This data set was compared to the data of Janev & Smith[90], see figure 22.0. The data of Janev & Smith[90] is believed to be more accurate and is taken as the preferred data. When Z0 = 2 and n = 2, the data employed was that reported by Fritsch & Lin[107]. This data set was compared to the new theoretical calculations of Toshima & Tawara[91], the results can be observed in figure 23.0 . Due to the uncertainty associated with the anomalous peaks shown in the data of Fritsch & Lin and Toshima & Tawara, a comparative data set was constructed from interpolating between the extremes of the two data sets. The comparative data set is taken as the preferred data for this process.

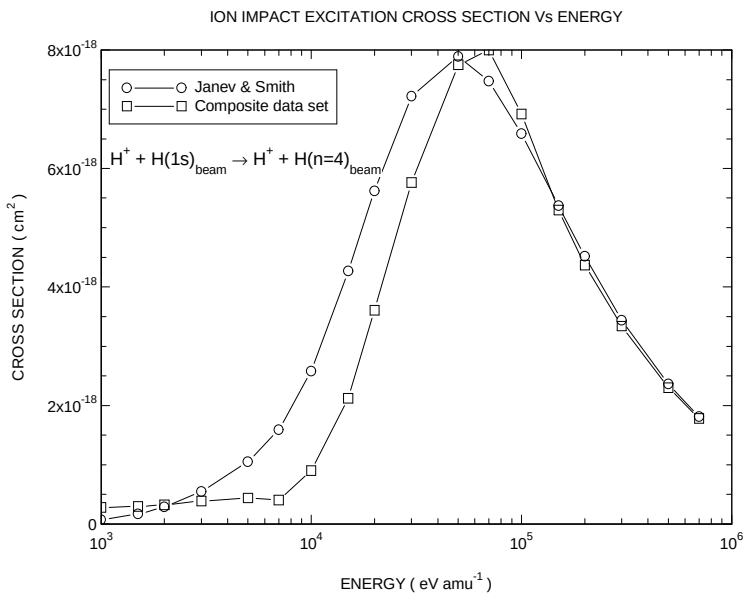

Figure 21.0 A plot of the ion impact excitation cross section Vs energy . The data of Janev & Smith[90] is taken as the preferred data set.

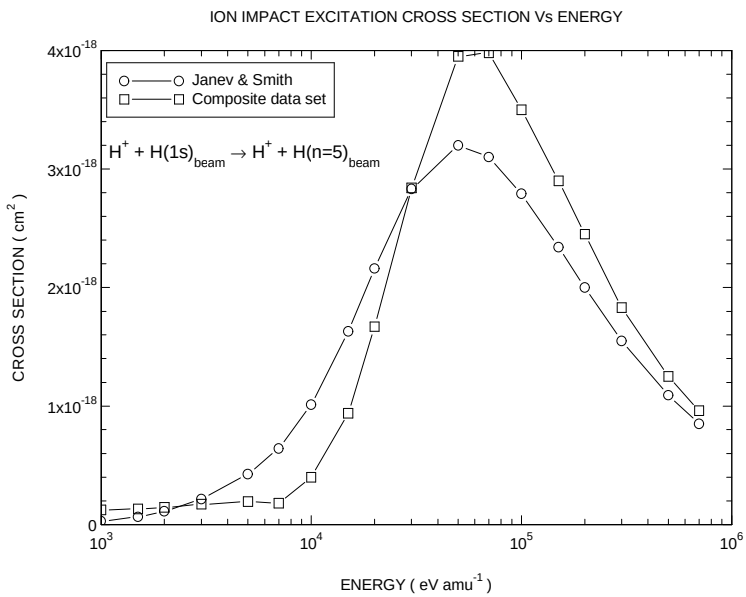

Figure 22.0 A plot of the ion impact excitation cross section Vs energy . The data reported by Janev & Smith[90] is taken as the preferred data for this particular process.

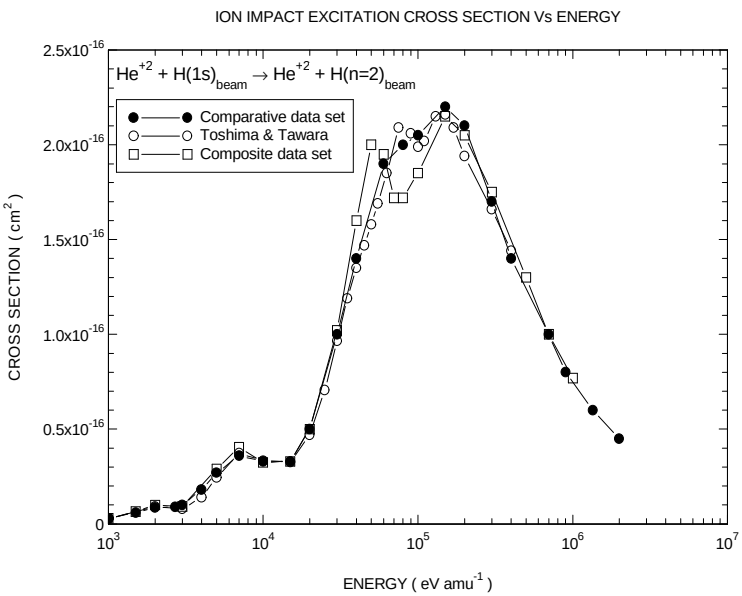

Figure 23.0 A plot of the ion impact excitation cross section Vs energy . Due to the uncertainty associated with the anomalous peaks in the data of Fritsch & Lin and Toshima & Tawara , the comparative data set is taken as the preferred data for this process.

For n = 3 and Z0 = 2 a composite data set based on the work of Fritsch[107] and Lodge[47] was used. This data set was compared to the data of Toshima & Tawara [91] as well as a comparative data set which has been constructed from interpolating between the extremes of the two data sets, see figure 24.0 . The comparative data set is the preferred data. When n = 4 and Z0 = 2, the data used is a general data set which is scaled according to the value of n and Z0. A comparison between this data set and the data of Toshima & Tawara[91] and Janev & Smith[90] is illustrated in figure 25.0. The data of Janev & Smith is taken as the best data as is referred to as the comparative data set. A general composite data set which is scaled according to the value of n and Z0 is used when Z0 = 3 and n = 2, 3 and 4. A comparison was made between these data sets and the calculations of Toshima & Tawara[91]. In the case of n =2 and 3, comparative data sets were constructed by interpolating through the data of neighbouring species, see figures 26.0 and 27.0. In each case the comparative data set is taken as the preferred data. The preferred data for n=4 is the general composite data which is scaled according to Z0 and n, this is shown in figure 28.0.

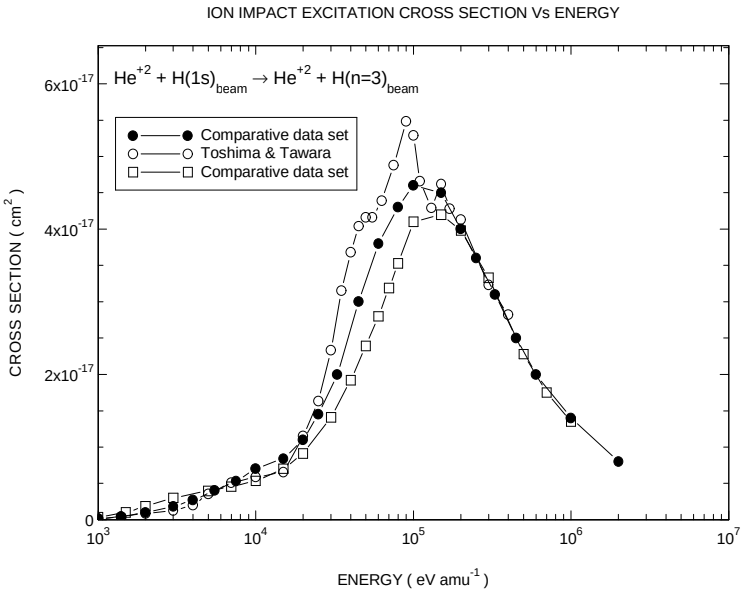

Figure 24.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data.

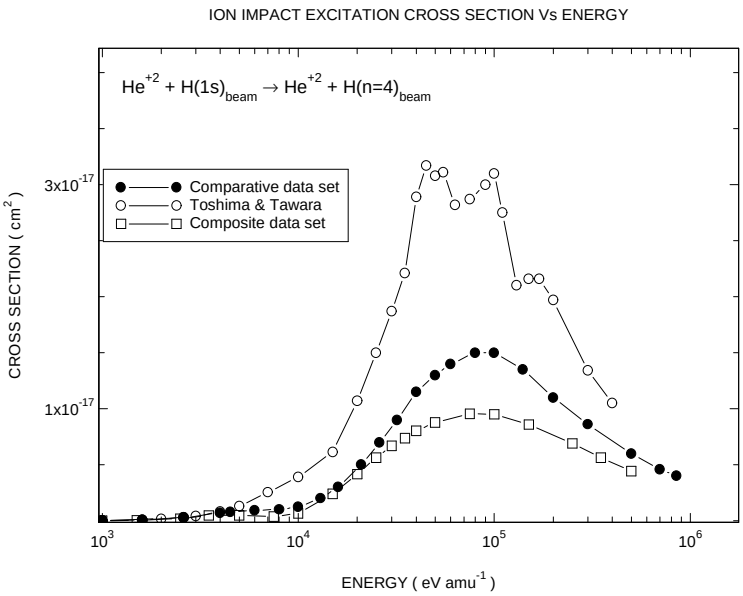

Figure 25.0 A plot of the ion impact excitation cross section Vs energy . The data reported by Janev & Smith[90] is taken as the preferred data. The calculation of Toshima & Tawara[91] only included states up to n = 4, ,therefore some over-estimation is present particular for the n = 4 shell.

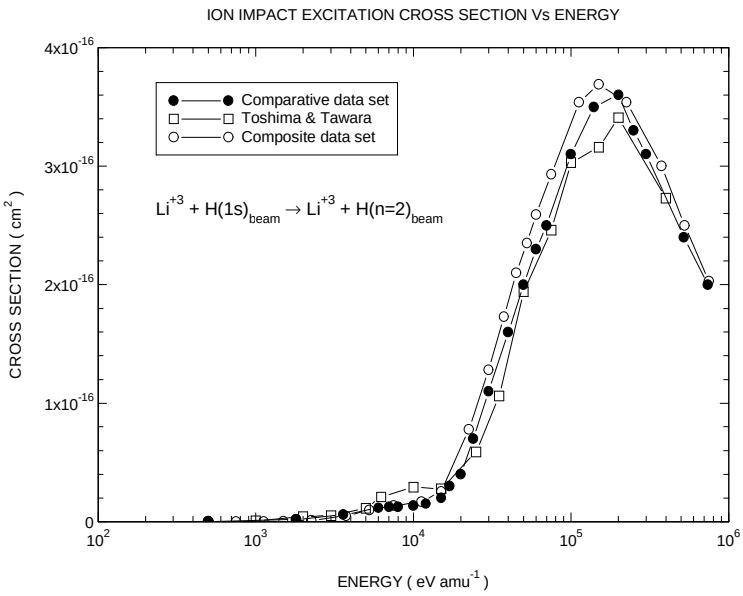

Figure 26.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data set.

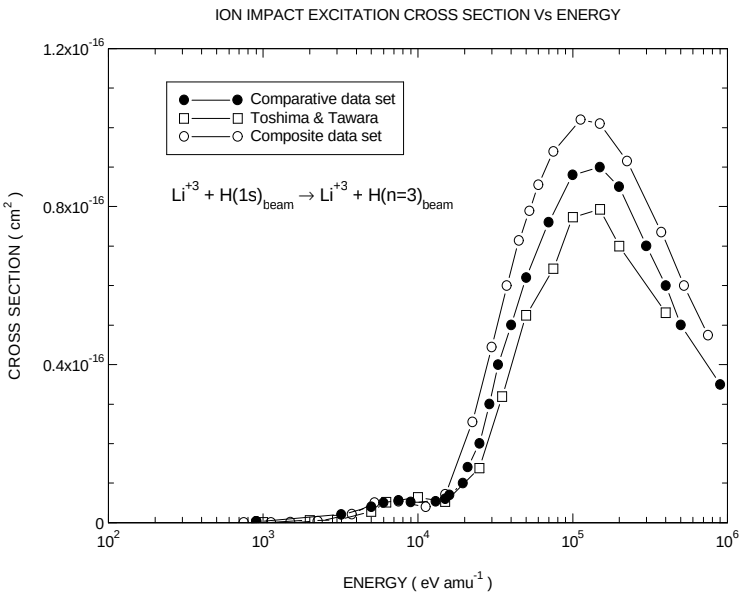

Figure 27.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data set.

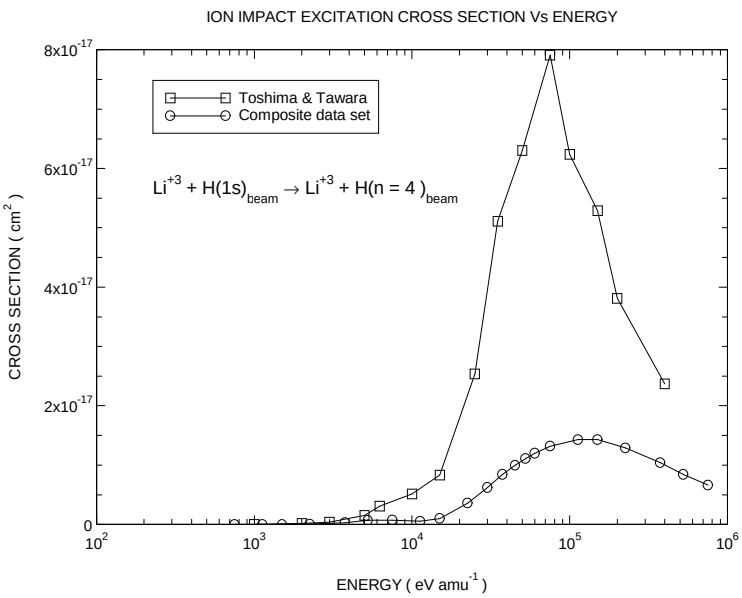

Figure 28.0 A plot of the ion impact excitation cross section Vs energy . The composite data set is taken as the preferred data set. The calculation of Toshima & Tawara only include states up to n = 4, therefore some over-estimation is present particular for the n = 4 shell .

In the case of Z0 = 4 and n = 2, the data which was used is based on the work of Fritsch[107] . A comparison was made between this data set and the work of Toshima & Tawara[91] as well as a comparative data set which was constructed by interpolating through the data of neighbouring species. The results can be observed in figure 29.0 . The comparative data set is taken as the preferred data.

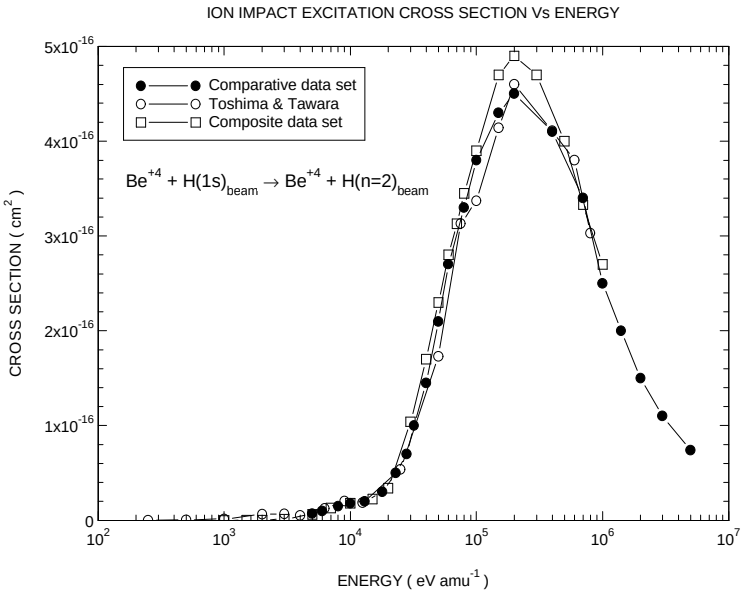

Figure 29.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data.

When Z0 =4 and n =3 the data which was used is based on the work of Fritsch[107]. This was compared to the data of Toshima & Tawara[91] and a comparative data set which was obtained by interpolating through the data of neighbouring species, see figure 30.0. The comparative data set is considered to be the best data for this process.

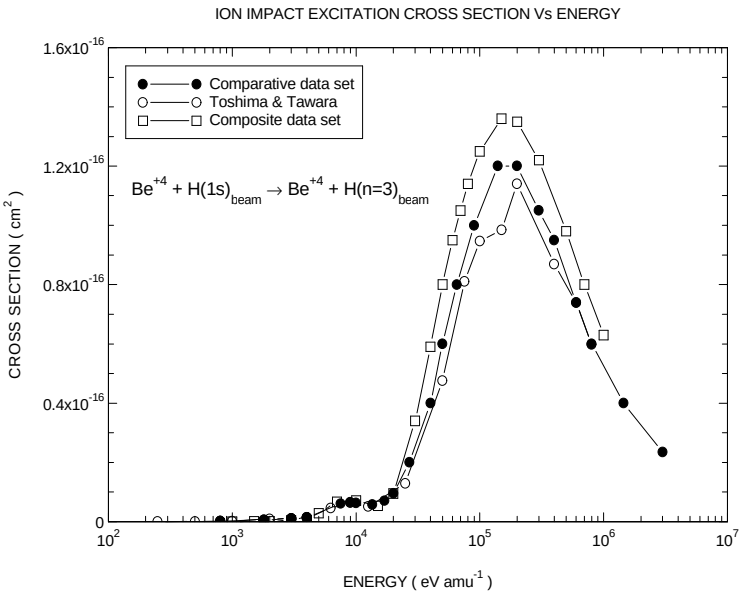

Figure 30.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data for this particular process.

For Z0 = 4 and n = 4, a general data set which is scaled according to the value of n and Z0 is employed. The results of the comparison between this data set and the data of Toshima & Tawara[91] can be observed in figure 31.0 . The general scaled data set, which is referred to as the composite data set, is the preferred data for this process. For all other value of Z0, a general data set was used which is scaled according to the value of n and Z0. The following figures illustrate the result of comparing the data of Toshima & Tawara[91] with the appropriately scaled data. Where possible a comparative data set, which is taken as the preferred data, was constructed by interpolating through the data of neighbouring species. In cases were it was not possible to construct a comparative data set, the general scaled data set is taken as the preferred data. The general scaled data set is referred to as the composite

data set. Finally, for Z0 = 9 and 10 the only data which existed was that of the general scaled data and a review of the literature failed to improve the situation.

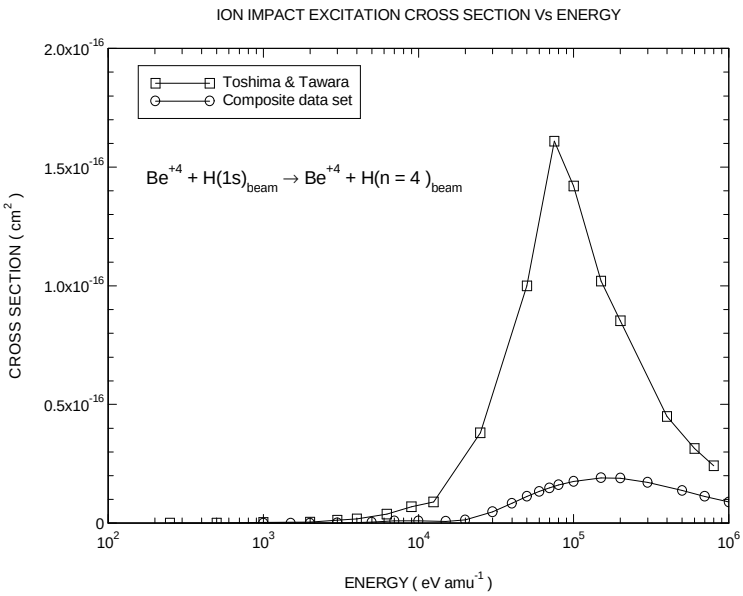

Figure 31.0 A plot of the ion impact excitation cross section Vs energy . The composite data set is taken as the preferred data. The calculation of Toshima & Tawara only include states up to n = 4, therefore some over-estimation is present particular for the n = 4 shell .

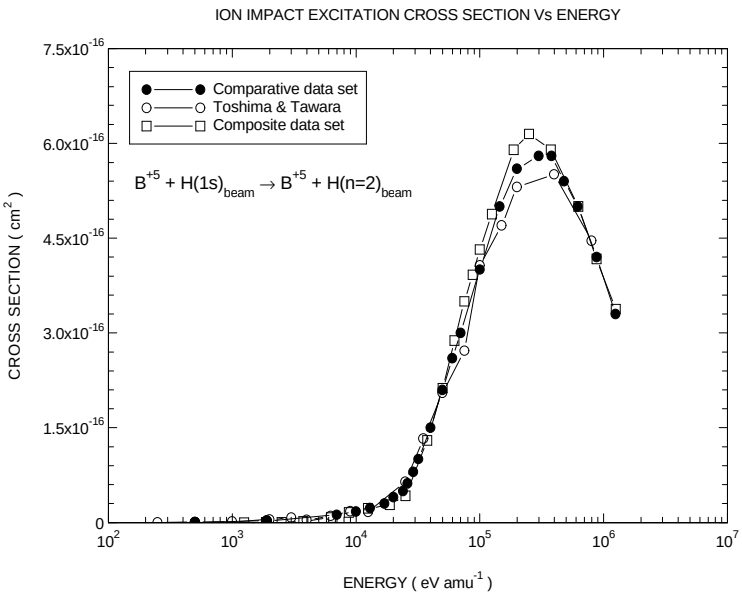

Figure 32.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data set for this process.

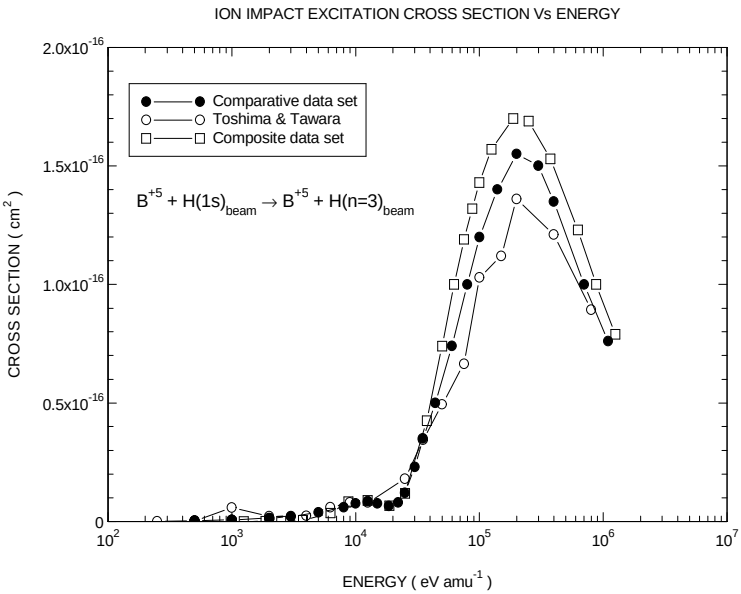

Figure 33.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data.

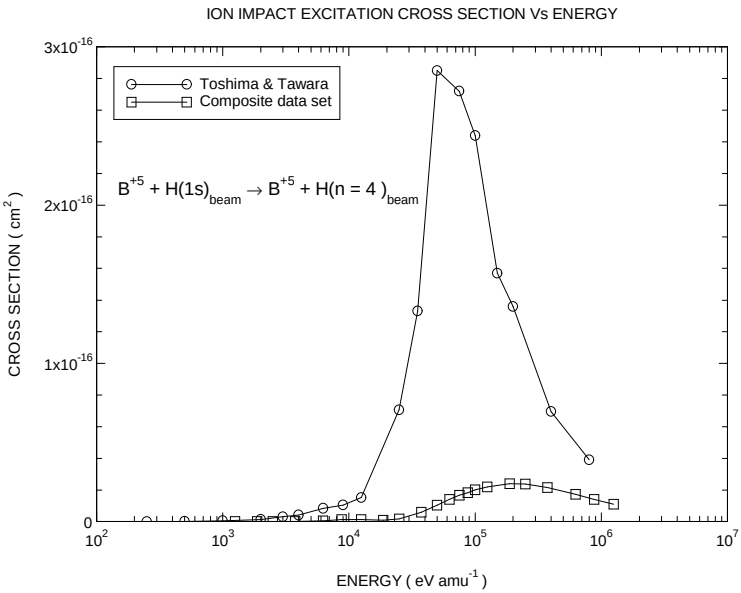

Figure 34.0 A plot of the ion impact excitation cross section Vs energy . The composite data set is taken as the preferred data. The calculation of Toshima & Tawara only include states up to n = 4, therefore some over-estimation is present particular for the n = 4 shell .

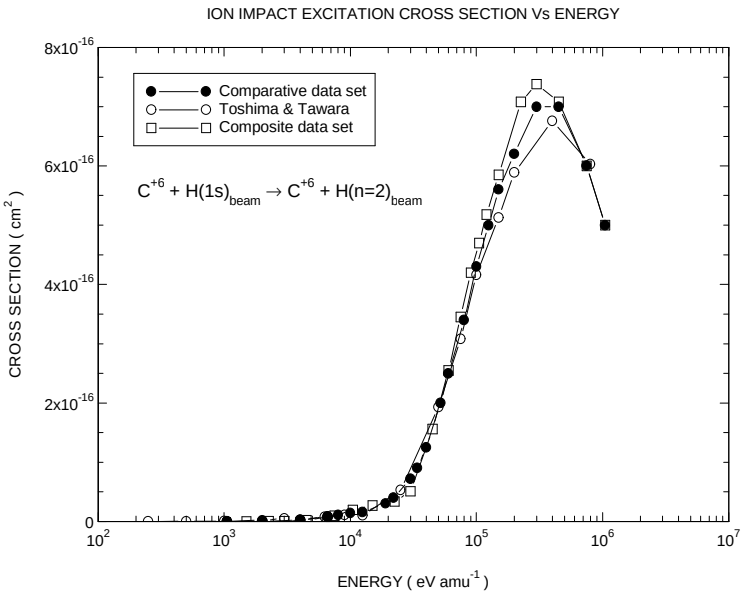

Figure 35.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data.

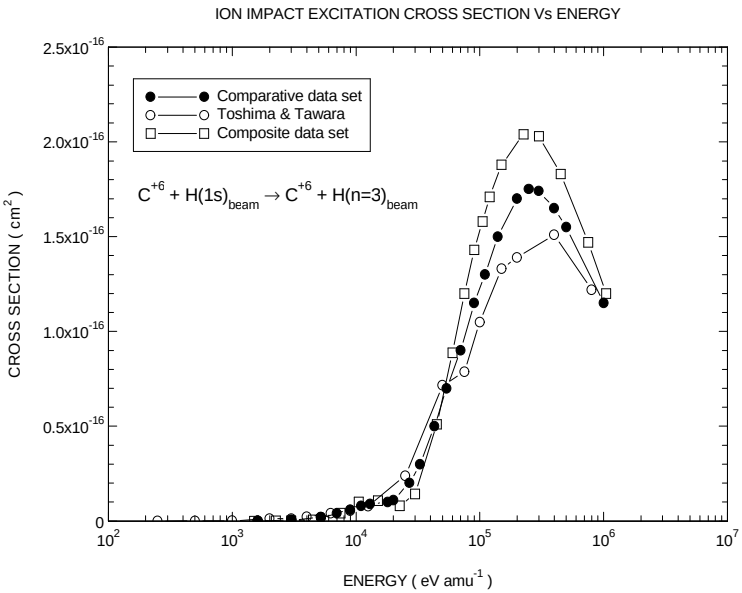

Figure 36.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data.

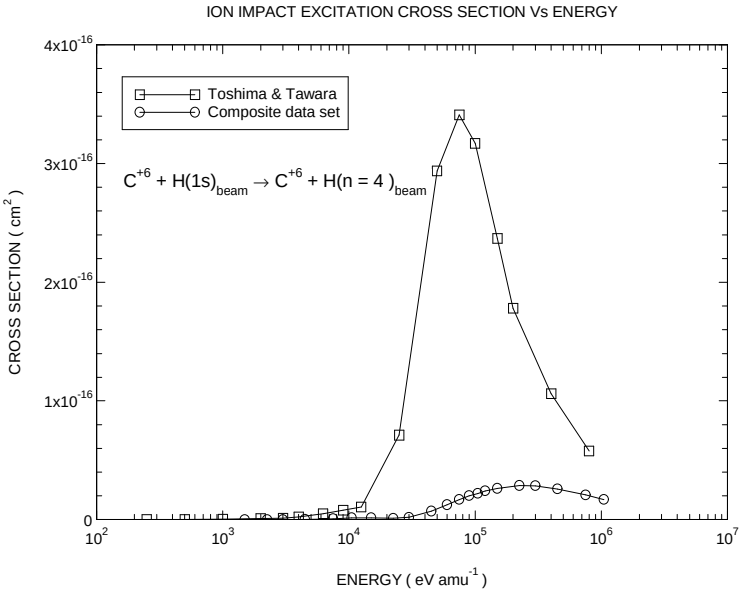

Figure 37.0 A plot of the ion impact excitation cross section Vs energy . The composite data set is taken as the preferred data. The calculation of Toshima & Tawara[91] only include states up to n = 4, therefore some over-estimation is present particular for the n = 4 shell .

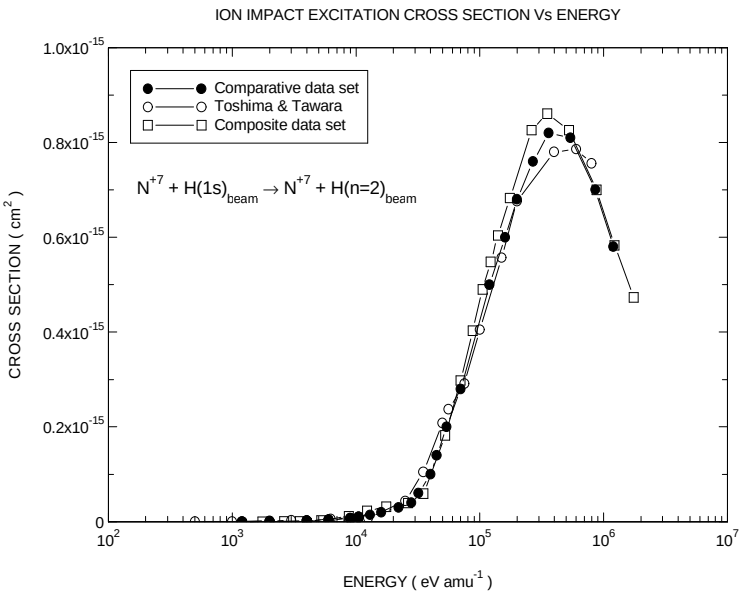

Figure 38.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data set.

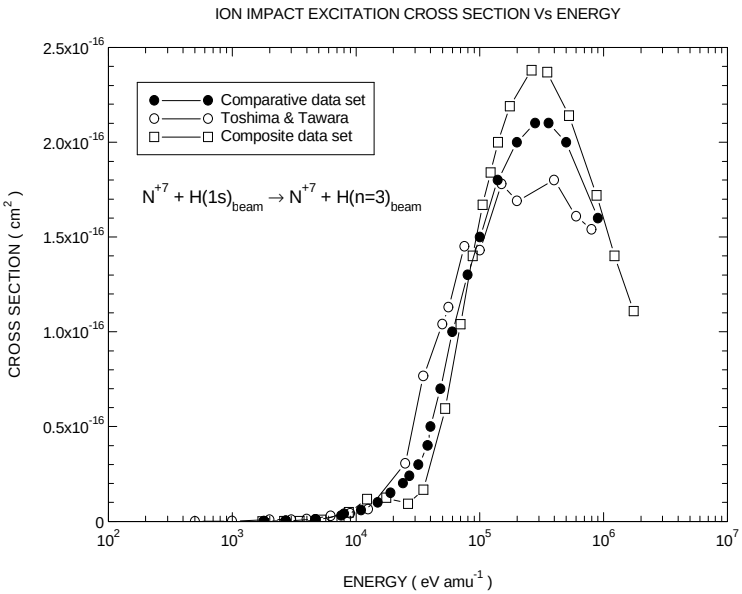

Figure 39.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data.

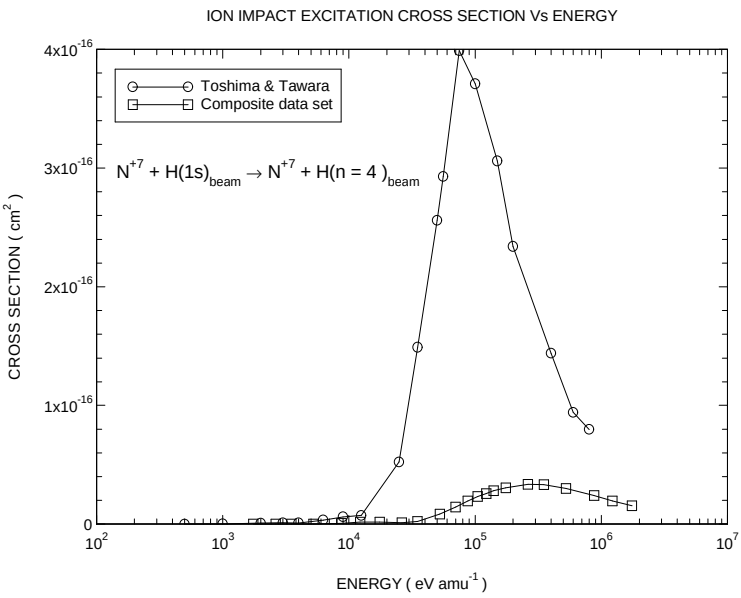

Figure 40.0 A plot of the ion impact excitation cross section Vs energy . The composite data set is taken as the preferred data. The calculation of Toshima & Tawara[91] only include states up to n = 4, therefore some over-estimation is present particular for the n = 4 shell .

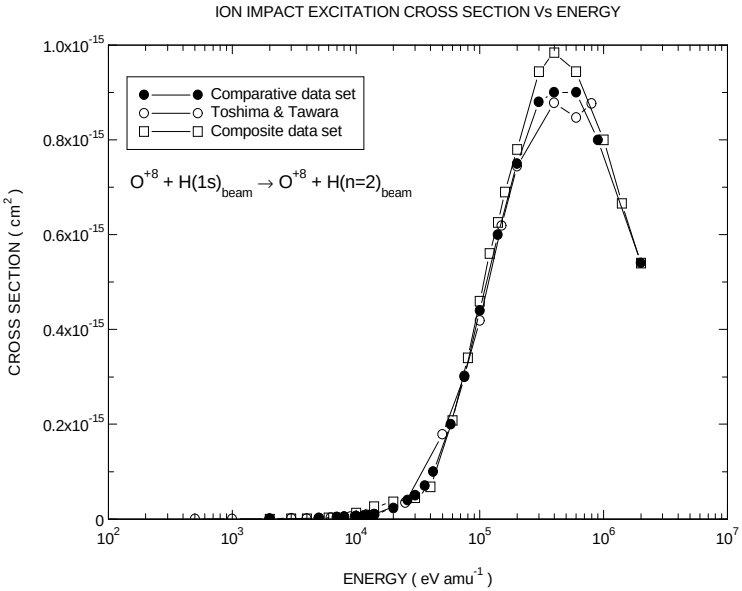

Figure 41.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data for this particular process.

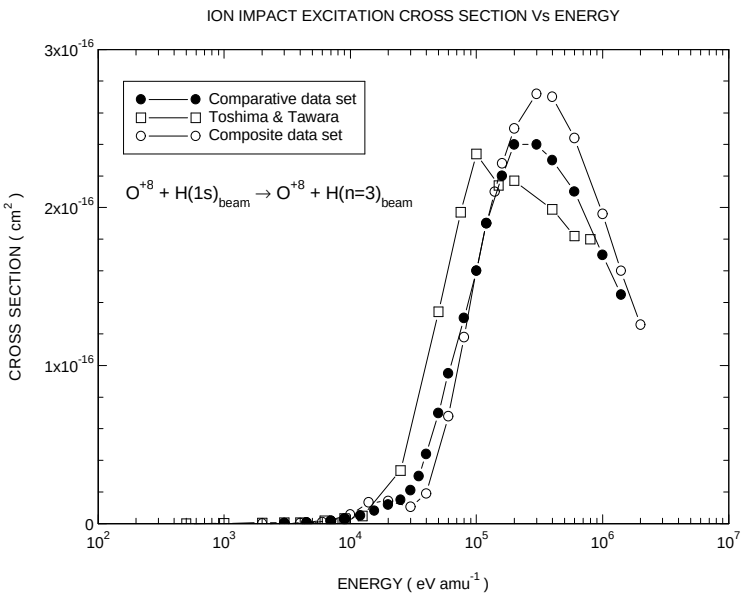

Figure 42.0 A plot of the ion impact excitation cross section Vs energy . The comparative data set is taken as the preferred data.

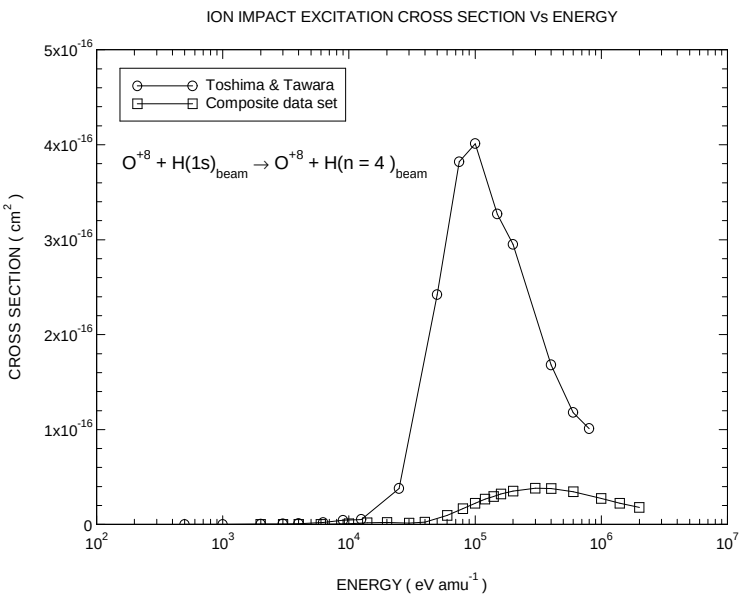

Figure 43.0 A plot of the ion impact excitation cross section Vs energy . The calculation of Toshima & Tawara[91] only include states up to n = 4, therefore some over-estimation is present particular for the n = 4 shell .

1.4 Review of ion impact ionisation from excited states of H

The database contains data for ion impact ionisation from excited states of the neutral beam particles as described by equation 1.4, where Z0 is the nuclear charge of the impurity and n is the principal quantum number.

$$X^{+Z0} + H(n)_{beam} \rightarrow X^{+Z0} + H^{+}_{beam} + e^{-} \qquad 1.4$$

The data which was used in all cases is a general data set which is scaled according to the value of Z0 and n. New data by Janev & Smith[90], for Z0 = 1 and n = 2, 3, 4 & 5 was compared to the results of using the general scaled data. The results can be seen in figures 44.0, 45.0, 46.0 and 47.0 . In all cases the data of Janev & Smith[90] is taken as the preferred data. An interesting point to note is the fairly large difference between the data of Janev & Smith[90] and the general scaled data in figure 45.0 . Ionisation from excited states by impurity ion impact is one of the least precisely known processes and so the more substantial deviations evident here are expected

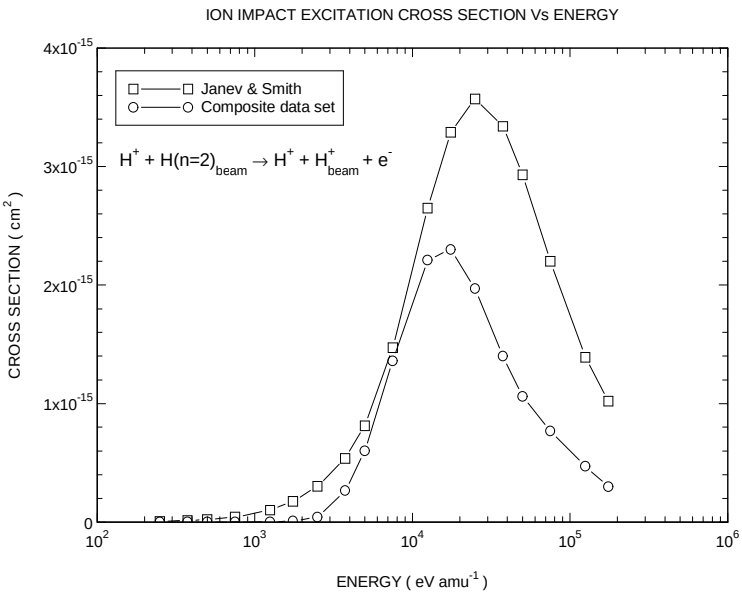

Figure 44.0 A plot of the ion impact ionisation cross section Vs energy . The data reported by Janev & Smith[90] is taken as the preferred data.

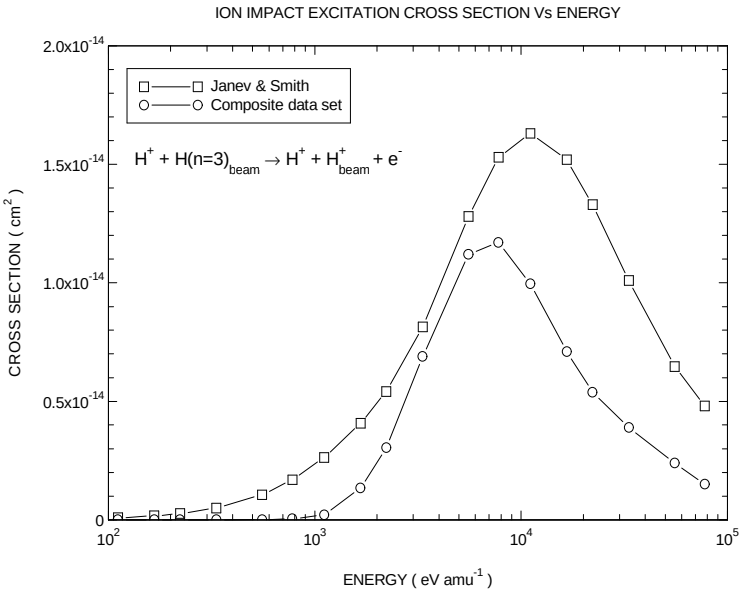

Figure 45.0 A plot of the ion impact ionisation cross section Vs energy . The data of Janev & Smith is taken as the preferred data. Interesting point to note is the significant difference between both data sets.

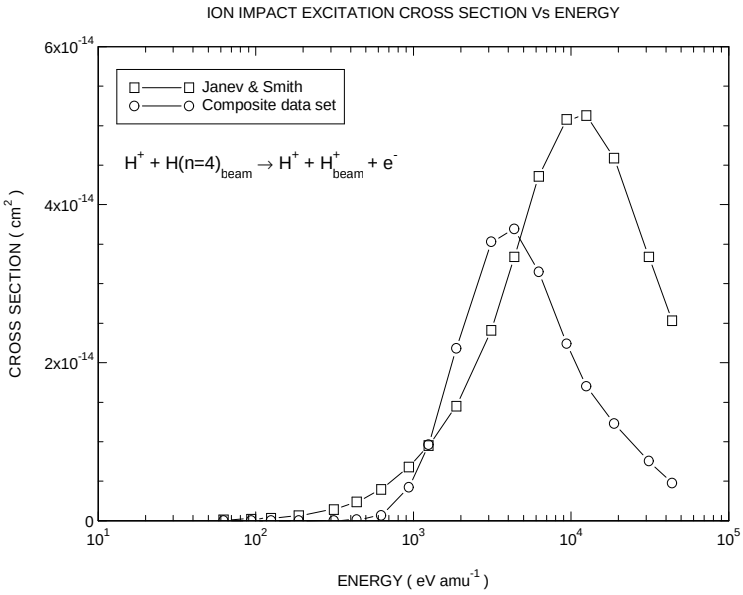

Figure 46.0 A plot of the ion impact ionisation cross section Vs energy . The data reported by Janev & Smith[90] is taken as the preferred data.

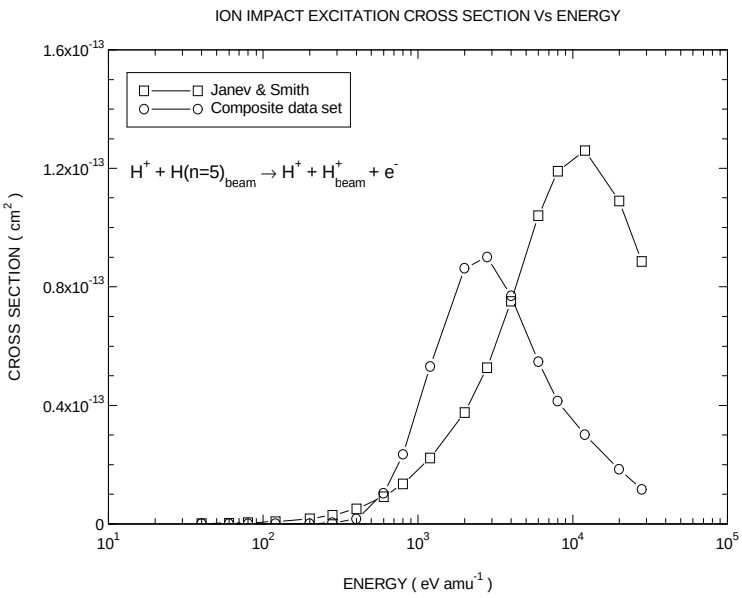

Figure 47.0 A plot of the ion impact ionisation cross section Vs energy . The data reported by Janev & Smith[90] is taken as the preferred data set.

1.5 Review of charge exchange data from excited states of H

The data base also contains data for charge exchange from excited states of the neutral beam particles as described by equation 1.5 .

$$X^{+Z0} + H(n)_{beam} \rightarrow X^{+Z0-1} + H^{+}_{beam} \qquad 1.5$$

Where all the symbols have there usual meaning. At the present, general scaled data is employed for this process and a survey of the literature failed to improve the situation.