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State-selective charge transfer cross sections for light ion impact of atomic hydrogen

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Abstract. Owing to the utility of diagnosing plasma properties such as impurity concentration and spatial distribution, and plasma temperature and rotation, by detection of photon emission following capture of electrons from atomic hydrogen to excited states of multiply charged ions, new calculations of state-selective charge transfer involving light ions have been carried out using the atomic orbital close-coupling and the classical trajectory Monte Carlo methods. By comparing these with results of other approaches applicable in a lower impact energy regime, and by benchmarking them using key experimental data, knowledge of the cross sections can be made available across the range parameters needed by fusion plasma diagnostics.

1. Introduction

Magnetic fusion experiments rely on a wide range of diagnostic techniques to understand important properties of the plasma such as the concentration of impurities, their transport within the plasma, and local plasma parameters such as density and rotation. One means of such diagnostics is the observation of photon emission when the electron from a hydrogen atom in a neutral heating beam is captured by a multiply charged impurity ion. Such collisions proceed with high probability to excited states of the ion and subsequent radiative relaxation yields photons of characteristic wavelengths (and other properties such as Doppler shift and line width and intensity) allowing identification of impurity species, motion, and density along the line of sight of the detector. This technique, commonly called charge exchange recombination spectroscopy (CHERS or CXRS) [1-4] is an important diagnostic tool implemented at many fusion research facilities.

As a contribution to the IAEA Coordinated Research Program on data for light ions, calculations were made for several common impurity ions (C^{5+}, N^{6+}, O^{6+}, and O^{7+}) colliding with atomic hydrogen in order to help create the database needed to derive cross sections over a broad range of impact energies and final captured states for CXRS diagnostics. This was carried out within a broad collaboration, consisting of work to provide benchmark measurements of the total charge transfer cross section at Oak Ridge National Laboratory [5] and theoretical work at several institutions including the University of Georgia, Bergische Universität Wuppertal, and the University of North Texas, using complementary methods for intercomparison and broad coverage of impact energies and final states. The complete results for C^{5+} + H [6], N^{6+} + H [7], and O^{6+} + H [8] have been published and those for O^{7+} + H are in final preparation.


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Here we describe some of the results and tabulate in detail a subset of data resulting from the calculations carried out by the first author who was a participant in the IAEA Coordinated Research Program. These calculations provide results for intermediate energy collisions, ~1 to 200 keV/u C^{5+}, N^{6+}, O^{6+}, and O^{7+} + H, using a method that is applicable particularly for capture to the low-lying excited states populated dominantly in these collisions (the atomic orbital close-coupling (AOCC) method) and another that is useful for prediction of results for the higher-lying excited states (the classical trajectory Monte Carlo (CTMC) method). When benchmarked by the total cross section measurements and combined with results applicable at lower collision energies (the molecular orbital close-coupling (MOCC) method) from our collaboration, recommended state-selective results can be derived for use in fusion plasma diagnostics and other applications.

2. Results and discussion

2.1. Total cross sections

At intermediate collisions energies (defined by collision velocities roughly comparable to those of the initially bound electron) the AOCC method should provide the most reliable results. As described in Refs. [6-8], we have employed the technique of Kuang and Lin [9,10] using very large basis sets to obtain state-selective charge transfer cross sections for all bound states in the calculation, and summed them to obtain the total cross section. Figures 1-2 show comparisons of the AOCC total cross sections with the benchmark measurements made at Oak Ridge. As these figures show, there is very good overall agreement between AOCC and the measurements regarding both the magnitude of the cross section and its behavior with energy throughout the overlapping energy ranges. Similar good agreement is also found with the to-be-published O^{7+} measurements. The limits of applicability of the AOCC method are reached below several hundred eV and so in that regime the results are the least reliable and another method, in particular, MOCC, is needed. The AOCC results are applicable to energies higher than those available in the experiment and are in generally good agreement with the results from CTMC [6-8] in this higher energy regime.

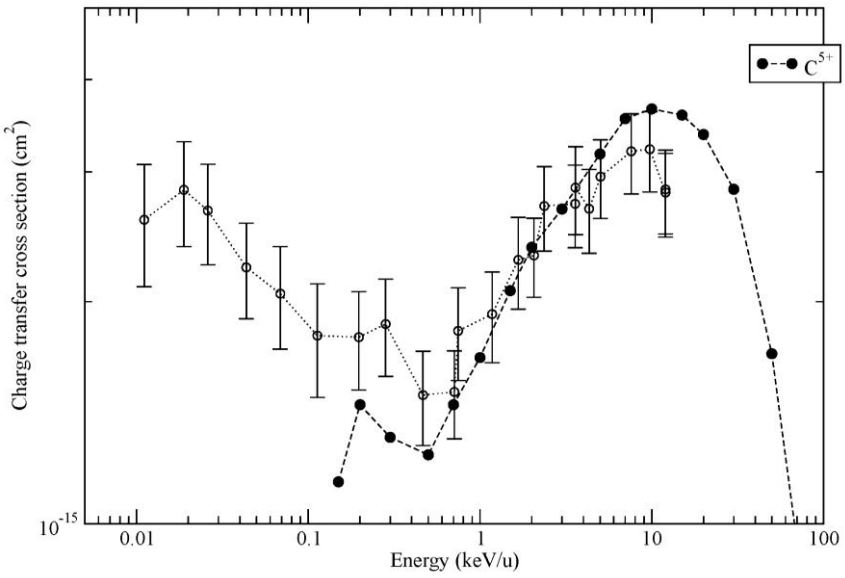


Figure 1. Comparison of the AOCC total cross section [6] (filled circles) for charge transfer in C^{5+} + H collisions with the benchmark measurements [5] (open circles).

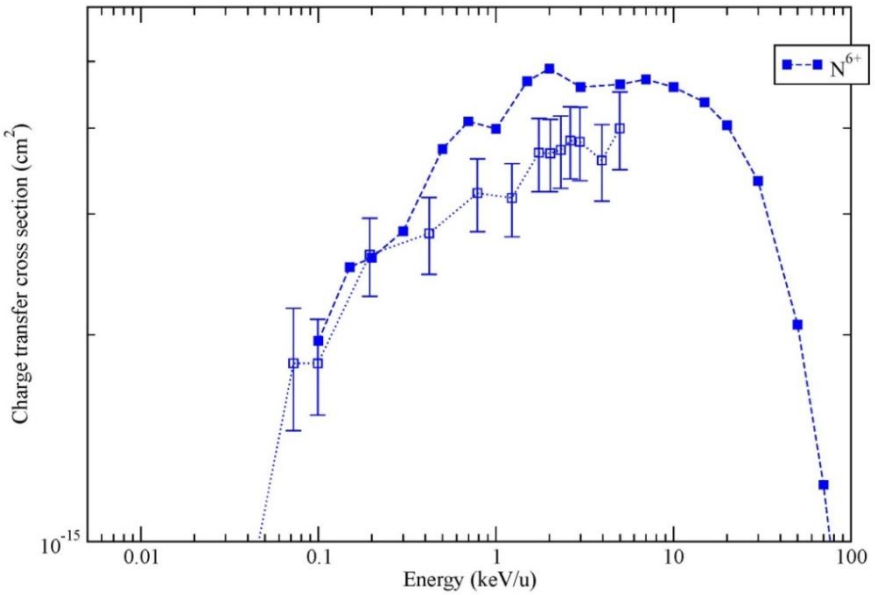


Figure 2. Comparison of the AOCC total cross section [7] (filled squares) for charge transfer in N^{6+} + H collisions with the benchmark measurements [7] (open squares).

2.2 State-selective cross sections

State-selective cross sections were computed using the AOCC method for the four collision systems at 19 impact energies between 0.15 and 200 keV/u and provide results for charge transfer up to principal quantum numbers of n=8. Since the AOCC formulation used is a one-electron model, resolution of the results by singlet and triplet spins is not possible and thus its results represent the sum of these channels that would be resolved by a two-electron treatment. The AOCC results are in generally good agreement with those obtained via the CTMC method and CTMC has been used to provide results for n levels higher than those contained in the AOCC basis sets. Together with analogous results of the MOCC method for lower energies, these data are being used to deduce recommended sets of data for use in plasma applications. To illustrate their behavior at intermediate energies, Tables 1-3 contain the AOCC state-selective charge transfer cross sections for $n< 6$ and those from CTMC for $n\geq 6$ at six energies between 0.5 and 100 keV/u for C^{5+}, N^{6+}, and O^{6+} + H.

Acknowledgement

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References

[1] R.J. Groebner, N.H. Brooks, K.H. Burrell, and L. Rottler, Appl. Phys. Lett. **43**, 920 (1983).
[2] R.C. Isler, Phys. Scr. **35**, 650 (1987).
[3] A. Boileau, M.G. von Hellerman, L.D. Horton, J. Spence, and H.P. Summers, J. Phys. B **31**, 779 (1989).
[4] O. Marchuk, Yu. Ralchenko, R.K. Janev, G. Berschinger, and W. Biel, J. Phys. B **42**, 165701 (2009).

[5] I.N. Draganić, D.G. Seely, and C.C. Havener, Phys. Rev. A 83, 054701 (2011) and references therein.
[6] J.L. Nolte, P.C. Stancil, H.P. Liebermann, R.J. Buenker, Y. Hui, and D.R. Schultz, J. Phys. B 45, 245202 (2012)
[7] Y. Wu, P.C. Stancil, H.P. Liebermann, P. Funke, S.N. Rai, R.J. Buenker, D.R. Schultz, Y. Hui, I.N. Draganić, and C.C. Havener, Phys. Rev. A 84, 022711 (2011).
[8] Y. Wu, P.C. Stancil, D.R. Schultz, Y. Hui, H.P. Liebermann, and R.J. Buenker, J. Phys. B 45, 235201 (2012).
[9] J. Kuang and C.D. Lin, J. Phys. B 29, 1207 (1996).
[10] J. Kuang and C.D. Lin, J. Phys. B 29, 5442 (1996).

Table 1. State-selective charge transfer cross sections (in units of 10^{-16} cm^2) for C^{5+} + H calculated by the present AOCC (n<6) and CTMC (n≥6) methods at selected intermediate collision energies (*E*).

C^{4+} state	*E*=0.5 keV/u	1 keV/u	5 keV/u	10 keV/u	50 keV/u	100 keV/u
2s	1.92E-05	1.21E-06	3.51E-04	7.11E-03	7.59E-02	3.72E-02
$2p_0$	1.29E-05	1.01E-06	3.65E-04	5.90E-03	5.87E-02	7.28E-02
$2p_1$	1.48E-05	3.27E-07	2.38E-04	2.81E-03	1.13E-01	8.16E-02
3s	9.05E-02	4.12E-01	1.87E+00	1.18E+00	1.56E-01	4.17E-02
$3p_0$	6.84E-02	2.96E-01	1.12E+00	1.79E+00	5.02E-01	1.17E-01
$3p_1$	8.68E-02	4.57E-01	3.14E+00	2.50E+00	3.44E-01	5.94E-02
$3d_0$	2.12E-02	7.02E-02	9.77E-01	1.46E+00	1.20E+00	3.41E-01
$3d_1$	2.37E-02	1.39E-01	9.28E-01	2.23E+00	1.65E+00	3.67E-01
$3d_2$	2.30E-02	1.10E-01	1.10E+00	1.50E+00	4.34E-01	6.19E-02
4s	1.02E+00	1.27E+00	9.55E-01	5.99E-01	1.11E-01	2.53E-02
$4p_0$	1.47E+00	1.64E+00	1.93E+00	1.29E+00	3.43E-01	9.82E-02
$4p_1$	1.13E+00	2.13E+00	1.14E+00	7.02E-01	1.41E-01	3.48E-02
$4d_0$	1.92E+00	1.83E+00	2.41E+00	2.73E+00	6.99E-01	1.96E-01
$4d_1$	2.24E+00	2.40E+00	3.34E+00	3.00E+00	7.26E-01	1.90E-01
$4d_2$	8.55E-01	8.00E-01	7.02E-01	6.19E-01	1.07E-01	2.40E-02
$4f_0$	1.02E+00	1.36E+00	3.01E+00	4.19E+00	1.21E+00	1.90E-01
$4f_1$	1.27E+00	2.08E+00	4.66E+00	6.46E+00	1.68E+00	2.31E-01
$4f_2$	6.01E-01	9.01E-01	2.08E+00	2.87E+00	5.22E-01	5.88E-02
$4f_3$	2.70E-01	3.17E-01	4.59E-01	5.61E-01	6.82E-02	5.74E-03
5s	3.50E-02	8.30E-02	6.72E-02	8.07E-02	7.30E-02	1.67E-02
$5p_0$	1.07E-02	2.72E-02	8.87E-02	1.51E-01	2.12E-01	7.42E-02
$5p_1$	4.56E-02	8.83E-02	3.62E-02	3.78E-02	7.93E-02	2.17E-02
$5d_0$	2.32E-02	6.63E-02	1.83E-01	1.53E-01	4.22E-01	1.30E-01
$5d_1$	3.56E-02	8.34E-02	1.33E-01	1.04E-01	3.65E-01	1.12E-01
$5d_2$	3.10E-02	2.49E-02	3.02E-02	2.03E-02	4.75E-02	1.25E-02
$5f_0$	3.40E-02	5.21E-02	2.64E-01	3.28E-01	5.39E-01	1.22E-01
$5f_1$	4.37E-02	4.20E-02	3.01E-01	3.55E-01	6.98E-01	1.48E-01
$5f_2$	1.50E-02	2.68E-02	1.22E-01	8.02E-02	1.82E-01	3.52E-02
$5f_3$	1.30E-02	1.94E-02	2.56E-02	1.38E-02	1.48E-02	3.22E-03
$5g_0$	1.80E-02	1.03E-02	1.53E-01	3.61E-01	3.34E-01	4.03E-02
$5g_1$	1.43E-02	1.49E-02	2.01E-01	5.21E-01	4.85E-01	5.71E-02
$5g_2$	2.96E-03	1.58E-02	8.28E-02	2.31E-01	1.90E-01	2.02E-02
$5g_3$	4.77E-03	1.33E-02	2.50E-02	5.16E-02	3.87E-02	3.60E-03
$5g_4$	7.81E-03	9.77E-03	3.58E-03	7.75E-03	4.20E-03	2.44E-04
n=6	8.8E-04	3.37E-03	3.89E-02	2.06E-01	1.74E+00	6.73E-01
n=7	-	6.4E-04	9.54E-03	7.28E-02	9.18E-01	4.69E-01
n=8	-	-	3.29E-03	3.78E-02	5.25E-01	3.36E-01
n=9	-	-	2.0E-03	2.03E-02	3.29E-01	2.46E-01
n=10	-	-	6.8E-04	1.29E-02	2.23E-01	1.84E-01
n=20	-	-	-	8.4E-04	2.19e-02	2.52E-02

Table 2. State-selective charge transfer cross sections (in units of 10^{-16} cm^2) for N^{6+} + H calculated by the present AOCC (n<6) and CTMC (n≥6) methods at selected intermediate collision energies (*E*).

N^{5+} state	*E*=0.5 keV/u	1 keV/u	5 keV/u	10 keV/u	50 keV/u	100 keV/u
2s	9.49E-05	1.16E-04	1.29E-05	2.20E-04	1.62E-02	1.82E-02
$2p_0$	6.71E-05	7.38E-05	6.72E-06	2.66E-04	8.18E-03	2.01E-02
$2p_1$	9.45E-05	1.70E-04	1.25E-05	5.41E-05	1.88E-02	2.73E-02
3s	1.11E-04	1.67E-03	2.72E-01	3.97E-01	1.54E-01	4.01E-02
$3p_0$	9.91E-05	1.73E-03	1.27E-01	3.09E-01	3.63E-01	1.02E-01
$3p_1$	1.52E-04	3.13E-03	3.16E-01	6.63E-01	3.58E-01	5.09E-02
$3d_0$	4.86E-05	1.04E-03	5.04E-02	2.41E-01	5.09E-01	2.64E-01
$3d_1$	9.23E-05	1.02E-03	1.01E-01	2.35E-01	8.19E-01	3.51E-01
$3d_2$	3.31E-05	6.13E-04	8.50E-02	2.81E-01	3.01E-01	7.59E-02
4s	2.71E+00	3.28E+00	1.73E+00	9.35E-01	1.17E-01	3.37E-02
$4p_0$	3.61E+00	3.61E+00	3.61E+00	1.97E+00	3.55E-01	8.23E-02
$4p_1$	2.62E+00	4.31E+00	3.22E+00	1.72E+00	1.65E-01	3.30E-02
$4d_0$	2.44E+00	2.65E+00	4.43E+00	3.68E+00	6.14E-01	1.67E-01
$4d_1$	3.55E+00	3.57E+00	6.55E+00	5.17E+00	6.86E-01	1.71E-01
$4d_2$	1.41E+00	2.21E+00	2.82E+00	1.67E+00	1.25E-01	3.14E-02
$4f_0$	4.30E+00	3.98E+00	3.64E+00	4.33E+00	1.52E+00	3.25E-01
$4f_1$	6.67E+00	6.17E+00	6.06E+00	6.74E+00	2.26E+00	4.47E-01
$4f_2$	2.62E+00	2.44E+00	3.25E+00	3.75E+00	8.76E-01	1.24E-01
$4f_3$	6.03E-01	9.47E-01	1.28E+00	1.10E+00	1.41E-01	1.30E-02
5s	5.99E-01	6.11E-01	1.15E-01	1.60E-01	7.64E-02	2.86E-02
$5p_0$	1.21E-01	6.07E-01	4.01E-01	4.36E-01	2.42E-01	5.01E-02
$5p_1$	8.14E-01	1.14E+00	1.84E-01	1.81E-01	9.30E-02	2.02E-02
$5d_0$	8.77E-01	8.03E-01	4.03E-01	5.19E-01	3.83E-01	1.46E-01
$5d_1$	6.83E-01	8.26E-01	5.73E-01	5.54E-01	3.59E-01	1.12E-01
$5d_2$	4.73E-01	3.05E-01	1.50E-01	1.08E-01	5.00E-02	1.54E-02
$5f_0$	1.33E+00	7.88E-01	7.38E-01	1.18E+00	6.60E-01	1.94E-01
$5f_1$	5.54E-01	4.79E-01	1.43E+00	1.55E+00	8.91E-01	2.38E-01
$5f_2$	2.27E-01	2.07E-01	5.13E-01	5.07E-01	2.61E-01	6.08E-02
$5f_3$	2.17E-01	1.83E-01	8.08E-02	7.76E-02	2.31E-02	5.32E-03
$5g_0$	3.84E-01	1.76E-01	1.12E+00	1.86E+00	8.62E-01	1.19E-01
$5g_1$	1.68E-01	1.86E-01	1.66E+00	2.87E+00	1.28E+00	1.80E-01
$5g_2$	7.39E-02	1.46E-01	6.72E-01	1.41E+00	5.52E-01	7.04E-02
$5g_3$	1.15E-01	1.48E-01	1.74E-01	4.08E-01	1.23E-01	1.33E-02
$5g_4$	1.26E-01	8.65E-02	3.63E-02	5.78E-02	1.29E-02	1.33E-03
n=6	6.89E-03	1.69E-02	1.47E-01	4.34E-01	3.30E+00	1.17E+00
n=7	2.8E-04	1.17E-03	1.95E-02	1.26E-01	1.23E+00	8.70E-01
n=8	-	2.4E-04	5.49E-03	5.20E-02	8.75E-01	6.31E-01
n=9	-	-	2.05E-03	2.79E-02	5.08E-01	4.71E-01
n=10	-	-	1.04E-03	1.50E-02	3.31E-01	3.52E-01
n=20	-	-	-	9.77E-04	2.86E-02	4.87E-02

Table 3. State-selective charge transfer cross sections (in units of 10^{-16} cm^2) for O^{6+} + H calculated by the present AOCC (n<6) and CTMC (n≥6) methods at selected intermediate collision energies (*E*).

O^{5+} state	*E*=0.5 keV/u	1 keV/u	5 keV/u	10 keV/u	50 keV/u	100 keV/u
2s	-	-	2.77E-05	8.10E-05	4.34E-03	1.88E-02
$2p_0$	-	-	1.40E-05	2.07E-04	4.97E-03	1.32E-02
$2p_1$	-	-	7.42E-06	9.34E-05	8.34E-03	3.34E-02
3s	1.19E-03	1.59E-03	6.61E-02	2.53E-01	1.55E-01	4.36E-02
$3p_0$	7.74E-04	4.87E-03	2.81E-01	1.97E-01	3.51E-01	9.31E-02
$3p_1$	5.44E-04	4.06E-03	4.77E-01	4.43E-01	2.72E-01	4.41E-02
$3d_0$	8.77E-04	4.44E-03	6.77E-02	2.51E-01	5.48E-01	3.33E-01
$3d_1$	4.20E-04	2.57E-03	7.43E-02	1.41E-01	7.88E-01	3.81E-01
$3d_2$	4.75E-04	7.80E-03	2.36E-01	2.33E-01	2.79E-01	6.32E-02
4s	6.85E+00	9.34E+00	7.22E+00	2.38E+00	9.68E-02	4.20E-02
$4p_0$	4.43E+00	6.72E+00	3.49E+00	2.47E+00	4.08E-01	7.00E-02
$4p_1$	1.18E+01	7.42E+00	2.75E+00	1.69E+00	1.21E-01	1.97E-02
$4d_0$	8.63E-01	9.22E-01	3.17E+00	3.45E+00	6.58E-01	2.55E-01
$4d_1$	6.19E-01	9.30E-01	3.01E+00	3.73E+00	7.12E-01	1.74E-01
$4d_2$	1.95E+00	1.83E+00	1.35E+00	1.06E+00	1.20E-01	2.22E-02
$4f_0$	2.10E+00	2.37E+00	3.08E+00	4.02E+00	1.52E+00	3.12E-01
$4f_1$	1.09E+00	2.81E+00	5.05E+00	6.32E+00	2.23E+00	4.06E-01
$4f_2$	5.47E+00	1.92E+00	2.43E+00	3.38E+00	8.77E-01	1.32E-01
$4f_3$	5.50E+00	4.95E+00	1.22E+00	8.80E-01	1.32E-01	1.91E-02
5s	1.62E-01	7.28E-01	4.41E-01	3.08E-01	6.17E-02	3.55E-02
$5p_0$	1.49E+00	4.04E-01	4.09E-01	5.27E-01	3.04E-01	4.96E-02
$5p_1$	7.93E-01	9.45E-01	2.43E-01	1.68E-01	5.90E-02	1.23E-02
$5d_0$	3.83E-01	8.82E-01	4.94E-01	6.03E-01	4.15E-01	1.90E-01
$5d_1$	7.44E-01	8.53E-01	5.53E-01	5.18E-01	3.94E-01	1.14E-01
$5d_2$	2.51E-01	1.85E-01	1.08E-01	7.11E-02	4.55E-02	1.26E-02
$5f_0$	2.42E-01	4.08E-01	9.94E-01	1.32E+00	7.39E-01	1.89E-01
$5f_1$	2.70E-01	3.47E-01	1.64E+00	1.80E+00	8.52E-01	2.14E-01
$5f_2$	1.29E-01	1.44E-01	5.62E-01	5.86E-01	2.56E-01	6.22E-02
$5f_3$	1.47E-01	1.45E-01	6.98E-02	7.35E-02	3.29E-02	7.47E-03
$5g_0$	8.73E-02	9.52E-02	1.24E+00	2.20E+00	9.03E-01	1.32E-01
$5g_1$	7.53E-02	1.75E-01	1.70E+00	3.25E+00	1.35E+00	1.92E-01
$5g_2$	4.46E-02	1.30E-01	7.34E-01	1.67E+00	6.10E-01	8.21E-02
$5g_3$	4.90E-02	7.38E-02	2.25E-01	4.64E-01	1.37E-01	1.60E-02
$5g_4$	1.26E-01	8.87E-02	3.36E-02	5.93E-02	1.19E-02	1.60E-03
n=6	4.36E-03	1.38E-02	1.48E-01	4.61E-01	3.34E+00	1.16E+00
n=7	-	1.63E-03	2.18E-02	1.33E-01	1.67E+00	8.66E-01
n=8	-	2.2E-04	6.66E-03	5.47E-02	9.02E-01	6.31E-01
n=9	-	-	3.02E-03	2.82E-02	5.30E-01	4.68E-01
n=10	-	-	1.41E-03	1.63E-02	3.44E-01	3.55E-01
n=20	-	-	1.0E-04	9.58E-04	2.91E-02	4.97E-02