ATOMIC AND PLASMA–MATERIAL INTERACTION DATA FOR FUSION

(Supplement to the journal Nuclear Fusion)

VOLUME 6

INTERNATIONAL ATOMIC ENERGY AGENCY, VIENNA, 1995

CONTENTS

Electron-Impact Ionization of Atomic Ions for ADAS

M. S. Pindzola

Department of Physics, Auburn University, Auburn, AL

D. C. Griffin

Department of Physics, Rollins College, Winter Park, FL

N. R. Badnell and H. P. Summers

Department of Physics and Applied Physics, University of Strathclyde, Glasgow, UK

Abstract

A progress report is made on efforts to calculate LS term and LSJ level resolved electron-impact ionization cross sections and rate coefficients for all the major impurity ions. This effort will extend the existing electron ionization data base found in the suite of computer codes for atomic data and analysis stucture (ADAS) developed at JET.

I. INTRODUCTION

The atomic data and analysis structure (ADAS) is an interconnected set of computer codes and data collections developed at JET for modelling the radiating properties of ions and atoms in plasmas and for assisting in the analysis and interpretation of spectral measurements [1]. An international consortium has been formed recently to distribute the entire set of codes, in a user friendly unix workstation format, to selected laboratory and astrophysical plasma research facilities. A key component of ADAS is its extensive atomic database. The fundamental part of the database includes electron-ion excitation, ionization, and recombi-

nation cross sections and rate coefficients, as well as atom-ion charge exchange recombination cross sections and rates. The database has a tiered structure, the lowest level inhabited by general semi-empirical formulae which provide at least some estimate of a scattering cross section or rate coefficient for any atomic ion, progressing through to the highest levels which contain the current best theoretical calculations and experimental measurements on selected atomic ions. Not infrequently, the validity of a given plasma spectral diagnostic will depend directly on the accuracy of the underlying atomic data.

In this paper we report on our efforts to calculate electron-impact ionization cross sections within the distorted-wave approximation for all the major impurity ions. The semi-empirical expression due to Burgess and Chidichimo [2] forms the current baseline for the ADAS atomic database, supplemented by cross sections for a small number of ions from either distorted-wave theory or experiment. For maximum predictive power over a variety of plasma conditions, the collisional-radiative modelling codes found in the ADAS package require LS term and LSJ level resolved ionization cross sections and rates coefficients. Since most experimental measurements count charge-changing events and thus sum over all final states of the ion, the distorted-wave codes developed in support of those experiments have had to be extensively modified to generate final state resolved ionization cross sections in the ADAS format. What remains of this paper is partitioned as follows: in Sec. II we review distorted-wave theory as applied to electron-impact ionization of atomic ions, in Sec. III we present results for O^{3+} in the ADAS format, while in Sec. IV we summarize our plans for the completion of the project.

II. THEORY

Major contributions to the electron-impact single-ionization cross section are made by the following two processes:

$$e^- + A^{q+} \rightarrow A^{(q+1)+} + e^- + e^- \ , \tag{1}$$

and

$$e^- + A^{q+} \rightarrow (A^{q+})^* + e^- \rightarrow A^{(q+1)+} + e^- + e^- \ , \tag{2}$$

where A represents an arbitrary ion with charge q. The first process is direct ionization while the second is excitation-autoionization. The total ionization cross section is given by:

$$\sigma_{tot} = \sum_f \sigma_{ion}(i \rightarrow f) + \sum_j \sum_f \sigma_{exc}(i \rightarrow j) B_{auto}(j \rightarrow f) \ , \tag{3}$$

where $\sigma_{ion}(i \rightarrow f)$ is the direct ionization cross section from an initial LS term or LSJ level i of the N-electron ion to a final term or level f of the (N-1)-electron ion, and $\sigma_{exc}(i \rightarrow j)$ is the inner-shell excitation cross section from an initial term or level i to a particular autoionizing term or level j. The branching ratio for autoionization from a term or level j is given by:

$$B_{auto}(j \rightarrow f) = \frac{A_a(j \rightarrow f)}{\sum_m A_a(j \rightarrow m) + \sum_n A_r(j \rightarrow n)} \ , \tag{4}$$

where $A_a(j \rightarrow m)$ is the autoionizing rate from a term or level j to a final term or level m, and $A_r(j \rightarrow n)$ is the radiative rate from a term or level j to a final bound term or level n.

A theoretical calculation of the total electron-impact ionization cross section for an arbitrary ion divides into three parts. The first part is a collisional ionization calculation for σ_{ion}, the second part is a collisional excitation calculation for σ_{exc}, and the third part is an atomic structure calculation for B_{auto}. We note that rate coefficients for an atomic database may be separately catalogued for σ_{ion} and σ_{exc} and then put together for applications. Future updates to the database are also easier due to the natural three part division.

The direct ionization cross sections are first calculated in a configuration average distorted-wave approximation, which is described in detail in the proceedings of a NATO advanced study institute [3]. The configuration average cross sections are resolved as to initial and final LS terms or LSJ levels by purely algebraic transformations [4]. Experimental threshold energies are then incorporated using a simple energy scaling of the resolved cross sections.

The inner-shell excitation cross sections may be calculated in a configuration average distorted-wave approximation. Although there is no pure algebraic transformation, the configuration-average cross section may be statistically partitioned over all terms or levels

of the final excited ion. For Fe^{5+} only 10 inner-shell configuration-average excitation cross sections were distributed over more than 5000 levels to produce a total ionization cross section in good agreement with crossed-beams experimental measurements [5].

More accurate inner-shell excitation cross sections may be calculated in a multi-configuration LS term or LSJ level resolved distorted-wave approximation. For some years we have calculated inner-shell excitation cross sections using an LSJ level resolved collisional excitation code [6] based on Cowan's atomic structure program [7]. For this project we have written an LS term and LSJ level resolved collisional excitation code based on Fischer's new atomic structure package [8].

The most accurate inner-shell excitation cross sections are calculated in a multi-configuration LS term or LSJ level resolved close-coupling approximation. We use the Breit-Pauli R-matrix codes [9] developed for the Iron Project [10]. The close-coupling formulation automatically includes the additional process of dielectronic capture followed by double autoionization:

$$e^- + A^{q+} \rightarrow (A^{(q-1)+})^{**} \rightarrow (A^{q+})^* + e^- \rightarrow A^{(q+1)+} + e^- + e^- \ . \qquad (5)$$

This process may enhance the total ionization cross section by as much as 50% in the threshold energy region. We have recently modified the Breit-Pauli R-matrix codes to include radiation-damping [11] and to eliminate pseudo-resonances associated with the use of approximate target wavefunctions [12].

The branching ratios for autoionization are calculated in a configuration interaction LS term or LSJ level resolved distorted-wave approximation using the AUTOSTRUCTURE code [13,14]. The ADAS format entails an added level of complexity since the branching ratios need to be resolved as to final LS term or LSJ level. For comparisons with experiments that measure charge-changing events, only branching ratios summed over all final states are required; i.e. $\sum_f B_{auto}(j \rightarrow f)$ in Eq.(3). Previously, to provide dielectronic recombination cross sections and rates in the ADAS format, we had to deal with the same increase in complexity. In that case, the branching ratio for radiative stabilization needed to be resolved

as to final state, although all ion storage-ring experiments to date require only the summed branching ratio.

III. RESULTS FOR O^{3+}

The total electron-impact ionization cross section for light impurity ions is dominated by the contribution from the direct ionization process of Eq.(1). As an example, we consider in detail the electron ionization of O^{3+}. The ground LS term is $2s^22p\ ^2P$ and the first metastable term is $2s2p^2\ ^4P$. We first calculated configuration-average distorted-wave cross sections for $2s^22p \rightarrow 2s^2$, $2s^22p \rightarrow 2s2p$, $2s2p^2 \rightarrow 2s2p$, and $2s2p^2 \rightarrow 2p^2$ at about 10 incident energies extending to 5 times the threshold energies. The cross sections were extrapolated to higher energies by calculation of Bethe constants from the energy-integrated configuration-average photoionization cross sections. Ionization cross sections for the transitions $2s^22p\ ^2P \rightarrow 2s^2\ ^1S, 2s2p\ ^3P, 2s2p\ ^1P$ are shown in Fig. 1, while the transitions $2s2p^2\ ^4P \rightarrow 2s2p\ ^3P, 2p^2\ ^3P$ are shown in Fig. 2. The LS term resolved ionization cross sections have been energy-scaled using experimental ionization potentials.

To compare with experiment, the LS term resolved ionization cross sections for the ground and metastable states of O^{3+} are summed over all final states. In Fig. 3 the ground and metastable ionization cross sections are compared with ORNL crossed-beams measurements [15]. For most electron ionization experiments, the fraction of metastables in the incident ion beam is unknown. As shown in Fig. 3, comparing theory and experiment has shed little light on the unknown metastable fraction problem.

The LS term resolved ionization cross sections for O^{3+} are entered into the ADAS atomic database in the form of Maxwell-averaged rate coefficients. Ionization rates for the transitions $2s^22p\ ^2P \rightarrow 2s^2\ ^1S, 2s2p\ ^3P, 2s2p\ ^1P$ are shown in Fig. 4, while the transitions $2s2p^2\ ^4P \rightarrow 2s2p\ ^3P, 2p^2\ ^3P$ are shown in Fig. 5. The numerical entry format for the O^{3+} rates in the ADAS database is presented in Table I. Initial and final states are identified by configuration, $2S+1$, L, WJ (statistical weight $= 2WJ+1$), and relative energy in cm^{-1}.

Ionization rates in cm^3 sec^{-1} from each initial LS term to each final LS term are tabulated as a function of electron temperature in Kelvin. Each entry format is signed and dated at the bottom with a short description of the theoretical or experimental procedure used to generate the atomic data.

IV. SUMMARY

In addition to O^{3+}, we have completed direct ionization cross section calculations in the ADAS format for all the light impurity ions; i.e. members of the Be, B, C, N, and O isonuclear sequences. We are currently engaged in calculating direct ionization and excitation-autoionization contributions to the total ionization cross section for Na- and Mg-like ions of the transition metal impurity ions; i.e. Ti, Cr, Fe, and Ni. Excitation-autoionization contributions for these ions are quite large. For example, the ionization cross sections for Ni^{16+} from the ground LSJ level $3s^2\ ^1S_0$ and the metastable levels $3s3p\ ^3P_0$ and $3s3p\ ^3P_2$ are enhanced by a factor of 3 due to excitation-autoionization contributions [16].

In summary, the atomic data needs of the current generation of plasma modelling codes, as found in ADAS, have pushed the data envelope beyond the accumulation of total ionization and recombination rate coefficients for each ionization stage of an important impurity ion. For population flows in non-equilibrium plasmas, LS term and LSJ level resolved rates are now needed for all the major impurity ions. This much more comprehensive atomic database seems only feasible in a purely electronic form. In addition, the turn towards level resolved ionization and recombination rate coefficients has forced us to make substantial changes in the way we carry out our theoretical calculations. In the future it may have an impact on the way electron-ion scattering experiments are carried out to test those theoretical predictions.

V. ACKNOWLEDGMENTS

This work was supported in part by the U.S. Department of Energy under Grant No. DE-FG05-86-ER53217 with Auburn University and Grant No. DE-FG05-93-ER54218 with Rollins College, and by U.K. EPSRC under Contract GR/K/14346 with the University of Strathclyde.

TABLE I. ADAS entry form for electron-impact ionization of O^{3+}.

```
seq ='B '    nucchl = 8                                                    ADF23

  final term indexing        bwnf =    918625.3     nprf =  6
  --------------------
  indf    code           S L   WJ       wnf
  ----    ----           - -   --  ------------
    1    2s22p0         (1)0( 0.0)          0.0
    2    2s12p1         (3)1( 4.0)       82413.1
    3    2s12p1         (1)1( 1.0)      158801.2
    4    2s02p2         (3)1( 4.0)      213928.8
    5    2s02p2         (1)2( 2.0)      231721.2
    6    2s02p2         (1)0( 0.0)      287913.4

  initial term indexing      bwni =    624106.8     nlev =  2
  --------------------
  indi    code           S L   WJ       wni
  ----    ----           - -   --  ------------
    1    2s22p1         (2)1( 2.5)          0.0
    2    2s12p2         (4)1( 5.5)       71331.1

------------------------------------------------------------------------------
meti*= 1

  ionis rates
  -----------
  indf Te= 3.20D+04  8.00D+04  1.60D+05  3.20D+05  8.00D+05  1.60D+06  3.20D+06  8.00D+06  1.60D+07  3.20D+07  8.00D+07  1.60D+08
  ---- ---
    1      5.51D-22  1.86D-14  6.78D-12  1.42D-10  9.47D-10  1.81D-09  2.42D-09  2.63D-09  2.44D-09  2.11D-09  1.62D-09  1.29D-09
    2      9.77D-24  3.16D-15  2.48D-12  7.75D-11  6.82D-10  1.46D-09  2.11D-09  2.44D-09  2.33D-09  2.06D-09  1.61D-09  1.28D-09
    3      1.02D-25  2.67D-16  4.19D-13  1.86D-11  2.04D-10  4.72D-10  7.15D-10  8.54D-10  8.29D-10  7.38D-10  5.82D-10  4.67D-10
    4      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    5      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    6      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00

------------------------------------------------------------------------------
meti*= 2

  ionis rates
  -----------
  indf Te= 3.20D+04  8.00D+04  1.60D+05  3.20D+05  8.00D+05  1.60D+06  3.20D+06  8.00D+06  1.60D+07  3.20D+07  8.00D+07  1.60D+08
  ---- ---
    1      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    2      7.03D-22  3.21D-14  1.29D-11  2.84D-10  1.96D-09  3.78D-09  5.09D-09  5.55D-09  5.16D-09  4.46D-09  3.43D-09  2.72D-09
    3      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    4      4.18D-25  7.00D-16  9.50D-13  3.91D-11  4.10D-10  9.36D-10  1.40D-09  1.66D-09  1.61D-09  1.43D-09  1.13D-09  9.02D-10
    5      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00
    6      0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00  0.00D+00

C  ---------------------------------------------------------------------------
C  Data generated by Donald C. Griffin   on 04/14/95
C
C  The rates were calculated using configuration-average ionization cross
C  sections, with non-relativistic wavefunctions , using the
C  frozen-core approximation, the prior form for the scattering
C  potentials, and the natural-phase approximation.
C  They were then multiplied by the appropriate angular coefficients.
C  ---------------------------------------------------------------------------
```

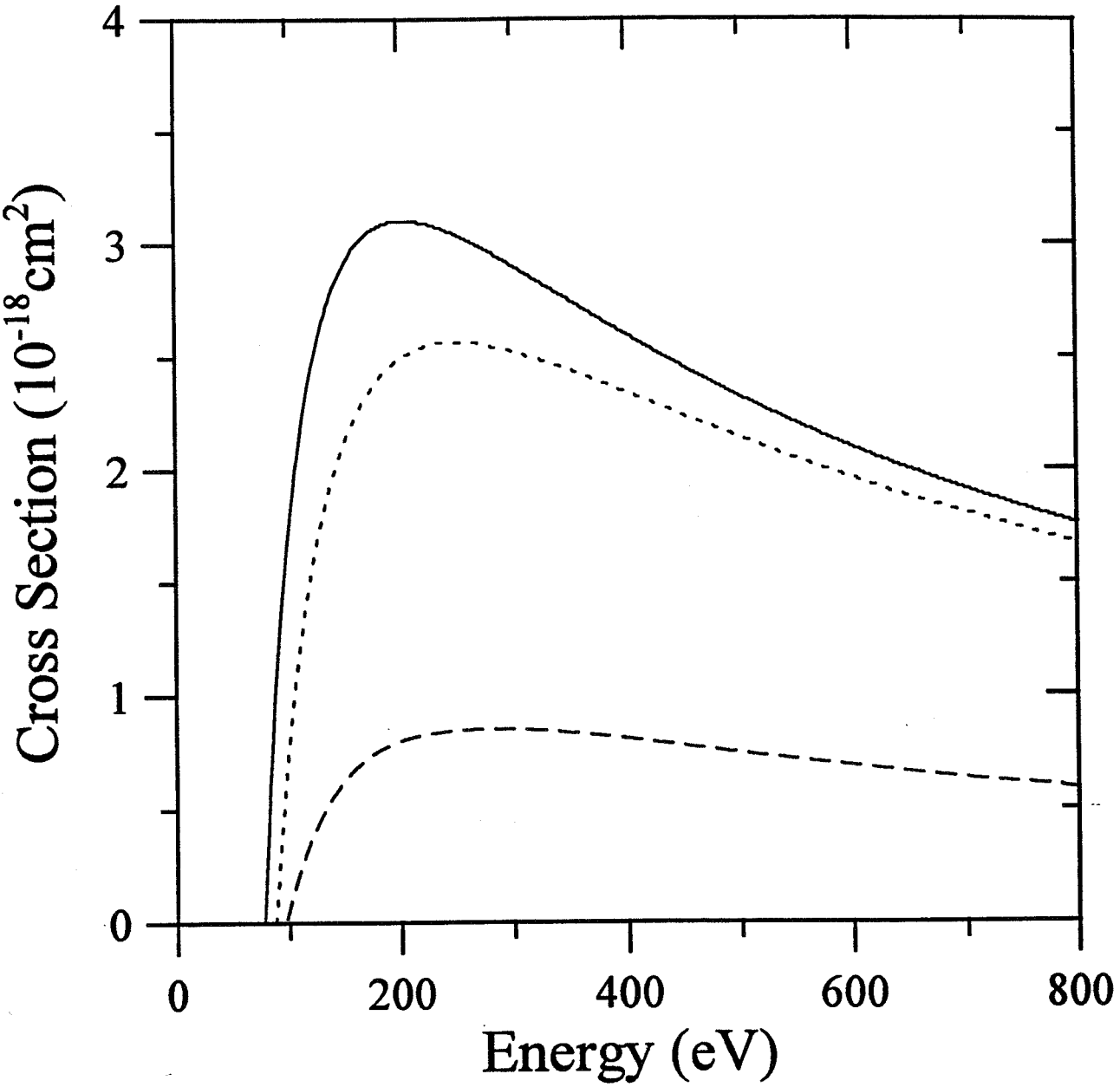

Figure 1. Electron-impact ionization of O^{3+} in the ground LS term $2s^2 2p\ ^2P$. Solid curve: $2s^2\ ^1S$ final term, short-dashed curve: $2s2p\ ^3P$ final term, and long-dashed curve $2s2p\ ^1P$ final term.

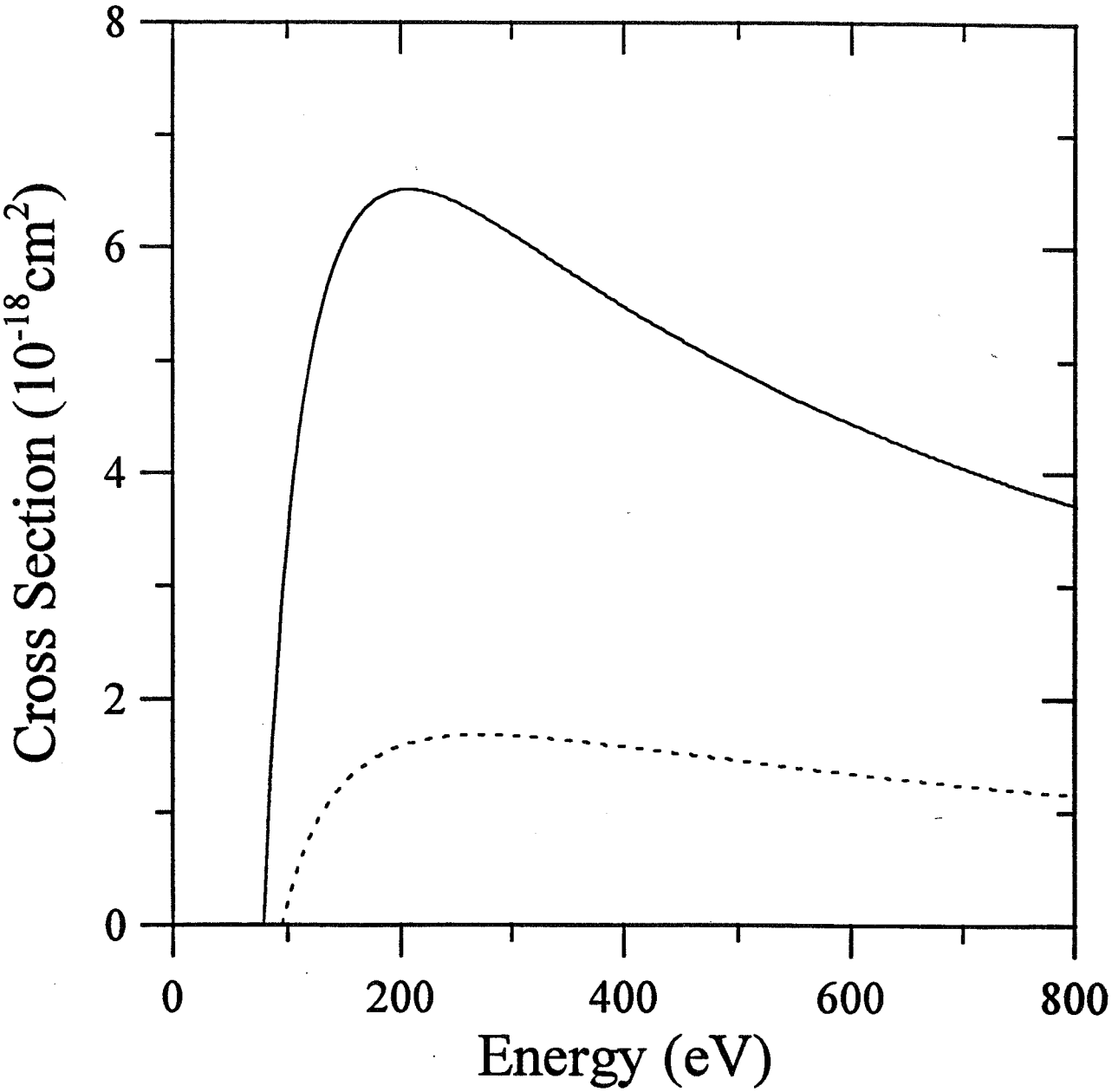

Figure 2. Electron-impact ionization of O^{3+} in the metastable term $2s2p^2\ ^4P$. Solid curve: $2s2p\ ^3P$ final term, and short-dashed curve: $2p^2\ ^3P$ final term.

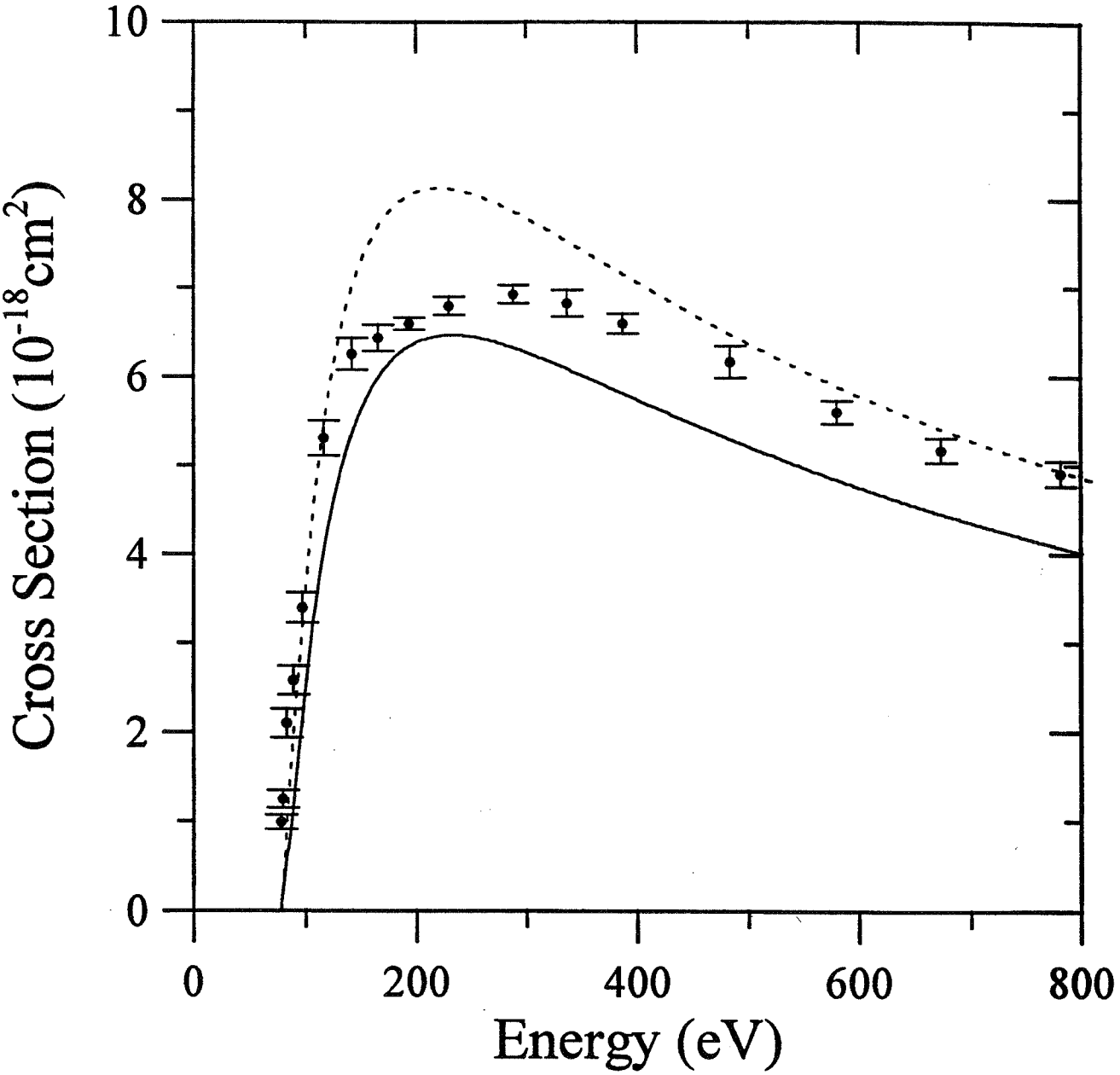

Figure 3. Electron-impact ionization of O^{3+}. Solid curve: $2s^2 2p\ ^2P$ ground term, short-dashed curve: $2s2p^2\ ^4P$ metastable term, solid circles: crossed-beams experiment.

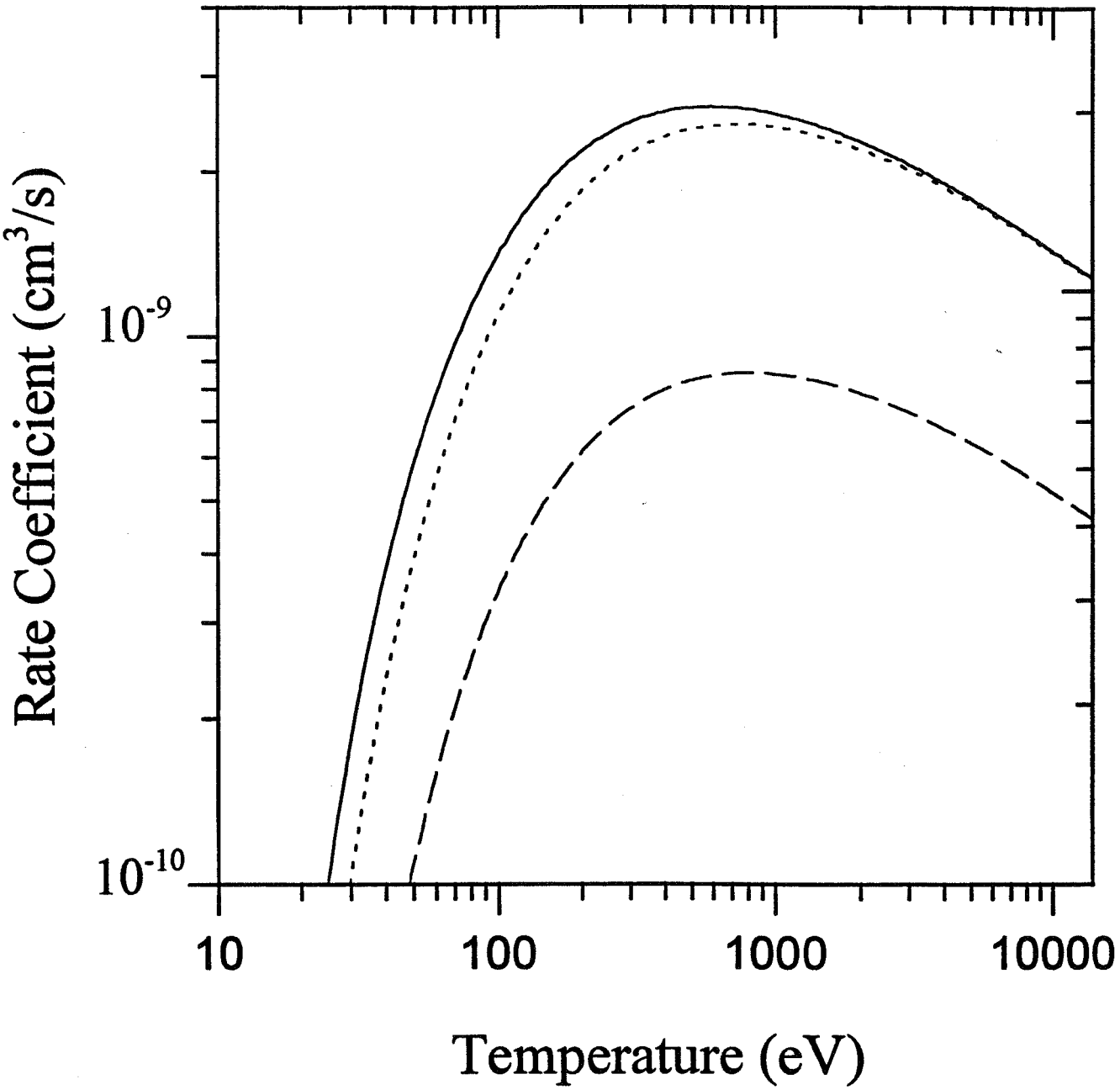

Figure 4. Electron-impact ionization of O^{3+} in the ground LS term $2s^2 2p\ ^2P$. Solid curve: $2s^2\ ^1S$ final term, short-dashed curve: $2s2p\ ^3P$ final term, and long-dashed curve $2s2p\ ^1P$ final term.

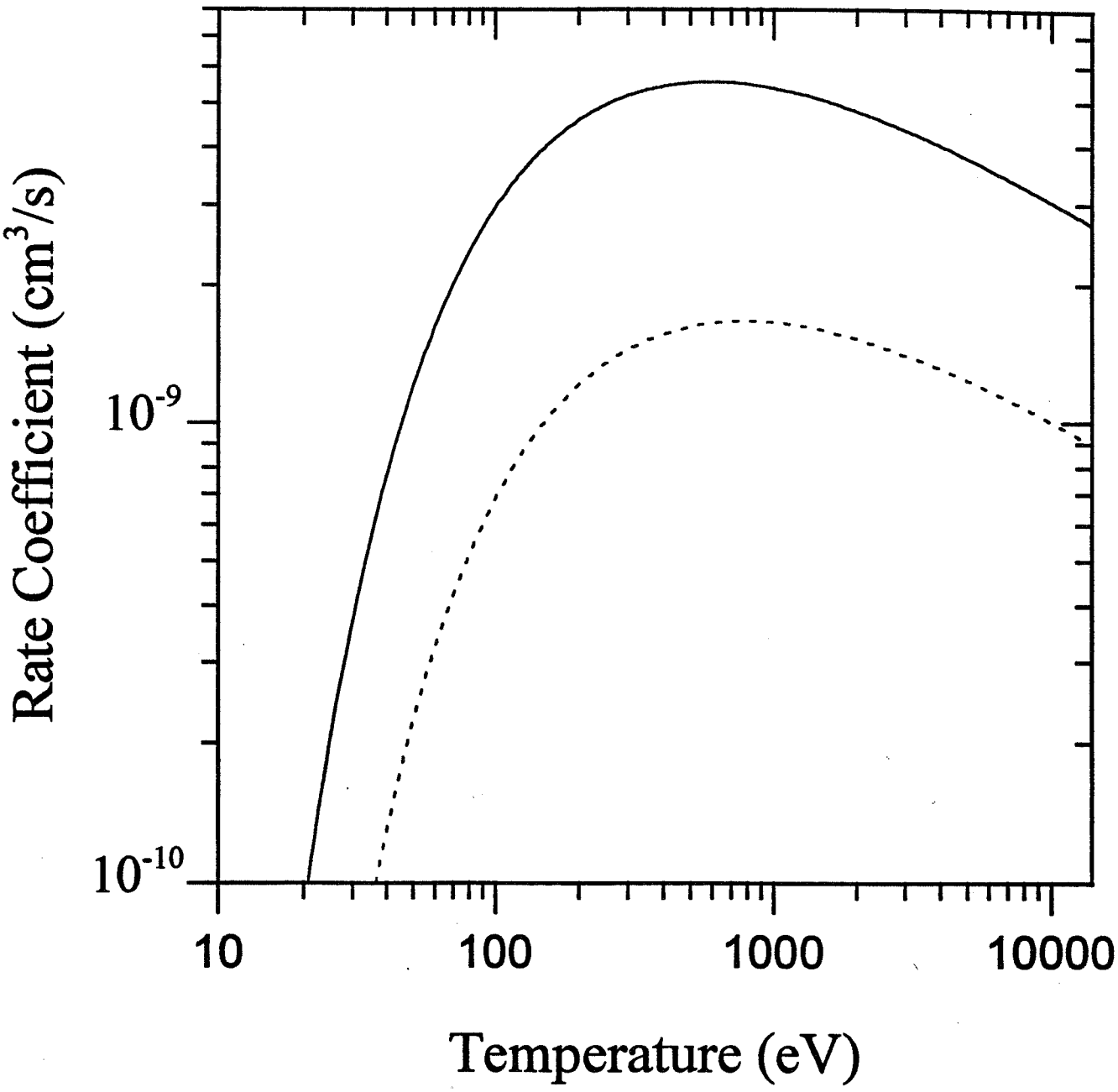

Figure 5. Electron-impact ionization of O^{3+} in the metastable term $2s2p^2\ ^4P$. Solid curve: $2s2p\ ^3P$ final term, and short-dashed curve: $2p^2\ ^3P$ final term.

REFERENCES

[1] H. P. Summers, *Atomic Data and Analysis Structure User Manual*, JET-IR(94)06.

[2] A. Burgess and M. C. Chidichimo, Mon. Not. R. Astron. Soc. **203**, 1269 (1983).

[3] M. S. Pindzola, D. C. Griffin, and C. Bottcher, in *Atomic Processes in Electron-Ion and Ion-Ion Collisions*, ed. F. Brouillard, NATO ASI B **145**, 75 (1986).

[4] D. H. Sampson, Phys. Rev. A **34**, 986 (1986).

[5] M. S. Pindzola, D. C. Griffin, and C. Bottcher, Phys. Rev. A **34**, 3668 (1986).

[6] D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A **36**, 3642 (1987).

[7] R. D. Cowan, *The Theory of Atomic Structure and Spectra*, (U. Calif. Press, 1981).

[8] C. F. Fischer, Comput. Phys. Commun. **64**, 369 (1991).

[9] P. G. Burke and K. A. Berrington, *Atomic and Molecular Processes: an R-matrix Approach*, (IOP Press, 1993).

[10] D. G. Hummer, K. A. Berrington, W. Eissner, A. K. Pradhan, H. E. Saraph, and J. A. Tully, Astron. Astrophys. **279**, 298 (1993).

[11] F. Robicheaux, T. W. Gorczyca, M. S. Pindzola, and N. R. Badnell, Phys. Rev. A **52**, 1319 (1995).

[12] T. W. Gorczyca, F. Robicheaux, M. S. Pindzola, D. C. Griffin, and N. R. Badnell, Phys. Rev. A (in press).

[13] W. Eissner, M. Jones, and H. Nussbaumer, Comput. Phys. Commun. **8**, 270 (1974).

[14] N. R. Badnell, J. Phys. B **19**, 3827 (1986).

[15] D. H. Crandall, R. A. Phaneuf, and D. C. Gregory, *Electron Impact Ionization of Multicharged Ions*, ORNL/TM-7020 (1979).

[16] D. C. Griffin and M. S. Pindzola, J. Phys. B **21**, 3253 (1988).