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PHYSICAL REVIEW A VOLUME 59, NUMBER 6 JUNE 1999

Reevaluation of experiments and new theoretical calculations for electron-impact excitation of C^{3+}

P. H. Janzen, L. D. Gardner, D. B. Reisenfeld,* D. W. Savin,† and J. L. Kohl
Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138

K. Bartschat
Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311

(Received 7 January 1999)

Experimental absolute-rate coefficients for electron-impact excitation of C^{3+} $(2s\ ^2S_{1/2}\rightarrow 2p\ ^2P_{1/2,3/2})$ near threshold [D. W. Savin, L. D. Gardner, D. B. Reisenfeld, A. R. Young, and J. L. Kohl, Phys. Rev. A **51**, 2162 (1995)] have been reanalyzed to include a more accurate determination of optical efficiency and revised radiometric uncertainties which reduce the total systematic uncertainty of the results. Also, new *R* matrix with pseudostates (RMPS) calculations for this transition near threshold are presented. Comparison of the RMPS results to those of simpler close-coupling calculations indicates the importance of accounting for target continuum effects. The reanalyzed results of Savin *et al.* are in excellent agreement with the RMPS calculations; comparisons are also made to other measurements of this excitation. Agreement with the RMPS results is better for fluorescence technique measurements than for electron-energy-loss measurements. [S1050-2947(99)07506-X]

PACS number(s): 34.80.Kw, 34.80.Lx

I. INTRODUCTION

Over the last quarter century, electron-impact excitation (EIE) of ions has been the subject of intense study, both experimental and theoretical, as it is the dominant mechanism for the formation of emission lines in many laboratory and astrophysical plasmas. Accurate knowledge of cross sections, and thus rate coefficients, is necessary for interpretation and modeling of the spectra of such plasmas. C^{3+} has particular importance as its EIE generated $2p\rightarrow 2s$ doublet at 155 nm is one of the most widely observed UV lines in astrophysics.

Several measurements of the electron-impact excitation cross section of C^{3+} $(2s\ ^2S_{1/2}\rightarrow 2p\ ^2P_{1/2,3/2})$ have been performed. In 1977 a crossed-beams fluorescence measurement was performed by Taylor *et al.* [1]. This measurement agrees very well with two-state close-coupling (2CC) theory [2], with later nine-state close-coupling (9CC) calculations [3,4], which agree with each other to better than 1% near threshold, and with a simpler Coulomb-Born with exchange (CBX) calculation [5], which gives values slightly larger than 2CC near threshold. Savin *et al.* [6] also used a crossed-beams fluorescence technique in 1995, reporting results that were lower: only the 9CC calculations fell within the experimental 90% confidence limits. In 1998 Bannister *et al.* [7] used a merged electron-ion-beams energy-loss technique to measure the same cross section, with the intent of resolving any discrepancy between the first two measurements. Their values are higher than CBX, although their 90% confidence limits overlap the 9CC theory. Greenwood *et al.* [8] also have measured this cross section using a merged-beams energy-loss technique; again, results are higher than CBX.

Recently, a subtle effect in a calibration technique used by Savin *et al.* was discovered that caused a small shift in the results. In addition, information about the uncertainties of calibrated photodiodes came to light allowing the total specified systematic uncertainty of this measurement to be reduced. In light of the perceived discrepancy between experimental results and the marginal agreement between the recent energy-loss experiments and 9CC theory, this paper presents reanalyzed results of Savin *et al.*, along with a 26-state *R* matrix with pseudostates (RMPS) calculation of greater sophistication than earlier calculations.

II. EXPERIMENT

The experimental apparatus and data collection techniques used by Savin *et al.* were discussed in detail in their original paper [6]; only the calibration of the optical system is relevant to this reanalysis. Briefly, an electron beam was sent across a carefully prepared C^{3+} beam at an angle of nominally 55°. The currents and shapes of both beams were measured. Photons were counted using beam chopping and synchronous detection to subtract background. A large mirror below the collision volume, which subtended slightly over π sr, concentrated photons onto a photomultiplier tube (PMT), which itself subtended ≈ 0.17 sr (see Fig. 1). The elements of the optical system were calibrated individually, and a ray-tracing code was used to determine the overall absolute photon detection efficiency of the system. The absolute quantum efficiency of the PMT was determined by referencing the PMT to a CsTe photodiode calibrated by the National Institute of Standards and Technology (NIST). In this manner an absolute rate coefficient was derived.

During the analysis of a recent $Si^{2+}(3s^2\ ^1S\rightarrow 3s3p\ ^1P)$ measurement [9], which used calibration techniques similar

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[*] Present address: Los Alamos National Laboratory, M/S-D466, Los Alamos, NM 87545.

[†] Present address: Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027.

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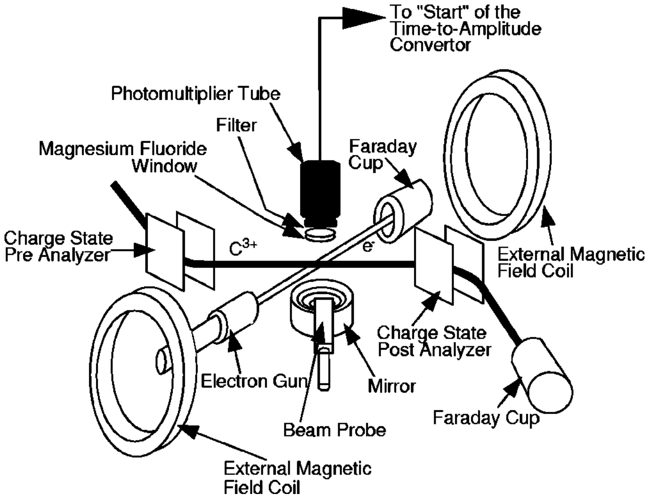

FIG. 1. Diagram of the experimental apparatus.

to those of the C^{3+} measurement, it was discovered that the analysis of the mirror calibration of Savin *et al.* had not fully accounted for multiple reflections particular to the calibration apparatus. Accounting for these reflections yields a mirror reflectivity 6% lower than that used by Savin *et al.* in their data reduction. All measured rate coefficients and statistical uncertainties then increase correspondingly. This correction is three times larger than the 90% confidence level assigned by Savin *et al.* to mirror reflectance uncertainty, and, therefore, it is not taken into account by their systematic error bars.

A separate matter in this reanalysis stems from the leading contribution to the total experimental uncertainty: the uncertainty in the absolute efficiency of the NIST-calibrated photodiode. The photodiode efficiency calibration immediately preceding the C^{3+} EIE measurement had a quoted uncertainty around 155 nm of 6% ''probable error,'' which was taken to be 15% at a confidence level considered to be equivalent to a statistical 90% confidence level. However, by the time of the follow-up photodiode calibration, NIST quoted an uncertainty of 9% at 2σ at the same wavelength. The reduction in uncertainty came largely from a reevaluation of the methodology used at NIST for assigning calibration uncertainties, rather than from changes in the calibration technique itself [10]. Therefore, it seems appropriate to use the more recent uncertainty value, along with an additional 0.5% to cover the 1% drop in the photodiode efficiency between calibrations. This reduces the total systematic uncertainty of the experiment from 26% to 22% (see Table I).

The reanalyzed C^{3+} $(2s\rightarrow 2p)$ data are listed in Table II and plotted in Fig. 2. Although the results were originally reported as rate coefficients $\langle v\sigma\rangle$ convolved over the experimental energy spread [a Gaussian with a full width at half maximum (FWHM) of 1.74 ± 0.37 eV], they are reported here as cross sections $\langle v\sigma\rangle/\langle v\rangle$ as well, in keeping with current convention. The error bars on the circles in Fig. 2 and the uncertainties quoted in Table II represent the statistical uncertainty at the 90% confidence level (1.65σ). The total experimental uncertainty $(\pm 23\%)$ is shown by the large error bar on the 10.10-eV data point in Fig. 2.

III. THEORY

The numerical calculations performed for this paper are based on the nonrelativistic *R*-matrix (close-coupling) approach. In addition to standard 2-state and 9-state calculations that were carried out for comparison with earlier work [2–4], the RMPS method was employed in order to account for coupling between both discrete and continuum parts of

TABLE I. Summary of systematic uncertainties. All uncertainties are quoted at a confidence level considered to be equivalent to a statistical 90% confidence level. Sources of uncertainty not discussed in this paper are discussed in the original paper by Savin *et al.* [6].

Sources of Uncertainty	Uncertainty
Uncertainty in beam densities	
aperture area of the ion probe	7%
ion-beam probe biasing procedure	2%
correction factor for O^{4+} contamination	1%
aperture area of the electron probe	4%
electron-beam probe biasing procedure	8%
Uncertainties in beams' geometric-overlap/ detection-efficiency factor	
spatial coordinates of the collision volume	5%
ion source fluctuations	4%
electron spiraling	8%
$C^{3+}(2p\ ^2P)$ lifetime	2%
computational error in overlap determination	1%
radiometric calibration	
NIST standard photodiode accuracy	7%
photodiode calibration variation	1%
PMT photocathode response map	9%
mirror reflectance	3%
crystalline quartz filter transmittance	2%
MgF_2 window transmittance	1%
computational error in ray tracing	1%
Uncertainty from normalizing the nonabsolute EIE data	10%
Total quadrature sum [a]	22%

[a] Total experimental uncertainty (in %) = $[22^2+(90\%\ \text{statistical uncertainty})^2]^{1/2}$.

TABLE II. Absolute C^{3+} $(2s\ ^2S\rightarrow 2p\ ^2P)$ electron-impact excitation results. Statistical uncertainty is given in parentheses at 1.65σ and does not include systematic uncertainty.

Energy (eV)	Rate coefficient $(10^{-8}\ cm^3\ s^{-1})$	Cross section $(10^{-16}\ cm^2)$
5.79	-0.12 (0.23)	-0.08 (0.16)
7.09	1.04 (0.21)	0.66 (0.13)
7.46	2.27 (0.37)	1.40 (0.23)
7.71	3.32 (0.64)	2.02 (0.39)
8.16	5.51 (0.40)	3.25 (0.24)
8.84	8.07 (0.84)	4.58 (0.48)
9.07	7.80 (0.35)	4.37 (0.20)
10.00	8.59 (0.50)	4.58 (0.27)
10.10	8.29 (0.63)	4.40 (0.33)
11.22	7.52 (0.53)	3.79 (0.27)
12.04	8.19 (0.51)	3.98 (0.25)

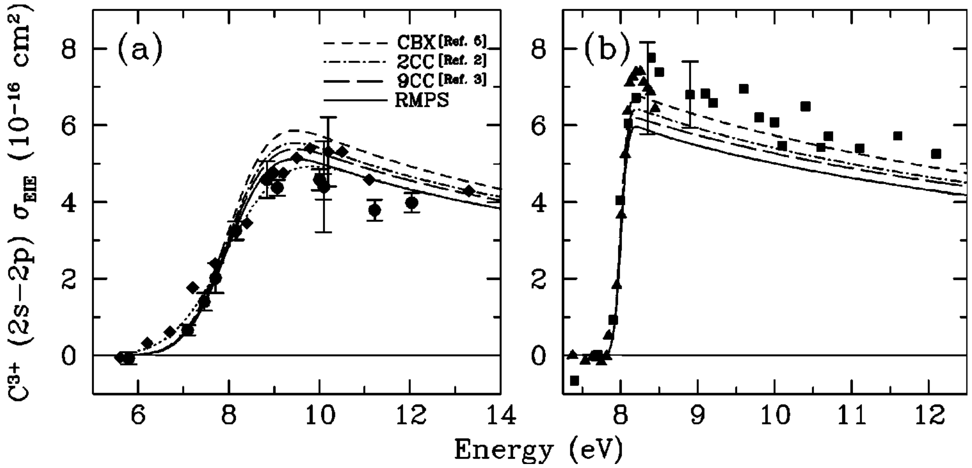

FIG. 2. Absolute C^{3+} $(2s\ ^2S \rightarrow 2p\ ^2P)$ electron-impact excitation cross sections. The circles in (a) are the reevaluated results of Savin *et al.* Error bars represent statistical uncertainty at the 90% confidence level, except for the large error bar on the 10.10-eV data point, which represents the total experimental uncertainty at a confidence level that is considered to be equivalent to a statistical 90% confidence level. The diamonds in (a) are from Taylor *et al.* [1,20]; the triangles and squares in (b) are the results of Bannister *et al.* [7] and Greenwood *et al.* [8], respectively. Error bars shown for these experiments represent the typical total uncertainties at a 90% confidence level. Four theoretical calculations are also presented, convolved with the experimental energy spreads [a 1.74-eV FWHM Gaussian in (a) and a 0.17-eV FWHM Gaussian in (b)]. Also in (a), the RMPS theory has been convolved with the 2.3-eV FWHM spread of Taylor *et al.* for a better comparison near threshold; this is shown by the dotted line.

the target spectrum. The RMPS calculation was very similar to the corresponding work on the Be^{+} [11] and B^{2+} [12] targets described before, and hence, we give only a very brief summary here.

To begin with, the Hartree-Fock orbitals $1s$-$4s$, $2p$-$4p$, $3d$-$4d$, and $4f$ were used to construct the lowest nine physical $(1s^2 n\ell)^2L$ states of the C^{3+} target. In addition, pseudoorbitals $\overline{n\ell}$ (up to $\overline{9}s$, $\overline{8}p$, $\overline{8}d$, and $\overline{7}f$) were constructed by taking the minimum linear combination of Sturmian-type orbitals $r^i e^{-\alpha r}$ orthogonal to the above-mentioned orbitals. The pseudostates were then obtained through diagonalization of the target Hamiltonian. Since we were interested in results for electron-impact excitation of the resonance $(2s \rightarrow 2p)$ transition, which are relatively insensitive to minor changes in the choice of α, we set $\alpha = 1.5$ in order to produce one pseudostate with negative energy per total target angular momentum, with the remaining pseudostates lying in the target continuum. All states could be fit into an R-matrix box of radius $20\,a_0$, and 25 basis functions per angular momentum of the projectile electron were sufficient to produce converged results for total collision energies up to 20 eV.

One indication about the quality of the target description can be obtained by investigating the theoretical results for the oscillator strength in both the length and the velocity forms of the dipole operator. In the present calculations, we obtained values of 0.292 and 0.322, respectively, essentially independent of the number of states included. This is not surprising, since the $2p$ orbital was optimized on the energy of the $^2P^o$ state while the core orbitals were kept fixed. Despite the remaining difference between the length and velocity results, we judge the target description to be sufficiently accurate, since the length form (which is generally preferred in such optimization procedures) predicts an A value of 2.75×10^8/s, in very good agreement with the experimental result of $(2.71 \pm 0.07) \times 10^8$/s obtained by Knystautas *et al.* [13] and also in other measurements. (A list of additional references can be found in Savin *et al.* [6].)

IV. DISCUSSION

Experimental data and theoretical calculations are shown in Fig. 2. Care must be taken to convolve the theory with the energy spread of each experiment for a valid comparison. The new RMPS values fall slightly below the 9CC results which, in turn, lie below the 2CC predictions. This trend of lowering the 9CC predictions by approximately 2–5% is not unexpected, since it was also seen in the corresponding work on Be^{+} [11] and B^{2+} [12]. Note that our 2CC and 9CC results agree very well with those of Refs. [2–4]. We believe that the RMPS results represent the most reliable theoretical predictions for the collision part of the problem; the structure results for this and simpler models such as CBX, 2CC, and 9CC are apparently very similar. If results from simpler models should indeed lie closer to experiment, this would be somewhat fortuitous. The reanalyzed results of Savin *et al.* and the measurement of Taylor *et al.* are in excellent agreement with the RMPS calculations. Although the RMPS theory agrees with the measurement of Bannister *et al.* within their 90% absolute error bars, the agreement is not as good as with either of the fluorescence technique measurements. Agreement with the energy-loss measurement of Greenwood *et al.* is, for the most part, outside their 90% absolute error bars.

The reanalysis of the Savin *et al.* EIE measurement also applies to the dielectronic recombination (DR) measurement using the same apparatus [14]. This measured absolute DR rate in an external electric field of $11.4 \pm 0.9(1\sigma)$ V cm^{-1}

goes from $(2.76\pm0.75)\times10^{-10}$ cm^3 s^{-1} to $(2.94\pm0.76)\times10^{-10}$ cm^3 s^{-1}, where the total experimental uncertainty is quoted at 1 σ. Thus the measurement no longer agrees as well with theory. The source of the discrepancy between these measurements and field-enhanced DR calculations [15–17] may be due to the presence of crossed electric and magnetic fields in the interaction region of the experiment [18,19].

ACKNOWLEDGMENTS

This work was supported by NASA Supporting Research and Technology Program in Solar Physics Grant Nos. NAGW-1687 and NAG5-5059, and by the Smithsonian Astrophysical Observatory. This paper was also supported by the National Science Foundation under Grant No. PHY-9605124 (KB).

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[1] P. O. Taylor, D. Gregory, G. H. Dunn, R. A. Phaneuf, and D. H. Crandall, Phys. Rev. Lett. **39**, 1256 (1977).
[2] J. N. Gau and R. J. W. Henry, Phys. Rev. A **16**, 986 (1977).
[3] V. M. Burke, J. Phys. B **25**, 4917 (1992).
[4] A. K. Pradhan (private communication).
[5] N. H. Magee, Jr., J. B. Mann, A. L. Merts, W. D. Robb, Los Alamos Scientific Laboratory Report No. LA-6691-MS, 1977 (unpublished).
[6] D. W. Savin, L. D. Gardner, D. B. Reisenfeld, A. R. Young, and J. L. Kohl, Phys. Rev. A **51**, 2162 (1995).
[7] M. E. Bannister, Y.-S. Chung, N. Djuric, B. Wallbank, O. Woitke, S. Zhou, G. H. Dunn, and A. C. H. Smith, Phys. Rev. A **57**, 278 (1998).
[8] J. B. Greenwood, S. J. Smith, A. Chutjian, and E. Pollack, Phys. Rev. A **59**, 1348 (1999).
[9] D. B. Reisenfeld, L. D. Gardner, P. H. Janzen, D. W. Savin, and J. L. Kohl (unpublished).
[10] L. R. Canfield (private communication).
[11] K. Bartschat and I. Bray, J. Phys. B **30**, L109 (1997).
[12] P. J. Marchalant, K. Bartschat, and I. Bray, J. Phys. B **30**, L435 (1997).
[13] E. J. Knystautas, L. Barette, B. Neveu, and R. Drouin, J. Quant. Spectrosc. Radiat. Transf. **11**, 75 (1971).
[14] D. W. Savin, L. D. Gardner, D. B. Reisenfeld, A. R. Young, and J. L. Kohl, Phys. Rev. A **53**, 280 (1996).
[15] D. J. McLaughlin and Y. Hahn, Phys. Rev. A **27**, 1389 (1983).
[16] K. J. LaGattuta, J. Phys. B **18**, L467 (1985).
[17] D. C. Griffin, M. S. Pindzola, and C. Bottcher, Phys. Rev. A **33**, 3124 (1986).
[18] F. Robicheaux and M. S. Pindzola, Phys. Rev. Lett. **79**, 2237 (1997).
[19] D. C. Griffin, F. Robicheaux, and M. S. Pindzola, Phys. Rev. A **57**, 2708 (1998).
[20] D. Gregory, G. H. Dunn, R. A. Phaneuf, and D. H. Crandall, Phys. Rev. A **20**, 410 (1979).