# Absolute cross sections for near-threshold electron-impact excitation of the dipole-allowed transitions $3s^{21}S \rightarrow 3s^{3}p^{1}P$ in $Cl^{5+}$ and $3s^{2}S \rightarrow 3p^{2}P$ in $Cl^{6+}$

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Experimental and theoretical cross sections for electron-impact excitation of the dipole-allowed transitions  $3s^{2} {}^{1}S \rightarrow 3s^{2}p^{1}P$  in  $Cl^{5+}$  and  $3s^{2}S \rightarrow 3p^{2}P$  in  $Cl^{6+}$  near the excitation thresholds are reported. Absolute cross sections are measured using the merged electron-ion beams energy-loss technique. The intermediate-coupling frame-transformation *R*-matrix method is used to obtain theoretical cross sections. The total cross sections, for the transitions studied in both ions, exhibit resonance structures near threshold. There is excellent agreement between theory and experiment with respect to both the shape and the magnitude of the cross section for the  $3s^{2}S \rightarrow 3p^{2}P$  transition in  $Cl^{6+}$ . For  $Cl^{5+}$ , structures and trends in both the present *R*-matrix calculation and the previous calculation of Baluja and Mohan [J. Phys. B **20**, 831 (1987)] agree well with the experimental results. However, the magnitudes of the theoretical cross sections for  $Cl^{5+}$  are significantly smaller than the measured cross section, which has been corrected for metastable contamination.

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# I. INTRODUCTION

Data for the electron-impact excitation of positive ions are necessary to model and diagnose high-temperature plasmas important in controlled-fusion research [1,2] and astrophysics [3]. Multiply charged ions occur in these environments and it is important to have knowledge of collision cross sections for the analysis and diagnostics of such plasmas. Most of the existing data for electron-impact excitation of positive ions come from theoretical calculations. Absolute experimental measurements are needed to provide tests of the theoretical methods.

We have previously reported on experimental cross section measurements for the dipole-allowed transitions in a few Na-like and Mg-like ions [4–7]. Here we present measurements and calculations of the excitation cross sections for the  $3s^{2} {}^{1}S \rightarrow 3s^{3}p {}^{1}P$  transition in Mg-like Cl<sup>5+</sup> and the  $3s {}^{2}S \rightarrow 3p {}^{2}P$  excitation of Na-like Cl<sup>6+</sup>.

Electron-impact excitation of atoms and ions can occur through both direct excitation and the indirect process of dielectronic capture of the incident electron into a doubly excited state, followed by autoionization to an excited state. For example, in  $Cl^{5+}$ , the processes that will contribute to the  $3s \rightarrow 3p$  excitation may be schematically represented as

$$e + \operatorname{Cl}^{5+}(3s^2) \rightarrow \operatorname{Cl}^{5+}(3s3p) + e,$$
  
 $e + \operatorname{Cl}^{5+}(3s^2) \rightarrow \operatorname{Cl}^{5+}(3snln'l') \rightarrow \operatorname{Cl}^{5+}(3s3p) + e.$  (1)

However, these processes are not independent, and the effects of the interactions between the various resonant states of the recombined ion as well as interference between the indirect and direct mechanisms are important, especially in lower-charge-state ions. These effects are included in any close-coupling calculation. For highly charged ions, these processes have been treated accurately using an independent processes approximation, in combination with the distortedwave method [8]. Although usually not so dominant as in the case of optically forbidden transitions, resonances may also be important for certain dipole-allowed transitions. We shall see that resonance structures appear in the near-threshold region of the excitation cross sections for both the ions studied here.

# **II. EXPERIMENTAL TECHNIQUE**

We have used the JILA/ORNL merged electron-ion beams energy-loss (MEIBEL) apparatus [9] for our experiment. The MEIBEL apparatus is designed to detect electrons that have lost most of their energy during inelastic collisions with ions. The ions were produced from CCl<sub>4</sub> gas in the ORNL Caprice electron-cyclotron resonance ion source, extracted and accelerated through about 15-kV potential, mass-to-charge analyzed, and directed into the MEIBEL apparatus. Since  ${}^{35}Cl^{5+}$  has the same mass-to-charge ratio as  ${}^{14}N^{2+}$ , the cross sections were measured using the  ${}^{37}Cl^{5+}$  isotope.

The MEIBEL apparatus shown in Fig. 1 is immersed in a uniform magnetic field ( $\sim 3$  mT) parallel to the direction of the incident ion beam. The merger, consisting of a pair of parallel plates producing a transverse electric field, is used to merge the electron beam with the ion beam. The electrons are produced in a dispenser-cathode electron gun, and initially they travel parallel to the ion beam. In the merger with crossed **E** and **B** fields ( $\mathbf{E} \times \mathbf{B}$ ), the electron motion is tro-



FIG. 1. Schematic view of the JILA/ORNL merged electron-ion beam energy-loss (MEIBEL) apparatus. The apparatus is immersed in a uniform magnetic field (in the z direction) and consists of three main units: merger, interaction region, and demerger.

The demerger also consists of a pair of parallel plates with a transverse electric field, and it disperses electrons according to their velocity component parallel to the **B** field. Thus, electrons that have lost energy in inelastic collisions with ions will be deflected at greater angles and directed onto a position sensitive detector (PSD). The PSD consists of a pair of microchannel plates and a resistive anode. The efficiency of the PSD was measured to be  $0.55\pm0.02$ , by alternately directing an electron beam ( $\sim 10^{-14}$  A) onto the detector and into a Faraday cup connected to a vibrating reed electrometer. The primary electron beam and electrons elastically scattered in the forward direction are deflected less by the E and **B** fields toward a Faraday cup. Electrons that are elastically scattered from ions at large angles may have the same range of longitudinal velocities as the inelastically scattered electrons, and thus could in principle reach the detector, causing an overestimate of the cross section. This is prevented by a set of five apertures mounted at the demerger entrance. Trajectory modeling [10] is used to verify that the apertures block elastically scattered electrons that would otherwise reach the detector. The ion beam is not significantly affected by the two fields; after continuing through the demerger it is deflected by 90° before reaching the ion Faraday cup.

A video beam probe [11] is inserted into the interaction region, and the xy beam density distributions are recorded at distinct positions (usually seven) as the probe is moved along the z direction. These data are used to compute the beam overlap as discussed below.

## A. Data

The relationship between the excitation cross section at the interaction energy in the center-of-mass (c.m.) system,  $E_{\rm c.m.}$ , with experimentally measured parameters is given by the well-known equation [12]

$$\sigma(E_{\text{c.m.}}) = \frac{Rqe^2}{\varepsilon I_e I_i} \left| \frac{v_e v_i}{v_e - v_i} \right| F, \qquad (2)$$

where *R* is the signal count rate of the inelastically scattered electrons;  $\varepsilon$  is the measured PSD efficiency;  $v_e$ ,  $v_i$ ,  $I_e$ , and  $I_i$  are laboratory velocities and currents of the electrons and ions of charge *e* and *qe*, respectively; and *F* is the form factor that represents the overlap of the two beams. The form factor *F* is given by

$$F = \frac{\int G(x,y,z)dxdy \int H(x,y,z)dxdy}{\int G(x,y,z)H(x,y,z)dxdydz},$$
(3)

where z is the direction of the magnetic field. As noted above, the current densities of the two beams G(x,y,z) and H(x,y,z) are measured using a two-dimensional video probe.

Despite careful tuning of both beams and residual pressure on the order of  $10^{-8}$  Pa, the signal collected at the PSD is accompanied by high background counts coming from both beams scattering from residual gas and surfaces. To extract the signal *R* coming from the inelastically scattered electrons in the studied transition, both beams are chopped in a phased four-way sequence. The counts from the PSD are directed to a position sensitive computer and further into four histogram memories. The signal spectrum is extracted by the appropriate subtraction and addition of the outputs of the four channels.

Typically, the data taking procedure starts with setting the laboratory energy of the electrons for the chosen ion energy, using the relation

$$E_{\text{c.m.}} = \mu \left[ \sqrt{\frac{E_e}{m_e}} - \sqrt{\frac{E_i}{m_i}} \right]^2, \tag{4}$$

where  $E_e$  and  $E_i$  are the laboratory energies of electrons and ions of mass  $m_e$  and  $m_i$ , respectively, and  $\mu$  is the reduced mass.

The next (and very tedious) step is to tune both beams to achieve minimum backgrounds, consistent with adequate beam overlaps. The goal is to make the beams overlap reasonably well in the interaction region and not overlap within and after the demerger apertures. This configuration prevents the production of a spurious signal at the detector from elastically scattered electrons (through large angle elastic scattering). Profiles of the two beams are then measured and the form factor is calculated. At this point, data taking starts and continues until the required statistical precision is obtained. The next c.m. energy is then set by scaling the voltages applied to the electrodes of the electron gun, the merger and the demerger, and the magnetic field for the new laboratory energy of electrons. The c.m. energy is changed by only a few percent in order to keep the same electron configuration, so that the determination of beam profiles for each data point is not necessary. This process continues until the cross section has been measured over a certain range of  $E_{c.m.}$ , when the form factor is again measured. The procedure is repeated several times over the energy region of interest, and the results are averaged for each energy.

#### B. Adjustments to data

### 1. Center-of-mass energy

In order to establish the absolute electron energy scale and also to compare theoretical data with experiment, we must determine the effective distribution of energies in the interaction region. Because of the Coulomb field in electron-ion collisions, the cross section for excitation is finite at threshold. For dipole-allowed transitions without strong resonant contributions, this often results in a near-step-function behavior of the cross section at threshold. Then, the adopted procedure [5,6] is to fit experimental data with a convolution of a Gaussian energy distribution of variable width, with a step function at the spectroscopic threshold value. In such cases, we have consistently found effective energy distributions between 0.18 and 0.20 eV. In the present case, resonances play a prominent role in the cross section near threshold, so this fitting routine is not appropriate. In order to compare theoretical calculations with experiments, we have used a Gaussian distribution of 0.18 eV full width at half maximum (FWHM), as has been employed in other recent measurements [13]. The energy has been shifted to agree with the spectroscopic threshold value.

#### 2. Below-threshold spurious signal

In all our experiments, we observed a spurious signal below each investigated threshold, which is probably due to the effect of space charge of one beam on the background of the other beam. Fortunately, this spurious signal of about 10% of maximum cross sections appeared to be constant with both energy and the time necessary for stepping through the relatively small threshold energy range; therefore its value could be subtracted from the measured cross sections.

#### 3. Path length

In evaluating the form factor F in Eq. (3), the geometric length of the merge path was used for integration over z.

However, if the electrons have any transverse velocity  $(v_t)$  upon exiting the merger, they will undergo helical trajectories about the **B** field (with radius  $r_e = mv_t/eB$ ) while in the interaction region. Thus, the collision path length is slightly lengthened, and the apparent measured cross section is slightly too large. However, the increase of the collision path length is only about 0.1% for the present experimental conditions, and therefore no correction to the data was applied.

#### 4. Backscattering

At the threshold energy for a given excitation and at electron energies just above the threshold, all inelastically scattered electrons travel in a forward direction in the laboratory frame. But, as the energy increases above threshold to the point that scattered electrons have velocity greater than the ion velocity, electrons scattered backward in the c.m. frame will also be traveling backwards in the laboratory frame and will not proceed to the PSD. Trajectory modeling [10] is used, as described in our earlier publications [5,9], to calculate and to correct for these losses. As corrections greater than 10% were considered to be unacceptable, backscattering limits the energy range of the experiment.

### 5. Metastable ions

In our previous work with Mg-like ions [6,7], we found that the ion beam consisted of ground state ions and a significant fraction of metastable ions in the 3s3p <sup>3</sup> $P_0$  and <sup>3</sup> $P_2$ states. Thus, we expected that the Cl<sup>5+</sup> ion beam would also be a mixture of ions in the ground and metastable states. In order to determine the metastable content, the  $Cl^{5+}$  ion beam was redirected into the ORNL crossed-beams apparatus used for electron-impact ionization measurements [14]. With metastable ions in the beam, one observes an ionization signal first at the threshold for ionizing metastables, then a second rise when ionization from the ground state is energetically possible. The ionization cross sections are first measured between 97.5 and 200.0 eV (Fig. 2 solid square points). Thus, by extrapolating the signal (apparent cross section) at low energy to the abscissa, we could determine the apparent threshold for ground state ionization with a spectroscopic value of 97.03 eV [15]. Data were then taken at only three c.m. energies: 80.0 eV, below the threshold for ionization from the metastable state; 91.0 eV, where there is a contribution only from the 3p electron of the metastable state; and 180.0 eV, where the mixed-state beam is contributing to the measured ionization cross section. This procedure was adopted to achieve the best possible statistical precision in a reasonable measurement time ( $\sim 30$  h), since the apparent ionization cross section of the 3p from the metastable initial state ions is only about  $10^{-19}$  cm<sup>2</sup>. To obtain the metastable-to-ground fraction we used the semiempirical single parameter Lotz formula [16] for the ionization from the metastable state and then from the ground state. The fitting procedure included spectroscopic ionization thresholds, as required by the Lotz formula, and an adjustable parameter for the metastable fraction  $f_m$ . The parameter  $f_m$ was adjusted until the ratio of cross sections at 91.0 eV and 180.0 eV agreed with the measured ratio. Thus, the assump-



FIG. 2. Electron-impact ionization cross sections for  $Cl^{5+}$  to determine the apparent ground state fraction in the target beam (see text).  $\blacksquare$ , absolute data measured between 97.5 and 200 eV;  $\blacktriangle$ , absolute data measured at three points with better statistical precision. The solid curve is from the single parameter Lotz [16] formula with an adjustable parameter  $f_m$  to make the ratio of values at 91.0 eV and 180.0 eV agree with the measured ratio, and then multiplied by 0.61 to agree with our absolute ionization measurements. Relative uncertainties, represented by the error bars, are at  $1\sigma$  C.L.

tion in this procedure is that the Lotz formula gives correct relative values from different electron subshells, even though the overall magnitude may be somewhat in error. The curve plotted in Fig. 2 has been multiplied by 0.61 so that the agreement of the Lotz and the measured ratios can be seen from the plot. The metastable fraction thereby determined from ionization data was  $0.23\pm0.12$ . The ground state fraction is then  $0.77\pm0.12$ , and a multiplicative correction of 1.30 is applied to the measured excitation cross section to give the cross section from the  $3s^{2} \, {}^{1}S$  ground state. An additional uncertainty in the absolute value of the cross section is incorporated in the total uncertainty quoted in Sec. IV. In the case of the Na-like Cl<sup>6+</sup> ion, no metastable ions should be present.

#### **III. THEORETICAL CALCULATIONS**

The accuracy of theoretical calculations for electronimpact excitation depends critically on the description of the target orbitals, as well as the states included in the closecoupling expansion and the details of the scattering calculation. For both ions, the multiconfiguration Hartree-Fock programs of Froese-Fischer [17] were used to generate the bound orbitals. In the case of Na-like  $Cl^{6+}$ , the target description was relatively simple; it included the 3*s* ground state and the 3*p*, 3*d*, 4*s*, 4*p*, 4*d*, and 4*f* excited states. The 1*s*, 2*s*, 2*p*, and 3*s* orbitals were generated from a Hartree-Fock (HF) calculation for the 3*s* ground state, while the 3*p*, 3*d*, 4*s*, 4*p*, 4*d*, and 4*f* orbitals were generated from a frozen-core HF calculation on the *nl* excited states. All seven terms and 12 levels resulting from these calculations were included in the close-coupling expansion for the scattering calculation and had energies within 0.5% of the spectroscopic values [15]. In addition, radiative rates calculated in the length and velocity gauges for all dipole-allowed transitions were in good agreement.

The target description for Mg-like Cl<sup>5+</sup> required a significantly more elaborate configuration-interaction expansion. It included all even-parity levels originating from the  $3s^2$ ,  $3p^2$ , 3s3d,  $3d^2$ , 3s4s, 3s4d, 3p4p,  $4s^2$ ,  $4p^2$ ,  $4d^2$ , 3s5s, 3s5d, 3p5p,  $5s^2$ ,  $5p^2$ , and  $5d^2$  configurations and the oddparity levels originating from 3s3p, 3p3d, 3p4s, 3p4d, 3p5s, and 3p5d. The 1s, 2s, 2p, 3s, and 3p orbitals were generated from a configuration-average Hartree-Fock (CAHF) calculation for the 3s3p configuration. The 3d, 4s, 4p, and 4d orbitals were generated from frozen-core CAHF calculations for the 3snl configurations. Finally, the 5s, 5p, and 5d were pseudo-orbitals, generated from multiconfiguration Hartree-Fock calculations designed to improve the description of both the  $3s^{2} {}^{1}S$  ground term and  $3s3p {}^{1}P$  term. Breit-Pauli configuration-interaction expansions involving these 16 even-parity configurations and six odd-parity configurations yielded energy levels in good agreement with spectroscopic energies. Spectroscopic energies exist for 32 levels of the 36 arising from the 20 terms included in the close-coupling expansion discussed below; of these, 29 were within 1% of the spectroscopic values. The exceptions were the  $3s3p {}^{1}P_{1}$ ,  $3p^{2} {}^{1}S_{0}$ , and  $3p3d {}^{1}P_{1}$  levels for which the average deviation from the spectroscopic energies, were 1.7%, 1.2%, and 5.4%, respectively. In addition, the length and velocity radiative rates for the stronger dipole-allowed transitions were in good agreement; for example, for the important  $3s3p^{1}P_{1} \rightarrow 3s^{2} {}^{1}S_{0}$  radiative transition, they agreed within 1.5%.

The scattering calculations for Cl<sup>5+</sup> and Cl<sup>6+</sup> were performed using the intermediate-coupling frametransformation (ICFT) *R*-matrix method [18]. With the ICFT method, one first employs multichannel quantum-defect theory (MODT) to generate unphysical K matrices in pure LS coupling [19]. These matrices are then transformed to intermediate coupling using term-coupling coefficients, and finally the physical K matrices are determined from the unphysical K matrices and the level energies using MQDT. This method has been shown to yield results in excellent agreement with a full Breit-Pauli R-matrix calculation [18,20].

In the case of  $\text{Cl}^{5+}$ , the 20 terms arising from the configurations  $3s^2$ , 3s3p,  $3p^2$ , 3s3d, 3p3d, 3s4s, 3s4p, and 3s4d were included in the close-coupling expansion for the *LS* portion of the calculation. In order to improve the accuracy of the scattering calculation, the theoretical energies were adjusted to the spectroscopic values, where known. The size of the *R*-matrix box was 11.3 a.u. and we used 15 basis orbitals to represent the continuum for each value of the angular momentum. All *LSII* partial waves from *L*=0 to 20 were included in the partial-wave expansion, which is more than enough to assure convergence for the energies considered here.

With  $Cl^{6+}$ , the seven terms mentioned above were included in the close-coupling expansion for the *LS* portion of the calculation; however, the agreement between the spectro-



FIG. 3. Cross section for the  $3s^{2} {}^{1}S \rightarrow 3s 3p {}^{1}P$  electron-impact excitation in Cl<sup>5+</sup> as a function of the c.m. energy. The absolute measurements, corrected for metastable contamination, are shown as solid points. Relative uncertainties, represented by the error bars, are at  $1\sigma$  C.L. The total expanded uncertainty at the 90% C.L. is shown by the bold error bar at 19.46 eV. The theoretical results are convoluted with a 0.18 eV FWHM Gaussian energy distribution. The present 20-term, 36-level ICFT *R*-matrix results are shown by the solid line. The dotted line is from the 11-term *LS R*-matrix calculation of Baluja and Mohan [22].

scopic and theoretical energies was sufficiently good in this ion that no adjustment of the theoretical energies was needed. The size of the *R*-matrix box was 9.7 a.u., and we again used 15 basis orbitals to represent the continuum for each value of the angular momentum, and all partial waves from L=0 to 20 were included.

#### **IV. RESULTS AND DISCUSSION**

Excitation cross sections, deduced from the measurements using Eq. (2) and the adjustments as described above, for the  $3s^2 \stackrel{i}{I}S \rightarrow 3s 3p \stackrel{1}{P}$  in  $Cl^{5+}$  and  $3s \stackrel{2}{S} \rightarrow 3p \stackrel{2}{P}$  transitions in Cl<sup>6+</sup> versus the center-of-mass interaction energy are plotted in Figs. 3 and 4, respectively. The energy range of the measurements (about 1.5 eV above thresholds for these transitions) was limited by the backscattering of electrons, as discussed previously. The points represent average experimental values, and the error bars display relative uncertainties (quadrature sum of statistical uncertainties and uncertainties due to trajectory modeling corrections) at the one standard deviation  $(1\sigma)$  level. The combined absolute uncertainty [21] U of the cross section at the 90% confidence level (C.L.) is obtained from the quadrature sum of statistical and all systematic uncertainties, where both are at 90% C.L. Typical values of U are 31% for excitation of  $Cl^{5+}$  and 23% for excitation of Cl6+. Experimental results above 18.9 eV and 15.75 eV for  $Cl^{5+}$  and  $Cl^{6+}$ , respectively, have been corrected for backscattering signal losses.

Also shown in Fig. 3 are the results of the present 20term, 36-level ICFT *R*-matrix close-coupling calculation and the results of an earlier 11-term *LS* coupling *R*-matrix calcu-



FIG. 4. Cross section for the  $3s \, {}^2S \rightarrow 3p \, {}^2P$  electron-impact excitation in Cl<sup>6+</sup> as a function of the c.m. energy. The absolute measurements are shown as solid points. Relative uncertainties, represented by the error bars, are at  $1\sigma$  C.L. The total expanded uncertainty at the 90% C.L. is shown by the bold error bar at 16.05 eV. The result of the present seven-term, 12-level ICFT *R*-matrix calculation convoluted with a Gaussian energy distribution of 0.18 eV FWHM is shown as the solid line.

lation by Baluja and Mohan [22] for the  $3s^{2} {}^{1}S \rightarrow 3s 3p {}^{1}P$  in Cl<sup>5+</sup>, both convoluted with an assumed Gaussian energy distribution of 0.18 eV FWHM. In Fig. 4, we compare the experimental results for the 3s  ${}^{2}S \rightarrow 3p {}^{2}P$  excitation in Cl<sup>6+</sup> with the corresponding theoretical cross section determined from the present seven-term, 12-level ICFT *R*-matrix calculation, also convoluted with a Gaussian distribution of 0.18 eV FWHM.

# A. Results for Cl<sup>5+</sup>

The experimental absolute cross sections of the  $3s^{2}$  <sup>1</sup>S  $\rightarrow 3s3p$  <sup>1</sup>P transition in Cl<sup>5+</sup>, corrected for the metastables fraction, are plotted in Fig. 3. As seen in this figure, the result of the present 20-term calculations are below those of the earlier 11-term calculations of Baluja and Mohan. We have found that the effect of intermediate coupling included in the present ICFT R-matrix calculations had very little effect on the results. The discrepancy between these two calculations, at the 20% level, is most likely due to differences in the descriptions of the target wave functions as well as the additional terms included in the close-coupling expansion in the present calculation. However, both theoretical calculations are significantly below the measured cross sections. The disagreement between theory and experiment in the energy region between 19 and 20 eV, where the cross section is dominated by direct excitation, is especially surprising. The discrepancy in the energy range below 19 eV, where the resonances contribute significantly to the cross section, is more understandable since the magnitudes of these resonances are very sensitive to the details of the calculations (see Griffin et al. [23]). We see from this figure that, despite the differences in magnitude, the general shape of the experimental resonance feature near 18.65 eV seems to be accurately predicted by both theoretical calculations, while the resonance feature near 18.85 eV appears to be more consistent with the present calculations. The experiment on the  $Cl^{5+}$  ion was repeated twice over a period of six months with no significant difference.

In our previous electron-impact excitation studies of the dipole-allowed  $3s^{2} S \rightarrow 3s 3p P$  transition in the Mg-like ions  $Ar^{6+}$  [6] and  $Si^{2+}$  [7], the agreement of the cross sections with the theory was mixed. The experimental values [6] and the convoluted theoretical curve [24] in Ar<sup>6+</sup>, where the direct mechanism dominates, agree within 10%. For the  $3s^{2} S \rightarrow 3s 3p P$  in Si<sup>2+</sup> where the resonances make a contribution to the excitation cross-section in the near-threshold region, the agreement between the theoretical curve [24] and the MEIBEL results [7] is reasonable. However, the theoretical data are slightly smaller near threshold, have a slower drop from the peak cross section, and are slightly higher at higher energies as compared to the MEIBEL data. The present discrepancies in magnitude between the theoretical and experimental cross sections for the same transition in Cl<sup>5+</sup> are significantly larger. This is surprising since coupling effects are expected to be much less important in a five-times ionized species than they are in a doubly ionized species, so that the inclusion of more states in the closecoupling expansion for Cl<sup>5+</sup> would be expected to have very little effect on the theoretical cross section.

# B. Results for Cl<sup>6+</sup>

The experimental cross section for the dipole-allowed  $3s^2S \rightarrow 3p^2P$  excitation in  $Cl^{6+}$  and the total theoretical cross section for the transitions from the  $3s^2S_{1/2}$  ground state to the  $3p^2P_{1/2}$  and  $3p^2P_{3/2}$  excited states, determined from the present ICFT *R*-matrix calculations, are presented in Fig. 4. Again, the effects of intermediate coupling included in the ICFT method are minimal for this transition and a very similar theoretical result would be expected from an *R*-matrix calculation in pure *LS* coupling. The separation between the  $3p^2P$  states is not large enough to be resolved within the given experimental uncertainties; however, the experimental data do show changes in the threshold slope at 15.25 eV (the threshold for  $3p^2P_{1/2}$  excitation) and at 15.5

eV (the threshold for  $3p {}^{2}P_{3/2}$  excitation). The agreement between theory and experiment is good in both magnitude and shape, with the ICFT *R*-matrix prediction being lower than the experimental results by about 10%.

In our earlier work with the dipole-allowed  $3s^2S \rightarrow 3p^2P$  transition in Na-like Si<sup>3+</sup> [4] and Ar<sup>7+</sup> [5] ions, the agreement between theoretical calculations [25] and the experimental data was also found to be very good. Direct excitation dominates in these transitions, at least through the energy range of the MEIBEL measurements.

# **V. CONCLUSIONS**

Experimental and theoretical cross sections are presented for the dipole-allowed transitions  $3s^{2} S \rightarrow 3s 3p P$  in  $Cl^{5+}$ and  $3s^2S \rightarrow 3p^2P$  in Cl<sup>6+</sup>. The merged electron-ion beams energy-loss technique is used to measure absolute excitation cross sections. The same transitions are studied using the ICFT R-matrix close-coupling method. There is good agreement between our theoretical calculations and our measurements for Cl<sup>6+</sup>. In the case of Cl<sup>5+</sup>, there is reasonable agreement between the present theoretical calculation and the earlier calculation of Baluja and Mohan [22]; but there is significant disagreement between the theoretical values and experimental data for the magnitude of the cross section. The discrepancy between theory and experiment is not just in the magnitude of the resonant contributions, as has occurred in other cases. Here the discrepancy is almost as large in the energy region dominated by the direct process. Causes for this discrepancy between theory and experiment are not evident.

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