Close-coupling cross sections for electron-impact excitation of Kr^{28+}

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(Received 21 October 1988; revised manuscript received 10 April 1989)

Coupling effects among the channels for collisional excitation of $2s^22p^4$, $2s2p^5$, and $2p^6$ configurations of oxygenlike krypton have been reinvestigated and found to be small. In an earlier publication, it was reported that coupling to the $2s2p^5\,{}^3P^\circ$ state has a strong influence on the cross section $\sigma(2s^22p^4\,{}^3P \rightarrow 2p^6\,{}^1S)$. That apparent coupling is shown to be due to an inconsistency involving orthogonality and correlation functions. We solve the correct set of coupled integrodifferential equations using the NIEM, IMPACT, and RMATRIX codes. All three calculations are performed using the same atomic states and the same configurations to describe the target. We find very good agreement among the cross sections obtained from all three codes. We also calculated distorted-wave cross sections for the same set of transitions. The distorted-wave results are nearly identical to the results obtained with the close-coupling codes.

I. INTRODUCTION

In this paper we present revised cross sections for electron-impact excitation of oxygenlike krypton. In an earlier publication[1] cross sections obtained in a six-state close-coupling calculation were reported for transitions among the $n=2$ states of Kr^{28+}. Those results were calculated using NIEM,[2] a computer code which uses a noniterative integral-equation method to solve the coupled integro-differential equations that arise in the scattering problem. When we calculated cross sections for the same transitions using IMPACT,[3] a close-coupling code developed at University College London, we found significant discrepancies with the results obtained with NIEM. As a further check, we used the RMATRIX code,[4] developed at Queen's University of Belfast, to calculate cross sections for the same six-state close-coupling expansion used in the NIEM and IMPACT calculations. The RMATRIX results where in good agreement with the results computed with IMPACT. While attempting to understand the reasons for the discrepancies between the NIEM results and the results from the other codes, we carried out an independent calculation of these cross sections using NIEM. The results of the new NIEM calculation are in agreement with the results obtained with RMATRIX and IMPACT. We have subsequently found a reason for the discrepancy in the earlier NIEM results, and here we report and compare the results of all four calculations.

There have been previous comparisons of IMPACT and RMATRIX cross sections, and in a recent publication, Berrington *et al.*[5] make a detailed comparison of results obtained for the $(C^{2+}+e)$ system using these two codes. We did not set out to do a detailed comparison study here, but to our knowledge this is the first time that all three of the major close-coupling codes (NIEM, IMPACT, and RMATRIX) have been applied to the same scattering problem employing the same target states and configurations.

II. THEORETICAL BACKGROUND

NIEM, RMATRIX, and IMPACT are codes which were developed to solve the coupled integro-differential equations which must be satisfied by the $N+1$ electron wave function Ψ which describes a system consisting of an N-electron target and a free (or scattered) electron. The wave function Ψ is written as an antisymmetrized product of a target wave function ψ_i and a continuum electron wave function

$$\Psi = A \sum_i \psi_i(X)\theta_i(\bar{x}) , \tag{1}$$

where X represents the coordinates of the bound target electrons and $\bar{x}$ represents the coordinates of the continuum electron.

The free electron functions $\theta_i(x)$ are products of a radial function $F_i(r)$ and a function $\chi_i(\hat{x})$ where $\hat{x}$ represents both spin and orbital angular momentum quantum numbers for the free electron

$$\theta_i(\bar{x}) = (1/r)F_i(r)\chi_i(\hat{x}) . \tag{2}$$

Vector-coupled products Θ_i are formed from the functions $\psi_i(X)$ and $\chi_i(\hat{x})$. The radial functions $F_i(r)$ are constrained to be orthogonal to the radial functions $P_\gamma(r)$ of the bound electron when the free electron and bound electron represented by $F_i(r)$ and $P_\gamma(r)$ have the same orbital angular momentum l, i.e.,

$$\langle F_i(r)|P_\gamma(r)\rangle = 0 \quad \text{if } l_i = l_\gamma . \tag{3}$$

This necessitates the addition of functions Φ_j which have the form of bound state functions of the $N+1$ electron

system and the total wave function Ψ then is

$$\Psi = A \sum_i \Theta_i(X,\hat{x}) \frac{1}{r} F_i(r) + \sum_j c_j \Phi_j(X,\hat{x}) \ . \quad (4)$$

The close-coupling equations satisfied by the function F_i and the coefficients c_j are then obtained from a variational procedure,

$$\langle \delta\Psi | H - E | \psi \rangle = 0 \ . \quad (5)$$

The discrepancies in the earlier NIEM calculation (which will be referred to as NIEMa), stem from the orthogonality constraint imposed on the scattering orbitals [see Eq. (3)]. An inconsistency was introduced into the NIEMa calculation when the $4s$, $4p$, $4d$, and $5s$ bound states were retained in the scattering calculation even though they were not used in the description of the target. The NIEM code automatically orthogonalizes the scattered electron wave function to all of the bound orbitals with the same orbital angular momentum. However, the correlation functions Φ_j which must be added [as in Eq. (4)] were not included in the earlier NIEMa calculation. The $4s$, $4p$, $4d$, and $5s$ orbitals were left out of the target description in the newer NIEM calculation, and from the IMPACT and RMATRIX calculations as well.

We give the following example in order to illustrate the potential effect of the orthogonality constraint. Consider the case of an electron scattered by an oxygenlike ion in its ground state which is represented by the $2p^4(^3P)$ configuration. If the scattered electron has orbital angular momentum $l=2$, the total wave function of target ion and scattered electron can have ^2D symmetry, and we may represent this by

$$\Psi = 2p^4(^3P)kd \ . \quad (6)$$

In general one would expect part of kd to be in the space spanned by $3d$ and $4d$, i.e.,

$$kd = \bar{k}\,\bar{d} + b_1 3d + b_2 4d \ . \quad (7)$$

Then the total wave function is

$$\Psi = 2p^4(^3P)\bar{k}\,\bar{d} + [b_1 2p^4(^3P)3d + b_2 2p^4(^3P)4d] \ . \quad (8)$$

Orthogonalization of $\bar{k}\,\bar{d}$ to $3d$ and $4d$ implies that kd is projected out of the space spanned by $3d$ and $4d$. Imposition of this orthogonality constraint excludes the terms in brackets in Eq. (8) from the total wave function. This exclusion can be corrected by adding terms of the type $2p^4(^3P)3d$ and $2p^4(^3P)4d$ in Eq. (6) [as is done in Eq. (4)]. In the NIEMa calculation reported in Ref. 1, correlation functions associated with the $4s$, $4p$, $4d$, and $5s$ orbitals were not added to the expansion for the total wave function.

III. RESULTS AND DISCUSSION

In LS coupling the $n=2$ complex of oxygenlike krypton consists of six levels and these are listed in Table I along with their computed energies. We show the energy levels calculated using SUPERSTRUCTURE,[6] along with the energy levels given in Table I of Ref. 1 which were calculated using Hibbert's code CIV3.[7] The energy of the $2p^4\,^1D$ level was incorrectly reported in Ref. 1, and the value given in Table I of this paper is the correct value. The configuration-interaction (CI) target wave functions for the IMPACT calculation are given in Table II(a). The target wave functions used in the RMATRIX calculation are identical to those used in the NIEM calculation and these are shown in Table II(b). Some of the CI coefficients in Table II(a) differ in sign from the corresponding CI coefficients in Table II(b) because the phase convention used in CIV3 differs from that used in SUPERSTRUCTURE.

TABLE I. Energy levels (a.u.) for Kr^{28+}.

State	SUPERSTRUCTURE	CIV3
$2s^2 2p^4\,^3P$	0.0	0.0
$2s^2 2p^4\,^1D$	0.6772	0.6759
$2s^2 2p^4\,^1S$	1.4220	1.4252
$2s2p^5\,^3P$	5.4678	5.4642
$2s2p^5\,^1P$	7.4757	7.4638
$2p^6\,^1S$	12.8523	12.8608

In Ref. 1 it was reported that the cross sections for excitation of transitions from the $2p^4\,^3P$ ground state of Kr^{28+} were strongly affected by coupling to the channel for the $2s2p^5\,^3P^\circ$ excitation. The reported coupling effects were most pronounced for the $2p^4\,^3P \rightarrow 2p^6\,^1S$ transition. It was reported that cross sections for this transition, obtained in a three-state close-coupling calculation, were reduced by a factor of 100 near threshold when the $2s2p^5\,^3P^\circ$ channel was included in a six-state close-coupling calculation. However, six-state close-coupling calculations with IMPACT did not show this dramatic reduction near threshold; nor did subsequent six-state calculations with RMATRIX or NIEM. In Fig. 1 we show the cross sections for the $2p^4\,^3P \rightarrow 2p^6\,^1S$ transition obtained in three separate six-state close-coupling calculations using NIEM, IMPACT, and RMATRIX, respectively. These are shown along with the results from the earlier calculation NIEMa. The cross sections from all three codes decrease smoothly and monotonically with increasing collision energy. This contrasts strongly with the behavior shown by NIEMa and reported in Ref. 1. The results from IMPACT, NIEM, and RMATRIX are all closer to each other than any of them are to the NIEMa results, and all of these newer results are higher than the NIEMa results. We note, however, that while the NIEM and IMPACT results are nearly identical, the RMATRIX cross sections are approximately 10% higher than the NIEM and IMPACT cross sections. Similar small discrepancies between RMATRIX results and results obtained using NIEM and LAM were found by Collins and Schneider in studies of electron-impact excitation of Li.[8] (LAM is a linear algebraic method for solving integral equations and was developed by Collins and Schneider.[9])

In Figs. 2 and 3 the cross sections for the $2p^4\,^3P \rightarrow 2p^4\,^1D$ and $2p^4\,^3P \rightarrow 2p^4\,^1S$ transitions are shown. In these figures we see again that the NIEMa results are distinctly below the results from the other three calculations. Again the IMPACT and NIEM results are nearly identical, and the RMATRIX results are slightly

TABLE II. Configuration-interaction wave functions for (a) IMPACT calculation and (b) NIEM and RMATRIX calculation.

(a)

$2p^4(^3P)=1.0000(2p^4)$

$2p^4(^1D)=0.9999(2p^4)+0.0017[2p^3(^2P)3p]+0.0034[2p^3(^2D)3p]+0.0006(2p^5 3p)$

$2p^4(^1S)=0.9881(2p^4)-0.1540(2p^6)-0.0004(2p^3 3p)-0.0003(2p^5 3p)$

$2s2p^5(^1P)=0.9997(2s2p^5)-0.0063(2p^5 3s)+0.0155(2p^5 3d)+0.0052(2p^3 3s)-0.0138[2p^3(^2P)3d]+0.0101[2p^3(^2D)3d]$

$2s2p^5(^3P)=0.9998(2s2p^5)-0.0049(2p^5 3s)-0.0038[2p^3(^2P)3d]+0.0163[2p^3(^2D)3d]+0.0002(2p^5 3s)-0.0051(2p^5 3d)$

$2p^6(^1S)=0.1540(2p^4)+0.9880(2p^6)-0.0003(2p^3 3p)+0.0078(2p^5 3p)$

(b)

$2p^4(^3P)=1.0000(2p^4)$

$2p^4(^1D)=0.9985(2p^4)-0.0006[2p^3(^2P)3p]-0.0547[2p^3(^2D)3p]-0.0008(2p^5 3p)$

$2p^4(^1S)=0.9881(2p^4)-0.1539(2p^6)-0.0019(2p^3 3p)+0.0063(2p^5 3p)$

$2s2p^5(^1P)=0.9999(2s2p^5)+0.0048(2p^5 3s)-0.0101(2p^5 3d)-0.0052(2p^3 3s)-0.0053[2p^3(^2P)3d]+0.0096[2p^3(^2D)3d]$

$2s2p^5(^3P)=0.9999(2s2p^5)-0.0050(2p^3 3s)-0.0054[2p^3(^2P)3d]+0.0093[2p^3(^2D)3d]$

$2p^6(^1S)=0.1539(2p^4)-0.9881(2p^6)+0.0002(2p^3 3p)+0.0063(2p^5 3p)$

higher. In this case, however, the RMATRIX results differ from the NIEM and IMPACT results by only 1% or less.

In the case of the $2s^2 2p^4\,^3P \rightarrow 2s2p^5\,^1P^\circ$ transitions the NIEMa results are still clearly lower than all of the other results. But Fig. 4 shows that in this case the NIEMa cross sections are somewhat closer to the other cross sections than they were in Figs. 1–3. The cross section for the electric-dipole-allowed $2s^2 2p^4\,^3P \rightarrow 2s2p^5\,^3P^\circ$ transition are shown in Fig. 5. In this figure, the NIEMa results are interspersed with the other results and differ very little from the newer NIEM results. The cross sections from all four calculations are within 5% of each other for this transition.

The three codes IMPACT, RMATRIX, and NIEM use different numerical methods to solve the same set of coupled integro-differential equations. In the case of IMPACT, the integro-differential equations are replaced by a system of linear algebraic equations using a finite difference approximation as discussed by Seaton.[10] The multiconfiguration target wave functions are generated in

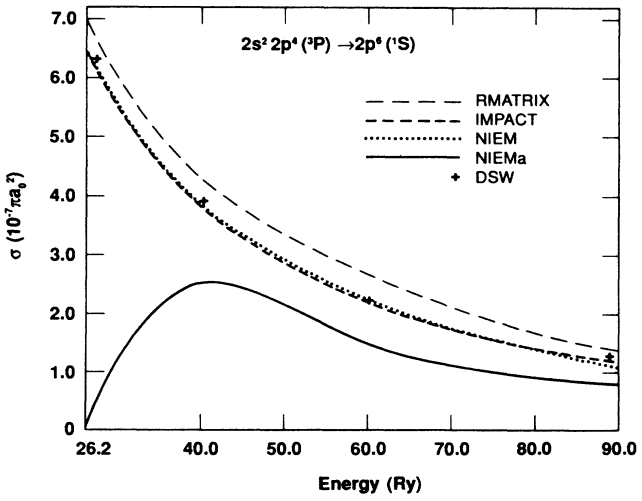

FIG. 1. Cross sections for the $2s^2 2p^4\,^3P \rightarrow 2p^6\,^1S$ transition in Kr^{28+}.

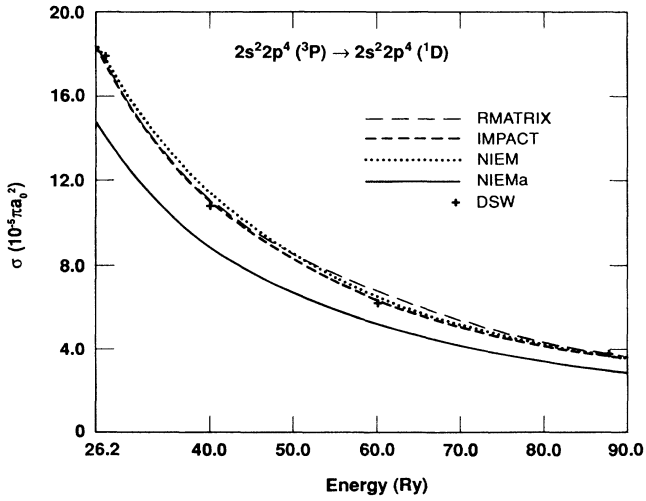

FIG. 2. Cross sections for the $2s^2 2p^4\,^3P \rightarrow 2s^2 2p^4\,^1D$ transition in Kr^{28+}.

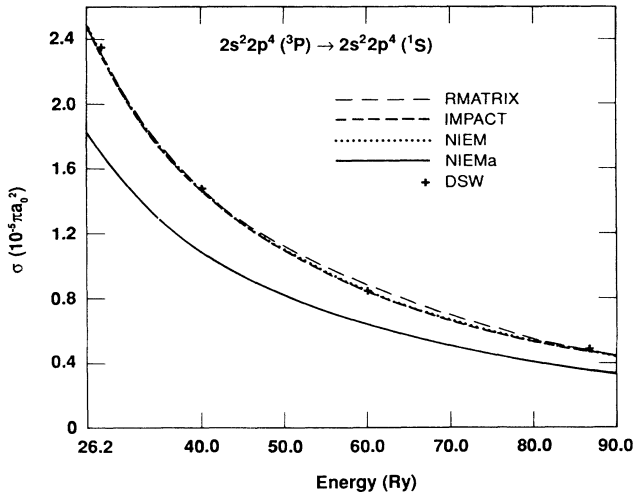

FIG. 3. Cross sections for the $2s^2 2p^4\,{}^3P \rightarrow 2s^2 2p^4\,{}^1S$ transition in Kr^{28+}.

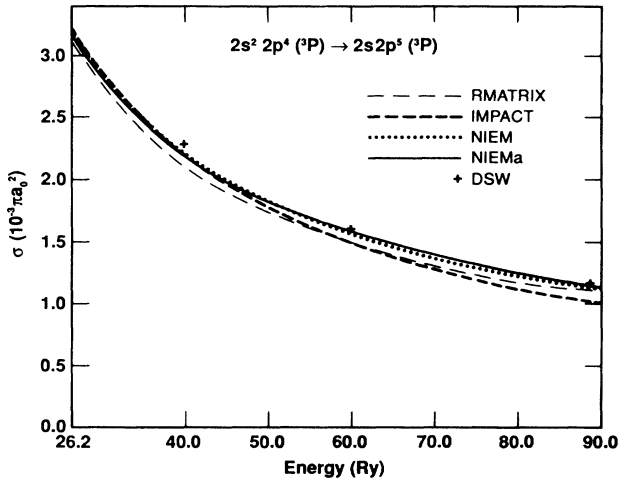

FIG. 5. Cross sections for the $2s^2 2p^4\,{}^3P \rightarrow 2s 2p^5\,{}^3P^\circ$ transition in Kr^{28+}.

a modified Thomas-Fermi potential using the atomic structure code SUPERSTRUCTURE. NIEM uses a noniterative integral-equation method to solve the coupled equations. In the RMATRIX calculation the collision space is divided into an inner region where correlation and exchange are important, and an outer region where electrostatic interaction dominates. At the boundary, the solution in the outer region is matched to the solution in the inner region.

The target wave functions for the NIEMa calculation were generated using Hibbert's program CIV3 as described in Ref. 11. The same target wave functions were used in the newer NIEM calculation. The $4s$, $4p$, $4d$, and $5s$ orbitals, however, were not included in the new calculations. The same CIV3 target wave functions were also used in the RMATRIX calculation. Although the target wave functions for the IMPACT calculation were generated in a Thomas-Fermi potential and the NIEM and RMATRIX calculations used target wave functions constructed with Hartree-Fock orbitals, we attempted to make the targets as much alike as possible by using the same atomic states and the same configurations to describe the target in each case. In all three cases we carried out explicit calculations for partial waves up to $L=10$. This was sufficient for convergence of the cross section for the dipole-forbidden transitions but not for the dipole-allowed $2p^4\,{}^3P \rightarrow 2s 2p^5\,{}^3P^\circ$ transition. For IMPACT the contribution of the higher partial waves was calculated using a Shank's extrapolation procedure.[12] For NIEM and RMATRIX, the higher partial wave contribution was computed using a scaled Coulomb-Bethe approximation. Exchange is neglected beyond a radius $r=3.0a_0$ in the RMATRIX calculation. In NIEM and IMPACT calculations exchange is neglected beyond $r=2.4a_0$ and $r=2.0a_0$, respectively. In the R-matrix calculation 25 continuum terms are included and this should be more than adequate for the accuracy needed here. It is impressive that the IMPACT and NIEM cross sections are so nearly identical for all of the transitions even though these two codes used target wave functions obtained from two entirely different methods. On the other hand, the target wave function input for the RMATRIX calculation is identical to that used in the NIEM calculation; yet the agreement between the RMATRIX results and the NIEM results is not as good as the agreement between the NIEM and IMPACT results. This notwithstanding, the good agreement among the results of all three calculations is nevertheless striking and encouraging. Even in the case of the $2p^6\,{}^1S$ transition the difference between RMATRIX and NIEM is less than 10%. This transition has a very small cross section and we would expect that differences would be most noticeable for such transitions.

In a separate earlier IMPACT calculation we included the additional correlation configurations in an effort to

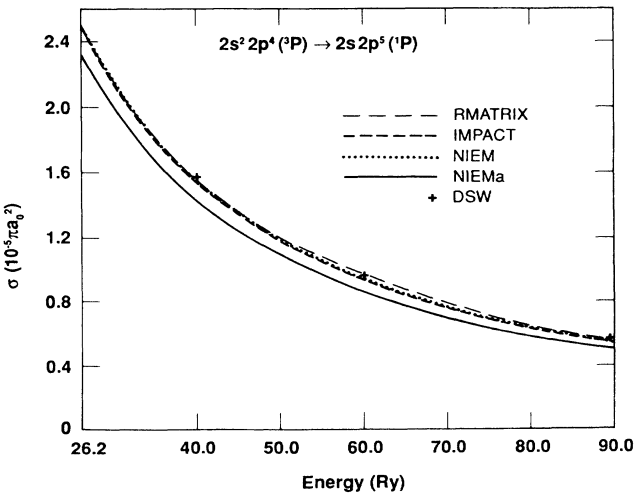

FIG. 4. Cross sections for the $2s^2 2p^4\,{}^3P \rightarrow 2s 2p^5\,{}^1P^\circ$ transition in Kr^{28+}.

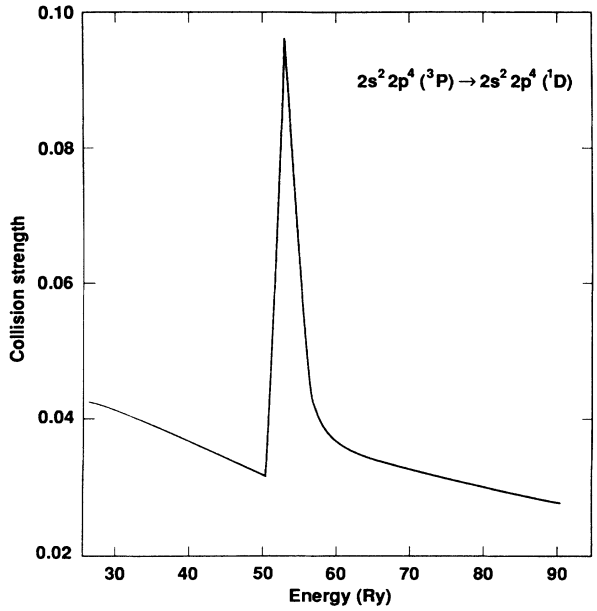

FIG. 6. Pseudoresonance in the cross section for the $2s^2 2p^4\,{}^3P \rightarrow 2s^2 2p^4\,{}^1D$ transition.

match the wave functions used in Ref. 11. But the needed correlation functions were not neglected. These additional orbitals, and the resulting additional configurations did not change the cross sections significantly, except in energy regions where these correlating configurations produced pseudoresonances. Figure 6 shows one of these pseudoresonances which occurred near 54 Ry in the $2p^4\,{}^3P \rightarrow 2p^4\,{}^1D$ channel.

In addition to the three six-state close-coupling calculations, we also used the University College London distorted wave code (DSW) to calculate cross sections for the transitions discussed above. Like IMPACT, this code uses multiconfiguration target wave functions calculated with SUPERSTRUCTURE and a modified Thomas-Fermi scattering potential. For this calculation we used the same target states and configurations that we used in the three six-state close-coupling calculations. These results are also shown in Figs. 1–5 along with the close-coupled results. The distorted-wave cross sections differ from the IMPACT cross sections by less than 5% in all of the transitions studied. The fact that the single channel distorted-wave results and the six-state close-coupling results are nearly the same, suggests that coupling among the excitation channels is negligible for these transitions.

IV. CONCLUSIONS

In conclusion, we have calculated cross sections for transitions from the ground state to the $n=2$ excited states of Kr^{28+} using three different close-coupling codes. We did not set out to make a detailed code comparison study. But all three calculations were performed using the same target configurations and the same six-state close-coupling expansion. Although these codes employ different methods for generating target wave functions, and different numerical techniques for solving the coupled integro-differential equations, the results from all three codes are in very good agreement for all of the transitions over the entire energy range considered. We note that the NIEM and IMPACT cross sections are nearly identical and that the RMATRIX cross sections are generally slightly above them. We also used a distorted-wave code to calculate these cross sections and the distorted-wave results did not differ significantly from the six-state close-coupling results. Our results differ markedly in behavior from the cross sections reported in an earlier publication, and the strong coupling effects noted in that study were apparently the result of an inconsistency introduced in the calculation by failure to include necessary correlation functions. Our newer results replace the cross sections reported in Ref. 1.

ACKNOWLEDGMENTS

We thank Dr. Karl Scheibner for assistance in using the RMATRIX code. We also thank Dr. Alfred Msezane for providing the input used in the NIEMa calculation; this helped us to determine the error in that calculation. Work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-ENG-48. One of us (R.J.W.H.) was supported in part by the U.S. Department of Energy, Division of Chemical Sciences.

[1]A. Z. Msezane, K. J. Reed, and R. J. W. Henry, Phys. Rev. A **34**, 2540 (1986).
[2]R. J. W. Henry, S. P. Rountree, and E. R. Smith, Comput. Phys. Commun. **23**, 233 (1981).
[3]M. A. Crees, M. J. Seaton, and P. M. H. Wilson, Comput. Phys. Commun. **15**, 23 (1978).
[4]K. A. Berrington, P. G. Burke, M. LeDourneuf, W. D. Robb, K. T. Taylor, and Vo Ky Lan, Comput. Phys. Commun. **14**, 367 (1978).
[5]K. A. Berrington, W. B. Eissner, H. E. Saraph, M. J. Seaton, and P. J. Storey, Comput. Phys. Commun. **44**, 105 (1987).
[6]W. Eissner, M. Jones, and H. Nussbaumer, Comput. Phys. Commun. **9**, 141 (1975).
[7]A. Hibbert, Comput. Phys. Commun. **9**, 141 (1975).
[8]L. A. Collins and B. I. Schneider, Phys. Rev. A **27**, 101 (1983).
[9]L. A. Collins and B. I. Schneider, Phys. Rev. A **24**, 1264 (1981).
[10]M. J. Seaton, J. Phys. B **7**, 1817 (1974).
[11]A. Z. Msezane, J. Lee, K. J. Reed, and R. J. W. Henry, Phys. Rev. A **34**, 3735 (1986).
[12]D. Shanks, J. Math. Phys. **34**, 1 (1955).