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Coupled-channels optical calculation of electron–helium scattering

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Abstract. Cross sections for electron impact excitation of the singlet $n = 1$ and 2 states of the helium atom at various energies ranging from 30–200 eV are calculated using the coupled-channels optical method with the half-on-shell polarization potential. The electron impact coherence parameters for the excitation to the 2^1P state are also calculated. Overall good, semi-quantitative agreement with experiment is achieved.

1. Introduction

The coupled-channels-optical (CCO) method with the half-on-shell polarization potential has proved to give useful descriptions of experimental data on electron scattering for hydrogen (Lower *et al* 1987), sodium (Mitroy *et al* 1987) and magnesium (McCarthy *et al* 1989).

A very strict test of details of the method is provided by helium, where a large number of experiments have been performed and where a converged calculation of the target bound states in a configuration interaction (CI) representation is not difficult. Preliminary CCO calculations for helium (Brunger *et al* 1990) have shown that theoretical estimates of scattering data depend critically on the polarization potential. The purpose of the present work is to test the CCO method on a broad range of data and to compare it with other methods as a simple and practical method of predicting scattering data.

In recent years, there have been a number of experimental and theoretical studies of the electron impact excitation of the ground-state helium atom to the $n = 2$ states (Beijers *et al* 1987, Csanak and Cartwright 1988, Fon *et al* 1988, Cartwright *et al* 1989, Brunger *et al* 1990). The most recent experimental and theoretical data can be found in Andersen *et al* (1988).

Most of the recent experimental studies have concentrated on measuring the electron-impact coherence parameters (EICP) for the transition 1^1S–2^1P (Beijers *et al* 1987, Andersen *et al* 1988). Besides these coherence studies, there have also been two recent measurements of the differential cross sections for the excitation to the $n = 2$ states at energies ranging from 29.6 to 100 eV (Cartwright *et al* 1989, Brunger

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et al 1990). These cross section measurements at 29.6 and 40.1 eV show favourable agreement with each other except in some details. Similar trends are obtained in comparing these measurements to the earlier data of Trajmar (1973) and Hall *et al* (1974). This seems to suggest that the definitive measurements at 29.6 and 40.1 eV have been made. At higher energies ($E > 40.1$ eV), there are the experiments reported by Suzuki and Takayanagi (1973), Chutjian and Srivastava (1975) and Cartwright *et al* (1989).

It seems that the measurements of the EICP have provided a very stringent test for the various theoretical methods. Among the various calculations, the R-matrix method (Fon *et al* 1979, 1980, 1988), the CCO calculation of Brunger *et al* (1990), the FOMBT (first-order many-body theory) (Csanak and Cartwright 1988) and the distorted-wave methods (Madison and Winters 1983, Beijers *et al* 1987) have given an extensive set of results for various energies in the range of 18–500 eV. The perturbative methods (FOMBT, DWBA) have solely concentrated on studying the 1^1S–2^1P transition in much detail. Their calculated differential cross sections and EICP show semi-quantitative agreement with most experimental data. The early R-matrix calculations of Fon *et al* (1979, 1980) had provided cross sections as well as angular correlation parameters ($\lambda, |\chi|$) for energies 30–200 eV. Their results at most energies except 30 eV showed reasonably good agreement with experiments. The recent 19-state R-matrix (Fon *et al* 1988), which included atomic states up to $n = 4$ in the basis, improved the agreement with experiment at 29.6 eV. Nevertheless there were differences for singlet states as well as for triplet states. The CCO calculation of Brunger *et al* (1990) shows semi-quantitative agreement with most experimental differential cross sections for the 2^1S and 2^1P states at 29.6 and 40.1 eV. Although the problem of the depth of the minimum for the 2^1S differential cross section at 29.6 eV may still remain unresolved, the overall descriptions of the 2^1S and 2^1P states have been very promising. The optical potentials are inadequate to give a satisfactory description for the triplet states (Brunger *et al* 1990). This can be explained by the rather crude treatment of the exchange part of the continuum optical potential. The more accurate direct part does not give spin flip.

The present work extends the CCO method to calculate differential cross sections, total cross sections and EICP for energies ranging from 30–200 eV.

2. Theory and details of calculations

A detailed description of the CCO method for electron–atom scattering has been given by McCarthy and Weigold (1990). Further details of the generalization of the CCO to allow for CI in the wavefunctions of many-electron targets have been given by Mitroy *et al* (1987) and Bray *et al* (1989). The optical potential for two valence electrons is calculated by the method of McCarthy *et al* (1988).

Essentially, the CCO method involves the solution of the set of coupled integral equations

$$\langle \boldsymbol{k}_i i|T|j\boldsymbol{k}_j\rangle = \langle \boldsymbol{k}_i i|V + V^{(Q)}|j\boldsymbol{k}_j\rangle + \sum_{l\in P}\int \mathrm{d}^3k\, \langle \boldsymbol{k}_i i|V + V^{(Q)}|l\boldsymbol{k}\rangle \times [E^{(+)} - \epsilon_l - \tfrac{1}{2}k^2]^{-1}\langle \boldsymbol{k}l|T|j\boldsymbol{k}_j\rangle \qquad (1)$$

where

$$\langle k_i i|T|jk_j\rangle = \langle k_i i|V|\Psi_j^{(+)}(k_j)\rangle \tag{2}$$

is the T-matrix element for the transition from the $(N+1)$-electron channel state $|jk_j\rangle$ to $|ik_i\rangle$. The ket $|\Psi_j^{(+)}\rangle$ is the formally exact solution of the $(N+1)$-electron Schrödinger equation with total energy E for entrance channel j while ϵ_l is the energy of the N-electron target state $|l\rangle$. The target states are described in a CI representation.

The first-order electron–target potential V includes the appropriate exchange operator. The complex polarization potential $V^{(Q)}$ is formally written as

$$PV^{(Q)}P = PVQ\frac{1}{[E^{(+)} - QHQ]}QVP \tag{3}$$

where the Feshbach operators P and Q project the explicitly coupled channels and the remaining channels respectively.

Using the notation of McCarthy *et al* (1988), the polarization potential $V^{(Q)}$ for continuum excitation of helium is given as

$$\begin{aligned}\langle k_i i|V^{(Q)}|jk_j\rangle = \int \mathrm{d}^3k' \int \mathrm{d}^3k\,(a_s + b_s P_r)\langle k_i i|V|\Psi^{(-)}(k_<)k_>\rangle \\ \times [E^{(+)} - \tfrac{1}{2}(k^2 + k'^2)]^{-1}\langle k_> \Psi^{(-)}(k_<)|V|jk_j\rangle\end{aligned} \tag{4}$$

where $\Psi^{(-)}(k_<)$, is a Coulomb wave, orthogonalized to the bound state in the same amplitude factor, which represents the slower electron. The spin coefficients a_s and b_s are given by McCarthy *et al* (1988). The half-on-shell polarization potential is given by the appropriate angular momentum projection of $V^{(Q)}$.

$$V_{l''l'l}(K) = \sum_{m''m'} C^{l''l'l}_{m''m'm} \int \mathrm{d}\hat{K}\,\langle k_i i|V^{(Q)}|jk_j\rangle i^{-l''} Y_{l''m''}(\hat{K}) \tag{5}$$

where $\boldsymbol{K} = \boldsymbol{k}_j - \boldsymbol{k}_i$, the orbital angular momentum quantum numbers l', m' and l, m belong to the target states i and j respectively, and $C^{l''l'l}_{m''m'm}$ denotes the Clebsch–Gordan coefficients. For the optical potential the target states are represented by the appropriate Hartree–Fock configuration. $V_{l''l'l}(K)$ is calculated with on-shell values of k_j.

The set of coupled integral equations (1) is solved in partial-wave expanded form with Gaussian quadratures used to make the integrals discrete. They need only to be solved for total angular momentum J up to the minimum value $J_{\min}$ for which the inelastic T-matrix elements for all J are computed by using the analytic Born approximation with the appropriate adjustments for $J < J_{\min}$. This is not good enough for the elastic channel where the Born approximation does not sufficiently account for dipole polarization. Here the T-matrix elements are given by using the phase shifts of O'Malley *et al* (1961) as an extrapolation.

The EICP were calculated following the notation introduced by Andersen *et al* (1988). The parameters $L_\perp$, P_l and γ are related to the Stokes parameters as follows.

$$\begin{aligned} L_\perp &= -P_3 \\ P_l &= (P_1^2 + P_2^2)^{1/2} \\ \gamma &= \frac{1}{2}\tan^{-1}\left(\frac{P_2}{P_1}\right) \end{aligned} \tag{6}$$

where the Stokes parameters P_1, P_2 and P_3 are

$$\begin{aligned} P_1 &= 2\lambda - 1 \\ P_2 &= -2[\lambda(1-\lambda)]^{1/2}\cos\chi \\ P_3 &= \left[1 - (P_1^2 + P_2^2)\right]^{1/2}. \end{aligned} \tag{7}$$

The angular correlation parameters λ and $|\chi|$ are related to the $\bar{P}_1$, $\bar{P}_2$, $\bar{P}_3$ by (7).

3. Comparison with experiment

In the present calculation the P space consists of ten channels; $1,2,3^1S$; $2,3^3S$; $2,3^1P$; $2,3^3P$; 3^1D. The Q space only includes the continuum. The basis used in the CI representation of these states consists of all allowed excitations of electrons in the 1,2,3,4s; 2,3,4p and 3d Hartree–Fock orbitals, with higher excitations allowed for by $\bar{s}$, $\bar{p}$ and $\bar{d}$ pseudo-orbitals. Polarization potentials are included for all couplings of the 1^1S ground state to the singlet and triplet $n = 2$ states and for the diagonal matrix elements for these states.

Table 1. Total cross sections for electron–helium scattering compared with the experimental values of Nickel *et al* (1985). Percentage experimental errors are given in parentheses. Units are 10^{-16}cm^2.

E (eV)	CCO	Experiment
30	2.69	2.391(0.1)
40	2.23	2.001(0.5)
50	2.06	1.715(0.9)
80	1.46	1.269(2.0)
100	1.38	1.120(0.6)
200	0.76	0.734(1.2)

The overall quality of the description is tested by comparing total cross sections with experiment at the energies of the calculation: 30, 40, 50, 80, 100 and 200 eV. The comparison is shown in table 1. The calculated total cross sections are somewhat too high, particularly at the lower energies. This is accounted for by an overestimate of the total ionization cross section (McCarthy and Stelbovics 1983). Since this affects the second and higher orders in the potential it is not expected to have a serious effect on the calculation of scattering to the $n = 2$ states.

Figures 1–6 show the differential cross section for elastic scattering, the $n = 2$ singlet differential cross sections and the EICPs $L_\perp$, γ and P_l for each of the six energies considered. The diagrams are labelled by the energy of the calculation. The experiments may be at a slightly different energy, e.g. those on the 30 eV figure are at 29.6 eV. The difference is not enough to invalidate the comparison.

The general trend for the elastic channel is that the calculated cross sections are somewhat higher than the experimental values but the shapes of the angular distributions are similar. The calculated elastic cross sections are insensitive to the details of the calculation and unrealistic changes would be necessary to agree with experiment at 100 and 200 eV.

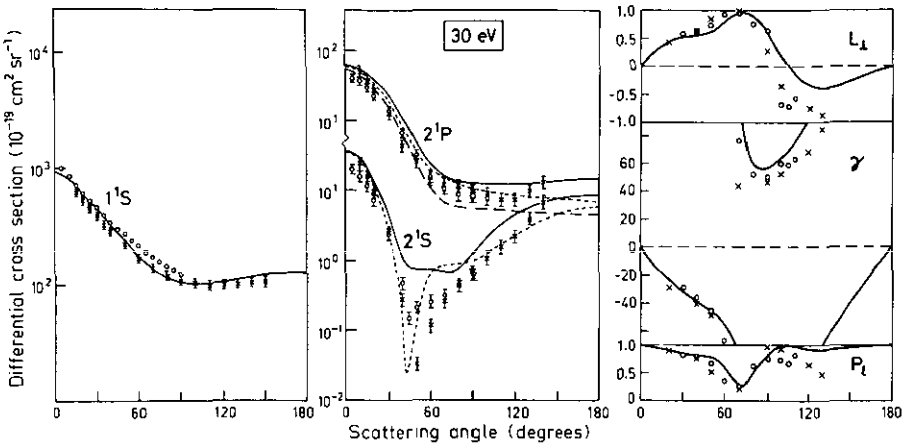

Figure 1. Angular distributions of scattering observables for the $n = 1$ and 2 singlet states of helium at 30 eV (see text). Experimental data for differential cross sections are shown by: circles, Brunger *et al* (1990); crosses, Register *et al* (1980) 1^1S, Trajmar (1973) 2^1S and Truhlar *et al* (1973) 2^1P. Experimental data for EICPs are shown by: crosses, McAdams *et al* (1980); circles, van den Heuvell *et al* (1982). Theoretical curves are: full curve, present CCO; broken curve, FOMBT (Cartwright *et al* 1991); dotted curve, 19-state R-matrix (Fon *et al* 1988).

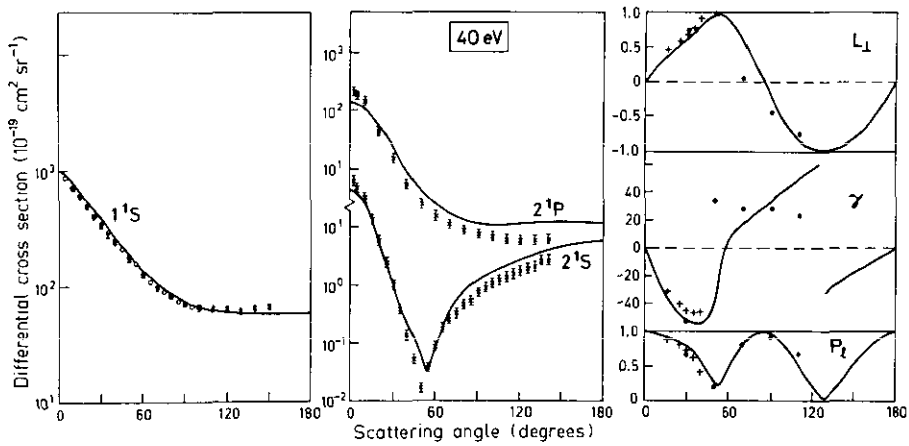

Figure 2. Variations from figure 1 are: energy 40 eV; EICPs: plus signs, Eminyan *et al* (1974); filled circles, Steph and Golden (1980).

The $n = 2$ differential cross sections show good agreement with experiment, particularly for the larger cross section values. Where there are discrepancies they are usually at larger angles, which are more sensitive to details of the calculation. The calculation does not agree in detail with experiment in the first minimum for 2^1S at most energies. At 30 eV the two available experiments disagree with each other and with the calculation in this minimum. Here the calculation does not agree as well with the data of Brunger *et al* (1990) as does the calculation reported in that article. The present numerical analysis is better and the previous apparently good agreement must be considered to be fortuitous.

Two other calculations of $n = 2$ differential cross sections are shown for

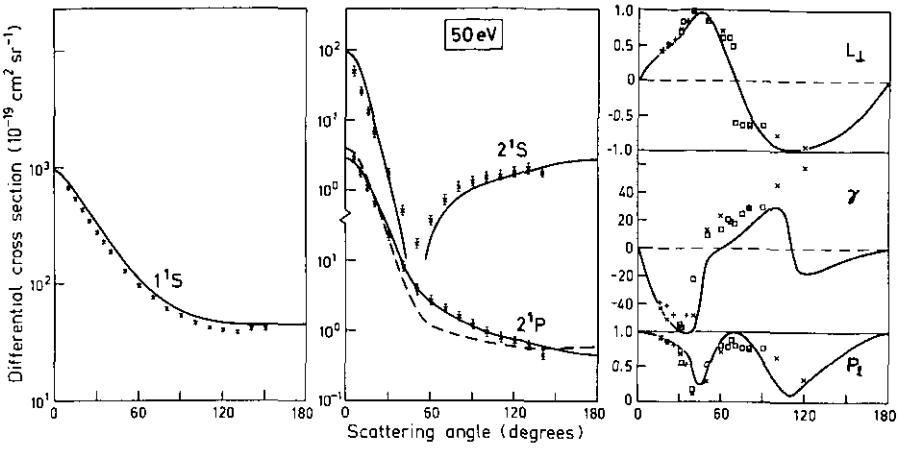

Figure 3. Variations from previous figures are: energy 50 eV; differential cross sections, crosses (Cartwright *et al* (1989) 2^1S, 2^1P); EICPs: squares, Beijers *et al* (1987).

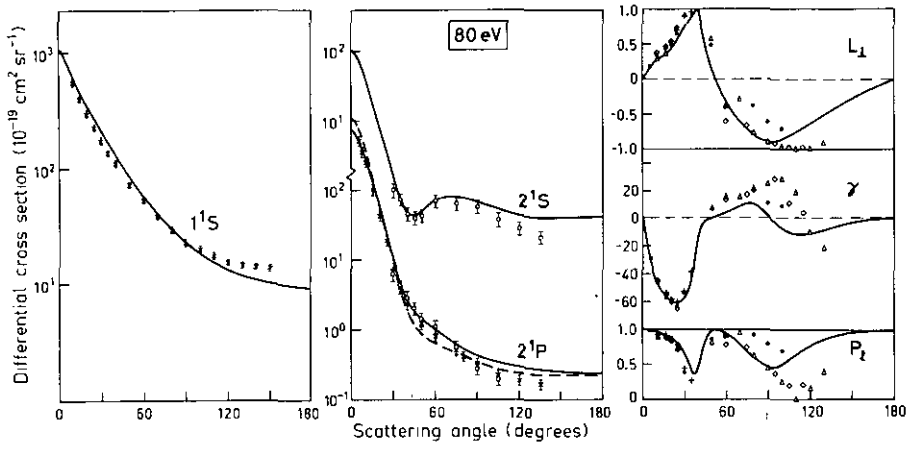

Figure 4. Variations from previous figures are: energy 80 eV; differential cross sections, circles (Opal and Beaty 1972); EICPs: diamonds (Slevin *et al* 1980); triangles (Hollywood *et al* 1979).

comparison. CCO gives a better overall description of the 2^1P excitation than FOMBT. For the $n = 2$ cross sections at 30 eV there is little to choose between CCO, the 19-state R-matrix calculation and FOMBT, none being really satisfactory. In the case of the 30 eV 2^1S excitation there is a deep minimum in the earlier experiment (Trajmar 1973) and a similar minimum in the R-matrix calculation at a smaller angle. The later experiment (Brunger *et al* 1990) shows a much shallower minimum but the corresponding minimum in the CCO calculation is too shallow. Sharp cross section minima require close cancellation of partial-wave contributions and it would be surprising if either method were accurate enough to reproduce such a minimum consistently.

The results for the EICPs are best studied in conjunction with the figures given in the review article of Andersen *et al* (1988). The experimental data and calculated curves are so numerous that they cannot be shown in detail here without confusion.

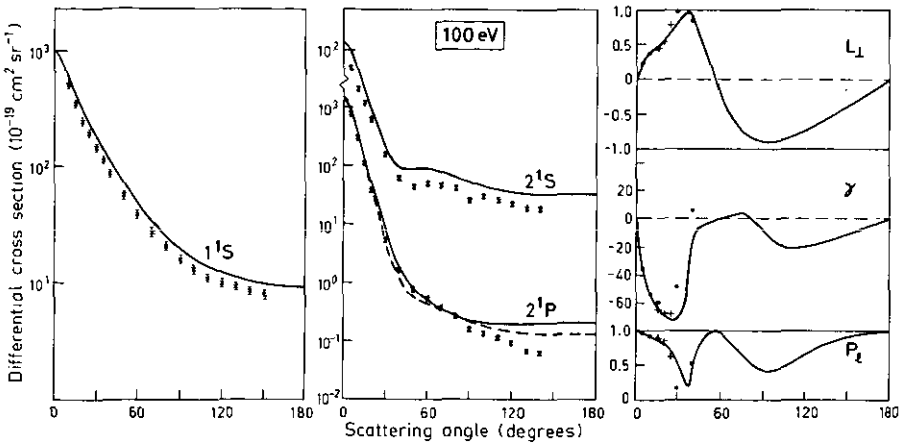

Figure 5. Variations from previous figures are: energy 100 eV.

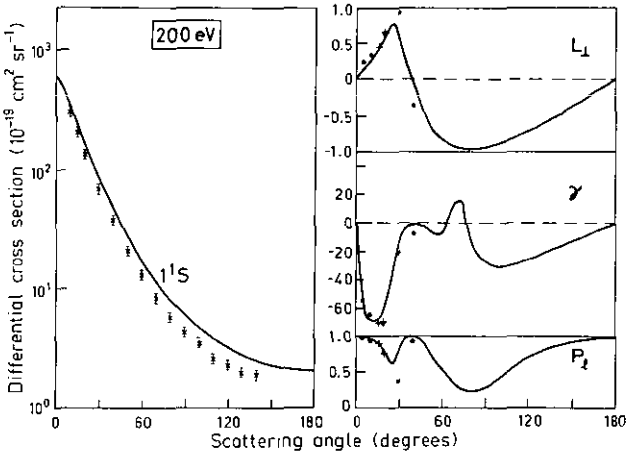

Figure 6. Variations from previous figures are: energy 200 eV.

Here we show only the central experimental points (error bars are given by Andersen *et al*) and the CCO curves. In some cases experiments disagree widely with each other. The present calculation describes the qualitative trends well, disagreeing in detail sometimes at larger angles.

4. Conclusions

It is interesting to compare the CCO method with the distorted-wave Born approximation (DWBA) and the R-matrix method. The DWBA may be considered as a single-excitation approximation to CCO in which the detailed calculation of the effects of other channels is replaced by local, central potentials for calculating distorted waves. It suffers from the conceptual disadvantage that the choice of distorting potentials is somewhat arbitrary. The FOMBT is a consistent first-order method of choosing real static potentials. Most distorting potentials that are normally used do not include the effects of virtual (polarization) and real (absorption) excitation of other channels, all

of which are accounted for by CCO. The price that CCO must pay is that it requires the calculation of a large number of amplitudes similar to the DWBA. In the present ten-state calculation there are about 1500 such amplitudes. The target states in each amplitude are calculated by CI. Computing time is correspondingly increased. The present calculation takes roughly 20 h on a 5-megaflop workstation, at least half of which is required for the polarization potentials.

The 19-state R-matrix calculation is also a major computation. Its 19 target states form the basis for a three-electron CI calculation in the internal region (cut off at 60 au). The internal wavefunctions are matched to the wavefunctions from a non-exchange coupled-channels calculation in the external region. Here exchange effects are negligible. The major conceptual problem with this method is that the target continuum has not been taken into account. It goes without saying that electron exchange is implemented where it is numerically necessary in all three methods, except usually in the DWBA distorting potentials.

The strength of the CCO method relative to the other two is that all channels, including the continuum, are taken into account. The present half-on-shell implementation of the polarization potential provides a broad semi-quantitative description of electron–helium scattering. It requires some drastic approximations for numerical feasibility. They are the half-on-shell approximation, the angular momentum projection (equivalent local) approximation, and the equivalent local exchange approximation. In view of the critical dependence of scattering data on the polarization potential these approximations are probably too crude for detailed agreement with experiment.

In the case of hydrogen (Bray *et al* 1990, 1991) detailed agreement with experiment had to await the calculation of the polarization potential without these approximations. This is an order of magnitude more difficult, but is the next step in the attempt to improve the calculation for helium.

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References

Andersen N, Gallagher J W and Hertel I V 1988 *Phys. Rep.* **165** 1

Beijers J P M, Madison D H, van Eck J and Heideman H G M 1987 *J. Phys. B: At. Mol. Phys.* **20** 167

Bray I, Konovalov D A and McCarthy I E 1991 *Phys. Rev.* A in press

Bray I, Madison D H and McCarthy I E 1990 *Phys. Rev.* A **41** 5916

Bray I, McCarthy I E, Mitroy J and Ratnavelu K 1989 *Phys. Rev.* A **39** 4998

Brunger M J, McCarthy I E, Ratnavelu K, Teubner P J O, Weigold A M, Zhou Y and Allen L J 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** 1325

Cartwright D C, Csanak G, Trajmar S and Register D F 1989 private communication

—— 1991 *Phys. Rev.* A to be published

Chutjian A and Srivastava S K 1975 *J. Phys. B: At. Mol. Phys.* **8** 2360

Csanak G and Cartwright D C 1988 *Phys. Rev.* A **38** 2740

Eminyan M, MacAdam K B, Slevin J, Standage M C and Kleinpoppen H 1974 *J. Phys. B: At. Mol. Phys.* **7** 1519

Fon W C, Berrington K A, Burke P G and Kingston A E 1979 *J. Phys. B: At. Mol. Phys.* **12** 1861

Fon W C, Berrington K A and Kingston A E 1980 *J. Phys. B: At. Mol. Phys.* **13** 2309

—— 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2961

Hall R I, Joyez G, Mazeau J, Reinhardt J and Schermann C 1973 *J. Physique* **34** 827
van den Heuvell H B V L, van Eck J and Heideman H G M 1982 *J. Phys. B: At. Mol. Phys.* **15** 3517
Hollywood M T, Crowe A and Williams J F 1979 *J. Phys. B: At. Mol. Phys.* **12** 819
Lower J, McCarthy I E and Weigold E 1987 *J. Phys. B: At. Mol. Phys.* **20** 4571
Madison D M and Winters K H 1983 *J. Phys. B: At. Mol. Phys.* **16** 4437
McAdams R, Hollywood M T, Crowe A and Williams J F 1980 *J. Phys. B: At. Mol. Phys.* **13** 3961
McCarthy I E, Ratnavelu K and Weigold A M 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 3999
McCarthy I E, Ratnavelu K and Zhou Y 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2597
McCarthy I E and Weigold E 1990 *Adv. At. Mol. Phys.* **27** 165
McCarthy I E and Stelbovics A T 1983 *Phys. Rev.* A **28** 1322
Mitroy J, McCarthy I E and Stelbovics A T 1987 *J. Phys. B: At. Mol. Phys.* **20** 4827
Nickel J C, Imre K, Register D F and Trajmar S 1985 *J. Phys. B: At. Mol. Phys.* **18** 125
O'Malley T F, Spruch L and Rosenberg L 1961 *J. Math. Phys.* **2** 491
Opal C B and Beaty E C 1972 *J. Phys. B: At. Mol. Phys.* **5** 627
Register D F, Trajmar S and Srivastava S K 1980 *Phys. Rev.* A **21** 1134
Slevin J, Porter H Q, Eminyan M, Defrance A and Vassilev G 1980 *J. Phys. B: At. Mol. Phys.* **13** 3009
Steph N C and Golden D E 1980 *Phys. Rev.* A **21** 759, 1848
Suzuki H and Takayanagi T 1973 *Proc. 8th Int. Conf. on Physics of Electronic and Atomic Collisions* (Beograd: Institute of Physics) Abstracts pp 286–7
Trajmar S 1973 *Phys. Rev.* A **8** 191
Truhlar D G, Trajmar S, Williams W, Ormonde S and Torres B 1973 *Phys. Rev.* A **8** 2475