Born Wave Calculation of Atom-Atom Inelastic Cross Sections: Description of Target Atoms by Elastic and Inelastic X-Ray Form Factors*

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Total electron-loss cross sections for H atoms in collision with He, Ne, Ar, Kr, C, N, and O over the range of incident energy 1 keV–100 MeV and total ($1s$-$2l$) excitation cross sections for H atoms in collision with He, Ne, Ar, and Kr over the range of incident energy 0.1 keV–10 MeV are calculated by using the first Born wave approximation and assuming closure. The relevant matrix elements for the target atoms are expressed in terms of elastic and inelastic x-ray form factors. The calculations agree, within experimental error, with high-energy measurements for He, N, and O targets. Good agreement between theoretical and experimental excitation cross sections is found at energies as low as 5 keV for He, Ne, and Kr targets when the Ne and Kr calculations are scaled with a velocity-dependent parameter calculated by matching theoretical and experimental ionization data. An explanation for the velocity-dependent scaling of the theoretical cross sections for many electron target atoms at energies up to 1 MeV is presented and discussed.

I. INTRODUCTION

Inelastic atom-atom and atom-molecule collisions are of great importance to the study of excitation and ionization in meteor trails, aurorae, and other atmospheric phenomena, and to the theory of stopping power in matter. Even the simplest theoretical model for these direct inelastic processes, the first Born wave approximation,[1] has only been applied to a few cross-section calculations[2-5] because the accurate evaluation of the necessary matrix elements becomes prohibitive for many electron atoms.

Recently, Green[6] suggested that calculations might be performed by the use of experimentally determined generalized oscillator strengths[7] to describe the projectile and target-atom excitations. The use of elastic and inelastic form factors to calculate electron-atom cross sections is well known[8] and has been extended by Dmitriev and Nikolaev[9] and Victor[10] to atom-atom ionization by the use of a free-electron model for the projectile. It is thus a logical extension to calculate total inelastic cross sections by use of calculated or experimental generalized oscillator strengths to describe the projectile, and elastic and inelastic form factors to describe the target.

This paper presents the calculation of ionization and ($1s$-$2l$) excitation cross sections for H scattered by a variety of atoms. Hydrogen is used as the projectile because the generalized oscillator strengths are available in analytic form[2] and many experimental data exist.[11-21] The effectiveness of the form-factor description of the target atom is then tested unambiguously by comparison with high-energy experiments, since the first Born approximation is correct in the limit of weak interaction and high velocity.[1] A comparison of theory and experiment at lower energies (1–100 keV) provides effective lower energy limits for the application of the first Born approximation for several target gases.

II. THEORY

The first Born wave approximation is a first-order time-independent perturbative treatment of a collision problem that uses plane waves to describe the initial and final relative motions of the two bodies, the Hamiltonian for the two isolated atoms as the zero-order Hamiltonian, the electrostatic interaction between the two systems as the coupling perturbation, and products of atomic wave functions without electron exchange as the total electronic wave functions.

Let us consider the collision $A_0+B_0\rightarrow A_n+B_{n'}$, where A, the projectile with Z_A electrons, and B, the target with Z_B electrons, are initially in their ground states, and following the collision are in states n and n' with the possibility that $n'=0$.

The first Born cross section in atomic units is[1]

$$\sigma(0,0-n,n') = (4\pi v_i^{2})^{-1}\int_{q_{\min}}^{q_{\max}} q\,dq\int_0^{2\pi} d\Phi\,\Big|\int e^{i\vec{q}\cdot\vec{R}}d\vec{R}\iint \psi_0^{A*}(\vec{r}_A)\psi_n^{A}(\vec{r}_A)$$
$$\times\psi_0^{B*}(\vec{r}_B)\psi_{n'}^{B}(\vec{r}_B)V(\vec{r}_A,\vec{r}_B,\vec{R})d\vec{r}_A\,d\vec{r}_B\Big|^2, \qquad (1)$$

where $\vec{r}_S = \vec{r}_{S1}, \vec{r}_{S2}, \ldots, \vec{r}_{SZ_S}, \vec{r}_{Si}$

is a vector from the nucleus of atom S to its ith electron, ψ_n^S is the electronic wave function for atom S in state n with energy ϵ_n^S, M is the reduced mass for the two-particle system, v_i is the initial velocity of relative motion, $\vec{R}$ is a vector from the center of atom A to the center of atom B,

$$V(\vec{r}_A, \vec{r}_B, \vec{R}) = \frac{Z_A Z_B}{R} - \sum_{i=1}^{Z_A} \frac{Z_B}{|\vec{R} - \vec{r}_{Ai}|} - \sum_{i=1}^{Z_B} \frac{Z_A}{|\vec{R} + \vec{r}_{Bi}|} + \sum_{i=1}^{Z_A} \sum_{j=1}^{Z_B} \frac{1}{|\vec{R} + \vec{r}_{Bj} - \vec{r}_{Ai}|}, \tag{2}$$

and the momentum-transfer vectors are defined in terms of the initial and final wave vectors $\vec{k}_i$ and $\vec{k}_j$ by $\vec{q} = \vec{k}_i - \vec{k}_f$.

Then $q_{\min} = k_i - k_f$, $q_{\max} = k_i + k_f$, $k_i = Mv_i$, and $k_f = [k_i^2 - 2M(\epsilon_n^A + \epsilon_{n'}^B - \epsilon_0^A - \epsilon_0^B)]^{1/2}$. (3)

Using Bethe's[8] integral and some straightforward manipulation, we find

$$\sigma(0, 0-n, n') = (4/v_i^2) \int_{q_{\min}}^{q_{\max}} q^{-3} dq \int_0^{2\pi} d\Phi |I_{0,n}^A(\vec{q})|^2 |I_{0,n'}^B(\vec{q}) - Z_B \delta_{0,n'}|^2, \tag{4}$$

with $$I_{0,n}^S(\vec{q}) = \sum_{i=1}^{Z_S} [\int \psi_0^{S*}(\vec{r}_S) \psi_n^S(\vec{r}_S) e^{i\vec{q} \cdot \vec{r}_{Si}} d\vec{r}_S]. \tag{5}$$

Equation (5) and the corresponding generalized oscillator strength are directly related by[22]

$$f^S(0\text{-}n|\vec{q}) = 2(\epsilon_n^S - \epsilon_0^S) |I_{0,n}^S(\vec{q})|^2 / q^2. \tag{6}$$

The ionization cross section for the projectile is

$$\sigma(0, 0-C, n') \int_0^{\vec{K}_{\max}} \sigma(0, 0-\vec{K}, n') d\vec{K}, \tag{7}$$

where $\vec{K}$ is the wave vector for the ionized electron, $\vec{K}_{\max}$ is determined by conservation of total energy, and

$$\int \psi_{\vec{K}}^{A*}(\vec{r}_A) \psi_{\vec{K}'}^A(\vec{r}_A) d\vec{r}_A = \delta(\vec{K} - \vec{K}'). \tag{8}$$

Total excitation and ionization cross sections for the projectile require summing over all possible final states of the target. Two basic cross sections are required.

The elastic cross section (no excitation of the target) is

$$\sigma_E(0,n) = (4Z_B^2/v_i^2) \int_{q_{\min}}^{q_{\max}} q^{-3} dq \int_0^{2\pi} d\Phi |I_{0,n}^A(\vec{q})|^2 |F_B(q) - 1|^2, \tag{9}$$

with the elastic form factor

$$F_B(q) = \frac{1}{Z_B} \sum_{i=1}^{Z_B} [\int |\psi_0^B(\vec{r}_B)|^2 e^{i\vec{q} \cdot \vec{r}_{Bi}} d\vec{r}_B]. \tag{10}$$

The inelastic cross section,

$$\sigma_I(0,n) = \sum_{n' \neq 0} \sigma(0, 0-n, n') \cong \frac{4Z_B}{v_i^2} \int_{\bar{q}_{\min}}^{\bar{q}_{\max}} q^{-3} dq \int_0^{2\pi} d\Phi |I_{0,n}^A(\vec{q})|^2 S_B(q), \tag{11}$$

with $$S_B(q) = \frac{1}{Z_B} \left[\sum_{j,k=1}^{Z_B} \int |\psi_0^B(\vec{r}_B)|^2 e^{i\vec{q} \cdot (\vec{r}_{Bj} - \vec{r}_{Bk})} d\vec{r}_B - |Z_B F_B(q)|^2 \right], \tag{12}$$

is derived[8] by using the property of completeness of $|\psi_n^B|$ and the approximation that $q_{\min}$ and $q_{\max}$ can be replaced by average values $\bar{q}_{\min}$ and $\bar{q}_{\max}$ for all n'. This assumption is valid over the energy range

of interest for q_{max} and is good for q_{min} at high energy.

The logarithmic mean energy $\epsilon_{Bethe}{}^{B}$, used in Bethe's[23] theory for the stopping power of heavy particles in matter, was substituted as an average excitation energy $\epsilon_{av}{}^{B}$ into Eq. (3) in place of $\epsilon_{n'}{}^{B}$ to calculate $\bar{q}_{min}$ and $\bar{q}_{max}$.

The energy $\epsilon_{Bethe}{}^{B}$ is weighted toward the continuum and tends to underestimate σ_I in the intermediate velocity region. The magnitude of the error depends on the importance of target excitations relative to target ionization in collisions that excite or ionize both atoms. Later, an empirical method of determining $\epsilon_{av}{}^{B}$ from excitation data will be proposed.

The total excitation cross section is

$$\sigma(0,n) = \sigma_E(0,n) + \sigma_I(0,n) \ , \tag{13}$$

and the total ionization cross section is

$$\sigma(0,C) = \int_0^{\vec{K}_{max}} \sigma(0,\vec{K}) d\vec{K} \ . \tag{14}$$

In the limit of high energy $q_{min} \to 0$ and q_{max}, $K_{max} \to \infty$. Thus, the integrals in Eqs. (9), (11), and (14) become independent of energy, and Eqs. (13) and (14) have the asymptotic form

$$\sigma(0,n) \to (Z_B{}^2 C + Z_B D)/v_i{}^2 \ , \quad \sigma(0,C) \to (Z_B{}^2 C' + Z_B D')/v_i{}^2 \ , \tag{15}$$

where C, D, C', and D' are constants depending upon the initial and final states of the projectile and on the elastic and inelastic form factors of the target.

The evaluation of Eq. (5) has been carried out by Bates and Griffing,[2] and an evaluation of $\int d\hat{K} |I_{0,\vec{K}}{}^{H}(\vec{q})|^2$ has been carried out by Landau and Lifschitz,[24] with the results

$$|I_{1s,2s}{}^{H}(q)| = (2^{\frac{17}{2}} q^2)/(4q^2+9)^3 \ , \quad |I_{1s,2p}{}^{H}(q)| = (2^{\frac{15}{2}} 3q)/(4q^2+9)^3 \ ,$$

$$\int d\hat{K} |I_{1s,\vec{K}}{}^{H}(\vec{q})|^2 = \frac{2^8 q^2 [q^2 + \frac{1}{3}(1+K^2)] \exp\{-(2/K)\tan^{-1}[2K/(1+q^2-K^2)]\}}{K[1-\exp(-2\pi/K)][1+(q-K)^2]^3[1+(q+K)^2]^3} \ . \tag{16}$$

The values of $F(q)$ and $S(q)$ for He have been calculated by Kim and Inokuti.[25] All other $F(q)$ values required have been calculated by Cromer and Mann.[26] The $S(q)$ values for Ne, Ar, Kr, and N have been calculated by Cromer and Mann,[27] and those for O and C have been calculated by Cromer.[28]

III. RESULTS AND DISCUSSION

A. Ionization

The current calculated electron-loss cross sections for H in collision with He are in Fig. 1. The earlier calculations of Bates and Williams[3] using a one-parameter variational He($1s^2$) wave function are in reasonable agreement at high and low energies with these more accurate results. The free-electron calculations of Dmitriev and Nikolaev[9] and Victor[10] tend asymptotically to the first Born calculation and are in good agreement with the present results for $E > 200$ keV.

There is excellent agreement between the calculated cross sections and the experimental data for $E > 100$ keV. The disagreement for $E < 100$ keV may be due to the contributions of indirect processes, such as level crossing, to the experimental cross section or due to the presence of H($2s$) in the initial H beam, or due to the effects of distortion and electron exchange.

The first possibility seems unlikely at energies as high as 100 keV, but the second is a distinct possibility and is supported by the large fluctuations among experimental data associated with different methods of initial beam preparation. Calculations for ionization of H($2s$) are in progress, and the discrepancy for $E < 100$ KeV will be discussed further in a future paper.

Distortion, which in the case of excitation[1,29] decreases the first Born cross-section maxima, has previously been suggested[3] as a source of increased ionization in H-He collisions. Electron exchange has been considered[30] in He-H excitation collisions and was found to reduce the first Born maxima for excitation of He(1^1s) to He(2^1s) while increasing the maxima for excitation to He(2^1p).

It is not clear what effect the various corrections to the first Born ionization cross section would have, and an impact-parameter calculation incorporating these improvements would be of great interest.

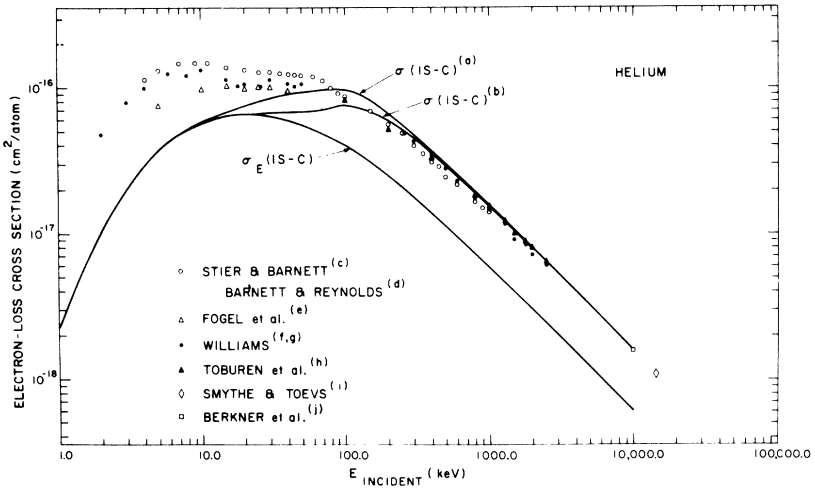

FIG. 1. Electron-loss cross sections for H in collision with He: (a) first Born calculation with ϵ_{av}^{He} = ionization potential of He, (b) first Born calculation with $\epsilon_{av}^{He} = \epsilon_{Bethe}^{He}$, (c) see Ref. 12, (d) see Ref. 13, (e) see Ref. 14, (f) see Ref. 16, (g) see Ref. 17, (h) see Ref. 18, (i) see Ref. 20, (j) see Ref. 19.

The calculations of σ_E and σ_1 for $\epsilon_{av}^{He} = \epsilon_{IP}^{He}$ (first ionization potential) and for $\epsilon_{av}^{He} = \epsilon_{Bethe}^{He}$ show that σ_E dominates the total cross section at low energies, that σ does not depend on ϵ_{Av}^{He} at high energies, and that significant fluctuations in σ, due to the indeterminacy of ϵ_{Av}^{He}, can occur in the intermediate velocity region.

The results for the other rare gases are plotted along with the experimental data in Fig. 2. The difference in slope at low energy is again present, presumably for the same reasons as in He, but the large differences in magnitude – the calculated cross sections being 10–50 times larger than experimental values at 10 keV, and 5–20 times larger than experiment at 100 keV – are at first glance surprising.

Distortion, electron exchange, and coupling to other states modify the first Born cross section in this region of energy, but it is not clear that they decrease the cross section. For H-He ionization it has been suggested that distortion increases[3] the first Born cross section, and the same arguments should apply to the other rare gases.

It may be that the Hartree-Fock calculations of $F(q)$ and $S(q)$ are not accurate enough, but Kim and Inokuti[25] found for He that correlation changed $F(q)$ very little and changed $S(q)$ at most 5%. Bonham,[31] using a highly correlated Ne wave function, also found little change in $F(q)$ and about 15% change in $S(q)$. Since the contribution of σ_I is already underestimated by the use of $\epsilon_{av}^{B} = \epsilon_{Bethe}^{B}$, the possible 15% error in its calculations does not justify decreasing the contribution of σ_I to σ.

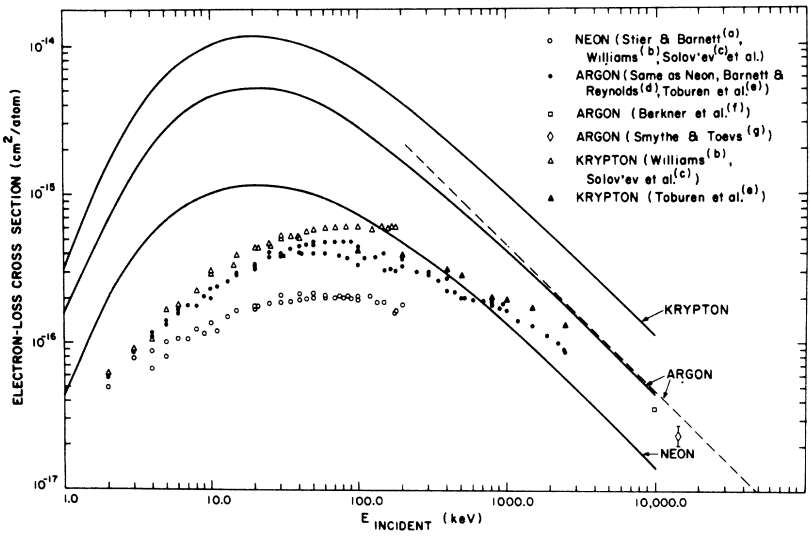

FIG. 2. Electron-loss cross sections for H in collision with Ne, Ar, and Kr: (a) see Ref. 12, (b) see Ref. 16, (c) see Ref. 15, (d) see Ref. 13, (e) see Ref. 18, (f) see Ref. 19, (g) see Ref. 20 – calculation by Victor (Ref. 10).

Equations (9), (11), and (15) show that differences in σ for the three targets are controlled by Z_B, since $F_B(q)$ is quite similar for all three, and suggest the following velocity-dependent scaling model for the target atom, which is independent of the particular projectile and inelastic process involved.

We replace Z_B by

$$\eta_B(v_i) \approx \sum_j N_j^B + \sum_k \alpha_k(v_i) N_k^B , \qquad (17)$$

where N_j^B is the number of electrons in the jth shell of the target with orbital velocity $v_j \ll v_i$, N_k^B is the number of electrons in shell k of atom B with $v_k \approx v_i$, and $\alpha_k(v_i)$ depends on the velocity distribution of the electrons in the kth shell. All electrons with $v \gg v_i$ are assumed to be completely unresolved by the projectile electrons. There is no obvious functional form for $\alpha_k(v_i)$, but as v_i decreases, a smaller fraction of the velocity distribution of the kth shell lies within v_i.

Table II presents a comparison of the values of $\eta_B(v_i)$ determined for Ne, Ar, and Kr by scaling the theoretical electron-loss cross sections to agree with experiment, and qualitative estimates, $\eta_B^{\text{est}}(v_i)$, based on the orbital velocities[32] listed in Table I. The $\eta_B^{\text{est}}(v_i)$'s are used merely to show the variation with v_i and the relative size of the scaling parameter. Considering the qualitative nature of the model and the variations in experimental data, the agreement in Table II is encouraging. In particular, the decrease of $\eta_B(v_i)$ with decreasing v_i and the increase for a given v_i in $\eta_B(v_i)$ with heavier B are expected. The upturn in $\eta_B(v_i)$ for $v_i < 0.5$ a.u. may be due to the low-energy effects mentioned earlier for He.

TABLE I. Average orbital velocities in a.u.

	Ne	Ar	Kr
ν_{1s}	8.1	15.4	32.3
ν_{2s}	2.0	5.0	11.8
ν_{2p}	1.3	4.4	11.2
ν_{3s}		1.6	4.7
ν_{3p}		1.0	4.1
ν_{3d}			3.3
ν_{4s}			1.5
ν_{4p}			1.0

The model neglects specific corrections to the first Born approximation, such as distortion, electron exchange, and coupling to other states, all of which depend on the particular projectile and inelastic process involved in the scattering, and it attempts to determine an over-all correction to the description of the target atom depending only on the incident velocity of the projectile.

The calculated electron-loss cross sections for C, N, and O targets are presented in Fig. 3. The experimental data for N_2 and O_2 were divided by 2 for comparison with the calculated values, and the experimental cross sections for C were estimated[18] by applying the rule of additivity – the molecular cross section is the sum of its constituent atomic cross sections – to the measured values for CO, CO_2, H_2, CH_4, C_2H_6, and C_4H_{10}.

The comparisons between calculation and experiment are similar to those for the rare gases in Fig. 2, although the calculated values for O at

TABLE II. Estimated and empirical velocity-dependent scaling factors for Ne, Ar, and Kr.

E (keV)	v_i (a.u.)	η_{Ne}^{est}	η_{Ne}	η_{Ar}^{est}	η_{Ar}	η_{Kr}^{est}	η_{Kr}
2.25	0.3	< 6	4.7	< 6	5.1	< 6	6.7
4.00	0.4	< 6	3.8	< 6	4.2	< 6	5.7
6.25	0.5	< 6	3.5	< 6	4.0	< 6	5.6
9.00	0.6	< 6	3.6	< 6	4.0	< 6	6.0
12.25	0.7	< 6	3.6	< 6	4.2	< 6	6.3
16.00	0.8	< 6	3.8	< 6	4.4	< 6	6.5
20.25	0.9	< 6	3.9	< 6	4.8	< 6	7.0
25.00	1.0	< 6	4.0	< 6	5.0	< 6	7.3
30.25	1.1	< 6	4.2	< 6	5.1	< 6	7.8
36.00	1.2	< 6	4.3	< 6	5.4	< 6	8.1
42.50	1.3	< 6	4.4	< 6	5.6	< 6	8.5
49.00	1.4	< 6	4.6	< 6	5.8	< 6	8.8
56.25	1.5	< 6	4.7	~6	6.1	~6	9.2
100.00	2.0	~6	5.2	< 8	6.8	~8	9.9
200.00	2.83	< 8	6.2	~8	8.3	> 8	12.6

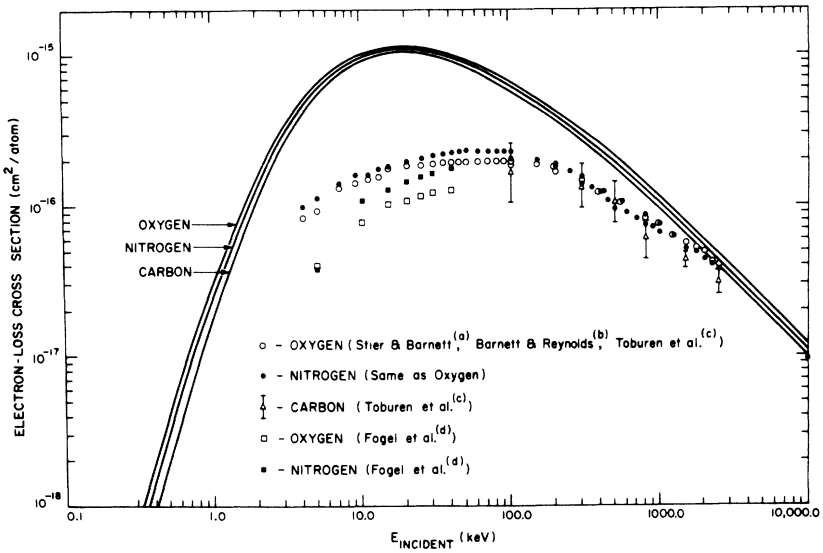

FIG. 3. Electron-loss cross sections for H in collision with C, N, and O: (a) see Ref. 12, (b) see Ref. 13, (c) see Ref. 18, (d) see Ref. 14.

14.6 MeV and for N at 10.0 and 14.6 MeV are within 15% of the experimental results of Berkner, Kaplan, and Pyle[19] and of Smythe and Toevs,[20] while the Ar calculation is off by 25% at 10.0 MeV. This is consistent with the model because the ν_{1s} for N and O (5.6 and 6.4 a.u., respectively) are much less than v_i at 10.0 and 14.6 MeV (20.0 and 24.2 a.u., respectively), while $\nu_{1s} = 15.0$ a.u. for Ar. A combination of errors in the experiment, errors in $S(q)$, and the effects of molecular binding would explain the O and N discrepancies, but η_B is needed to explain the Ar discrepancy. The N electron-loss cross sections exceed the O cross sections for $E < 500$ keV. This could be explained by the model if $(\eta_O/\eta_N)^2 < \frac{64}{49}$, but it might also be due to the use of $|\langle F_0(p)\rangle_{av}|^2$ rather than $\langle |F_0(q)|^2\rangle_{av}$. The error is only in the contribution of the single $2p$ electron outside the half-filled shell, but it increases with decreasing energy where, according to the velocity-dependent scaling model, the $2p$ orbitals are responsible for most of the scattering. The correction for this error could be incorporated into the target parameter η_O.

B. Excitation

Calculated and experimental values for $\sigma(1s\text{-}2s)$, $\sigma(1s\text{-}2p)$, and the sum of the two, $\sigma(1s\text{-}2s, 2p)$, for the excitation of H(1s) by He are shown in Fig. 4. The calculated values of $\sigma(1s\text{-}2s, 2p)$ are in excellent agreement with the experimental results of Ankudinov, Andreev, and Orbeli.[33] The data of Dose, Gunz, and Meyer[34] and of Ankudinov *et al.*[33] for $\sigma_{expt}(1s\text{-}2p)$ bracket $\sigma(1s\text{-}2p)$, but $\sigma_{expt}(1s\text{-}2s)$ and $\sigma(1s\text{-}2s)$ are in definite disagreement. This disagreement may be due to the neglect of distortion, for Flannery[29] has found that

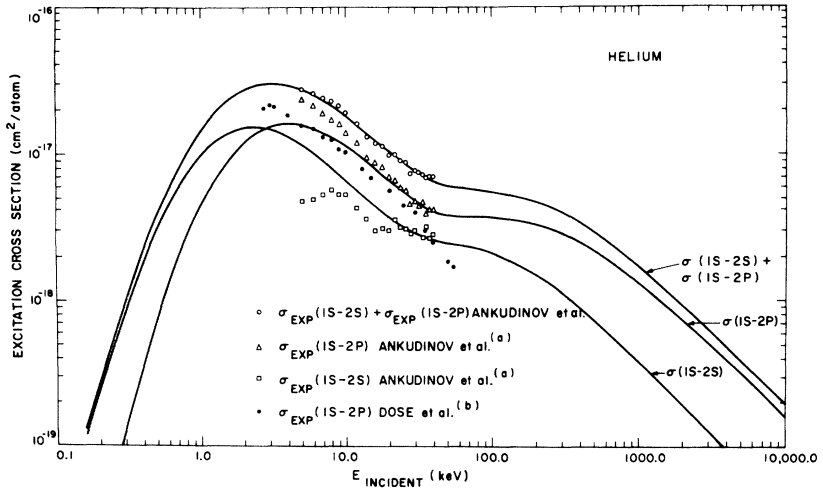

FIG. 4. Excitation cross sections for H in collision with He: (a) see Ref. 33, (b) see Ref. 34.

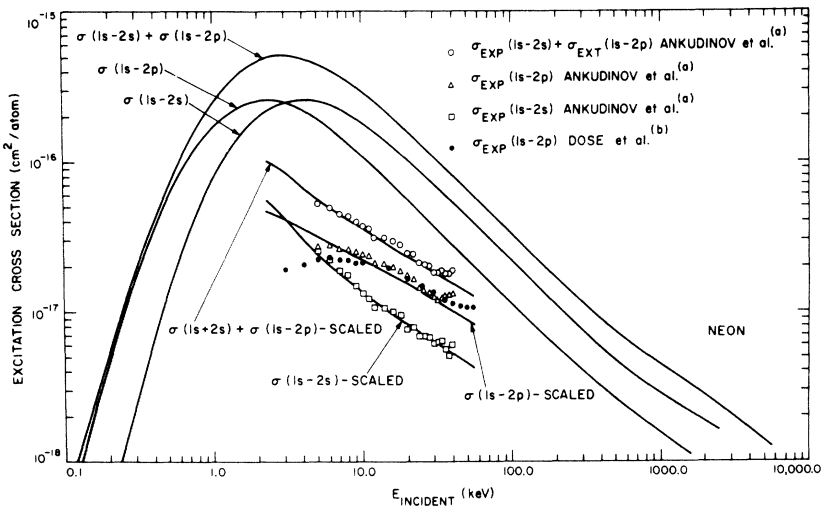

FIG. 5. Excitation cross sections for H in collision with Ne: (a) see Ref. 33, (b) see Ref. 34.

distortion decreases first Born cross-section maxima for both $\sigma(1s\text{-}2s)$ and $\sigma(1s\text{-}2p)$ when H is the target; but, considering the excellent agreement found for the sum of the two cross sections, and the fact that the experiment measures $\sigma_{\text{expt}} \times (1s\text{-}2s, 2p)$ and $\sigma_{\text{expt}}(1s\text{-}2p)$, accidental mixing of $H(2s)$ and $H(2p)$ final states by stray electric fields may also have occurred.

An interesting feature of the data is their leveling off for $E > 30$ keV. This can be attributed to the onset of significant contributions to σ from σ_I. It is observed to occur at slightly higher energy in the theoretical calculations. Bates and Griffing[2] previously noted the effect in their calculations for the H-H system. This phenomenon is readily observable in excitation cross sections where σ_E peaks at a low energy, but less so in ionization cross sections, which tend only to broaden (see Fig. 1). Given accurate excitation cross sections in the energy region where the leveling appears, the target-gas parameter ϵ_{av}^{B} could be determined empirically so that the theoretical cross sections $\sigma_E + \sigma_I$ reproduce the measured values. The average excitation energy of the target is probably insensitive to the projectile and probably insensitive to the particular process. Accordingly, the semiempirical calculations may well provide accurate predictions of the cross sections for a wide range of processes.

The excitation cross sections for $H(1s)$ in collision with Ne, Ar, and Kr, both scaled and unscaled, are compared with experimental results in Figs. 5–7.

The scaled calculations for a Ne target are in good agreement with experiment for $\sigma(1s\text{-}2s)$, $\sigma(1s\text{-}2p)$, and $\sigma(1s\text{-}2s, 2p)$, although again the agreement is less good with the data of Dose

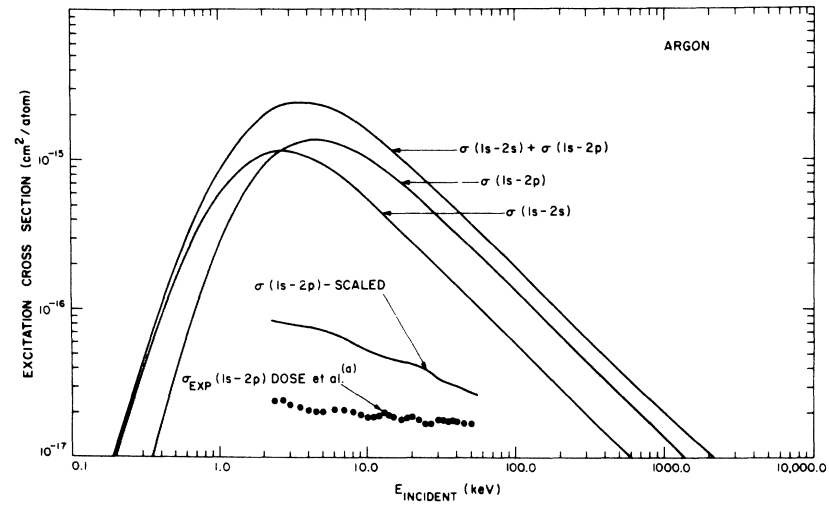

FIG. 6. Excitation cross sections for H in collision with Ar: (a) see Ref. 34.

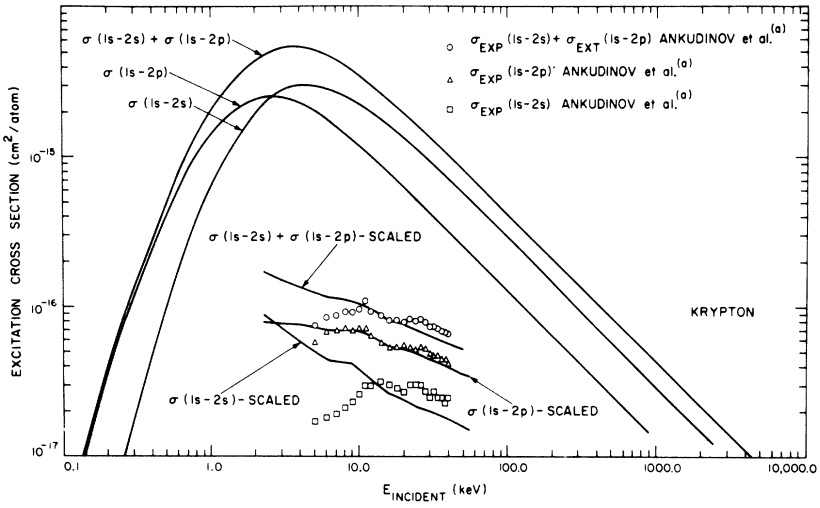

FIG. 7. Excitation cross sections for H in collision with Kr: (a) see Ref. 33.

et al.[34] The breakdown in the determination of η_B for low energies (see Table II) is apparent in the lack of maxima in the scaled calculations. The leveling off of the experimental data at high energy is again observed, but the calculated results do not show the same effect. This implies that $\epsilon_{\text{Bethe}}^{\text{Ne}}$ is too large a value for $\epsilon_{\text{av}}^{\text{Ne}}$.

The scaled calculations for Ar do not agree well with the experimental values of Dose *et al.*[34] Further experimental measurements would be instructive.

The scaled calculations for Kr show fair agreement for $E > 10$ keV, although again the breakdown in the determination of η_B at low energies occurs. The Ar and Kr data both show the possibilities of oscillations that are not present in the first Born calculations. Whether these are molecular effects, as Dose *et al.* suggest,[34] or velocity-dependent variations in the polarization of the emitted radiation is not clear.

C. Conclusions

Good agreement between first Born wave cross sections and experimental data down to 5-keV incident energy was found for excitation of H(1*s*) by He.

Velocity-dependent scaling parameters were determined for Ne, Ar, and Kr target atoms by fitting calculated first Born electron-loss cross sections for H projectiles to experimental data. These parameters were used to scale first Born excitation cross sections for H(1*s*) scattered by Ne, Ar, and Kr. Good agreement was found with experiment for Ne and Kr, but the Ar results were approximately three times greater than the experimental data.

The range of applicability of the scaling model is not known, but for H-rare-gas collisions it appears that the empirical determination of ϵ_{av}^{B} and $\eta_B(v_i)$ for a given target B allows one to obtain cross sections for the collision system quite accurately from scaled first Born approximation calculations.

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[1]D. R. Bates, in Atomic and Molecular Processes, edited by D. R. Bates (Academic Press Inc., New York, 1962), Chap. 14.

[2]D. R. Bates and G. W. Griffing, Proc. Phys. Soc. (London) A66, 961 (1953); A67, 663 (1954); A68, 90 (1955).

[3]D. R. Bates and A. Williams, Proc. Phys. Soc. (London) A70, 306 (1957).

[4]B. L. Moiseiwitsch and A. L. Stewart, Proc. Phys. Soc. (London) A67, 1069 (1954).

[5]J. Adler and B. L. Moiseiwitsch, Proc. Phys. Soc. (London) A70, 117 (1957).

[6]T. A. Green, Phys. Rev. 157, 103 (1967).

[7]E. N. Lassettre and E. A. Jones, J. Chem. Phys. 40, 1222 (1964).

[8]N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Clarendon Press, Oxford, 1965), 3rd ed., pp. 87, 493.

[9]I. S. Dmitriev and V. S. Nikolaev, Zh. Eksperim. i Teor. Fiz. 44, 660 (1963) [English transl.: Soviet Phys. – JETP, 17, 447 (1963)].
[10]G. A. Victor, Phys. Rev. (to be published).
[11]S. K. Allison, Rev. Mod. Phys. 30, 1137 (1958).
[12]P. M. Stier and C. F. Barnett, Phys. Rev. 103, 896 (1956).
[13]C. F. Barnett and H. K. Reynolds, Phys. Rev. 109, 355 (1958).
[14]Ia. M. Fogel', V. A. Ankudinov, D. V. Pilipenko, and N. V. Topolia, Zh. Eksperim. i Teor. Fiz. 34, 579 (1958) [English transl.: Soviet Phys. – JETP 7, 400 (1958)].
[15]E. S. Solov'ev, R. N. Il'in, V. A. Oparin, and N. V. Fedorenko, Zh. Eksperim. i Teor. Fiz. 42, 659 (1962) [English transl.: Soviet Phys. – JETP 15, 459 (1962)].
[16]J. F. Williams, Phys. Rev. 153, 116 (1967).
[17]J. F. Williams, Phys. Rev. 157, 97 (1967).
[18]L. H. Toburen, M. Y. Nakai, and R. A. Langley, Phys. Rev. 171, 114 (1968).
[19]K. H. Berkner, S. N. Kaplan, and R. V. Pyle, Phys. Rev. 134, A1461 (1964).
[20]R. Smythe and J. W. Toevs, Phys. Rev. 139, A15 (1965).
[21]L. M. Welsh, K. H. Berkner, S. N. Kaplan, and R. V. Pyle, Phys. Rev. 158, 85 (1967).
[22]N. F. Mott and H. S. W. Massey, The Theory of Atomic Collisions (Clarendon Press, Oxford, 1965), 3rd ed., p. 478.
[23]A. Dalgarno, in Atomic and Molecular Processes, edited by D. R. Bates (Academic Press Inc., New York, 1962), Chap. 15.
[24]L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Pergamon Press, Inc., Oxford, 1965), 2nd ed., p. 579
[25]Y.-K. Kim and M. Inokuti, Phys. Rev. 165, 39 (1968).
[26]D. T. Cromer and J. B. Mann, Los Alamos Scientific Laboratory Report No. LA-3816, 1968.
[27]D. T. Cromer and J. B. Mann, J. Chem. Phys. 47, 1892 (1967).
[28]D. T. Cromer (private communication).
[29]M. R. Flannery, Phys. Rev. (to be published).
[30]D. R. Bates and D. S. F. Crothers, Proc. Phys. Soc. (London) 90, 73 (1967).
[31]R. A. Bonham (private communication).
[32]E. Clementi, IBM J. Res. Develop., Suppl. 9, 2 (1965).
[33]V. A. Ankudinov, E. P. Andreev, and A. L. Orbeli, in Proceedings of the Fifth International Conference on the Physics of Electronic and Atomic Collision, edited by I. P. Flaks (Publishing House "Nauka", Leningrad, USSR, 1967), p. 312.
[34]V. Dose, R. Gunz, and V. Meyer, Helv. Phys. Acta 41, 269 (1968).