PHYSICAL REVIEW A VOLUME 46, NUMBER 11 1 DECEMBER 1992

Elastic scattering of hydrogen atoms at low temperatures

M. J. Jamieson,* A. Dalgarno, and J. N. Yukich†
Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138

(Received 1 June 1992)

The elastic scattering of two hydrogen atoms interacting at very small energies is explored numerically using the most accurate potential-energy curves available for the $X\,^1\Sigma_g^+$ and $b\,^3\Sigma_u^+$ states of H_2. The scattering lengths and low-temperature-averaged cross sections are determined and compared with previous calculations. The scattering lengths are $0.41a_0$ for the singlet case and $1.91a_0$ for the triplet. The predicted total triplet cross section at 2 K is 5.5×10^{-15} cm^2 but it could be lower, at 4.8×10^{-15} cm^2, with a different fit to the triplet potential between $12a_0$ and $15a_0$. A more accurate triplet-state potential is needed at these separations.

PACS number(s): 34.40.+n

I. INTRODUCTION

Recent developments in low-temperature physics, such as the study of Bose gases [1,2], have renewed interest in H-H scattering. Atomic hydrogen can be described at low temperatures as a dilute hard-sphere Bose gas and low-temperature scattering data provide a criterion for finding an upper limit to the densities for which the model is valid [1]. There is also a long-standing application of low-temperature spin-change scattering in astrophysics [3]. In the scattering process, the atoms interact via the potentials of the lowest single ($X\,^1\Sigma_g^+$) and triplet ($b\,^3\Sigma_u^+$) states of the hydrogen molecule. The triplet potential is appropriate for the Bose-gas model. These potentials have been studied in detail and incrementally improved over the past three decades [4–8]. Cross sections used in diffusion and viscosity calculations [9,10] and for spin change have been evaluated [11,12] with the 1965 potentials of Kolos and Wolniewicz (KW65) [4]. The scattering lengths, which enable the zero-energy limits of the cross sections to be inferred, have been calculated [1] for the triplet state with an analytic (Silvera) fit to the KW65 triplet modified by the 1974 improvement (KW74) [5]. (Note that the coefficient of the second exponential term in the Silvera fit is printed with the wrong sign in Ref. [1].) The low-energy limits of the cross sections are sensitive to the potential; the inclusion of the KW74 improvement caused significant changes. Koyama and Baird [13] incorporated a further improvement (KW75) [6] to the singlet potential and then calculated scattering lengths, effective ranges, and spin-change cross sections. Recently there have been new calculations of the singlet [7] and triplet [8] potentials and corrections to the singlet potential arising from nuclear motion and relativistic effects have been obtained [14,15]. The experimental measurement [2] of the cross sections at low temperatures suggests the need for a numerical reevaluation of the theoretical predictions of low-temperature scattering properties, to be made with the latest representations of the potentials.

We present calculations for the scattering lengths and give a comparison of the temperature-averaged diffusion, viscosity, and spin-change cross sections with earlier results. For the singlet potential we used the Born-Oppenheimer potential of Kolos, Szalewicz, and Monkhorst (KSM86) [7] and obtained results with and without the nuclear motion and relativistic corrections [14,15]. Frye, Lie, and Clementi [8] demonstrated that although their triplet potential (FLC89) is slightly better at long and short range than the combination of KW65 and KW74, nevertheless the Kolos-Wolniewicz potentials are very precise. We used both to explore the effect of the improvement FLC89.

We fitted the potentials at long range to the form given by Kolos [16], which is reliable at internuclear distances R greater than $15a_0$ [16]. The tabulated potentials [5,7,8] are given out to $12a_0$. The long-range part of the singlet potential is relatively unimportant and we made the fit at $12a_0$ by adjusting the coefficient of R^{-6}. The triplet potential has a shallow well starting at $R=7a_0$ with a maximum depth at around $R=8a_0$ and extending beyond $R=12a_0$. We made a fit between $12a_0$ and $15a_0$. We found that the scattering length was quite sensitive to the details of the fit so that there is a need for accurate calculations of the triplet potential in this range. We examined the effect of including the R^{-11} term of Chan and Dalgarno [17] in the triplet potential.

II. THEORY

The radial part $u_l(R)$ of the lth partial wave is the solution, finite at the origin, of the differential equation

$$[d^2/dR^2-l(l+1)/R^2+2\mu/\hbar^2\{E-V(R)\}]\{Ru_l(R)\}=0\ , \qquad (1)$$

with boundary condition, at large R,

$$u_l(R)\simeq R^{-1}\sin(kR-l\pi/2+\eta_l)\ , \qquad (2)$$

where μ is the reduced mass, E is the energy of relative motion, $V(R)$ is the (asymptotically vanishing) interatomic potential, $k=\sqrt{2\mu E}/\hbar$ is the wave number, and η_l is the phase shift that also satisfies the integral equation for the normalization (2),

TABLE I. Quantities for Eqs. (4) and (5).

Type	f	θ_1	θ_2	ω_1 (l even)	ω_2 (l even)	ω_1 (l odd)	ω_2 (l odd)	p
total	$2l+1$	η_l^s	η_l^t	$\frac{1}{8}$	$\frac{9}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	1
diffusion	$l+1$	$\eta_{l+1}^s-\eta_l^s$	$\eta_{l+1}^t-\eta_l^t$	$\frac{1}{8}$	$\frac{9}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	2
viscosity	$\frac{l+1)(l+2)}{(2l+3)}$	$\eta_{l+2}^s-\eta_l^s$	$\eta_{l+2}^t-\eta_l^t$	$\frac{1}{8}$	$\frac{9}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	3
spin change	$2l+1$	$\eta_l^s-\eta_l^t$		$\frac{3}{32}$	0	$\frac{3}{16}$	0	1

$$\sin\eta_l = \frac{-2\mu}{\hbar^2}\int_0^\infty R^2 j_l(kR)V(R)u_l(R)dR \ , \tag{3}$$

where $j_l(kR)$ denotes the regular spherical Bessel function. We solved Eq. (1) by Numerov's method [18] and Eq. (3) provided a useful check. The singlet and triplet potentials produce phase shifts on which the cross sections depend [9,10].

The total, diffusion, and viscosity cross-section formulas [10] require modification to include nuclear symmetry effects because the colliding atoms are identical; the necessary changes are detailed for general spin by Hirschfelder, Curtiss, and Bird [9]. The cross section for spin change has been given by Dalgarno [19] and modified to include nuclear symmetry by Smith [20]. The cross sections can be summarized by

$$\sigma = \frac{4\pi}{k^2}\sum_l f(l)(\omega_1\sin^2\theta_1+\omega_2\sin^2\theta_2) \ , \tag{4}$$

where the quantities to be summed are given in Table I. Of interest are the cross sections averaged over a Maxwellian distribution at temperature T,

$$\langle\sigma(T)\rangle = (kT)^{-(p+1)}\int_0^\infty \sigma(E)E^p\exp(-E/kT)dE \ , \tag{5}$$

where the values of p are shown in Table I and k is Boltzmann's constant. The diffusion and viscosity integrals are proportional to the collision integrals of transport theory [9]. The rate coefficient for the change of hyperfine-state quantum number F from 1 to 0 is given by [12,20]

$$\mathcal{R}(1-0) = \tfrac{1}{3}\left[\frac{8kT}{\pi\mu}\right]^{1/2}\langle\sigma_{\text{sp}}(T)\rangle \ , \tag{6}$$

the subscript indicating the spin-change cross section. We evaluated the integrals (5) by the generalized Gauss-Laguerre quadrature formula [18], described in more detail in the Appendix. At small energies or wave numbers the phase shifts are given by effective range expansions [10] and the $l=0$ contribution dominates the cross sections. Hence the low-energy scattering is described by the $l=0$ scattering length a and the effective range r and $\cot\eta_0$ may be expanded in the form

$$k\cot\eta_0 = -\frac{1}{a}+\frac{1}{2}rk^2+\cdots \ . \tag{7}$$

We determined these parameters by numerically fitting the phase shifts at small k to Eq. (7).

III. RESULTS AND DISCUSSION

The temperature-averaged cross sections for diffusion and viscosity, calculated using the potentials described earlier (KSM86, including the relativistic and nuclear-motion correction for the singlet, and FLC89 for the triplet) are shown in Table II. Comparison with previous results of Allison and Smith [11] shows that use of the present potentials has a slightly larger effect on the diffusion than on the viscosity cross sections. The previous results [11] did not include the relativistic and nuclear motion corrections, but in a separate calculation, we found that these corrections changed the cross sections by less than 0.25% over the range of temperatures quoted. We found also, in a comparison with calculations using the KW65 and KW74 triplet potentials, that the improvement FLC89 increases these cross sections by about 10% at the lower temperatures but has little effect above 6 K. We see below that there is a more substantial change to the low-energy limits of the cross sections.

The rate coefficients $\mathcal{R}$(1-0) for spin change are shown in Table III. We found in separate calculations that the improvement FLC89 increases these cross sections substantially (by a factor of 3) at 1 and 2 K, makes little difference at 6 K, and reduces the cross sections by about 8% at 8 K. We also found in separate calculations increases of around 18% due to the relativistic and

TABLE II. Temperature-averaged cross sections (10^{-16} cm^{-2}).

Temperature (K)	Diffusion	Diffusion[a]	Viscosity	Viscosity[a]
1	94.5	89.8	199	186.7
2	98.3	97.0	224	220.7
4	90.2	90.56	211	212.5
6	83.6	84.15	196	197.3
8	80.5	80.45	188	191.5

[a] Reference [11].

TABLE III. Rate coefficients for spin change.

Temperature (K)	$\mathcal{R}(1\text{-}0)$ (10^{14} cm^3 s^{-1})	$\mathcal{R}(1\text{-}0)$ (10^{14} cm^3 s^{-1})[a]
1	23.6	2.2
2	23.6	4.2
4	24.9	18
6	42.0	51
8	93.3	120

[a] Reference [12].

TABLE V. Scattering lengths and effective ranges in units of a_0 for various interaction potentials for (a) singlets and (b) triplets.

Potentials	Scattering length	Effective range
	(a) Singlet	
KW65,74 [4,5]	0.32 [22]	
	0.595 [13]	1820
KSM86[a] [7]	0.5425	2300
KSM86[b] [7]	0.4109	4120
	(b) Triplet	
KW65,74 [4,5]	1.36[c] [1]	
	1.370[c] [24]	
	1.335 [24]	323 [24]
	1.36[c] [22]	
	1.339 [25]	327 [25]
	1.34 [26]	
	1.34 [13]	302 [13]
FLC89[d]	1.91	120

[a] Without relativistic and adiabatic corrections.

[b] With relativistic and adiabatic corrections.

[c] Silvera analytic fit.

[d] Based on FLC89 (with the smooth fit of Fig. 1) from Ref. [8].

nuclear-motion corrections at the lower temperatures, but the differences fell rapidly with increasing temperature.

A variety of cross sections occurs in the analysis of spin-exchange frequency shifts in hydrogen masers [21,22]. It may be valuable to present our values for them, though only graphical values are available, so a useful comparison is not possible. In what Koelman *et al.* [22] call the degenerate internal-states approximation, the cross sections are

$$\lambda_0=\frac{\pi}{2k^2}\sum_{\text{even}\,l}(2l+1)\sin(2\eta_l^t-2\eta_l^s)\ , \tag{8}$$

$$\sigma_1=\frac{\pi}{k^2}\sum_{l}(-)^l(2l+1)\sin^2(\eta_l^s-\eta_l^t)\ , \tag{9}$$

$$\sigma_2=\frac{\pi}{k^2}\sum_{\text{odd}\,l}(2l+1)\sin^2(\eta_l^s-\eta_l^t)\ . \tag{10}$$

We present the thermally averaged cross sections corresponding to $p=1$ in Eq. (5) for temperatures up to 6 K in Table IV. Allison [23] reported a value of -27.3×10^{-16} cm^2 at 10 K for a quantity λ_+, equivalent to $-4\lambda_0$ of Eq. (8). Our corresponding value is -14.4×10^{-16} cm^2.

There have been many previous calculations of scattering lengths and effective ranges for the $l=0$ partial waves. Table V(a) lists the results of Friend and Etters [1], Koelman *et al.* [22], Koyama and Baird [3], and those we obtained. The inclusion of the nuclear-motion and relativistic corrections has a substantial effect. Together with the small improvement in the adiabatic interaction potential in KSM86 the corrections change the singlet scattering length from $0.595a_0$ to $0.4109a_0$ and the effective range from $1820a_0$ to $4120a_0$.

Table V(b) lists the results of Friend and Etters [1], Uang and Stwalley [24], Gutiérrez, de Llano, and Stwalley [25], Lhuiller [26], Koelman *et al.* [22], and those we obtained. The triplet interaction potential has to be fitted in the region between the tabulated points of $12a_0$ and $15a_0$. Beyond $15a_0$ the asymptotic long-range form $V_L(R)$ [16,17] is adequate. Uang and Stwalley [24] noted that the KW74 potential fits the long-range form of Hirschfelder and Meath [27] at $12a_0$ and they used this long-range potential for all interatomic separations exceeding $12a_0$. The FLC89 potential differs considerably from the KW74 potential at $12a_0$ and cannot be matched to any of the long-range forms [16,17,27]. We made a fit with a continuous derivative by modifying the cubic-spline approximation between $12a_0$ and $15a_0$. This smooth potential is illustrated in Fig 1, is tabulated in Table VI, and was used in our results presented in the various tables. In the absence of data on the potential between $12a_0$ and $15a_0$ it is possible to construct other plausible smooth-looking fits. We also tried a fit for all interatomic separations greater than $12a_0$ with the expression

TABLE IV. Thermally averaged cross sections (10^{-17} cm^2) defined in Eqs. (8)–(10) as functions of temperature T.

T (K)	λ_0	σ_1	σ_2
0	$-\infty$	19.7	0
1	-102	8.08	0.370
2	-54.1	5.00	0.503
4	-14.9	2.89	0.653
6	7.61	2.17	1.51

TABLE VI. Smooth fit triplet potential.

Interatomic distance (a_0)	Potential (10^{-6} a.u.)
12.0	-1.77
12.5	-1.34
13.0	-1.14
13.5	-0.980
14.0	-0.852
14.5	-0.726
15.0	-0.624

TABLE VII. Accumulated scattering length (in a_0) for the triplet potential from Eq. (3)

R (a_0)	Smooth (Fig. 1)	$d=0$ (Fig. 2)	$d=2$ (Fig. 2)
4	0.31	0.32	0.33
5	3.02	3.07	3.15
6	7.01	7.12	7.31
7	8.30	8.44	8.66
10	5.07	5.16	5.30
12	3.85	3.91	4.01
15	3.02	2.85	2.80
20	2.38	2.20	1.87
30	2.05	1.87	1.47
40	1.96	1.78	1.39
50	1.93	1.76	1.36
60	1.92	1.74	1.35

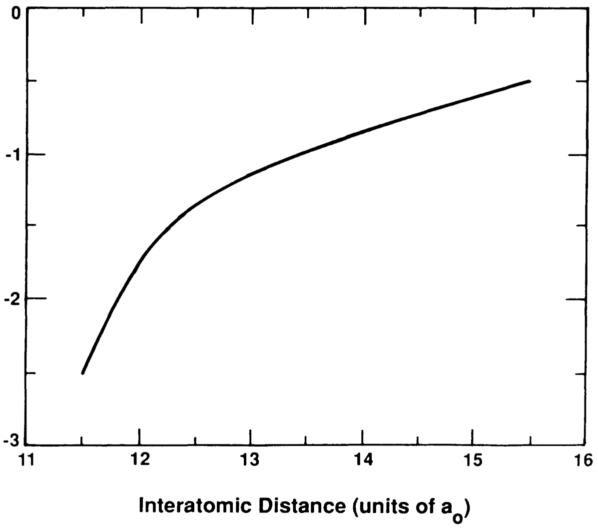

FIG. 1. The adopted ${}^3\Sigma_u^+$ potential between $12a_0$ and $15a_0$.

$$V(R)=V_L(R)+\{V_T(12)-V_L(R)\}\exp\{-(R-12)/d\}\ , \tag{11}$$

where $V_t(12)$ denotes the tabulated value and d is an arbitrary damping constant. We included in $V_L(R)$ the R^{-11} term of Chan and Dalgarno [17], but its effect is negligible. We illustrate in Fig. 2 the interaction potentials (11) for values of damping constant ranging from $0a_0$ to $3a_0$. The potential with no damping is discontinuous at $12a_0$. The fit (11) ensures that for any positive damping there is no discontinuity and the long-range form is correct; however, the derivative is discontinuous at $12a_0$. The scattering length is very sensitive to the potential. With the smooth fit it is $1.91a_0$ and with the fit (11) it changes from $1.73a_0$ to $0.667a_0$ as the damping constant d varies from $0a_0$ to $3a_0$. For $d=2a_0$ the scattering length is $1.33a_0$ with effective range $305a_0$ in good, but misleading, agreement with the published values quoted in Table V(b). There is a need for an accurate potential between $12a_0$ and $15a_0$.

The sensitivity of the scattering length and the corresponding low-energy cross sections to the triplet potential arises from the presence of the shallow well. In Table VII we show the incremental contributions to the triplet scattering length a_t by using the integral formula (3) for $ka_0=10^{-3}$, and the FLC89 potential with the smooth fit and also with the fit (11) for $d=0a_0$ and $2a_0$. The contribution is largest around $R=7a_0$, where the integrand changes sign corresponding to the left-hand side of the well. Cancellation makes the scattering length ill-conditioned toward small changes in the potential and enhances the importance of the integrand at long range.

A measurement of the total triplet scattering cross section has been carried out by Hershcovitch [2] at 2 K. We present in Table VIII the partial cross sections

$$\sigma_l=\frac{4\pi}{k^2}(2l+1)\sin^2_{\eta_l}\ , \tag{12}$$

for singlet and triplet scattering at low energies E. With increasing E the $l=0$ cross sections grow rapidly as do the cross sections for the higher partial waves. The agreement of the singlet and triplet cross sections for $l=2$ is fortuitous.

Table IX presents the thermally averaged values of the total scattering cross sections

TABLE VIII. Partial cross sections $\sigma_l(E)$ (10^{-16} cm^2) for singlet and triplet scattering as functions of relative energy E.

l	Singlet			Triplet		
E(10^{-6} a.u.)	0	1	2	0	1	2
0	0.59	0.00	0.00	12.6	0.00	0.00
1	2.83	0.30	0.00	17.3	0.21	0.00
2	5.35	0.84	0.01	20.8	0.54	0.01
3	7.93	1.37	0.02	23.8	0.84	0.02
4	10.4	1.80	0.05	26.5	1.05	0.05
5	12.8	2.10	0.08	28.7	1.16	0.08
6	15.1	2.26	0.12	30.8	1.19	0.12
7	17.2	2.31	0.17	32.5	1.15	0.17
8	19.1	2.25	0.23	34.1	1.05	0.23

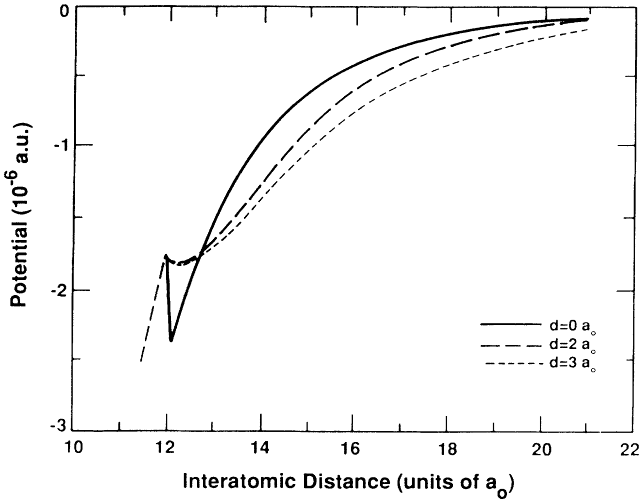

FIG. 2. The ${}^3\Sigma_u^+$ potential between $10a_0$ and $20a_0$ using the fit in Eq. (11) with $d=0$, $2a_0$, and $3a_0$.

$$\sigma_s = \frac{1}{2}\frac{4\pi}{k^2}\sum_{\text{even}\, l}(2l+1)\sin^2\eta_l + \frac{3}{2}\frac{4\pi}{k^2}\sum_{\text{odd}\, l}(2l+1)\sin^2\eta_l\ , \tag{13}$$

$$\sigma_t = \frac{3}{2}\frac{4\pi}{k^2}\sum_{\text{even}\, l}(2l+1)\sin^2\eta_l + \frac{1}{2}\frac{4\pi}{k^2}\sum_{\text{odd}\, l}(2l+1)\sin^2\eta_l\ , \tag{14}$$

as functions of temperature. The cross sections at $T = 2K$ are considerably larger than the zero-temperature limits.

With the smooth potential of Fig. 1 at 2 K the triplet cross section is 5.5×10^{-15} cm^2. With the fit (11) and a damping factor d of $2a_0$ the cross section is 5.0×10^{-15} cm^2. For $d=0a_0$, the cross section is 5.3×10^{-15} cm^2 and for $d=3a_0$ it is 4.8×10^{-15} cm^2. The measured value is probably close to but below 1×10^{-14} cm^2 [2]. The agreement is acceptable. A more accurate triplet potential is needed to limit the theoretical uncertainty.

APPENDIX: GENERALIZED GAUSS-LAGUERRE QUADRATURE

We summarize the generalized Gauss-Laguerre quadrature, which we used to evaluate integrals (5), because it is less well known than the ordinary Gauss-Laguerre formula. It allows exactly for the exponentials and the power terms of the integrands and can be used when there are no important regions where the cross sections

TABLE IX. Thermally averaged total singlet and triplet cross section (10^{-16} cm^2) as functions of temperature.

$T(K)$	Singlet	Triplet	Mean
0	0.297	18.8	14.2
1	9.71	44.8	36.0
2	14.0	54.6	44.4
4	21.1	60.6	50.7
6	29.0	60.6	52.7
8	37.5	59.1	53.7

TABLE X. Weights and pivots for generalized Gauss-Laguerre quadrature.

p	n	Weight	Pivot
1	3	0.588 681 48	0.935 822 23
		0.391 216 06	3.305 407 29
		0.020 102 46	7.758 770 48
1	4	0.446 870 59	0.743 291 93
		0.477 635 77	2.571 635 01
		0.074 177 78	5.731 178 75
		0.001 315 85	10.953 894 31
1	5	0.348 014 54	0.617 030 85
		0.502 280 67	2.112 965 96
		0.140 915 92	4.610 833 15
		0.008 719 89	8.399 066 97
		0.000 068 97	14.260 103 07
1	6	0.277 650 14	0.527 668 12
		0.493 910 58	1.796 299 81
		0.203 004 30	3.876 641 52
		0.024 668 82	6.918 816 57
		0.000 763 04	11.234 610 43
		0.000 003 12	17.645 963 55
2	3	1.037 494 96	1.517 387 08
		0.905 750 00	4.311 583 13
		0.056 755 03	9.171 029 79
2	4	0.725 525 00	1.226 763 26
		1.063 424 29	3.412 507 36
		0.206 696 13	6.902 692 61
		0.004 354 58	12.458 036 77
2	5	0.520 917 40	1.031 109 14
		1.066 705 93	2.837 212 82
		0.383 549 72	5.620 294 27
		0.028 564 23	9.682 909 84
		0.000 262 71	15.828 473 92
2	6	0.384 353 81	0.889 941 02
		0.997 127 47	2.433 144 23
		0.536 086 20	4.766 203 58
		0.079 539 53	8.048 254 75
		0.002 879 55	12.600 413 87
		0.000 013 45	19.262 042 55
3	3	2.836 328 20	2.141 216 28
		2.951 294 31	5.315 517 13
		0.212 377 48	10.543 266 60
3	4	1.860 334 07	1.755 521 65
		3.356 891 02	4.265 605 87
		0.764 453 97	8.057 940 68
		0.018 320 93	13.920 931 80
3	5	1.250 983 61	1.490 554 95
		3.238 557 19	3.581 333 81
		1.390 185 24	6.626 996 30
		0.119 041 17	10.944 418 00
		0.001 232 78	17.356 696 94
3	6	0.865 313 49	1.296 419 20
		2.901 275 13	3.093 988 38
		1.893 145 31	5.661 285 22
		0.326 801 88	9.167 097 27
		0.013 394 41	13.941 345 37
		0.000 069 77	20.839 854 55

are very oscillatory. It is

$$\int_0^\infty f(x)x^p \exp(-x)dx = \sum_{j=1}^{n} H_j f(a_j) , \tag{A1}$$

where the pivots a_j are the zeros of the associated Laguerre polynomial

$$L_n^p(x) = \sum_{j=0}^{n} \frac{(n+p)!n!(-x)^j}{(n-j)!(p+j)!j!} , \tag{A2}$$

and the weights H_j are given by

$$H_j = \frac{(n+p)!n!}{a_j[L_n^{pI}(a_j)]^2} , \tag{A3}$$

where in the notation of Kopal [18], $L_n^{p\mathrm{I}}(a_j)$ denotes the polynomial evaluated at a_j after the factor $(x-a_j)$ has been removed. The error is proportional to the $(2n)$th derivative of $f(x)$ evaluated at some point in the range of integration. Fletcher *et al.* [28] cited sources of the weights and pivots from Burnett [29] for $p=2,3,4$ and $n=2,3$ (with few decimal places) and Rabinowitz and Weiss [30] for $p=1,2,3,4,5$ and $n=4,8,12,16$. At the low temperatures we considered, the cross sections at energies where the integrands are important vary slowly. Use of small values of n avoids need for cross sections at higher energies where oscillations occur (see for example the spin-change cross sections of Ref. [12]). We calculated weights and pivots for $p=1,2,3$ and $n=3,4,5,6$, the pivots being found by repeated bisection and the Newton-Raphson method with a tolerance of 10^{-12}; the data were checked against those of Rabinowitz and Weiss for $n=4$. We used six pivots in the temperature averages given in the various tables, but quote our calculated data in Table X as they are not readily available elsewhere. We note that this quadrature method is unsuitable at higher temperatures where the cross sections oscillate in regions that make significant contributions to the integrals.

ACKNOWLEDGMENTS

This work was done while M.J.J. and J.N.Y. were visiting the Institute for Theoretical Atomic and Molecular Physics at the Harvard-Smithsonian Center for Astrophysics. It has been supported by the U.S. Department of Energy, Division of Chemical Sciences, Office of Basic Energy Sciences.

---

[*] Permanent address: Department of Computing Science, University of Glasgow, Glasgow, Scotland.

[†] Current address: Department of Physics, University of Virginia, Charlottesville, VA 22901.

[1] D. G. Friend and R. D. Etters, J. Low Temp. Phys. **39**, 409 (1980).

[2] A. Hershcovitch, Phys. Rev. Lett. **63**, 750 (1989).

[3] E. M. Purcell and G. B. Field, Astrophys. J. **124**, 542 (1956).

[4] W. Kolos and L. Wolniewicz, J. Chem. Phys. **43**, 2429 (1965).

[5] W. Kolos and L. Wolniewicz, Chem. Phys. Lett. **24**, 457 (1974).

[6] W. Kolos and L. Wolniewicz, J. Mol. Spectrosc. **54**, 303 (1975).

[7] W. Kolos, K. Szalewicz, and H. J. Monkhorst, J. Chem. Phys. **84**, 3278 (1986).

[8] D. Frye, G. C. Lie, and E. Clementi, J. Chem. Phys. **91**, 2366 (1989).

[9] J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (Wiley, New York, 1964).

[10] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford University Press, Oxford, 1965).

[11] A. C. Allison and F. J. Smith, At. Data **3**, 317 (1971).

[12] A. C. Allison and A. Dalgarno, Astrophys. J. **158**, 423 (1969).

[13] N. Koyama and J. C. Baird, J. Phys. Soc. Jpn. **55**, 801 (1986).

[14] W. Kolos and L. Wolniewicz, J. Chem. Phys. **41**, 3663 (1964).

[15] L. Wolniewicz, J. Chem. Phys. **78**, 6173 (1983).

[16] W. Kolos, Int. J. Quantum Chem. **1**, 169 (1967).

[17] Y. M. Chan and A. Dalgarno, Mol. Phys. **14**, 101 (1968).

[18] Z. Kopal, *Numerical Analysis* (Chapman and Hall, London, 1961).

[19] A. Dalgarno, Proc. R. Soc. London Ser. A **262**, 132 (1961).

[20] F. J. Smith, Planet. Space Sci. **14**, 929 (1966).

[21] L. C. Balling, R. J. Hanson, and F. M. Pipkin, Phys. Rev. **133**, A607 (1964); **135**, AB1 (1964).

[22] J. M. V. A. Koelman, S. B. Crampton, H. T. C. Stoof, O. J. Luiten, and B. J. Verhaer, Phys. Rev. A **38**, 3535 (1988).

[23] A. C. Allison, Phys. Rev. A **5**, 2695 (1972).

[24] Y. H. Uang and W. C. Stwalley, J. Phys. (Paris) Colloq. **41**, C7-33 (1980).

[25] G. Gutierrez, M. de Llano, and W. C. Stwalley, Phys. Rev. B **29**, 5211 (1984).

[26] C. Lhuillier, J. Phys. **44**, 1 (1983).

[27] J. O. Hirschfelder and W. J. Meath, Adv. Chem. Phys. **12**, 3 (1967).

[28] A. Fletcher, J. C. P. Miller, L. Rosenhead, and L. J. Comrie, *An Index of Mathematical Tables,* 2nd edition (Blackwell Scientific Publications, Oxford, 1962).

[29] D. Burnett, Proc. Cambridge Philos. Soc. **33**, 359 (1937).

[30] P. Rabinowitz and G. Weiss, Math. Tables Other Aids Comput. **13**, 285 (1959).