Use of the Van Regemorter formula for collision strengths or cross sections

Douglas H. Sampson and Hong Lin Zhang
Department of Astronomy and Astrophysics, The Pennsylvania State University, University Park, Pennsylvania 16802
(Received 16 May 1991)

The accuracy of the widely used Van Regemorter formula [Astrophys. J. **136**, 906 (1962)] for calculating the collision strengths needed in applications to high-temperature plasmas is tested by comparison with numerous more accurate calculations. It is found to be frequently a very poor approximation, especially for $\Delta n \geq 1$ excitation transitions from levels with $l < n-1$, and the recommendation is made that with the recent advances in calculational procedures and available accurate atomic data use of the Van Regemorter formula should be discontinued.

PACS number(s): 34.80.Kw

I. INTRODUCTION

In general, it is much more lengthy and consuming of computer time to calculate electron-impact excitation cross sections or collision strengths than it is to calculate radiative oscillator strengths or decay rates. Hence, about 30 years ago when Van Regemorter [1,2], Burgess [3], and Seaton [4] obtained an approximate, simple, formula, commonly called the Van Regemorter formula, in which the electron-impact excitation cross section was expressed in terms of the electric-dipole radiative oscillator strength f and an effective Gaunt factor $\bar{g}$, the formula became very widely used almost immediately in the modeling of high-temperature plasmas and its use has continued to the present time. However, recently the picture has drastically changed from that existing a few years ago due to advances in computers and the development of very rapid procedures for calculating collision strengths, such as is done in the work of Refs. [5–7] and applied to large-scale calculations of atomic data in Refs. [8–13]. Hence, it is no longer a prohibitive task to make accurate, direct, calculations of the collision strengths needed in nonlocal thermodynamic equilibrium plasma applications. Moreover, it is now clear that the Van Regemorter formula is often a much worse approximation than was earlier expected. Our principal purpose here is to illustrate this and to determine more precisely than previously the conditions for which use of the Van Regemorter formula is an especially poor approximation. We concentrate on highly charged ions satisfying Eq. (8) below, but expect that the conclusions apply approximately to somewhat less highly ionized atoms, as well.

First we briefly review the Van Regemorter method. Then we discuss its accuracy based on many comparisons with more accurate calculations and we give some illustrative examples of these comparisons.

II. SUMMARY OF THE VAN REGEMORTER PROCEDURE

The Van Regemorter formula [2] expresses the cross section Q_{if} for a transition $i \rightarrow f$ in terms of the electric-dipole oscillator strength f_{if} for the transition and an effective Gaunt factor $\bar{g}$. Specifically,

$$Q_{if}=\frac{8\pi}{\sqrt{3}}\frac{1}{k_i^2}\frac{f_{if}}{\Delta E(\mathrm{Ry})}\bar{g}\pi a_0^2 , \tag{1}$$

where $\Delta E(\mathrm{Ry})$ is the transition energy in Rydbergs, a_0 is the Bohr radius, and k_i is the wave number of the impact electron. In the nonrelativistic limit

$$k_i^2=E_i(\mathrm{Ry}) , \tag{2}$$

where $E_i(\mathrm{Ry})$ is the impact electron energy in Rydbergs. The relativistic expression for k_i^2 contains an extra factor, see Eq. (2) of Ref. [7], but that factor is negligible for most conditions of interest. The well-known relationship between the cross section Q and collision strength Ω is

$$Q_{if}=\frac{\pi a_0^2}{k_i^2 g_i}\Omega_{if} , \tag{3}$$

where g_i is the statistical weight of the initial level. Hence, one sees that Eq. (1) corresponds to using

$$\Omega_{if}=\frac{8\pi}{\sqrt{3}}\frac{g_i f_{if}}{\Delta E(\mathrm{Ry})}\bar{g} \tag{4}$$

as the Van Regemorter formula for the collision strength.

Van Regemorter [2] assumed the $\bar{g}$ for every optically allowed transition in any positive ion could be represented by one universal function of x, where x^2 is the scattered electron energy in threshold units

$$x^2=E_f/\Delta E . \tag{5}$$

Of course, if $\bar{g}$ could be represented as a function of x, it could also be given as a function of ε, where ε is the impact electron energy in threshold units

$$\varepsilon=E_i/\Delta E \tag{6}$$

because obviously ε must equal x^2+1. For very high energies for which $\varepsilon \simeq x^2 \gg 1$, $\bar{g}$ is given accurately by

$$\bar{g}=\frac{\sqrt{3}}{2\pi}\ln(x^2)=\frac{\sqrt{3}}{2\pi}\ln\varepsilon . \tag{7}$$

For lower energies, where $\bar{g}$ is *a priori* unknown, Van Re-

gemorter chose $\bar{g}$ such that Eq. (1) gave approximate agreement with the best theoretical and experimental results available at that time. His choice for $\bar{g}(x)$ is given in Table I of Ref. [2]. For the region $\varepsilon \leq 3$, or $x^2 \leq 2$, which is usually the most important energy region for $\Delta n \geq 1$ transitions, he simply used $\bar{g}=0.2$ for positive ions.

III. ACCURACY OF THE VAN REGEMORTER FORMULA

Now we consider the accuracy of the Van Regemorter formula. The error due to use of this formula can obviously be considered to be a consequence of one or the other of the following two causes: (1) the optically forbidden transitions are omitted or (2) the optically allowed transitions are not treated with sufficient accuracy by the Van Regemorter formula.

In testing the importance of (1) and (2) we have used the very rapid relativistic distorted-wave approach and associated computer programs that have been developed recently in Refs. [6,7] and applied to large-scale production of atomic data in Refs. [8–13]. The results in Refs. [9–11] for Li-like, Na-like, and Cu-like ions, which are not complicated by configuration and intermediate coupling mixing effects, are particularly helpful for these purposes. However, we expect the conclusions reached to apply for transitions involving principally the same orbital transitions nlj-$n'l'j'$ in more complex ions, as well, and this has been verified by several test calculations.

As discussed in Refs. [6–13], the approach appears to be accurate for

$$Z \geq 2N \ , \tag{8}$$

where Z is the nuclear charge number and N is the number of bound electrons per ion. However, we have found that it is moderately accurate for most transitions in considerably less highly ionized ions, as well. Also, with the use of judiciously chosen effective Z's, the nonrelativistic Z-scaled Coulomb-Born exchange results of Refs. [14–17] for hydrogenic ions apply approximately for most transitions in ions somewhat more nearly neutral than those satisfying Eq. (8). Since the general conclusions we reach also apply to the scaled hydrogenic results, we expect that these conclusions apply approximately for considerably more nearly neutral atoms, as well as those satisfying Eq. (8).

It should be noted that the programs of Refs. [6,7] have recently been expanded to include the effect of resonances treated as a two-step process of electron capture followed by autoionization with the possibility of radiative decay of the doubly excited intermediate levels included. However, the results in Refs. [8–13] do not include resonance effects. Nevertheless, the resonance contributions are expected to be small except for the weak transitions, and we expect the inclusion of resonance effects would not greatly affect the conclusions reached here.

On the basis of comparison of results using the Van Regemorter formula with those of Refs. [9–11] plus additional test calculations, we have reached the following conclusions:

(i) For the $\Delta n \equiv n'-n=0$ transitions, we find, as has been found by others, that the allowed transitions greatly dominate. Hence, the error due to cause (1) above is not very significant for these transitions. However, the error due to cause (2) is rather large for the energies of principal interest if one uses the original $\bar{g}$ values of Van Regemorter given in Table 1 of Ref. 2. On the other hand, since this error is generally in the same direction and quite similar for all of these transitions, it appears that for them moderately accurate results, to within about 30 or 40%, could be obtained by choosing a larger $\bar{g} \simeq 0.8$ at and near threshold that increases with energy and goes into the form given by Eq. (7) only for very high energies.

(ii) In contrast to this, for the $\Delta n \geq 1$ transitions the error due to both causes (1) and (2) above is frequently very large. Moreover, that due to cause (2) is not in a single direction. In fact, we find that, for $\Delta n \geq 1$ transitions, use of the Van Regemorter formula leads to near threshold results too small by as much as an order of magnitude in some cases and too large by nearly as big a factor in others. Thus, although Van Regemorter's choice for $\bar{g}$ is probably about as good as can be made for the $\Delta n \geq 1$ transitions assuming a single $\bar{g}(x)$ applies for all of them, it appears there is no way one can, in general, choose a single, convenient $\bar{g}(x)$ that will lead to generally accurate results for all $\Delta n \geq 1$ transitions in complex ions. However, in the very special case of $n-n'$ transitions in hydrogenic ions, where all transitions are optically allowed, we have been successful in choosing a moderately simple form for $\bar{g}$ that leads to accurate results, see Eqs. (17) and (18) of Ref. [18].

(iii) Finally, we have found the interesting result that, in all of the very numerous cases we considered, the sum of the collision strengths for the optically forbidden transitions from a given sublevel nlj to upper sublevels with a given $n' \geq n+1$ exceeds (generally by a wide margin) the sum of the collision strengths for all the allowed transitions from nlj to the sublevels with the same n' value, with the exception of the transitions from the sublevels nlj with $l=n-1$. Hence, for this reason, use of the Van Regemorter formula tends to be a very poor approximation for all sublevels with a given n value that satisfy $l<n-1$. Thus, for $n=1$, where there is only the single sublevel $1s_{1/2}$, the allowed transitions do dominate. However, for $n=2$, the forbidden transitions dominate the transitions from $2s_{1/2}$ to the $n' \geq 3$ sublevels, while the allowed transitions dominate the transitions from $2p_{1/2}$ and $2p_{3/2}$ to the $n' \geq 3$ sublevels. For $n=3$, the forbidden transitions dominate the transitions from $3s_{1/2}$, $3p_{1/2}$, and $3p_{3/2}$ to the $n' \geq 4$ sublevels, while the allowed transitions dominate the transitions from $3d_{3/2}$ and $3d_{5/2}$ to these same sublevels, etc. Thus, the error from use of the Van Regemorter formula due to cause (1) above becomes greater the higher the n values of the sublevels one is considering.

The points we have been making are illustrated by the comparisons made in Tables I and II of collision strengths for a sample of the transitions among the $n=3$ sublevels and from the $n=3$ sublevels to those with $n'=4$ and 5 in Na-like iron ($Z=26$) and for a sample of the

TABLE I. Comparison of collision strengths for Na-like iron ($Z=26$). Here $nl*$ and nl mean nlj with $j=l-\frac{1}{2}$ and $j=l+\frac{1}{2}$, respectively. For the allowed transitions the upper entries are the relativistic distorted-wave values (Ref. [10]), while the lower entries are obtained with the Van Regemorter formula (Ref. [2]). These are followed by the ratio of lower to upper entries. The single entries for fobidden transitions are also from Ref. [10]. Entries labeled nlj A and nlj T are the sums of the preceeding collision strengths for the allowed transitions and for all the transitions, respectively, from sublevel nlj. This is followed by their ratios. Finally, E' is the scattered electron energy in units of Z_{eff}^2 Rydbergs, where $Z_{\text{eff}}=Z-8.34$.

Transition	E' = 0.0025	E' = 0.04	E' = 0.40
$3s$ $3p^*$	1.19	1.42	2.19
	2.84×10^{-1}	5.36×10^{-1}	1.52
	0.238	0.377	0.696
$3s$ $3p$	2.34	2.78	4.31
	5.72×10^{-1}	1.03	3.04
	0.245	0.371	0.704
$3s$ $3d^*$	1.20×10^{-1}	1.27×10^{-1}	1.40×10^{-1}
$3s$ $3d$	1.79×10^{-1}	1.91×10^{-1}	2.10×10^{-1}
$3s$ A	3.53	4.20	6.50
$3s$ T	3.83	4.51	6.85
	0.922	0.930	0.949
$3p^*$ $3s$	1.19	1.42	2.19
	2.84×10^{-1}	5.36×10^{-1}	1.52
	0.238	0.377	0.696
$3p^*$ $3p$	2.21×10^{-1}	1.96×10^{-1}	1.75×10^{-1}
$3p^*$ $3d^*$	1.73	2.04	3.18
	4.65×10^{-1}	6.86×10^{-1}	2.40
	0.269	0.336	0.757
$3p^*$ $3d$	4.55×10^{-2}	3.65×10^{-2}	3.11×10^{-2}
$3p^*$ A	2.92	3.46	5.37
$3p^*$ T	3.19	3.70	5.57
	0.916	0.937	0.963
$3d$ $3s$	1.79×10^{-1}	1.91×10^{-1}	2.10×10^{-1}
$3d$ $3p^*$	4.55×10^{-2}	3.64×10^{-2}	3.11×10^{-2}
$3d$ $3p$	3.20	3.77	5.85
	8.40×10^{-1}	1.28	4.37
	0.262	0.340	0.747
$3d$ $3d^*$	2.32×10^{-1}	$1.50\times^{-1}$	8.02×10^{-2}
$3d$ A	3.20	3.77	5.85
$3d$ T	3.66	4.15	6.17
	0.875	0.909	0.948
$3s$ $4s$	9.86×10^{-2}	1.05×10^{-1}	1.15×10^{-1}
$3s$ $4p^*$	5.93×10^{-3}	9.22×10^{-3}	3.86×10^{-2}
	2.56×10^{-2}	2.56×10^{-2}	6.10×10^{-2}
	4.313	2.772	1.582
$3s$ $4p$	1.13×10^{-2}	1.70×10^{-2}	7.08×10^{-2}
	4.75×10^{-2}	4.75×10^{-2}	1.13×10^{-1}
	4.222	2.796	1.597
$3s$ $4d^*$	1.64×10^{-2}	1.93×10^{-2}	3.25×10^{-2}
$3s$ $4d$	2.43×10^{-2}	2.87×10^{-2}	4.83×10^{-2}
$3s$ $4f^*$	3.38×10^{-2}	3.44×10^{-2}	3.79×10^{-2}
$3s$ $4f$	4.51×10^{-2}	4.58×10^{-2}	5.05×10^{-2}
$3s$ A	1.72×10^{-2}	2.62×10^{-2}	1.09×10^{-1}
$3s$ T	2.35×10^{-1}	2.59×10^{-1}	3.94×10^{-1}
	0.073	0.101	0.278
$3p^*$ $5s$	1.96×10^{-3}	2.31×10^{-3}	6.51×10^{-3}
	3.23×10^{-3}	3.23×10^{-3}	6.75×10^{-3}
	1.649	1.401	1.037
$3p^*$ $5p^*$	2.20×10^{-2}	2.28×10^{-2}	2.42×10^{-2}
$3p^*$ $4s$	9.02×10^{-3}	1.39×10^{-2}	4.70×10^{-2}
	2.39×10^{-2}	2.39×10^{-2}	6.54×10^{-2}
	2.655	1.727	1.393
$3p^*$ $4p^*$	1.14×10^{-1}	1.19×10^{-1}	1.27×10^{-1}
$3p^*$ $4p$	1.58×10^{-2}	1.62×10^{-2}	2.22×10^{-2}
$3p^*$ $4d^*$	3.50×10^{-2}	5.53×10^{-2}	1.88×10^{-1}
	1.02×10^{-1}	1.02×10^{-1}	2.55×10^{-1}
	2.929	1.852	1.362
$3p^*$ $4d$	1.53×10^{-2}	1.35×10^{-2}	1.21×10^{-2}
$3p^*$ $4f^*$	1.07×10^{-1}	1.30×10^{-1}	2.03×10^{-1}
$3p^*$ $4f$	2.35×10^{-2}	1.71×10^{-2}	1.42×10^{-2}
$3p^*$ A	4.40×10^{-2}	6.92×10^{-2}	2.34×10^{-1}
$3p^*$ T	3.20×10^{-1}	3.65×10^{-1}	6.13×10^{-1}
	0.138	0.190	0.383
$3d$ $4s$	2.20×10^{-2}	2.23×10^{-2}	2.77×10^{-2}
$3d$ $4p^*$	1.43×10^{-2}	1.08×10^{-2}	7.49×10^{-3}
$3d$ $4p$	4.59×10^{-2}	5.73×10^{-2}	1.43×10^{-1}
	5.68×10^{-2}	5.68×10^{-2}	1.75×10^{-1}
	1.239	0.991	1.220
$3d$ $4d^*$	4.47×10^{-2}	2.86×10^{-2}	1.68×10^{-2}
$3d$ $4d$	4.65×10^{-1}	4.58×10^{-1}	4.57×10^{-1}
$3d$ $4f^*$	1.43×10^{-1}	1.27×10^{-1}	1.89×10^{-1}
	5.41×10^{-2}	5.41×10^{-2}	1.53×10^{-1}
	0.379	0.426	0.808
$3d$ $4f$	1.33	1.66	3.37
	1.08	1.08	3.06
	0.816	0.652	0.907
$3d$ A	1.52	1.85	3.70
$3d$ T	2.06	2.37	4.21
	0.735	0.780	0.879
$3s$ $5s$	1.88×10^{-2}	1.98×10^{-2}	2.19×10^{-2}
$3s$ $5p^*$	1.78×10^{-3}	2.36×10^{-3}	8.66×10^{-3}
	5.66×10^{-3}	5.66×10^{-3}	1.09×10^{-2}
	3.181	2.402	1.254
$3s$ $5p$	3.41×10^{-3}	4.42×10^{-3}	1.62×10^{-2}
	1.08×10^{-2}	1.08×10^{-2}	2.06×10^{-2}
	3.149	2.434	1.269
$3s$ $5d^*$	5.66×10^{-3}	6.16×10^{-3}	9.42×10^{-3}
$3s$ $5d$	8.46×10^{-3}	9.19×10^{-3}	1.41×10^{-2}
$3s$ $5f^*$	7.76×10^{-3}	7.08×10^{-3}	6.95×10^{-3}
$3s$ $5f$	1.04×10^{-2}	9.45×10^{-3}	9.28×10^{-3}
$3s$ $5g^*$	4.29×10^{-3}	3.64×10^{-3}	3.85×10^{-3}
$3s$ $5g$	5.36×10^{-3}	4.55×10^{-3}	4.81×10^{-3}
$3s$ A	5.20×10^{-3}	6.78×10^{-3}	2.49×10^{-2}
$3s$ T	6.59×10^{-2}	6.67×10^{-2}	9.52×10^{-2}
	0.079	0.102	0.261
$3d^*$ $5s$	3.50×10^{-3}	2.83×10^{-3}	2.65×10^{-3}
$3d^*$ $5p^*$	4.41×10^{-3}	4.53×10^{-3}	9.45×10^{-3}
	3.44×10^{-3}	3.44×10^{-3}	8.04×10^{-3}
	0.780	0.758	0.851

TABLE I. (*Continued*)

Transition	E' 0.0025	0.04	0.40	Transition	E' 0.0025	0.04	0.40
$3p^*$ $5p$	4.71×10^{-3}	4.18×10^{-3}	4.77×10^{-3}	$3d^*$ $5p$	6.75×10^{-3}	4.73×10^{-3}	3.67×10^{-3}
$3p^*$ $5d^*$	1.16×10^{-2}	1.65×10^{-2}	4.81×10^{-2}		6.56×10^{-4}	6.56×10^{-4}	1.53×10^{-3}
	2.45×10^{-2}	2.45×10^{-2}	4.95×10^{-2}		0.097	0.139	0.418
	2.101	1.479	1.029	$3d^*$ $5d^*$	5.87×10^{-2}	5.61×10^{-2}	5.47×10^{-2}
$3p^*$ $5d$	5.64×10^{-3}	4.43×10^{-3}	3.30×10^{-3}	$3d^*$ $5d$	1.72×10^{-2}	9.96×10^{-3}	3.84×10^{-3}
$3p^*$ $5f^*$	2.11×10^{-2}	2.35×10^{-2}	3.35×10^{-2}	$3d^*$ $5f^*$	1.73×10^{-1}	2.04×10^{-1}	3.69×10^{-1}
$3p^*$ $5f$	7.08×10^{-3}	4.64×10^{-3}	2.79×10^{-3}		1.02×10^{-1}	1.02×10^{-1}	2.32×10^{-1}
$3p^*$ $5g^*$	9.71×10^{-3}	1.08×10^{-2}	1.45×10^{-2}		0.591	0.500	0.628
$3p^*$ $5g$	5.03×10^{-3}	3.13×10^{-3}	1.93×10^{-3}	$3d^*$ $5f$	2.75×10^{-2}	1.43×10^{-2}	4.01×10^{-3}
$3p^*$ A	1.36×10^{-2}	1.88×10^{-2}	5.46×10^{-2}	$3d^*$ $5g^*$	3.36×10^{-2}	4.10×10^{-2}	7.44×10^{-2}
$3p^*$ T	8.89×10^{-2}	9.23×10^{-2}	1.40×10^{-1}	$3d^*$ $5g$	1.24×10^{-2}	6.08×10^{-3}	2.54×10^{-3}
	0.153	0.204	0.391	$3d^*$ A	1.84×10^{-1}	2.14×10^{-1}	3.82×10^{-1}
				$3d^*$ T	3.37×10^{-1}	3.44×10^{-1}	5.24×10^{-1}
					0.546	0.621	0.729

TABLE II. Comparison of collision strengths for Cu-like gadolinium ($Z=64$). Notation as in Table I except that $Z_{\text{eff}}=Z-23.3$ and Ref. [11] replaces Ref. [10].

Transition	E' 0.001	0.015	0.18	Transition	E' 0.001	0.015	0.18
$4s$ $5s$	4.87×10^{-2}	5.06×10^{-2}	5.58×10^{-2}	$4d^*$ $5s$	1.07×10^{-2}	1.17×10^{-2}	1.60×10^{-2}
$4s$ $5p^*$	2.40×10^{-3}	3.22×10^{-3}	1.34×10^{-2}	$4d^*$ $5p^*$	2.01×10^{-2}	2.72×10^{-2}	7.74×10^{-2}
	1.07×10^{-2}	1.07×10^{-2}	2.35×10^{-2}		3.54×10^{-2}	3.54×10^{-2}	1.04×10^{-1}
	4.473	3.332	1.761		1.759	1.301	1.340
$4s$ $5p$	5.11×10^{-3}	5.49×10^{-3}	1.51×10^{-2}	$4d^*$ $5p$	8.86×10^{-3}	9.30×10^{-3}	1.55×10^{-2}
	1.19×10^{-2}	1.19×10^{-2}	2.55×10^{-2}		4.78×10^{-3}	4.78×10^{-3}	1.36×10^{-2}
	2.325	2.163	1.686		0.540	0.514	0.877
$4s$ $5d^*$	3.86×10^{-3}	4.28×10^{-3}	7.06×10^{-3}	$4d^*$ $5d^*$	1.43×10^{-1}	1.46×10^{-1}	1.54×10^{-1}
$4s$ $5d$	5.44×10^{-3}	5.98×10^{-3}	9.74×10^{-3}	$4d^*$ $5d$	9.66×10^{-3}	8.55×10^{-3}	8.02×10^{-3}
$4s$ $5f^*$	4.09×10^{-3}	4.32×10^{-3}	5.44×10^{-3}	$4d^*$ $5f^*$	5.40×10^{-2}	7.12×10^{-2}	2.10×10^{-1}
$4s$ $5f$	5.39×10^{-3}	5.67×10^{-3}	7.11×10^{-3}		1.16×10^{-1}	1.16×10^{-1}	2.87×10^{-1}
$4s$ $5g^*$	6.82×10^{-3}	6.65×10^{-3}	7.70×10^{-3}		2.158	1.637	1.364
$4s$ $5g$	8.53×10^{-3}	8.31×10^{-3}	9.62×10^{-3}	$4d^*$ $5f$	9.69×10^{-3}	7.88×10^{-3}	5.38×10^{-3}
$4s$ A	7.51×10^{-3}	8.71×10^{-3}	2.85×10^{-2}	$4d^*$ $5g^*$	1.19×10^{-1}	1.35×10^{-1}	2.08×10^{-1}
$4s$ T	9.03×10^{-2}	9.45×10^{-2}	1.31×10^{-1}	$4d^*$ $5g$	1.44×10^{-2}	1.07×10^{-2}	7.04×10^{-3}
	0.083	0.092	0.217	$4d^*$ A	8.30×10^{-2}	1.08×10^{-1}	3.03×10^{-1}
				$4d^*$ T	3.90×10^{-1}	4.28×10^{-1}	7.02×10^{-1}
$4p^*$ $5s$	3.80×10^{-3}	5.28×10^{-3}	1.88×10^{-2}		0.213	0.252	0.432
	1.17×10^{-2}	1.17×10^{-2}	2.90×10^{-2}				
	3.070	2.210	1.542	$4f^*$ $5s$	5.51×10^{-3}	4.97×10^{-3}	4.38×10^{-3}
$4p^*$ $5p^*$	5.36×10^{-2}	5.54×10^{-2}	5.97×10^{-2}	$4f^*$ $5p^*$	1.25×10^{-2}	1.33×10^{-2}	1.67×10^{-2}
$4p^*$ $5p$	5.05×10^{-3}	5.36×10^{-3}	7.75×10^{-3}	$4f^*$ $5p$	7.62×10^{-3}	6.79×10^{-3}	6.13×10^{-3}
$4p^*$ $5d^*$	4.39×10^{-3}	5.44×10^{-3}	2.11×10^{-2}	$4f^*$ $5d^*$	2.49×10^{-2}	3.05×10^{-2}	7.34×10^{-2}
	1.76×10^{-2}	1.76×10^{-2}	3.83×10^{-2}		2.86×10^{-2}	2.86×10^{-2}	9.16×10^{-2}
	3.997	3.231	1.820		1.147	0.937	1.247
$4p^*$ $5d$	3.46×10^{-3}	3.33×10^{-3}	3.62×10^{-3}	$4f^*$ $5d$	1.15×10^{-2}	9.05×10^{-3}	7.95×10^{-3}
$4p^*$ $5f^*$	1.00×10^{-2}	1.17×10^{-2}	2.09×10^{-2}		1.84×10^{-3}	1.84×10^{-3}	5.84×10^{-3}
$4p^*$ $5f$	3.46×10^{-3}	2.98×10^{-3}	2.39×10^{-3}		0.160	0.203	0.735
$4p^*$ $5g^*$	2.20×10^{-2}	2.35×10^{-2}	2.83×10^{-2}	$4f^*$ $5f^*$	2.43×10^{-1}	2.42×10^{-1}	2.41×10^{-1}
$4p^*$ $5g$	6.04×10^{-3}	5.03×10^{-3}	3.79×10^{-3}	$4f^*$ $5f$	2.21×10^{-2}	1.49×10^{-2}	6.51×10^{-3}
$4p^*$ A	8.19×10^{-3}	1.07×10^{-2}	3.99×10^{-2}	$4f^*$ $5g^*$	8.36×10^{-1}	9.76×10^{-1}	1.91
$4p^*$ T	1.12×10^{-1}	1.18×10^{-1}	1.66×10^{-1}		6.29×10^{-1}	6.29×10^{-1}	1.77
	0.073	0.091	0.240		0.753	0.645	0.931
				$4f^*$ $5g$	3.45×10^{-2}	2.26×10^{-2}	9.19×10^{-3}
				$4f^*$ A	8.72×10^{-1}	1.02	1.99
				$4f^*$ T	1.20	1.32	2.27
					0.728	0.769	0.875

transitions from the $n=4$ sublevels to the $n'=5$ sublevels in Cu-like gadolinium ($Z=64$). Here nl^* designates nlj with $j=l-\frac{1}{2}$, while nl designates nlj with $j=l+\frac{1}{2}$. For example,

$$3s=3s_{1/2},\quad 3d^*=\ 3d_{3/2},\quad 4f=4f_{7/2},\ etc. \tag{9}$$

Results are given as a function of scattered electron energy E' in units of $Z_{\rm eff}^2$ Rydbergs [19], where $Z_{\rm eff}=Z-8.34$ for Na-like ions and $Z_{\rm eff}=Z-23.3$ for Cu-like ions. The range of energies covered includes those needed to obtain collision rates for the temperatures ordinarily of interest for plasma applications, with the two lower-energy points ordinarily being of more importance. Of course, for determining accurate rates more energy points, as given in Refs. [10,11], are needed, but this is not necessary for our present purposes.

For each of the allowed transitions in the tables the first entries are the relativistic distorted-wave values given in Ref. [10] or [11]. The second entries are those obtained with the Van Regemorter formula [Eq. (4)] using the values for the transition energies ΔE and oscillator strengths f also given in Ref. [10] or [11]. The values of $\bar{g}$ used are those given in Table 1 of Ref. [2] supplemented by Eq. (7) for very large ε or x. The third entries are the ratios of the second entries to the first, or upper, entries and hence give an indication of the error in use of the Van Regemorter formula for allowed transitions; that is, the error due to cause (2) above. Inspection of the results in Table I for transitions among the $n=3$ sublevels in Na-like iron indicates, as noted in point (i) above, that this error, although quite substantial, could be largely eliminated by using a larger value for $\bar{g}$ starting with about 0.8 at threshold. In contrast to this, as noted in point (ii) above, for the $\Delta n\geq 1$ transitions, one sees from the tables that this type error is in various directions for different transitions. Hence, it cannot be removed by using a single, different choice for $\bar{g}(x)$. Extreme examples of this type of error for the $\Delta n\geq 1$ transitions are given by the near threshold results for the $3s_{1/2}$-$4p_{1/2}$, $3s_{1/2}$-$4p_{3/2}$, and $3d_{3/2}$-$5p_{3/2}$ transitions in Na-like iron and the $4s_{1/2}$-$5p_{1/2}$, $4p_{1/2}$-$5d_{3/2}$, and $4f_{5/2}$-$5d_{5/2}$ transitions in Cu-like gadolinium, where one sees from Tables I and II that the ratios of the near threshold results of the Van Regemorter formula to the relativistic distorted-wave collision strengths are 4.313, 4.222, 0.097, 4.473, 3.997 and 0.160, respectively.

The single entries for the forbidden transitions in Tables I and II are the relativistic distorted-wave collision strengths of Ref. [10] or [11]. The entries labeled A and T that follow the results for all the transitions from a sublevel nlj to the sublevels with a given n' value are the sum of the relativistic distorted-wave collision strengths for the allowed transitions and for all of these transitions, respectively. These entries are followed by the ratio A/T, which indicates directly the error due to cause (1) above; that is, the neglect of the forbidden transitions by the Van Regemorter formula. The results for the transitions among the $n=3$ sublevels in Table I illustrate the point made in (i) above that this type error is small for $\Delta n=0$ transitions. However, the results for the $\Delta n\geq 1$ transitions in Tables I and II illustrate the points made in (ii) and (iii) above that this type error is generally large for these transitions with the exception of those from the sublevels nlj with $l=n-1$. In fact, even for the latter the error is usually not negligible. Some extreme examples of this type error are given by the near threshold results for transitions from the $3s_{1/2}$ sublevel in Na-like iron to the sublevels with $n'=4$ and 5 and from the $4s_{1/2}$ and $4p_{1/2}$ sublevels in Cu-like gadolinium to the sublevels with $n'=5$, where one sees from Tables I and II that the "allowed" contributions to the total collision strengths are only 7.3, 7.9, 8.3, and 7.3 %, respectively.

In summary, we find that the Van Regemorter formula is frequently a very poor approximation for the $\Delta n\geq 1$ transitions because the forbidden transitions omitted by it are dominant and/or because it gives a poor approximation for results for the allowed transitions. It is a considerably better approximation for the $\Delta n=0$ transitions if a larger $\bar{g}$ than originally recommended in Ref. [2] is used. However, with the very rapid procedures now available for more accurate calculations, such as those of Refs. [5–7], and the large amount of accurate atomic data now available, for example, at the Belfast Atomic Data Bank [20], which is being continuously updated and expanded, there appears to be little reason to continue use of the Van Regemorter formula for either kind of transitions.

ACKNOWLEDGMENTS

This research was supported in part by the Department of Energy under Grant No. DE-FG02-90ER54104 and a Lawrence Livermore National Laboratory Subcontract and by the Innovative Science and Technology Office of the Strategic Defense Initiative Organization.

[1] H. Van Regemorter, Mon. Not. R. Astron. Soc. **121**, 213 (1960).
[2] H. Van Regemorter, Astrophys. J. **136**, 906 (1962).
[3] A. Burgess, Mém. Soc. R. Sci. Liége **4**, 299 (1961).
[4] M. J. Seaton in *Atomic and Molecular Processes,* edited by D. R. Bates (Academic, New York, 1962), Chap. 11.
[5] A. Bar-Shalom, M. Klapisch, and J. Oreg, Phys. Rev. A **38**, 1773 (1988).
[6] D. H. Sampson, H. L. Zhang, A. K. Mohanty, and R. E. H. Clark, Phys. Rev. A **40**, 604 (1989).
[7] H. L. Zhang, D. H. Sampson, and A. K. Mohanty, Phys. Rev. A **40**, 616 (1989).
[8] H. L. Zhang and D. H. Sampson, At. Data Nucl. Data Tables **43**, 1 (1989).
[9] H. L. Zhang, D. H. Sampson, and C. J. Fontes, At. Data Nucl. Data Tables **44**, 31 (1990).
[10] D. H. Sampson, H. L. Zhang, and C. J. Fontes, At. Data Nucl. Data Tables **44**, 209 (1990).
[11] H. L. Zhang, D. H. Sampson, and C. J. Fontes, At. Data Nucl. Data Tables **44**, 273 (1990).
[12] D. H. Sampson, H. L. Zhang, and C. J. Fontes, At. Data Nucl. Data Tables, **48**, 25 (1991).

[13] H. L. Zhang, D. H. Sampson, and C. J. Fontes, At. Data Nucl. Data Tables **48**, 91 (1991).
[14] A. Burgess, D. G. Hummer, and J. A. Tully, Philos. Trans. R. Soc. London, Ser. A **266**, 225 (1970).
[15] L. B. Golden and D. H. Sampson, Astrophys. J. Suppl. **38**, 19 (1978).
[16] L. B. Golden, R. E. H. Clark, S. J. Goett, and D. H. Sampson, Astrophys. J. Suppl. **45**, 603 (1981).
[17] R. E. H. Clark, D. H. Sampson, and S. J. Goett, Astrophys. J. Suppl. **49**, 545 (1982).
[18] D. H. Sampson and H. L. Zhang, Astrophys. J. **335**, 516 (1988).
[19] Actually, E' is the initial electron energy for transitions among the $n=3$ sublevels from an upper to a lower sublevel, such as $3d_{5/2}$-$3s_{1/2}$.
[20] J. G. Hughes, F. J. Smith, K. A. Berrington, K. M. Aggarwal, and M. Elder, Comput. Phys. Commun. **33**, 99 (1984).