ELSEVIER

Formula for the calculation of integral excitation cross sections of the electron-molecular collision at small scattering angles

Z. Chen*, A.Z. Msezane

Center for Theoretical Studies of Physical Systems, Department of Physics, Clark Atlanta University, Atlanta, GA 30314, USA

Abstract

A new method has been developed to evaluate the excitation cross sections for the electronic dipole-allowed transitions of electron-molecular collision. The formula for the calculation of the contribution from each vibronic state in the small scattering angles has been derived and tested in the $X^1\Sigma^+ \rightarrow A^1\Pi$ transition of e-CO scattering. The results show a better agreement between the theoretical results and the experimental data than the previous evaluation. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Charge-s-chemical reaction; Electron co-electron spe

1. Introduction

Experimental small angle electron differential cross sections (DCSs) for electronic transitions of electron-molecular collision are difficult to obtain due to their rapid variation with decreasing scattering angle θ, particularly when impact energies are high. The error in the measurement will propagate to the integral cross sections (ICSs). Due to this, experimentalists began their measurements at small angle $\theta_{min}^°$ to avoid the region where the measurement may have large errors [1–3]. DCS data in the region of $0 - \theta_{min}^°$ are then obtained by several extrapolating methods. Srivastava and Jensen [1] extrapolated the DCS data to 0° by continuing the slope between the last two measured points. Khakoo and Trajmar [2] used theoretical DCS, whenever they were available, to extrapolate their data to 0°. Their extrapolation, according

to our calculation, uses a slope that is approximately three times steeper than the slope achieved from continuing the last two measured points. Obviously, the ICS obtained by this kind of extrapolating are bound to contain large uncertainties.

In this paper, we introduce a new method to evaluate the ICS from measured DCS for the electronic dipole-allowed transition in electron-molecular scattering. The formula for the calculation of the contribution from each vibronic state in the small scattering angles has been derived and tested in the $X^1\Sigma^+ \rightarrow A^1\Pi$ transition of e-CO scattering.

2. Method

The method takes two steps to calculate the ICS. First, in the angular range $(\theta_{max}^° > \theta > \theta_{min}^°)$, $\theta_{min}^°$ and $\theta_{max}^°$ are, respectively, the minimum and maximum angles measured in the experiment, a cubic spline function is used to fit the experimental data and integrate to give the ICS of $\theta_{min}^° - \theta_{max}^°$.

* Corresponding author. Tel.: + 1-404-880-8631; fax: +1-404-880-8360.

E-mail address: zchen@ctsps.cau.edu (Z. Chen).

Table 1
Excitation energy $w_{v'}$ (eV), oscillator strength $f_{v'}$, and Franck–Condon factors $q_{v'}$ for the fourth positive band of carbon monoxide

v'	$w_{v'}$	$f_{v'}$	$q_{v'}$
0	8.03	0.0162	0.1151
1	8.21	0.0351	0.2204
2	8.39	0.0402	0.2347
3	8.56	0.0347	0.1828
4	8.74	0.0242	0.1173
5	8.90	0.0145	0.06621

Secondly, Frank–Condon factors are utilized to obtain the DCS for every vibronic state at each measured point. The DCS are then transferred to the generalized oscillator strengths (GOS) according to Eq. (1).

$$f_G = \frac{K_i}{2K_f} K^2 w \frac{d\sigma}{d\Omega} \tag{1}$$

where K_i and K_f are, respectively, the incident and scattered momenta, w is the excitation energy, and K_2 is the momentum transfer squared given by

$$K^2 = 2E\left[2 - \frac{w}{E} - 2\sqrt{1 - \frac{w}{E}}\cos\theta\right] \tag{2}$$

where θ and E are, respectively, the scattering angle, and the impact energy. GOS and optical oscillator strength (OOS) for each vibronic state are fitted with Lassettre series [4]

$$f(x) = \frac{1}{(1+x)^6}\sum_{n=0}^{n=\infty} f_n\left(\frac{x}{1+x}\right)^n \tag{3}$$

where f_0 is the OOS, $x = K^2/\alpha^2$, $\alpha = \sqrt{2I} + \sqrt{2(I-w)}$ with I the ionization energy. The coefficients are determined by the least square calculation. Substituting Eq. (3) into the equation below

$$\sigma = \frac{\pi}{Ew}\int_{K_0^2}^{K_{min}^2} f(K^2)\frac{dK^2}{K^2} \tag{4}$$

and integrating from $K_0^2(\theta = 0°)$ to $K_{min}^2(\theta = \theta_{min}°)$,

we obtain the following formula (keeping up to f_5):

$$\sigma = \frac{\pi}{Ew}\left[f_0\left(\frac{1}{5(1+x)^5} + \frac{1}{4(1+x)^4} + \frac{1}{3(1+x)^3}\right.\right.$$
$$+ \frac{1}{2(1+x)^2} + \frac{1}{(1+x)} + \left.\ln\left(\frac{x}{1+x}\right)\right)$$
$$- \frac{f_1}{6(1+x)^6} - \frac{f_2}{(1+x)^7}\left(\frac{x}{6} + \frac{1}{42}\right)$$
$$- \frac{f_3}{(1+x)^8}\left(\frac{x^2}{6} + \frac{x}{21} + \frac{1}{168}\right)$$
$$- \frac{f_4}{(1+x)^9}\left(\frac{x^3}{6} + \frac{x^2}{14} + \frac{x}{56} + \frac{1}{504}\right)$$
$$- \frac{f_5}{(1+x)^{10}}\left(\frac{x^4}{6} + \frac{2x^3}{21} + \frac{x^2}{28} + \frac{x}{126} + \frac{1}{1260}\right)\cdots\left.\right]_{x_0}^{x_{min}}; \tag{5}$$

Eq. (5) can be used to evaluate the contribution to the ICS in the region of $0°-\theta_{min}°$ for each vibronic state. The total electronic excitation cross section is the sum of the ICS from the first step and the results from Eq. (5).

3. Results

The method is demonstrated in ICS calculations for $X^1\Sigma^+ \rightarrow A^1\Pi$ transition in e-CO scattering. DCS are taken from the measurements of Zetner et al. [3] at impact energies of 12.5 and 15 eV with $\theta_{min}° = 9$ and 14°, respectively. The difference in using Eq. (3) in comparison with the usual Lassetre fitting procedure is that we include not only the GOS data but also the OOS in the least square calculation. This is dictated by the Lassettre limit theorem [5]; namely the GOS will converge to the OOS regardless of whether the first Born approximation is applicable or not.

Table 1 lists the Frank–Condon factors [4], $q_{v'}$, excitation energy [6], $w_{v'}$ (eV), and OOSs [7], $f_{v'}$ for the vibronic states $v' = 0 - 5$ for the fourth bands of carbon monoxide. Table 2 gives the results of ICS in 10^{-18} cm^2 from Eq. (5), $\sigma_{v'}$, the ICS of $\theta_{min} - \theta_{max}$, σ_b, and the total ICS, σ_t together with the R-matrix calculation by Morgan and Tennyson [8] and the

Table 2
ICS (10^{-18} cm^2) for the $X^1\Sigma^+ \rightarrow A^1\Pi$ process in e-CO scattering at 15.0 and 12.5 eV impact energies, $\theta^\circ_{min} = 9$ and $14°$, respectively

	v'	15 eV	12.5 eV
$\sigma_{v'}$	0	2.293	0.6793
	1	4.529	1.304
	2	4.733	1.328
	3	3.743	1.026
	4	2.380	0.6349
	5	1.314	0.3419
$\Sigma\sigma_{v'}(0°-\theta^\circ_{min})$		18.99	5.311
$\sigma_b(\theta > \theta^\circ_{min})$		55.36	42.49
σ_t		74.35	47.80
Morgen and Tennyson [8]		80.0	52.2
Zetner et al. [3]		64.95	45.83

initial ICS data by Zetner et al. [3]. The comparison shows that our results are closer to the theoretical *R*-matrix calculation [8] than the previous Zetner et al. evaluations [3] using the same DCS data. The difference between the results of *R*-matrix and the evaluation of Zetner is 18.8 (15 eV) and 12.2% (12.5 eV). After using Eq. (5) and reevaluating the ICS the differences between the theoretical results and experimental data are reduced to 7.0 (15 eV) and 8.4% (12.5 eV).

4. Conclusions

In conclusion, a new method has been developed to evaluate the excitation cross sections for the electronic dipole-allowed transitions of the electron-molecular collision. The method has been tested with the $X^1\Sigma^+ \rightarrow A^1\Pi$ transition in e-CO scattering. A better agreement between the theoretical results and the experimental data has been obtained by using the new method.

References

[1] S.K. Srivastava, S. Jensen, J. Phys. B 10 (1977) 3341.
[2] M.A. Khakoo, S. Trajmar, Phys. Rev. A 34 (1986) 146.
[3] P.W. Zetner, I. Kanik, S. Trajmar, J. Phys. B 31 (1998) 2395.
[4] E.N. Lassettre, A. Skerbele, J. Chem. Phys. 54 (1971) 1597.
[5] E.N. Lassettre, A. Skerbele, M.A. Dillon, J. Chem. Phys. 50 (1969) 1829.
[6] V.D. Meyer, A. Skerbele, E.N. Lassettre, J. Chem. Phys. 43 (1965) 805.
[7] W.F. Chan, G. Cooper, C.E. Brion, Chem. Phys. 170 (1993) 123.
[8] L.A. Morgen, J. Tennyson, J. Phys. B 26 (1993) 2429.