

## SHORT COMMUNICATIONS

INTEGRAL INELASTIC CROSS SECTIONS FOR THE ROTATIONAL ENERGY TRANSFER IN CO<sub>2</sub>-Ar SYSTEM

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THE study of rotational energy transfer (RET) is important to the efficient operation of the short pulsed (1 n. second or less) CO<sub>2</sub> lasers currently being used in and designed for laser-induced fusion experiments<sup>1</sup>. The results of the computed integral inelastic cross sections (IICS),  $\sigma(j_i \rightarrow j_f)$ , for RET in CO<sub>2</sub> in (001) vibrational state due to collision with Ar are presented here. The conclusion that the cross sections can be fitted into an empirical relation known as the power-gap (PG) law<sup>2</sup> is presented in this paper. The most important result of this paper is a new equation that gives the variation of a fitting parameter with the collision energy.

The modified form of the infinite order sudden approximation<sup>3</sup> (IOSAM) given by Agrawal and Raff<sup>4</sup> and the 'electron-gas' potential energy surface computed by Parker, Snow and Pack<sup>5</sup> have been used to calculate the cross sections. Calculations have been performed over a wide range of initial energy,  $T_i$  ( $0.069 \leq T_i \leq 0.425$  eV). The number of phase shifts computed varies with energy. At 0.425 eV, 660 phase shift have been considered. Phase shifts were calculated using a 10 point Gauss-Mehler Quadrature of the WKB phase-shift equation<sup>6</sup>. A 200-point Gauss-Legendre quadrature has been used to integrate over the angle variable [Eq. (21) of Ref. (7)].

The cross sections,  $\sigma(j_i \rightarrow j_f)$ , for initial rotational state  $j_i = 19$ , and final rotational state  $j_f$  in the range  $1 \leq j_f \leq 65$  are reported here. The interesting aspect of the results is that all the computed cross sections (except those with  $|\Delta j| = 2$ ) can be represented fairly well by the following empirical relation known as power-gap (PG) Law<sup>2</sup>.

$$\sigma(j_i \rightarrow j_f)(T_i/T_f)^{1/2}/(2j_f + 1) = a|\Delta E|^{-\gamma} \quad (1)$$

where  $\Delta E$  = rotational energy gap between  $j_i$  and  $j_f$  levels,  $T_f$  is the final translation energy,  $a$  and  $\gamma$  are the fitting parameters.

Log of the left hand side of (1) has been plotted against  $\ln |\Delta E|$ .  $a$  and  $\gamma$  have been determined from the

knowledge of the slope and the intercept of the straight line plot so obtained, for each value of  $T_i$ . Further, it has been observed that  $\ln a$  vs  $\ln T_i$ , and  $\gamma$  vs  $\ln T_i$  plots are also straight lines, i.e., the variation of  $a$  and  $\gamma$  with  $T_i$  is governed by the following equations:

$$a = \beta T_i^{-\alpha} \quad (2)$$

$$\text{and} \quad \gamma = \gamma_0 + d \ln T_i \quad (3)$$

For  $\Delta E$  and  $T_i$  in eV, and  $\sigma$  in Å<sup>2</sup> the slopes and intercepts of the plots give following values of the parameters:

$$\beta = 0.00086, \quad \alpha = 0.596 \\ \gamma_0 = 0.795, \quad \text{and} \quad d = 0.081 \quad (4)$$

The data reported in table 1 clearly demonstrates the success of relations (1)–(4). Except for the transitions with  $|\Delta j| = 2$ , the other values show good agree-

Table 1. Cross sections for CO<sub>2</sub>-Ar system ( $j_i = 19$ )

$j_f$	$\sigma(j_i \rightarrow j_f)(T_i/T_f)^{1/2}$ values in Å <sup>2</sup>					
	$T_i = 0.425$ eV		0.19 eV		0.069 eV	
	(a) IOSAM	(b) PG Law	(a) IOSAM	(b) PG Law	(a) IOSAM	(b) PG Law
1	0.085	0.079	0.11	0.10	0.15	0.13
3	0.20	0.19	0.25	0.23	0.34	0.31
7	0.47	0.44	0.57	0.54	0.80	0.71
11	0.84	0.82	1.00	0.99	1.34	1.26
13	1.14	1.14	1.32	1.35	1.71	1.69
15	1.66	1.68	1.89	1.96	2.48	2.37
17	3.76	3.01	4.78	3.36	7.59	3.87
21	4.18	3.43	5.32	3.86	8.46	4.49
23	2.09	2.19	2.39	2.59	3.16	3.19
25	1.63	1.71	1.91	2.09	2.51	2.67
27	1.40	1.45	1.70	1.81	2.29	2.38
29	1.25	1.29	1.55	1.63	2.16	2.19
31	1.15	1.17	1.45	1.50	2.06	2.05
35	1.01	1.01	1.31	1.33	1.90	1.88
39	0.92	0.91	1.21	1.22	1.79	1.76
43	0.85	0.84	1.14	1.14	1.67	1.68
47	0.80	0.78	1.08	1.08	—	—
51	0.76	0.74	1.02	1.03	—	—
55	0.72	0.70	0.97	0.99	—	—
59	0.69	0.67	0.93	0.96	—	—
63	0.66	0.64	0.88	0.93	—	—
65	0.65	0.63	0.86	0.92	—	—

(a) Computed using IOSAM formulation of Agrawal and Raff<sup>3</sup>.

(b) Evaluated using the PG law and the parameters given by Eqs. (1)–(4)

ment. ICS for CO<sub>2</sub>-Ar system can thus be computed at least in the range of present study using three simple equations (1)-(3) and four parameters given by (4).

Equation (2) is not new. For N<sub>2</sub>-Ar system also Koura<sup>8</sup> noted such behaviour. The variation of  $\gamma$  according to (3) has been noted here for the first time.

Table I shows that the PG law underestimates the cross-sections for  $|\Delta j| = 2$ . Further, the difference between  $\sigma_{PG}$  and  $\sigma_{IOSAM}$  for  $|\Delta j| = 2$  increases with decrease in  $K_1$ . This behaviour may be related with the magnitude of the torque required for changing the angular momentum of the molecule. Change in angular momentum roughly depends on the product of the torque and the collision time. As the collision time, approximately, varies as  $T_i^{-1/2}$  the torque,  $\tau$ , required to cause particular transition would be proportional to  $|\Delta j| \times \sqrt{T_i}$ . Therefore,  $\tau$  would be low for low values of  $|\Delta j|$  and  $T_i$ . Thus we note that the power-gap law underestimates the efficiency of those transitions which require low value of torque. It may be mentioned that the PG law overestimates<sup>9</sup> the efficiency of those transitions which require high value of torque. It is therefore inferred that the empirical power-gap law works well in the 'medium range' of  $\tau$ . The details are being investigated further.

The dependence of  $\beta$ ,  $\alpha$ ,  $\gamma_0$  and  $d$  on the parameters of the colliding system is also being investigated further. Such a study may lead to the better understanding of the mechanism of RET also.

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## POLAROGRAPHIC STUDIES ON ACTIVE CONSTITUENTS OF *SIDA CORDIFOLIA*

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POLAROGRAPHIC method has been used widely for the identification and estimation of active components of plants. Thus, the optimum conditions for the isolation of anthocyanins<sup>1</sup> from fruits of *Sambucus nigra* were established by this method. Similarly, juglone and hydrojuglone contents of different parts of walnut trees and fruits were estimated<sup>2</sup>. Several tropolone derivatives similar to colchicine, were detected and isolated from the seeds of meadow saffron and characterized by polarographic methods<sup>3</sup>.

The present investigation of the plant, *Sida cordifolia* (Malvaceae), has been undertaken from this point of view. The plant is of considerable medicinal importance and is said to contain an alkaloid, ephedrine, known to have wide therapeutic values<sup>4-7</sup>.

Polarograms have been recorded (298K) with a Radiometer pen-recording polarograph, Polariter PO4g. A Kaloušek cell with a saturated calomel electrode as reference electrode has been used. The dme made from sargent capillary has the following characteristics:  $m = 0.952 \text{ mgs}^{-1}$  and  $t = 4.3 \text{ s}$  at 60 cm height of mercury reservoir in potassium chloride solution ( $0.5 \text{ mol dm}^{-3}$ ) at zero applied potential (sce). The pH-values of the solutions have been measured before and after recording each polarogram on an ELICO model LI-10 pH-meter with an accuracy of  $\pm 0.1$  pH unit.

All the chemicals used are of A. R. grade. The stems and roots of the plant *sida cordifolia* have been separately dried in air, powdered and 11.0g of each are kept immersed in 1% perchloric acid (200 ml) at room temperature and after allowing to stand for a week, the extracts are filtered before use. Preliminary tests show that these extracts are too concentrated for polarographic work and have been diluted 100 times in the test solution. The extract (1 ml) is first diluted to 10 ml; 1 ml of this solution is added to 5 ml of acetic acid-tetra-ethylammonium acetate ( $0.1 \text{ mol dm}^{-3}$ ) buffer; 1 ml of tetra-ethylammonium bromide ( $1.0 \text{ mol dm}^{-3}$ ) is added and the solution is made up to 10 ml with conductivity water. A 1.5 ml of 0.2% gelatin is also added before making up to volume wherever required to suppress maxima.

A stock solution of ephedrine hydrochloride ( $10.0 \text{ mol dm}^{-3}$ ) has been used for comparison.

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