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Quasi-classical Trajectory Study of Ba+HI→BaI+H Reaction

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The quasi-classical trajectory calculations based on extended London-Eyring-Polanyi-Sato potential energy surface have been used to study the reaction of Ba+HI→BaI+H system. The rotational, vibrational, translational, and angular distributions of the product BaI have been calculated. The calculated results are in good agreement with the experimental ones.

Key words: Quasi-classical trajectory calculation, London-Eyring-Polanyi-Sato potential energy surface, Ba+HI reaction

I. INTRODUCTION

Laser induced fluorescence (LIF) has made possible the detailed study of the state-to-state reaction dynamics of alkaline earth metal atoms with hydrogen halides *e.g*

$$\mathrm{M} + \mathrm{HI} \rightarrow \mathrm{MI} + \mathrm{H} \tag{1}$$

Specific reactions have been investigated experimentally under single collision conditions for the following reactions: Sr+HI [1], Ca+HI [1], Ba+HF [2–7], Ba+HCl [4, 8, 9], Ba+HI [1, 4, 10], and so on.

Recently, Han and co-workers performed some experimental studies and the quasi-classical trajectory (QCT) calculations on the reactions of the alkaline earth metal with hydrocarbon halides [11–15]. The dynamics of this reaction family are quite interesting, because of the mass combination heavy/heavy-light (H+H′L) to form heavy-heavy+light (HH′+L), the orbital angular momentum of the collision is expected to be channeled almost exclusively into rotational-angular momentum of the diatomic product [11, 16]. Although gaseous reaction of group IIa alkaline earth atoms have apparently not yet been studied by conventional kinetic techniques, a number of molecular beam laboratories [17-25] have become interested in reactions of these atoms. Furthermore, impact parameter dependence [10], angular distributions [1], internal state distributions [4] and relative total reactive cross sections for title reaction have been studied.

It was one of the most important progress that, using selectively LIF, Zare and coworkers measured the rotational state distribution of the beam-gas reaction Ba+HI→BaI(v=8)+H [10]. Owing to the highly constrained kinematics of these systems, these measurements can be used to derive the reaction probability as a function of the impact parameter for this channel, called the "specific" opacity function, once the reaction probability as a function of velocity has been determined. In contrast to a large number of experimental studies, no comprehensive theoretical and/or dynamical features of this class of reaction have emerged. In this work, we report the effectiveness of vibrational, rotational, angular distributions on the exothermic reaction of Ba+HI→BaI(v=8)+H using the QCT method based on the extended London-Erying-Polanyi-Sato (LEPS) potential energy surface (PES).

II. THEORY

The extended LEPS PES is employed in this calculation [26–29]:

$$V(r_1, r_2, r_3) = Q_1 + Q_2 + Q_3 - ({J_1}^2 + {J_2}^2 + {J_3}^2 - J_1J_2 - J_2J_3 - J_1J_3)^{1/2} \tag{2}$$

$$Q_i = \frac{{}^{I}E_i + {}^{3}E_i}{2} \tag{3}$$

$$J_i = \frac{{}^{1}E_i + {}^{3}E_i}{2} \tag{4}$$

${}^{1}E_i$ is defined as the diatomic Morse potential and ${}^{3}E_i$ stands for the anti-Morse function.

$${}^{1}E_i = D_i(\{1 - \exp[-\beta_i(r - r_o)]\}^2 - 1) \tag{5}$$

$${}^{3}E_i = {}^{3}D_i(\{1 + \exp[-\beta_i(r - r_o)]\}^2 - 1) \tag{6}$$

$${}^{3}D_i = \frac{D_i(1 - S_i)}{2(1 + S_i)} \tag{7}$$

S_i is an adjustable parameter (the so-called Sato parameter), D_i, β_i, and r_i represent Morse parameters of the diatom, subscript i=1, 2, 3, indicates BaI, HI, and BaH respectively. The parameters of D_i, β_i, and r_i for PES are taken from the Ref.[30] (Table I).

The QCT calculations are standard [26, 31–35], the classical Hamilton's equations were integrated numer-

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TABLE I The parameters used in the LEPS of the Ba + HI reaction.

Species	$D^a/10^{-12}$eV	$\beta^a/10^8$A^{-1}	$r^a/10^{-8}$Å	S
BaI	7.08084	0.79888	3.08476	0.496
HI	4.89251	1.79205	1.60916	−0.225
BaH	3.12390	1.13520	2.23175	0.940

[a] The results from Ref.[30].

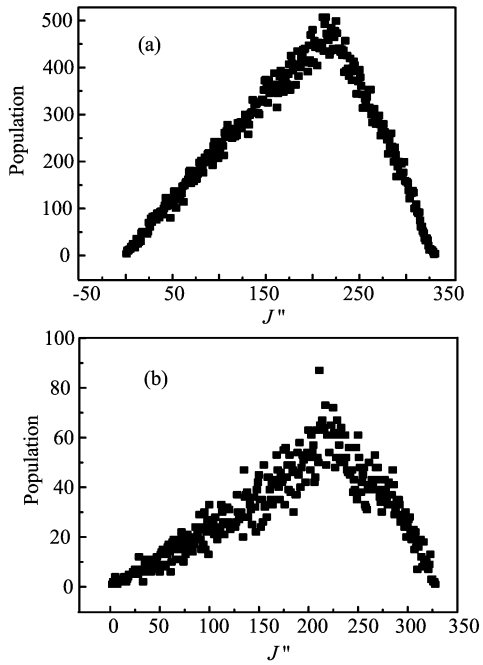

FIG. 1 Rotational distribution of the BaI (v=8) product. (a) Experimental results taken from Ref.[10] and (b) theoretical results in this work.

ically for motion in three-dimensions. In our calculations, 10^5 trajectories were sampled and the trajectories were initiated with Ba-HI internuclear distance of 15 Å. The intergration step size in the trajectories was chosen to be 0.1 fs. In order to confirm the correction of this calculation, we have reproduced the work of Han *et al.* [11].

III. RESULTS AND DISCUSSION

Figure 1 shows the rotational distribution of the BaI (v=8) product obtained in the Ba+HI reaction from the QCT calculations. In order to compare with experimental results [10], collision energy was chosen as 15.05 kJ/mol. Clearly the calculated rotational distribution of the BaI product in v=8 produced by the Ba+HI are in good agreement with the experimental measurements. The highest J obtained is 330.

Figure 2 shows the plot of the vibrational distribution for the product BaI with a peak at 9. The product

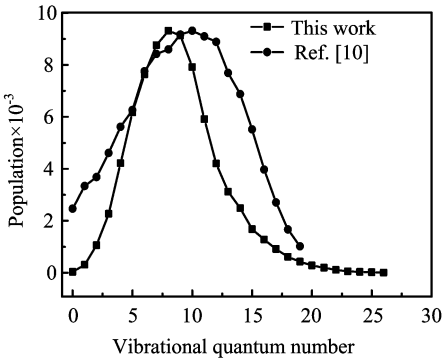

FIG. 2 Vibrational distribution of the BaI product.

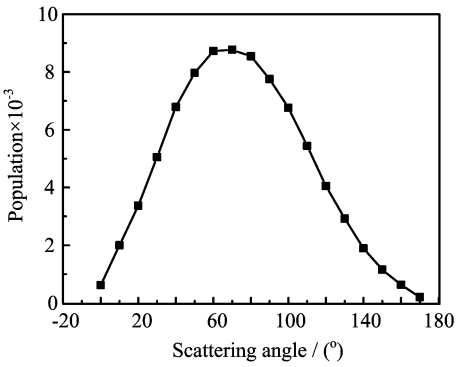

FIG. 3 Angular distribution of the BaI product.

vibrational distribution with a peak at 10 was reported experimentally by Noda *et al.* [10]. The calculated vibrational distributions are consistent with experimental ones very well. The product angular distribution is shown in Fig.3. From the plot it is indicative to see the distribution to be highest between 70–80. This is in agreement with the experimental one [1], in which Mims *et al.* have studied this reaction by measuring the BaI angular distribution produced under crossed-beam conditions [1]. Both predict that it is sideway scattering.

IV. CONCLUSION

It is shown that the QCT calculated results agree well with the experimental results for the exothermic reactions of Ba+HI. The calculated results show very close resemblance in the vibrational and rotational as well as angular distributions with experimental ones [1, 10].

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