IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861. Volume 3, Issue 3 (Mar. - Apr. 2013), PP 24-29
www.iosrjournals.org

Maximum Limit of Rotational energy transfers in C_2 - He system and Power gap law

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Abstract: *Theoretical importance of the classical limit of the maximum rotational energy transfer, $(\Delta E)_{max,}$ it has been reviewed for a two dimensional hard ellipsoid potential model over a wide range of energies, reduced mass of the system. It has been found that $(\Delta E)_{max}$, is comparable with a well-known parameter $l\Delta El^*$ given by the two parameter Power- gap law. The numerical equivalence of $(\Delta E)_{max}$ and $l\Delta El^*$ has been verified for different collision energy of the atom - diatom system. Such equivalence suggests that the value of $(\Delta E)_{max}$ can be used as one parameter $l\Delta El^*$ of the power -gap law. The salient feature of the research helps to develop several techniques in field of rotationally energy transfer inelastic collision in atom- diatom systems.*
Keywords:- *Rotational energy transfer, Diatomic collision and scattering cross section.*

I. Introduction

The study of rotational inelastic scattering between molecules and neutral atoms at low collision energies is a fast developing field in collision dynamics [1-2].The nature of rotational energy transfer (RET) in collisions of molecules with He, Ar and Ne were studied experimentally [3-4] and theoretically [5-7] .

In several papers Mccaffery and co-workers [8-10] explored various aspects of the RET by treating the conversion of orbital angular momentum to the angular momentum of the molecule at the repulsive wall of anisotropic intermolecular potential. However they point out that the maximum change in rotational momentum might be limit either by energy conservation or by momentum conservation, developing on detail of the particular collision system. They obtain the maximum classical limit of RET by using a hard ellipsoid potential model. This model treats a molecule as a hard core ellipsoid and the collision between the atom and the hard core ellipsoid.

The relationship between the shape of the potential surface and the energy transfer is crucial idea for giving technique to understanding collision processes of molecules and rare gases i. e. He, Xe, Ne and Ar. The link between the two is provided by the general quantum theory of collision for hard shapes and classical approach of hard ellipsoid model. The problem of the rotationally inelastic collision of a particle with a hard ellipsoid potential [11-14] can be solved by using the three principles of conservation; the total energy conservation, linear momentum conservation and the angular momentum conservation. Agrawal and co-workers [15-17] have noted that the classical limit of rotational energy transfer $(\Delta E)_{max,}$ predicted by the hard ellipsoid model is comparable to a well known parameter $l\Delta El^*$ given by power -gap law [18] and the RET cross – sections computed on the real potentials.

It would be important to perform an elaborate test of the expression for the maximum limit of angular momentum transfer so obtained, such a test would be useful for the RET cross- sections computed using the realistic potential.

In this study, in addition to the validity of the hard ellipsoid potential model we shall also reconfirm that the division between the classically allowed and forbidden transitions given by the power-gap law is excellent. Further, we show that the equivalence of the $l\Delta El^*$ and $(\Delta E)_{max,}$ not only provide the physical meaning to $l\Delta El^*$ given by the RET data and the power -gap law but is also valuable for determination of some features of intermolecular interaction potential from knowledge of RET data.

In Section 2, we formulate the procedure for determination of $l\Delta El^*$ and $(\Delta E)_{max}$. The numerically results are presented and discussed in Section 3. Finally the conclusions are summarised in Section 4.

II. Fomulation

2.1. DETERMINATION OF lΔEl*

The parameter lΔEl* is determined with the help of cross sections obtained from scattering calculations and the power gap law.

For the computation of cross sections the homonuclear diatomic molecule, C_2, is treated as a rigid rotor and the interaction between the molecule and the atom, He, is taken as a pairwise sum of the potential terms,

$$V = V(r_1) + V(r_2), \quad (1)$$

where r_1 and r_2 are the C^1-He and C^2-He distances, respectively, as shown in Fig.1.

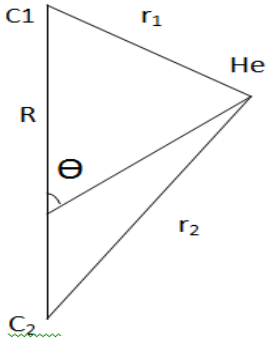


Fig. (1) Coordinates for the rigid rotor C_2-He system.

For V (r_i) the general form of the Lennard–Jones (L-J) potential is taken with different values of n and m:

$$V(r_i) = \varepsilon[\{m/(n-m)\}(r_o/r_i)^n - \{n/(n-m)\}(r_o/r_i)^m], \quad (i = 1, 2), \quad (2)$$

where r_0 and ε are taken [19] as 1.925Å and 1.2437meV, respectively .

In addition to the above-mentioned potential functions, purely repulsive terms of the potential functions have also been investigated. It is convenient to denote such potentials by the notation $V_R(n)$, which has been obtained by deleting the attractive term from the potential V (n, m). The cross sections have been computed using the modified infinite order sudden approximation method (IOSAM), [19]. The phase shifts have been computed using a 10- point Gauss – Mehler quadrature of the WKB phase shift equation as described by Pack [20].

According to the power gap law [19] the cross sections, $\sigma(j_i \rightarrow j_f)$ can be expressed as

$$\sigma(j_i \rightarrow j_f) = a(2j_f + 1)(T_f/T_i)^{1/2} \left| \Delta E \right|^{-\gamma}, \quad (3)$$

where j_i and j_f are the initial and final rotational quantum numbers, a and γ are the fitting parameters, T_f and T_i are the final and initial translational energies and lΔEl is the energy gap between initial and final rotational levels. Eq. (3) gives the following equation which can be used to separate the two regions.

$$Y = -\gamma X + \ln a, \quad (4)$$

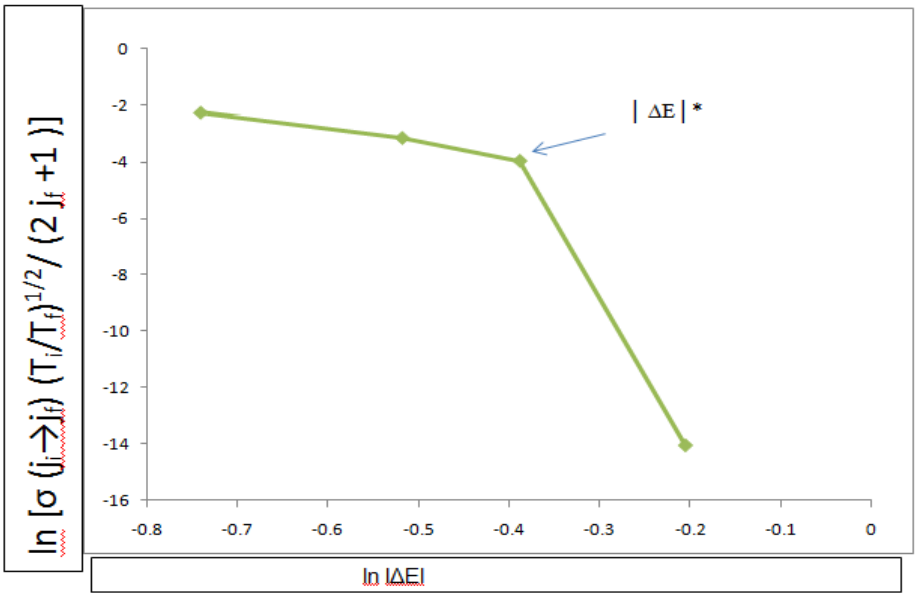
where

$$Y = \ln[\sigma(j_i \rightarrow j_f)(T_i/T_f)^{1/2}/(2j_f + 1)], \quad (5)$$

and

$$X = \ln l\Delta El. \quad (6)$$

A typical X-Y plot which shows the existence of two straight lines signifying the two regions is given in Fig. (2). The location of the critical point has been marked as lΔEl* in the figure. For all sets of the computed cross sections, lΔEl* has been obtained by such plots.



Graph - (1) ln $[\sigma\ (j_i \rightarrow j_f)\ (T_i/T_f)^{1/2}/\ (2\ j_f +1\ )]$ versus ln lΔEl for j_i=0 at E= 0.1 eV for V(12,6) potential. lΔEl* point is shown by an arrow. The unit of ΔE and σ are eV and Å , respectively

2.2. DETERMINATION OF $(\Delta E)_{max}$

For the maximum limit of angular momentum transfer the hard ellipsoid potential model was discussed in detailed by Agrawal and co-workers. He found the following relation for the classical limit of the angular momentum transfer

$$(\Delta J)_{max} = \sqrt{(2\mu)}(\sqrt{E}+\sqrt{E'})\ (A-B), \qquad (7)$$

where μ is the reduced mass of the colliding system, E and E$'$ are the initial and final translational energies of the system, respectively and A and B are the lengths of the semi – major and semi-minor axes of ellipsoid, respectively.

From the above expression the limit of the rotational energy transfer in the molecule can easily be obtained. For simplicity, if the diatomic molecule is considered initially in the ground state, then the expression for the maximum amount of rotational energy transfer would be

$$(\Delta E)_{max} = [(\Delta J)_{max}\ ]^2 / 2I,$$
$$(\Delta E)_{max} = (\mu/ I)\ (A-B)^2\ \ [E+E' + 2\sqrt{(EE')}] \qquad (8)$$

where I is the moment of inertia of the diatomic molecule. Eq. (8) together with the following energy conservation equation

$$E' = E - (\Delta E)_{max}, \qquad (9)$$

can be used to compute $(\Delta E)_{max}$ from knowledge of E, A, B, μ and I.

III. Results And Discussion

3.1 EFFECT OF ENERGY

Table 1 list γ_{low}, γ_{high} and lΔEl* given by the scattering calculations for the potential V (12, 6) and V_R (6) as a function of the initial translational energy for C_2- He system. For comparison the value of $(\Delta E)_{max}$ given by Eq. (8) are also shown in the Table 1. A comparison of the values of $(\Delta E)_{max}$ given by the hard ellipsoid model and lΔEl* given by the scattering method shows that they are in very good agreement. This excellent agreement shows that lΔEl* can be considered as $(\Delta E)_{max}$.

The data reported in Table 2 also shows that $(\Delta E)_{max}$ is approximately proportional to E : $(\Delta E)_{max}$ / E varies from 0.047 to 0.189 as E increases from 0.1 to 0.4 eV. The variation of $(\Delta E)_{max}$ / E with E can be analyzed by the two factors $(A-B)^2$ and $[E+E' + 2\sqrt{(EE')}]$ / E, occurring in Eq. (8). The factor $(A-B)^2$ increases from 0.7334 to 0.7775 and letter factor decreases from 1.6052 to 1.4086 as E increases from 0.1 to

0.4eV. For a perfectly hard ellipsoid potential, $(A-B)^2$ would not depend on E and as such the variation in $(\Delta E)_{max}$ / E would be given by the later factor only. Another important parameter is, **γ**. For a given potential we see that γ_{low} is insensitive to the change in the collision energy. The values of γ_{high}, however, shows a different trend. The energy dependence of these parameters is a matter of further studies.

Table-1

Comparing of maximum amount of rotational energy transfer $(\Delta E)_{max}$ values by the hard ellipsoid potential model and those obtained by using the scattering cross sections and the power- gap law for the C_2-He system. Where the L-J Potential Parameter σ and ϵ are 1.925Å and 0.0012437eV respectively.

Potential	**Energy (eV)**	$\gamma_{low}^{(a)}$	$\gamma_{high}^{(a)}$	$(\Delta E)_{max}$ **eV.**	
				Ellipsoid Model	**Scattering**
V (12 ,6)	**0.10**	**0.749**	**6.19**	**0.051**	**0.047**
	0.15	**0.793**	**8.27**	**0.077**	**0.078**
	0.20	**0.802**	**9.96**	**0.104**	**0.111**
	0.25	**0.816**	**11.07**	**0.130**	**0.143**
	0.30	**0.803**	**9.03**	**0.158**	**0.162**
	0.35	**0.799**	**7.1**	**0.178**	**0.181**
	0.40	**0.792**	**4.21**	**0.213**	**0.189**
V_R(12)	**0.10**	**0.817**	**6.95**	**0.049**	**0.046**
	0.15	**0.816**	**7.94**	**0.075**	**0.072**
	0.20	**0.858**	**10.34**	**0.102**	**0.109**
	0.25	**0.833**	**10.53**	**0.129**	**0.133**
	0.30	**0.846**	**9.84**	**0.155**	**0.160**
	0.35	**0.815**	**4.48**	**0.182**	**0.178**
	0.40	**0.825**	**4.94**	**0.191**	**0.188**

(a) The unit of γ_{low} and γ_{high} are such that in Eq. (3) cross section is in $(Å)^2$ and ΔE is in eV.

Table-2

Comparing of maximum amount of rotational energy transfer $(\Delta E)_{max}$ values by the hard ellipsoid potential model and those obtained by using the scattering cross sections for the C_2-He system. Where the L-J Potential Parameters σ and ϵ are 1.925Å, .0012437eV respectively.

Potential	**Energy (eV.)**	**A Å**	**B Å**	**A-B Å**	$(\Delta E)_{max}$ **eV.**	
					Ellipsoid Model	**Scattering**
V (12 ,6)	**0.10**	**2.4616**	**1.6052**	**0.8564**	**0.051**	**0.047**
	0.15	**2.4108**	**1.5478**	**0.8630**	**0.077**	**0.078**
	0.20	**2.3750**	**1.5070**	**0.8680**	**0.104**	**0.111**
	0.25	**2.3474**	**1.4752**	**0.8722**	**0.130**	**0.143**
	0.30	**2.3252**	**1.4494**	**0.8758**	**0.158**	**0.162**
	0.35	**2.3190**	**1.4392**	**0.8798**	**0.178**	**0.181**
	0.40	**2.2904**	**1.4086**	**0.8818**	**0.213**	**0.189**
	0.10	**2.4912**	**1.6530**	**0.8382**	**0.049**	**0.046**

$V_R(12)$	**0.15**	**2.4342**	**1.5860**	**0.8482**	**0.075**	**0.072**
	0.20	**2.3948**	**1.5394**	**0.8554**	**0.102**	**0.109**
	0.25	**2.3648**	**1.5040**	**0.8608**	**0.129**	**0.133**
	0.30	**2.3408**	**1.4514**	**0.8654**	**0.155**	**0.160**
	0.35	**2.3208**	**1.4514**	**0.8694**	**0.182**	**0.178**
	0.40	**2.3036**	**1.4408**	**0.8628**	**0.191**	**0.188**

3.1 EFFECT OF MASS

Table 3 gives the results for C_2-X system having r_0 and Є value of C_2-He system and the masses of X are 2.0, 4.0, 8.0, 12.0, 16.0, 20.2 and 39.95 amu. for the potential V(12,6) at different collision energies.

A very good agreement between the $(\Delta E)_{max}$ values given by the hard ellipsoid model and scattering calculations is seen from Table 3. Further a decrease in $(\Delta E)_{max}$ values with increase in mass of the atomic molecule, X, is also seen from the table.

For a system to exhibit angular momentum constraint the final rotational state of the molecule must be energetically accessible to eliminate any energetic restrictions. Thus the $(\Delta E)_{max}$ values must be smaller than the available translational energy E.

We have

$$(\Delta E)_{max} / E < 1,$$

or

$$(\mu / I) \ (A-B)^2 < 1, \qquad \text{[using Eq. (8)]}$$

or

$$(\mu / \mu_m) \ [(A-B) / R_e]^2 < 1, \qquad (10)$$

where μ_m and R_e are the reduced mass and bond length of the molecules. Thus the ratio μ / μ_m is an important factor in determining whether a collision system is momentum or energy constrained. In C_2-He system the order of (A-B) is 0.8564 and the bond length of C_2 is $R_e = 1.54$ Å. Hence $[(A-B) / R_e]^2$ is ≈ 0.7. Therefore the ratio μ / μ_m should be smaller than 2 for the inequality in Eq. (10) to hold. In other cases all the transitions permitted by the energy conservation constraint would be possible.

Table-3

Comparing of maximum amount of rotational energy transfer $(\Delta E)_{max}$ values by the hard ellipsoid potential model and those obtained by using the scattering cross sections for the C_2-X system at the potential V(12,6).

Where X = 2.0, 4.0, 8.0, 12.0 and 16.0 amu.

Mass of X (amu)	μ	μ / μ_m	A (Å)	B (Å)	γ_{low} [a]	γ_{high} [a]	$(\Delta E)_{max}$ (eV)	
							Ellipsoid Model	**Scattering**
2.0	**1.85**	**0.31**	**2.4616**	**1.6052**	**0.904**	**9.20**	**0.032**	**0.034**
4.0	**3.0**	**0.50**	**2.4616**	**1.60452**	**0.749**	**6.19**	**0.051**	**0.047**
8.0	**6.0**	**1.00**	**2.4616**	**1.60452**	**0.746**	**2.63**	**0.072**	**0.0697**
12.0	**8.0**	**1.33**	**2.4616**	**1.60452**	**0.737**	**0.92**	**0.083**	**0.0537**
16.0	**9.6**	**1.60**	**2.4616**	**1.60452**	**0.738**	**1.28**	**0.089**	**0.0714**

IV. Conclusion

The maximum amount of rotational energy transfer in collisions of C_2 with He has been investigated over a wide range of energies, reduced mass of the system, potential functions and potential parameters. Further, the classical limit of maximum rotational energy transfer has been reviewed for a hard ellipsoid potential model.

$|\Delta E|^*$ and $(\Delta E)_{max}$ also suggest that the classical limit of angular momentum transfer given by the hard ellipsoid potential model is meaningful even for the cross sections computed on the real potentials provided the classical turning point surface of the soft potential is assumed as the hard potential surface. The $|\Delta E|^*$ values

given by the scattering results are also found to be in good agreement with the $(\Delta E)_{max}$ values obtained by using the hard ellipsoid model.

Acknowledgements

The support of the university grant commission, central regional office, Bhopal under grant No. MS-49/107029/10-12/CRO (2) is gratefully acknowledged.

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