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RESEARCH COMMUNICATIONS

The dependence of rotationally inelastic cross-sections on the parameters of the potential

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The dependence of cross-sections, $\sigma(0 \rightarrow j)$, on the parameters of the intermolecular potential for rotational transitions in a diatomic molecule due to collision with an atom has been investigated. It is found that a 300% increase in the potential leads to only about 33% increase in the cross-sections. It is explained on the basis of the importance of the torque at the classical turning point, range of the potential and the collision time.

THE study of rotational energy transfer (RET) is important to many areas[1], such as lasers, astrophysics, molecular-beam experiments, spin–lattice relaxation of NMR signals, ultrasonic absorption and dispersion, thermal conductivity and transpiration, shock-wave propagation, microwave broadening, and intermolecular interaction. In many situations, it is useful to have an estimate of a set of cross-sections from a few parameters that can be obtained from some known cross-sections. Scaling and fitting laws such as the power-gap law[2] and the exponential-gap law[3] serve such a purpose. Further, it would also be worthwhile to arrive at some semiempirical expressions that give the dependence of cross-sections on the parameters of the intermolecular potential. In this paper we present one such empirical relationship, obtained by investigating a set of computed cross-sections. We also discuss the physical explanation.

A system of a homonuclear diatomic molecule and an atom has been considered, and the following form of the intermolecular potential has been used:

$$V(r,\theta) = v(r)\left[1 + \sum_{l=2}^{10} a_l P_l(\cos\theta)\right] \quad (1)$$

with

$$v(r) = C e^{-\alpha r}, \quad (2)$$

where r is the distance between the centre of mass of the molecule and the atom, θ the angle between vector **r** and the bond, and P denotes the Legendre polynomial. Due to symmetry of the homonuclear molecule odd terms in the summation in eq. (1) would be zero. The masses of the molecule and atom are taken as 28.0 and 4.0 amu. The bond length of the molecule is chosen as 1.0 Å.

The computations have been performed at relative translational energy $E = 0.1$ eV by using the modified infinite-order sudden approximation (IOSAM) given by Agrawal and Raff[4]. IOSAM is a modification of the well-known infinite-order sudden approximation[5] (IOSA) to the solution of the Schrödinger equation.

Table 1 gives the variation of the cross-sections, $\sigma(0 \rightarrow j)$, with the parameter C of eq. (2). As the magnitude of the torque ($= \partial V/\partial\theta$) acting on the molecular is proportional to C, one may expect a strong dependence of cross-sections on C. However, only about 33%

Table 1. Computed cross-sections $\sigma(0 \rightarrow j)$ in Å^2 and r_0^2/σ values as a function of j and C in eV. ($a_2 = a_4 = a_6 = a_8 = a_{10} = 0.1$, and $\alpha = 3.0$ Å^{-1}).

	$\sigma(0 \rightarrow j)$ when $C =$			r_0^2/σ when $C =$		
j	200	400	800	200	400	800
2	0.949	1.109	1.281	6.76	6.89	7.00
4	0.510	0.596	0.684	12.59	12.82	13.12
6	0.358	0.417	0.481	17.93	18.33	18.65
8	0.248	0.288	0.332	25.88	26.53	27.03
10	0.140	0.163	0.187	45.85	46.89	47.99
12	0.126	0.150	0.176	50.94	50.95	50.99

increase in the cross-sections corresponding to the 300% increase in the value of C is observed.

Table 1 also lists the corresponding values of r_0^2/σ, where r_0 is the distance of the classical turning point and can be estimated[6] by the relation:

$$v(r_0) \sim E. \quad (3)$$

The values of r_0^2/σ reported in the table show that a 33% variation in the cross-sections reduces to less than 5% variation in r_0^2/σ. One may thus infer that r_0^2/σ almost remains unchanged with the increase in the potential parameter C.

The torque acting on the molecule when the atom is at the classical turning point is proportional to $a_i v(r_0)$. The collision time may be considered[6] as $\sim 2r_0/v_{rel}$ where v_{rel} is the average relative speed; and the variation in the effective range of the potential with the change in C may be considered proportional to r_0 corresponding to a fixed value of incident energy. Thus the increase in C does not alter the torque acting at the classical turning point [see eq. (3)] but increases the time of collision and the effective range of the potential. The assumption of linear dependence of cross-sections on the torque, the range as well as the collision time, and the assumption that at a fixed incident energy the average torque is proportional to the torque at the classical turning point, would thus explain the observed variation, $\sigma \propto r_0^2$, as reported in Table 1. Computation of all such quantities by using the classical trajectory method[7] is required for explicit verification of these assumptions. It may be mentioned that the present system is suitable for the classical calculations and the IOSAM results are found to be in close agreement with the classical ones for such systems[3,8].

The dependence of σ on a_l, α, E and the masses of the molecule and the atom is being investigated further. Such a study may lead to better understanding of the RET process, and to an explanation of the scaling and fitting laws and the dependence of the fitting parameters on the parameters of the potential and the colliding system.

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Fine-scale microwave radio refractivity measurements over Bombay area of the Indian subcontinent

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Radio-refractivity measurements obtained using aircraft-borne microwave refractometer reveal fine structure in refractivity profiles. Measurements made over the Bombay area in the morning hours in August 1987 show large fluctuations of the vertical refractivity gradients. These fluctuations may be associated with the occurrence of inversion layers.

RADIO-refractivity profiles derived from radiosonde measurements have long been used for assessment of electromagnetic propagation effects, even though their validity is seriously compromised[1]. In order to assess electromagnetic propagation effects of the lower atmosphere on radar and communication systems (for reliable and efficient operation for strategic and tactical needs), fine-structure information on radio refractivity is required. These environmental data (radio refractive index) are usually obtained from airborne microwave refractometers since the latter provide reliable data (on a real-time basis) to permit assessment of propagation conditions (however complicated the case may be). I have therefore started collecting fine-scale microwave radio-refractivity data on a moderate scale for various seasons at different locations in the Indian subcontinent. The present communication deals with the data collected over Bombay. The present measurements were made in a variety of meteorological conditions, from strong subsidence and advection inversions to neutral, unstable atmospheric conditions. The high-speed data were analysed on a real-time basis by computer.

The microwave refractometer was installed on a Dakota aircraft of the National Remote Sensing Agency (NRSA), Hyderabad. The aircraft flew spiral trajectories in altitude with constant ascent and descent rates. The vertical resolution was typically of the order of a few tens of centimetres. The aircraft's spiral trajectory had a radius of about one kilometre. Altitude information was obtained from the inertial navigation system of the aircraft. The microwave radio-refractivity data obtained during aircraft sorties are presented as vertical profiles. The refractivity data collected from such sorties indicated that near-standard propagation conditions prevailed over Bombay (land–sea interface) during the observational period. The measurements, made in the morning hours in August 1987, compare well with radiosonde measurements taken over Bombay airport at 5.30 a.m. Throughout the observation there were no clouds over Bombay. It may be mentioned that