PHYSICAL REVIEW LETTERS

VOLUME 20 19 FEBRUARY 1968 NUMBER 8

INFORMATION ON THE $^1\Sigma^+$ AND $^3\Sigma^+$ POTENTIALS OF NaCs FROM TOTAL SCATTERING CROSS-SECTION MEASUREMENTS*

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(Received 27 December 1967)

The velocity dependence of the total elastic cross section for the scattering of a fast Na atomic beam by a thermal-energy Cs beam has been investigated in the energy range 14-2300 eV. Detailed information on the interatomic potential for both the singlet and triplet state of NaCs has been obtained from an analysis of the experimental data.

The velocity dependence of the total scattering cross section has previously been studied only for atom-atom or atom-molecule collisions for which the interaction is determined by a single potential.[1] In contrast, for alkali-alkali scattering two very different interaction potentials are involved: the potential for the $^1\Sigma^+$ state of the collision pair, in which a stable molecule can be formed, and the potential of the $^3\Sigma^+$ state which results from repulsive valence forces and has a shallow well at a large equilibrium distance. Without state selection both potentials contribute to the measured total scattering cross section. If Q_S and Q_T are the scattering cross sections determined by the potential V_S of the singlet state and the potential V_T of the triplet state, respectively, then the measured cross section Q is given by

$$Q = \tfrac{1}{4}Q_S + \tfrac{3}{4}Q_T. \qquad (1)$$

Both $Q_S(v)$ and $Q_T(v)$ exhibit the familiar form for the dependence of the total scattering cross section on the velocity v. This curve is divided into two regions by the characteristic velocity $v_c = \epsilon r_m/\hbar$ (where ϵ is the potential well depth and r_m is the equilibrium distance); for $v < v_c$ the total scattering cross section oscillates about an average cross section $Q_m \sim v^{-2/5}$ which results from the attractive part of the potential; for $v > v_c$ the scattering cross section exhibits a monotonic behavior which is increasingly dependent upon the repulsive term of the potential as the ratio v/v_c increases. Since the characteristic velocities of $Q_S(v)$ and $Q_S(v)$, v_c^S and v_c^T, are quite different, there is a velocity region ($v_c^T < v < v_c^S$) in which Q_T already shows monotonic behavior while Q_S still oscillates. For alkali-alkali scattering, this velocity region corresponds to energies of a few to several thousand eV. Our measurements for the collision pair Na-Cs were made in this energy region, in which it should be possible in an experiment without state selection to separate the contributions of both potentials and thus to obtain information about both V_S and V_T.

The apparatus used for these experiments and the measurement procedure are described in detail elsewhere.[2,3] Figure 1 shows the measured velocity dependence of the total scattering cross section for Na-Cs. The glory oscillations of Q_S with the indices $N = 1, 1.5, \cdots, 7$ (the indexing follows the notation of Bernstein[4])

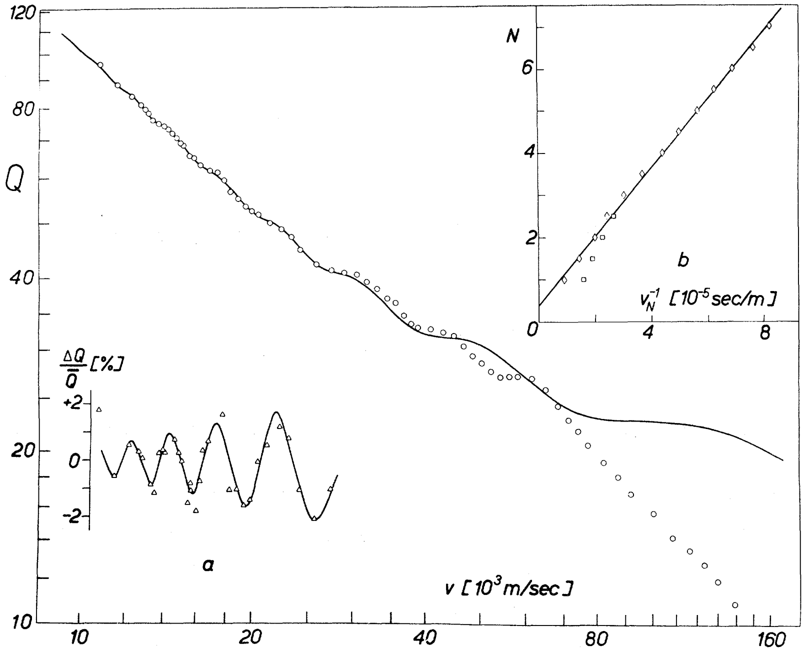

FIG. 1. The velocity dependence of the total scattering cross section for Na-Cs. The curve drawn through the measurements is calculated under the assumption of modified Lennard-Jones potentials and equal van der Waals interaction in both states. Insert (a) shows the singlet-state glory undulations with the indices $N = 3.5, 4, \cdots, 7$ on an enlarged scale in the form $\Delta Q/\bar{Q}$. ΔQ is the difference between the measured cross section and the mean cross section $\bar{Q}$, which is obtained by averaging over the undulations. Insert (b) shows a plot of N vs $1/v_N$. The deviations of the points denoted by squares from the straight line at small values of $1/v_N$ are a result of the finite angular resolution of the apparatus. The points denoted by diamonds are corrected for this effect. For $N > 2.5$ the correction is negligibly small, so that the measured points coincide with the corrected points.

can clearly be seen. In Fig. 1(a) the oscillations with $N < 3.5$ are shown on a larger scale in the form $\Delta Q/\bar{Q}$, where ΔQ is the difference between the measured scattering cross section and the cross section $\bar{Q}$ which is found by averaging over the oscillations. In addition to the experimental data, calculated curves for $Q(v)$ and $\Delta Q/\bar{Q}$ are also shown. These curves are found from formula (1) by assuming modified Lennard-Jones (4,12; 72,6) potentials[5] and equal van der Waals interaction in both states. The discrepancy between measured and calculated cross sections at high velocities is due to the finite angular resolution of the apparatus. One result of the finite angular resolution is a systematic decrease in the measured cross section. This effect increases with increasing velocity. It is discussed in a number of publications.[6-8] In addition, for glory scattering at higher energies a displacement of the extrema towards smaller velocities is observed. This displacement can be explained by the relation between the glory effect and the rainbow structure in the differential scattering cross section. The effect is observed when the angular separation of the rainbow structure is of about the same size as the angular resolution of the experimental setup. As will be discussed more thoroughly in a future publication,[9] it is possible to correct for this effect. This can be seen in Fig. 1(b), where N is plotted as a function of v_N^{-1}. The corrected points (diamonds) show the linear relationship which has been observed for other collision pairs, while the uncorrected points (squares) show a systematic deviation from the line at higher velocities.

The analysis of the experimental data yields the product $\epsilon r_m a_1$ for the potentials V_S and V_T, where a_1 is an expansion coefficient of the maximum phase shift[10] which depends upon the potential. For the singlet state this product can be calculated from the slope of the line in the N vs v_N^{-1} plot. For the triplet state the product is determined by comparing the measurements with theoretical curves, as is described in detail in another publication.[3]

In consequence of the monotonic behavior of

Q_T, the product $\epsilon r_m a_1$ cannot be ascertained as precisely for the triplet state as for the singlet state. The results obtained are

$$(\epsilon r_m a_1)_S = 0.85 \text{ [eV Å]},$$

$$(\epsilon r_m a_1)_T = 0.039 \text{ [eV Å]}.$$

Since the van der Waals constant $C = [n/(n-6)] \times \epsilon r_m{}^6$ [n is the exponent of the repulsive term of a Lennard-Jones (n, 6) potential] has been measured for the system Na-Cs,[11] it is possible to calculate ϵ and r_m separately for both V_S and V_T. Prerequisite for this is the assumption of a model potential which fixes the constants a_1 and n. The potential used for these calculations was a Lennard-Jones (8, 6) for both V_S and V_T. Assuming equal van der Waals interaction for both states, the following potential parameters are obtained:

$$\epsilon_S = 0.69 \text{ eV}, \quad \epsilon_T = 1.7\times10^{-2} \text{ eV},$$

$$r_m{}^S = 2.6\times10^{-8} \text{ cm}, \quad r_m{}^T = 4.9\times10^{-8} \text{ cm}.$$

The parameters of the triplet potential V_T are of the same order of magnitude as those which are found for alkali–inert-gas scattering (for example, for Na:Xe [12]). The only data available for comparison with the parameters of the singlet-state potential V_S are from spectroscopic studies of Na_2 and Cs_2 molecules.[13] The dissociation energies yield the following values for ϵ_S:

$$\text{for } Na_2, \ \epsilon_S = 0.74 \text{ eV};$$

$$\text{for } Cs_2, \ \epsilon_S = 0.46 \text{ eV}.$$

The potential well depth ϵ_S of NaCs lies between these values, as is expected from the usual combination rules.

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*Work supported by the Deutsche Forschungsgemeinschaft.

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POSSIBILITY OF THE FORMATION OF THE MUONIUM WATER MOLECULE

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(Received 5 January 1968)

The possibility of the formation of muonic (μ^+) molecules has been investigated by several researchers.[1] In this paper we consider specifically the possibility of the formation of muonic water[2] molecule and its probable fundamental vibrational frequencies. The formation of (μ_2O) molecule would be in general more difficult than that of (μHO) molecule, and in the following we confine our discussion to the latter case only.

When positive muons slow down in water, muonium water molecules may be formed either via muonium or through direct replacement of a proton by a positive muon:

$$\mu^+ + e^- = \text{muonium}, \ \text{muonium} + H_2O \rightarrow H + (\mu HO), \quad (1)$$

or

$$\mu^+ + H_2O \rightarrow H^+ + (\mu HO). \quad (2)$$

In the second case, a large momentum transfer is involved, whereas the first case is really a two-step process and in either case the probability for the formation of muonium water should be small. One may estimate the rate of the four-atom reaction, muonium $+ H_2O \rightarrow H + (\mu HO)$, by applying the method developed by Alter and Eyring.[3] However, such a calculation is not expected to give a very reliable result, and the great labor involved in such a calculation does not appear to be worthwhile at this time.[4]