Study of differential scattering of He atoms in CO and N_2

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Results are presented of the measurement of the differential scattering of He atoms in CO and N_2 in the detector angle interval $(0–5)\times 10^{-2}$ rad and at an He beam energy $E = 800$ eV. The experimental scattering picture is compared with the relation calculated for the theoretical potential-energy surfaces for the two systems, and a difference between them is noted.

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Interest in molecular-collision effects that determine the population of rotational-vibrational levels of molecules has greatly increased in recent years. In view of the difficulty of direct measurements of the cross sections of definite molecular transitions, the greatest promise of obtaining the necessary information is offered by scattering theory, which makes possible the solution of the dynamic scattering problem when the interaction potential is known. By the same token, the determination of the anisotropic intermolecular forces becomes the key to the solution of the resultant problems.

We present here the results of measurements of the differential elastic scattering (DS) of the isoelectronic pairs He—N_2 and He—CO. The main purpose of the investigation was to compare the experimental DS curves with those calculated for the theoretical potential energy surfaces (PES) proposed in[1,2]. This comparison permits an estimate of the reliability of the predictions of[1,2] on the basis of the popular so-called statistical model (SM) and to establish the feasibility of an empirical correlation of the SM approximations. The data obtained make it also possible to obtain independently the parameters of a model potential, say of the additive type.

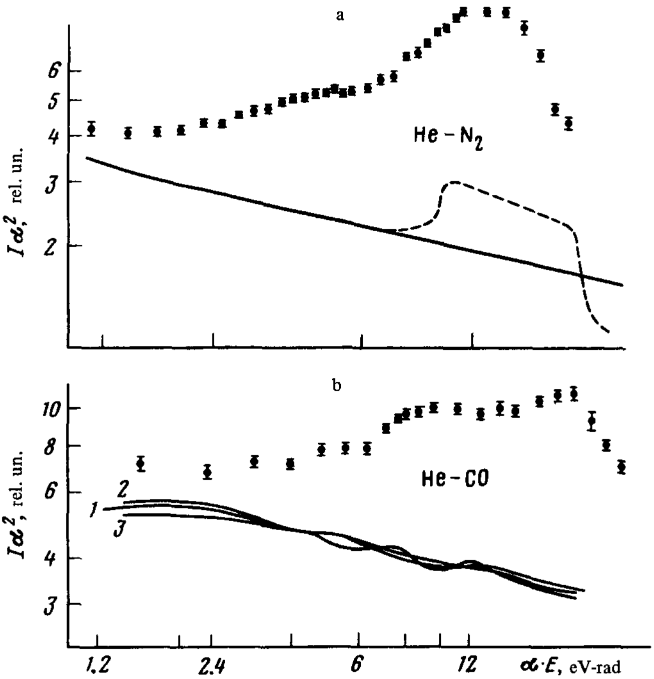

FIG. 1.

The apparatus and procedure of the automatized measurements of the DS of fast beams are described in detail in[3,4]. The measurements were made in detector-angle (α) intervals from 0 to 5×10^{-2} rad and at an He beam energy $E = 800$ eV. The measured intensities $I(\alpha)$ of the scattered beam are illustrated in Fig. 1 in terms of the relative coordinates $I\alpha^2$ and αE; the error bars represent the rms errors of the individual measurements. The obtained DS pictures differ substantially from those expected for an interaction described by the usual exponential or power-law potentials.

The classical-approximation calculation of the scattering picture is based on the use of a simple relation for the convolution of the differential cross section

$$\sigma(\theta) = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|$$

namely,

$$I(\alpha) = C \int_{\langle\Omega\rangle} \int_{(b)} f_\alpha(\theta) b \, db \, d\Omega \,, \qquad (1)$$

where b is the impact distance, Ω is the assembly of angles characterizing the molecule spatial orientation, which is effectively frozen during the collision time, $\theta(b, \Omega)$ is the deflection function, $f_\alpha(\theta)$ is the instrumental function, and C is a known constant. According to (1), the task of calculating the DS picture reduces to finding the deflection function $\theta = \theta(b, \Omega)$ for scattering by an anisotropic PES.

The PES of the investigated systems have been proposed in the form of an additive potential for He—N_2[1] and of an expansion in Legendre polynomials (up to fifth order) in the case of He—CO. [2] The method of calculating the deflection function for such potentials was discussed in[4,5].

To calculate $I(\alpha)$ from (1), a P-40 computer was used with a Monte Carlo procedure ensuring a statistical accuracy 1—2% in a realization of 10^5 trajectories with random sets of b and Ω.

The calculations in the He—CO case were made for a number of successive approximations to the theoretical PES[2]: 1) for a potential $\bar{V}(r)$ averaged over the orientations (curve 1, Fig. 1b): 2) for an expansion containing radial components with $l=1$ and 2 (curve 2, Fig. 1b); 3) for an expansion containing components with $l=0$, 1 and 2 (curve 3, Fig. 1b). Although the complete PES of[2] contains components up to $l=5$, the good convergence of the calculations (Fig. 1b, curves 1, 2, and 3) allow us to confine ourselves to $l=2$.

A comparison of the calculated $I\alpha^2$ relations (continuous curves) for both investigated systems with the measured ones shows them to differ strongly.

This difference (analogous differences were observed by us for other systems, e.g., Ar—CO_2 and Ar—N_2) allow us to conclude that the DS in its present form is not accurate enough for use in dynamic calculations aimed at predicting quantitatively the cross sections of elastic scattering and impact excitations of molecular degrees of freedom. At the same time, the results presented uncover a possibility of an improvement, coordinated with experiment, in the DS procedure.

The experimental curves for the isoelectronic systems He—Co and He—N_2 reveal the presence of well pronounced singularities in the region $\alpha E > 10$. The angle position of the $I\alpha^2$ peak makes it possible to relate these singularities with perturbation of the elastic scattering by an inelastic channel; in particular, the energywise accessible channel is the channel of excitation into triplet $A^3\Sigma^+(N_2)$ and $a^3\Pi(CO)$ states as a result of the intersection of the corresponding PES. This interpretation is supported by the results of recent direct measurements[6] of the inelastic losses in scattering in the system $Li^+ - N_2$(Li^+ is electronwise similar to He).

A model-dependent calculation of the picture of scattering in a system of two intersecting terms of the He—N_2 systems (one of which, $\bar{V}$, is the average potential of[1], and $V^*(r) = 63.6\exp(-2.5r)$) has shown that the observed singularities is qualitatively accounted for if the position of the intersection point is $r_{\text{int}} = 1.15$ Å (dashed curve of Fig. 1a).

This effect of excitation in collisions (which is forbidden by the rule for conservation of the total spin) of the triplet state uncovers a new interesting research object and may apparently also be of aeronomic interest. Indeed, the inverse process of deactivation leads to a conversion of the electron energy $\Delta V = V^*(\infty) - V(\infty)$ into a kinetic recoil energy carried away mainly by the atom He ($E_{\text{He}} = (m_{N_2}/(m_{N_2} + m_{\text{He}})\Delta\nu$). This deactivation process in the upper atmosphere can therefore serve as a source of a non-thermal flux of runaway helium atoms.

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