SCATTERING AND DEACTIVATION OF METASTABLE $N_2(A^3\Sigma_u^+)$ MOLECULES

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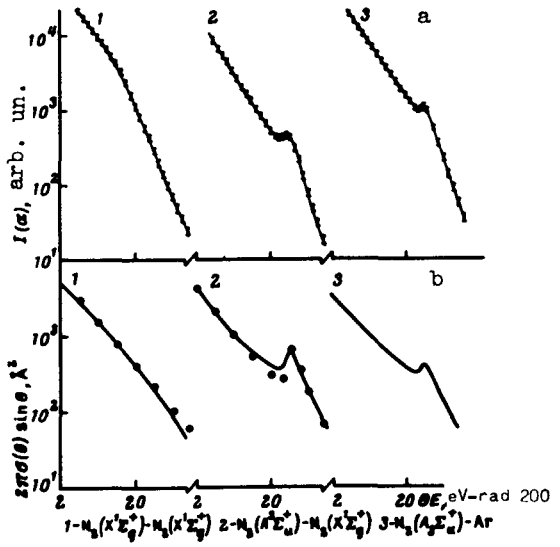
We have investigated, on the basis of measurements of the differential scattering cross sections, the features of the interaction of metastable $N_2(A^3\Sigma_u^+)$ molecules with $N_2(X^1\Sigma_g)$ and Ar molecules in the region of close approach distances.

The cross sections were measured with the aid of fast beams (E = 2000 eV) in the reduced-angle range $\theta E \sim 1 - 10^2$ rad-eV using a modified setup described in [1]. This range of reduced angles, by virtue of the fact that $\theta E \sim V$, yields information on the interaction potential in the region 1 - 100 eV.

The use of a secondary-electron multiplier of the channel type as the detector has made it possible to increase greatly the sensitivity and to improve appreciably the resolution of the detector. A quantitative characteristic of the resolution is the apparatus function f_α, a calculation of which is described in [2].

A beam of fast $N_2(A^3\Sigma_u^+)$ molecules was obtained by charge exchange of N_2^+ ions in Cs vapor. Random resonance ensures a large cross section for charge exchange in triplet states, which then go over spontaneously into the metastable $A^3\Sigma_u^+$ state (cf., e.g., [3]). In these measurements we investigated also the scattering cross sections for the system $N_2(X^1\Sigma_g^+) - N_2(X^1\Sigma_g^+)$.

The angular distribution of the charged particles $I(\alpha)$ (α is the angle of inclination of the detector to the beam axis) is connected with the differential scattering cross section $\sigma(\theta)$ by a relation [2] that makes it possible to invert the measured $I(\alpha)$ distribution shown in Fig. a, provided f_α is known. The $\sigma(\theta)$ relations obtained for the investigated systems by inversion are shown in Fig. b (solid lines). It is seen from the figure that the scattering of the metastable molecules is characterized by a sharply pronounced singularity.



From the relative locations of $\sigma(\theta)$ for the molecules in the ground and metastable states it is clear that the observed singularity is not connected with the presence in the $N_2(A^3\Sigma_u^+)$ of an admixture of ground-state molecules. The admixture can only weaken the observed effect, and there are grounds for assuming its influence to be negligible.

The amplitude and the position ($\theta E \sim V$, where V is the potential energy of the interaction at the closest-approach distance r_0, which is equal to the

impact parameter b) of the observed peak, and its presence in the case of the N* - Ar system, exclude the possibility of rainbow scattering.

A sufficiently obvious cause of the singularity is the presence of a channel of impact deactivation of the excited state in parallel with the elastic channel. In this case the excitation energy (electronic and vibrational) goes over into recoil energy, and at the same impact distance the deactivated molecules will be deflected by a larger angle than the elastically-scattered molecules. The measured cross section will be the sum of two cross sections, elastic σ_{el} and inelastic σ_{in} ($\sigma(\theta) = (1 - p)\sigma_{el}(\theta) + p\sigma_{in}(\theta)$), where p is the probability of the transition (assumed henceforth to be independent of the orientation).

The localization of the observed peak allows us to conclude a sufficiently abrupt "turning on" of the inelastic-channel probability, a fact perfectly understandable within the framework of the notion of quasi-intersection of the surfaces of the potential interaction energy of the molecules of the ground state $V^0(N_2 - N_2)$ and of the excited state $V^*(N_2^* - N_2)$. To obtain a quantitative interpretation of the observed $\sigma(\theta)$ relations, we used the BESM-4 computer to calculate the differential scattering cross sections for single-channel (purely elastic) and two-channel scattering; superposition of the calculated and measured relations makes it possible to solve the inverse problem - to determine the potential-energy surface and the probability of the inelastic channel. To simplify the calculations, the angle of scattering with deactivation was assumed to equal the sum of the elastic-scattering angle θ and of an increment $\theta^*[\theta^* \sim (\Delta q_\infty/E)]$, determined by the value of the recoil energy Δq_∞ (it was assumed in practice that $\Delta q_\infty = 7.4$ eV and $\theta^* = 1.35 \times 10^{-2}$).

The differential scattering cross sections $\sigma(\theta)$ in the classical approximation were found by using the expressions for the inclination function $\theta(b)$ [4, 5] using the obvious expression for small scattering angles

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

In practice the calculation of the values of $\sigma(\theta)$ averaged over the orientation reduced to an evaluation of the integral

$$\sigma(\theta) = \frac{1}{16\pi^2}\iint_{(\phi)} d^2\phi_i \iint_{(\chi)}\left|\frac{\Delta b^2}{\theta\Delta\theta}\right| d^2\cos\chi_i$$

at fixed $\Delta\theta$. The angles ϕ_i and χ_i describe the relative orientation of the approaching molecules, the force field of which is described by the additive potential $V(N_2 - N_2) = \sum_{i=1}^{4} V_i(N - N)$ with exponential interaction of the atoms, $V(N - N) = A\exp(-\gamma r)$. The aforementioned averaging was carried out by a Monte Carlo procedure and the typical number of calculated trajectories for the $\sigma(\theta)$ relations given below reached 10^4.

The cross section $\sigma(\theta)$ calculated for the system $N_2(X^1\Sigma_g^+) - N_2(X^1\Sigma_g^+)$, using the corrected values of the parameters of [5] ($A^0 = 367$ eV, $\gamma^0 = 3.27$ $Å^{-1}$), is shown by the points of Fig. b. The agreement with the measured values (continuous line) is perfectly satisfactory. In the calculation of the random trajectories for the system $N_2(A^3\Sigma_u^+) - N_2(X^1\Sigma_g^+)$, the "turning on" of the inelastic channel was effected for closest-approach distances $r_0 = b$ ensuring a real intersection in accord with the condition $V^0(b) \geq V^*(b) + \Delta q_\infty$, it being assumed that the vibrational excitation of the $N_2(X^1\Sigma_g^+)$ molecule does not

change the parameters A^0 and γ^0. A comparison of the measured (continuous line) and calculated (dark points) relations for two-channel scattering (Fig. b) shows sufficiently good agreement, making it possible to assume that the values of the parameters of the potential energy surface ($A^* = 230$ eV, $\gamma^* = 3.8$ Å^{-1}) and of the probability ($p = 0.4$) are reliable. Some discrepancy in the region of the peak is apparently due to the approximate character of the calculation, and in particular to the neglect of the existence of distributions of the quantities Δq_∞ and θ^*, due to the real population of the vibrational levels of the excited and de-activated molecules.

In conclusion, we summarize the main results.

1. We measured the differential scattering cross section of the molecules N_2 in the ground and metastable states. We observed for the first time effects connected with impact de-activation of $N_2(A^3\Sigma_u^+)$.

2. We reconstructed the surface of the potential energy of the interaction of $N_2(X^1\Sigma_g^+)$ with $N_2(A^3\Sigma_u^+)$ and obtained its intersection with the surface for the ground-state molecules.

3. The results enable us to estimate the total cross section for impact deactivation of the $A^3\Sigma_u^+$ state of N_2, namely $Q \approx 3.3$ Å^2; this value disagrees with $Q \approx 1$ Å^2 obtained in [6].

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ANISOTROPY OF THE MOSSBAUER EFFECT IN ANTIMONY SINGLE CRYSTALS

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Of greatest interest in the investigation of the Mossbauer-effect anisotropy in pure elements are single crystals of tin, tellurium, and antimony. Single crystals of tin and tellurium were investigated in [1 - 4]. We report here the results of a study of the anisotropy of the probability of resonant absorption of 37.2-keV γ quanta by Sb^{121} nuclei in antimony single crystals at liquid-nitrogen temperature.

Crystalline antimony has rhombohedral syngony, space group $R\bar{3}m$, and lattice parameters $a = 4.4928$ Å and $\alpha = 57°12'$ at liquid-nitrogen temperature [4]. Each unit cell has two atoms located on the spatial diagonal [111] of the rhombohedron, which is the inversion of the threefold axis C. Each atom has three nearest neighbors at a distance 2.87 Å, and is bound to them covalently, forming a folded layer. The shortest distance between atoms of different layers is 3.47 Å, and the binding forces between layers are much weaker. Therefore the greatest strength of the crystal is observed in the (111) planes parallel to the folded layers of the atoms, and the crystal is relatively easily damaged in directions perpendicular to these layers. Antimony exhibits