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He⁰+N₂ collisions at 1.0 keV

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He⁰+N₂ collisions are studied at an energy of 1.0 keV and in an angular range from 0.2° to 2°. Time-of-flight techniques are used to identify the dominant collision processes. Electronically elastic collisions are found to dominate the scattering for angles out to 1.3°. In He⁰+N₂, H₂, and O₂ collisions the electronically elastic processes were found to be weak beyond the smallest angles, in sharp contrast to the present results. Excitation of N₂ (*a* ¹Π_g) is found to be the dominant small-angle inelastic process. Our results also show excitation of N₂⁺ (*A* ²Π_u and *B* ²Σ_u⁺) but at most very weak excitation of the N₂⁺ (*X* ²Σ_g⁺) ground state. The excitation of an electron from the 3σ_g molecular orbital of N₂ is found to be generally quite specific and takes place primarily through a transition to a 1π_g orbital. [S1050-2947(98)01402-4]

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INTRODUCTION

Experimental studies of collisions at low keV energies generally show that the electronically elastic channel is dominant in the direct scattering (no change in projectile charge state) at small angles. In recent work [1,2] on H⁰ collisions with N₂, H₂, and O₂ molecules the electronically elastic processes were, however, found to be weak beyond the smallest scattering angles. As examples in terms of τ, the reduced scattering angle (=Eθ, the beam energy × scattering angle), the inelastic channels were found to dominate the collisions for values greater than 0.2, 0.2, and 0.3 keV deg for N₂, H₂, and O₂, respectively. Such low keV energy collisions occur in the aurora [3] and since the underlying theory is complex it is useful to have a simple model applicable to the basic interactions.

The unusual weakness of the elastic scattering found with H⁰ was consistent with a model [1,2,4] attributing inelastic processes to the excitation of intermediate ionic states during the collisions. If ionic states are excited, they could populate the observed inelastic channels via surface crossings and also because they lie close in energy to them at large interparticle separation. Since the ionic forces are attractive, the projectiles would also be scattered through smaller angles, as indeed was found in the H⁰ cases. To test this simple model we are studying He⁰+N₂ collisions. He provides a limiting case because it has the largest energy difference (at infinite separation) between the ionic and incident channels and only a single (He⁺+N₂⁻) intermediate ionic state. The He⁻+N₂⁺ intermediate state can be neglected since He⁻ is a quartet state. He⁰+N₂ collisions have not been investigated in detail to date but they are both of theoretical and practical applied interest.

THE EXPERIMENTAL RESULTS AND CONCLUSIONS

The small-angle direct scattering in He⁰+N₂ is studied at a beam energy E=1.0 keV. The basic experimental techniques are outlined in Refs. [1] and [2]. Briefly, He⁺ is generated in an ion source floated at 1.0 kV. The ions are extracted, focused, and then pass between two small plates where the beam is “chopped,” by an electric field, for time-of-flight energy measurements. The beam is mass analyzed and then enters a charge exchange cell containing He gas, and resonant electron capture generates a He⁰ beam at 1.0 keV. Residual He⁺ ions are deflected and a collimated He⁰ beam enters the target N₂ gas cell. After scattering through an angle θ it traverses a 4.2-m-long flight tube to a detector. The arrival time spectra are then acquired at each scattering angle. Since the direct scattering does not involve a change in charge state, the incident He⁰ beam provides the energy reference from which the states are identified.

The angular distribution and energy spectra of the scattered He⁰ are studied in an angular range from 0.2° to 2.1° (2.5° for the energy spectra). Figure 1 shows spectra at an energy E=1.0 keV and scattering angles of (a) 1.5° and (b) 2.3°. The peak labeled *A* results from electronically elastic collisions. On the basis of Gilmore’s potential energy curves for N₂ [5] and assuming that the collisions involve “Franck-Condon” transitions, the peak labeled *B* at an energy loss near 9 eV can be attributed to He⁰+N₂ (*X* ¹Σ_g⁺)→He⁰+N₂ (*a* ¹Π_g). The excitation of N₂ (*w*¹Δ_u or *a*¹Σ_u⁻) cannot be ruled out but an analysis of all our results shows that these states are only weakly excited. Although there are low-lying triplet states (*A* ³Σ_u⁺ and *B* ³Π_g), which would result in energy losses near 8 eV, in the Franck-Condon region, these are not excited by the singlet He projectile in accordance with the Wigner spin conservation rule. The rule requires the

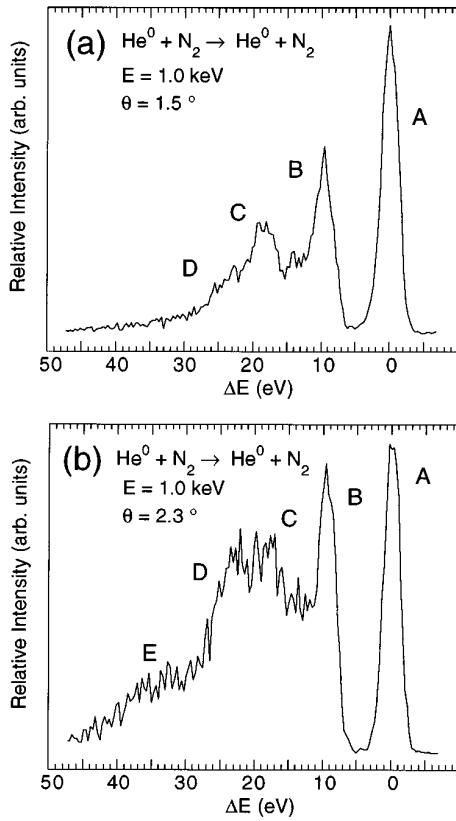


FIG. 1. Energy spectra from $E=1.0$ keV energy He^0+N_2 collisions at angles of (a) 1.5° and (b) 2.3° . Peak A results from electronically elastic collisions. Peak B having an energy loss near 9 eV is attributed to He^0+N_2^+ ($a^1\Pi_g$). Peak C contains contributions from He^0+N_2 ($A^2\Pi_u$ and $B^2\Sigma_u^+$). The structures (D and E) at higher energy losses include contributions from excited He as well as from excitation of both the He^0 and N_2 .

total electron spin angular momentum to remain constant in a collision (very weak coupling between the orbital and spin angular momenta is assumed). There are a number of states that can give rise to the structure near 14 eV, clearly seen in the 1.5° spectrum, but an assignment is not possible. Similar structure was seen in H^++N_2 [6]. The data over a range of angles shows that peak C contains contributions from N_2^+

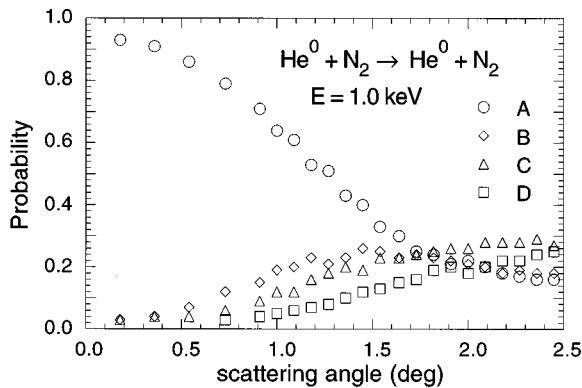


FIG. 2. The probabilities for the excitation of processes corresponding to A, B, C, and D (E is not shown for clarity) in Fig. 1. The elastic channel (A) is seen to be dominant for scattering angles less than 1.3° .

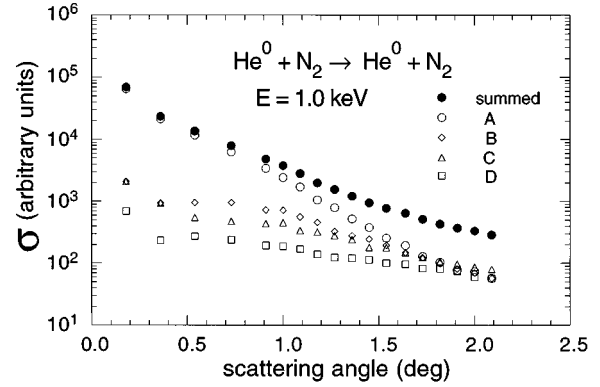


FIG. 3. The differential cross sections for both the ‘‘summed’’ (A, B, C, D, and E) and the A, B, C, and D processes.

($A^2\Pi_u$) and N_2^+ ($B^2\Sigma_u^+$). The structure at higher energy losses (D and E) includes contributions from He^* as well as from the excitation of both the projectile and target where triplet He^0 and N_2 states may be simultaneously excited.

Figure 2 is a plot of the probabilities, as a function of scattering angle, for the excitation of processes corresponding to the peaks labeled A, B, C, and D in Fig. 1 (E is not shown for clarity). The elastic channel is seen to be dominant for scattering angles $\theta < 1.3^\circ$ (corresponding also to $\tau < 1.3$ keV deg for $E=1.0$ keV). The differential cross sections for the ‘‘summed’’ and ‘‘A,B,C,D’’ channels are shown as a function of angle in Fig. 3. These differential cross sections can provide a rigorous test of approximations used in calculations.

The present results show that the elastic channel is dominant in small angle He^0 collisions with N_2 . In earlier work on He^0+D_2 [H_2] [7,8] the elastic channel was shown to be dominant at the small angles. This was also found [9] to be the case in He^0+CO and He^0+NO collisions. All these results are consistent with the proposed role of intermediate ionic states. When compared to H^0 , the larger energy difference between the incident and intermediate ionic states (15 eV for H^0 , 26 eV for He^0 —at infinite separation) corresponds to a crossing at smaller interparticle distance with He^0 projectiles. Therefore weaker excitation at small angles is expected in He^0+N_2 collisions than in H^0+N_2 .

The N_2 ($X^1\Sigma_g^+$) ground state [5] has a $(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^2(2\sigma_u)^2(1\pi_u)^4(3\sigma_g)^2$ molecular-orbital configuration. The dominant electronically inelastic process (for $\theta < 1.5^\circ$) in He^0+N_2 results in N_2 ($a^1\Pi_g$), which requires a $3\sigma_g$ to $1\pi_g$ electron transition. The same N_2 state was found to be dominant in the direct scattering in H^++N_2 [4]. For H^0 [1], Ar^+ [10], and He^+ [9] projectiles where excitation of triplet states of N_2 is allowed, the N_2 ($B^3\Pi_g$) state (involving again a $3\sigma_g$ to a $1\pi_g$ transition) was strongly excited. The N_2 ($A^3\Sigma_u^+$), involving a $1\pi_u$ to a $1\pi_g$ transition, has an excitation energy very close to that of the $B^3\Pi_g$ state but is weakly excited. The present results show only weak contributions from the lowest lying N_2^+ ($X^2\Sigma_g^+$) state. The X state involves the ionization of a $3\sigma_g$ electron from N_2 . Weak excitation of the X state was also found with H^+ [6], He^+ [9], and H^0 [1] projectiles. Excitation of the N_2^+ ($A^2\Pi_u$) state found requires the ionization of a $1\pi_u$ electron. Collisions leading to N_2^+ ($B^2\Sigma_u$) involve

contributions from two configurations: (i) a $3\sigma_g$ to $1\pi_g$ excitation with the ionization of a $1\pi_u$ electron and (ii) the ionization of a $2\sigma_u$ electron. It may be concluded that there is generally a preferred $3\sigma_g$ to $1\pi_g$ electron excitation in collisions with N_2 molecules.

ACKNOWLEDGMENTS

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