found shortly. HD^+ pure rotational spectra ($v = v'$) and overtone spectra ($|v - v'| \geq 2$) may appear in other laser frequency ranges. It also seems likely that the equipment can be used to study other molecular ions possessing adequate oscillatory dipole moments, as well as the vibrational-state dependence of molecular-ion collision processes.

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He(3^3P) States Excited in 1.5- and 3.0-keV He^+-H_2 Charge-Transfer Collisions*

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The linear polarization of 3889-Å radiation in coincidence with scattered neutral particles has been measured for 1.5- and 3.0-keV He^+-H_2 collisions at selected scattering angles. At one scattering angle the measurements show a stronger polarization than is presently observed in He^+-He at any scattering angle; this is surprising in view of the many final states available to the recoiling H_2^+ ion.

The introduction of coincidence techniques to atomic collision measurements has focused attention on processes where one determines the maximum information concerning the state of the entire collision system, for example the excitation of He atoms by electron impact when the emitted radiation is detected in delayed coincidence with the scattered electrons.[1] Such measurements are known to deal with pure atomic states, i.e., states represented by a density matrix which has only one nonzero diagonal element of unit magnitude in a representation of eigenstates. On the other hand, collisions with complex targets generally produce excited atoms or ions in mixed states because of the averaging over a large number of degrees of freedom of the target. The excited He atoms resulting from collisions of He ions with a tilted foil, as first measured by Berry and Subtil,[2] are a noteworthy example of such mixed states. Although the excited He atoms from the foil were oriented and aligned, the relative magnitudes of these parameters demonstrated that the atoms were in mixed states as would be expected of atoms interacting with a complex system.

The excitation of atoms by diatomic molecules, however, represents a case of intermediate complexity, even though the averaging over all orientations of the molecule would indicate the production of mixed states. In this note we report mea-

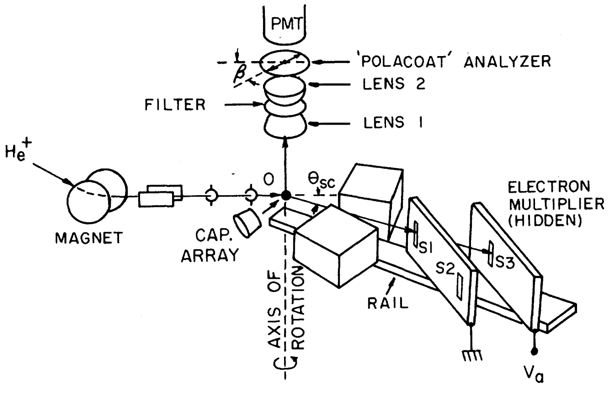

FIG. 1. Schematic diagram of the apparatus.

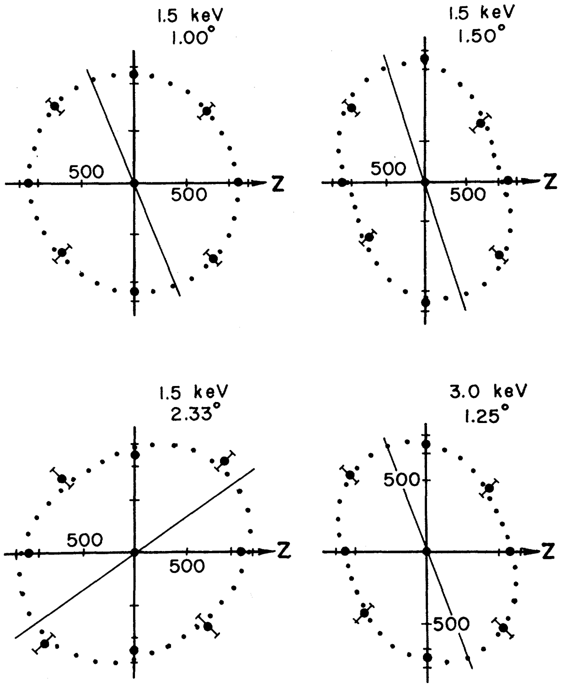

FIG. 2. Polar plots of the average number of real coincidences per 10^9 scattered neutral particles versus β for three scattering angles at 1.5 keV and one angle at 3.0 keV. The data are shown by solid dots with error bars and the dots without error bars are best fits to the data as described in Ref. 3. In all the plots, the incident-beam direction is along the z axis (to the right in the figure) and the neutral particles are detected above the z axis.

surements of the alignment of He(3^3P) states excited in 1.5- and 3.0-keV He^+-H_2 charge-transfer collisions. Rather surprisingly, for at least one scattering angle, we find more nearly maximal alignment than for any of the scattering angles studied previously[3] in He^+-He; the large alignment suggests that along an appropriate axis of quantization the excited atoms are close to being pure states with $m_l = 0$. Furthermore, the momentum-transfer axis appears to play an important role in this system, whereas recent results indicate it has little or no relevance in He^+-He collisions.

A brief description of the apparatus has been given elsewhere,[3] and no changes in the equipment or the experimental procedure have been incorporated. Referring to Fig. 1, a He^+ ion beam interacts with a thermal beam of H_2 molecules near the scattering center 0. Scattered neutral particles passing through slits $S1$ and $S3$ are detected by a secondary electron multiplier, and 3889-Å photons are analyzed according to their linear polarization and detected by a conventional photomultiplier tube (PMT). The detector signals are counted in delayed coincidence as a function of the polarizer angle β, the laboratory scattering angle θ, and the incident kinetic energy T_0. Our results for four combinations of incident energy and scattering angle are shown in Fig. 2. At least two 24-h, and in some cases two 36- or two 48-h, determinations of the coincidence count rate are made for each of the polarizer angles 0°, 45°, 90°, and 135°. The error bars represent estimates of the standard deviation of the random counting error.

The excited atoms in this experiment represent a source characterized by three alignment parameters ($A_0'^{\,\mathrm{col}}$, $A_{1+}'^{\,\mathrm{col}}$, and $A_{2+}'^{\,\mathrm{col}}$) and one orientation parameter ($O_{1-}'^{\,\mathrm{col}}$), as defined in a frame with a z' axis along the maximum of the polarization pattern.[4] Since the light is not analyzed for circular polarization, our measurements do not determine $O_{1-}'^{\,\mathrm{col}}$. Also, $A_{1+}'^{\,\mathrm{col}}$ is zero in this coordinate system, so the intensity of the emitted radiation is

$$I=\tfrac{1}{3}CS\{1+\tfrac{1}{4}h^{(2)}G^{(2)}[A_0'^{\,\mathrm{col}}+3A_{2+}'^{\,\mathrm{col}}+3(A_0'^{\,\mathrm{col}}-A_2'^{\,\mathrm{col}})\cos2(\beta-\alpha)]\}, \tag{1}$$

where β is the angle between the axis of the linear polarizer and a plane Σ (the plane Σ is defined by the incident-beam axis and the light-detector axis), α is the angle between the Σ plane and the z' axis, $h^{(2)} = -2$, and C and S are constants as defined in Ref. 4. The factor $G^{(2)}$, equal to $\frac{5}{18}$, accounts for the light depolarization due to the fine structure of the 3^3P level. In general, Eq. (1) represents an hourglass-shaped pattern and there are three undetermined parameters. We have determined least-squares best fits of our data by an equation equivalent to Eq. (1),[3] the fits being shown in Fig. 2 as dotted lines.

The ratio R of the intensity at the minimum ($\beta - \alpha = 90°$) to the intensity at the maximum ($\beta - \alpha = 0°$) is determined from Eq. (1):

$$R = \frac{I_{\mathrm{min}}}{I_{\mathrm{max}}} = \frac{1 - G^{(2)}[3A_{2+}'^{\,\mathrm{col}} - A_0'^{\,\mathrm{col}}]}{1 - 2G^{(2)}A_0'^{\,\mathrm{col}}}. \tag{2}$$

The minimum value of this ratio is $\frac{13}{28}$, equal to 0.46, and obtains when $A_0'^{\,\mathrm{col}} = -1$ and $\frac{1}{2}(3A_{2+}'^{\,\mathrm{col}} - A_0'^{\,\mathrm{col}}) = \frac{1}{2}$, that is $A_{2+}'^{\,\mathrm{col}} \simeq 0$. Note that in the absence of the fine-structure depolarization, $G^{(2)} = 1$ and the minimum value of R is zero. Thus, in the absence of fine structure, a minimum value of $R = 0$ would imply only $\frac{1}{2}(3A_{2+}'^{\,\mathrm{col}} - A_0'^{\,\mathrm{col}}) = \frac{1}{2}$, whereas with the depolarization included one is able to draw a stronger conclusion, namely, $A_0'^{\,\mathrm{col}} \approx 1$ *and* $A_{2+}'^{\,\mathrm{col}} \approx 0$, characteristic of a pure state.

Table I lists the values of the ratio R determined for our data. Since the polarization analyzer accepts some light intensity perpendicular to its axis, the measure values of R are slightly too large. We have used the specifications of the manufacturer (transmission of crossed polarizers of 1.4%, transmission of parallel polarizers 26%) to correct our values of R as shown in Table I.

These data are startling when compared to the values of R observed in He^+-He collisions. The smallest value of R observed in 3.0-keV He^+-He collisions is 0.72 ± 0.06 (Ref. 3). Recently reported measurements[5] in our laboratory at 1.5 keV, 1.25°, and unreported measurements at 1.50° and 2.0° show the smallest R to be 0.72. Thus, the ratio 0.6 ± 0.05 at 1.5 keV, 1.5°, is significantly smaller than any for He^+-He, and the ratio 0.72 ± 0.1 at 3.0 keV, 1.25°, is as small as any seen in He^+-He. Also, the ratio 0.6 is close to the minimum value of 0.46, suggesting the excitation of nearly pure He(3^3P) states.

TABLE I. Measured and corrected values of the ratio R. T_0 and θ are the laboratory incident kinetic energy in keV and laboratory scattering angle in degrees, respectively. The correction to R is explained in the text.

T_0 (keV)	θ (deg)	R_{meas}	R_{corr}
3.0	1.25	0.72 ± 0.1	0.70 ± 0.1
1.5	1.00	0.90 ± 0.1	0.88 ± 0.1
1.5	1.50	0.62 ± 0.05	0.60 ± 0.05
1.5	2.33	0.80 ± 0.1	0.78 ± 0.1

Another important feature of the data is shown in Table II. We have calculated the direction of the momentum-transfer axis for several inelastic energy losses ΔQ, assuming that the entire H_2^+ molecule recoils as a single particle. This assumption is not unreasonable in light of recent measurements.[6] Table II compares the direction of the momentum-transfer axis to the direction of either the major or the minor axis of the polarization pattern. Denote by θ_{mom} the angle from the incident beam direction to the momentum-transfer axis, and by θ_{symm} the angle from the incident-beam direction to the relevant symmetry axis of the polarization patterns. For the data at 3.0 keV, 1.25°; 1.5 keV, 1.00°; and 1.5 keV, 1.50°, the major axis lies along the momentum-transfer axis. For the data at 1.5 keV, 2.33°, the minor axis lies along the momentum-transfer axis. This correlation is somewhat surprising since the momentum-transfer axis is known to be of little significance in He^+-He collisions.[3]

In the approximation that the H_2 internuclear axis is rigidly fixed during the collision, our results imply that the orientation of this axis plays little role in the relative population of the magnetic sublevels. Alternatively, one can consider the reaction

$$He^+ + H_2 \rightarrow He^*(3^3P) + (H_2^+)^*, \tag{3}$$

TABLE II. A comparison of angles θ_{mom} and θ_{symm} as defined in the text. The inelastic energy loss is denoted ΔQ, and three values of ΔQ were selected to show the dependence of θ_{mom} on ΔQ.

T_0 (keV)	θ (deg)	θ_{sym} (deg)	ΔQ (eV)	θ_{mom} (deg)
3.0	1.25	109 ± 11	13.6	98
		(major)	27.8	104
			41.7	110
1.5	1.00	112 ± 10	13.6	107
		(major)	27.8	120
			41.7	130
1.5	1.50	107 ± 9	13.6	102
		(major)	27.8	112
1.5	2.33	125 ± 23	13.6	100
		(minor)	27.8	106
			41.7	112

where there is electronic and/or rotational-vibrational excitation of the H_2^+ ion. Since the measurement averages over all states of H_2^+, our results show that the particular magnetic substate excited in the collision is independent of the rotational-vibrational excitation of the H_2^+ ion. Another possible conclusion, namely that only one final state of the H_2^+ ion contributes to the excitation, seems unlikely, although selection rules may play a role in reducing the number of final states.

At 1.5 keV, 2.33°, and 1.5 keV, 1.00°, the alignment is considerably less than maximal but the atoms could still be in pure states if there is a definite phase relation between the eigenstates $m_l = 0$ and $m_l = \pm 1$. Further measurements of the three alignment parameters and the single orientation parameter are needed to fully characterize these states and show that they are pure states.

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Calculation of the Structure Factor of Liquid Metals*

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We suitably modify the scheme of Singwi *et al.* for calculating the density response function of interacting electron gas to take into account the fact that the pair correlation function vanishes in the highly repulsive hard-core region of the potential for classical liquids. This modified self-consistent iterative scheme is applied to calculate the structure factor for liquid sodium and rubidium. Both equilibrium and dynamical properties of classical liquids can now be calculated from a single theory.

The static structure factor $S(q)$ and the pair correlation function $g(r)$ have been successfully calculated by use of a perturbation theory due to Weeks, Chander, and Andersen (WCA)[1] for the Lennard-Jones fluid.[2] More recently, this scheme has been applied to calculate thermodynamic properties of liquid metals.[3]

For the calculation of dynamical properties, on the other hand, one uses either the generalized hydrodynamics[4-6] or the theory of Singwi *et al.*[7] (STLS), which introduces correlations between particles through the equilibrium pair correlation function. In both these schemes, the equilibrium structure given by $S(q)$ or $g(r)$ is assumed to be given.

In the STLS theory,[7] the dynamical density response function $\chi(q, \omega)$ is expressed as

$$\chi(q, \omega) = \chi_0(q, \omega)/[1 - \psi(q)\chi_0(q, \omega)]. \tag{1}$$

Here, $\chi_0(q, \omega)$ is the dynamical density response function of a free (noninteracting) system and the $\psi(q)$ is defined by

$$d\psi(r)/dr = g(r)d\varphi(r)/dr, \tag{2}$$

$\varphi(r)$ being the pair potential of the system. The fluctuation-dissipation theorem leads to a further relation between the structure factor and the ef-