THEORETICAL STUDIES OF INTERSTELLAR PROCESSES

Final Report

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A. Progress Under NASA Grant NAGW 2832

During the current reporting period we have continued our studies of the dissociative recombination (DR) of HeH^+ with an electron with the goal of calculating accurate cross sections and rate coefficients to allow for the accurate modelling of the abundance of HeH^+ in planetary nebulae and supernova envelopes. We have also started studies of the DR of H_3^+, a process of great importance in the interstellar medium.

1. Dissociative Recombination of HeH^+

Dissociative recombination of HeH^+ with an electron is described by:

$$HeH^+ + e^- \rightarrow He + H.$$

Our prior calculations of the DR of HeH^+ had considered dissociative routes of $^2\Sigma^+$ symmetry only (Guberman, 1994). During the current reporting period we have determined potential curves for the B and E $^2\Pi$ dissociative routes. There are no experimental data on these states. However, we have used the same approach to calculate these states as was used for the accurately determined $^2\Sigma^+$ states. Therefore we expect the potential curves for the B and E states to be highly accurate. These potential curves are shown with all the previously determined potential curves in Figure 1. The dissociative states going to the He + H(n=1,2) limits are shown as solid lines as is the ground state of the ion. The dissociative routes going to the He + H(n=3) limit are shown as dashed lines. For the B state, the calculated spectroscopic constants are 3319.6cm^{-1} for ω_e, 149.2cm^{-1} for $\omega_e x_e$, and 1.4513a_0 for the equilibrium internuclear separation. A common feature of all the dissociative curves is that they do not cross the ground state of the ion. However, we have shown previously (Guberman, 1994) that as long as there are large Born-Oppenheimer breakdown couplings DR can proceed with high rates even though there is no curve crossing with the ion. These large breakdown couplings correspond to an exchange of character between these adiabatic states. In order to assess the importance of the Π states we have calculated the derivative couplings as a function of internuclear distance, between the B state and the E state. From these couplings, the coupling of the B state to the electron ion continuum can be found by multiplying the B-E coupling by a density of states for the E state. The calculated B-E coupling has a maximum of only 0.03a_0^{-2} compared to the dominant coupling between the $C^2\Sigma^+$ and $D^2\Sigma^+$ states which reaches

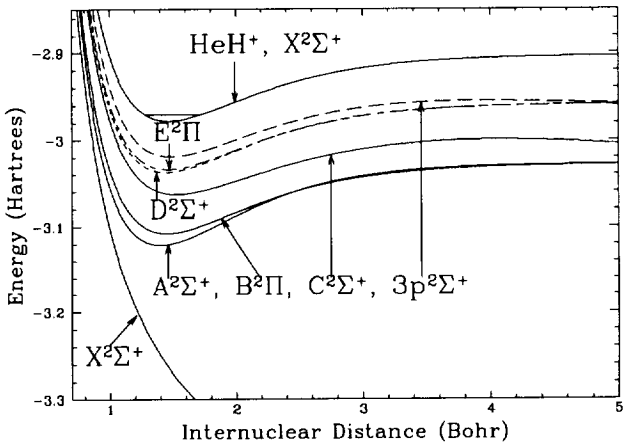

Figure 1. Potential curves for HeH and HeH^+.

a maximum of $2.1a_o^{-2}$. Therefore the B state is not expected to play an important role in DR by derivative coupling.

2. Dissociative Recombination of H_3^+

During the current reporting period, we have begun the calculation of potential surfaces needed for the study of the DR of H_3^+. The three Jacobi coordinates needed for the description of the potential surfaces are shown in Figure 2. For the potential surfaces described here, one coordinate, Θ, is held constant and the remaining coordinates, r and R, are plotted versus the calculated total energy. These calculations make use of a [4s,3p,2d,1f] Gaussian basis set centered on each atom. For the description of Rydberg states, the basis set is supplemented with six diffuse s and six diffuse p functions placed at the center of mass. Orbitals are determined in Hartree-Fock calculations on H_3^+ and the final energies are obtained form configuration interaction (CI) wave functions calculated by taking all single and double excitations to the virtual orbitals from a large set of reference configurations. To date, our calculations have been in C_{2v} symmetry in which the H_3 molecule takes the form of an isosceles triangle. For these calculations, Θ is fixed at 90 degrees.

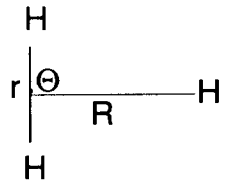

Figure 2. Jacobi coordinates for H_3.

Surfaces calculated under current NASA support are shown in Figure 3. The upper surface is that for H_3^+ and is composed of 748 calculated points, i.e. 748 CI, HF and integral calculations. The ground state of H_3^+ is an equilateral triangle having $^1A_1'$ symmetry in D_{3h}. In Figure 3, the zero point energy is about 1/16" above the bottom of the well in the upper surface.

The lower repulsive surface is the ground state of H_3 and it consists of 836 calculated points. Note that the lowest surface and the ion surface do not cross each other and the

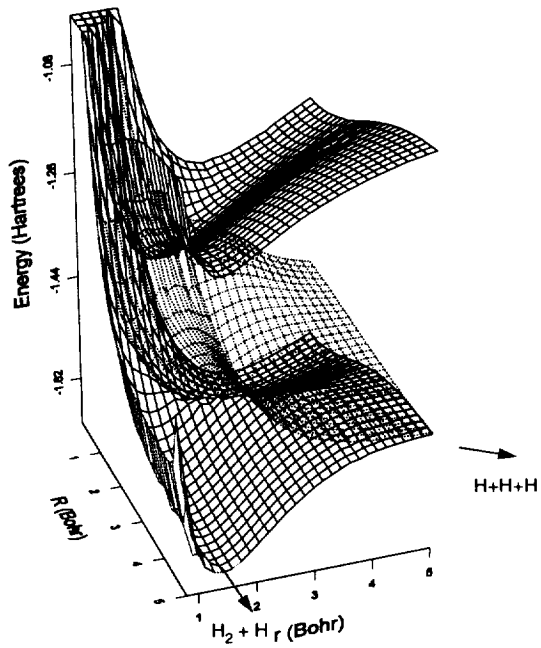

Figure 3. Potential energy surfaces calculated under current NASA support for H_3^+ and H_3.

situation is analogous to that for HeH. Dissociation along the ground state can yield either H_2 + H or H + H + H depending upon the direction travelled on the lower surface. Note also that for R held fixed at 6 Bohr, the energy versus r potential curve resembles the H_2 potential curve, as expected. In isosceles triangle geometries, the lowest surface is nondegenerate. However, at equilateral triangle geometries, the ground state is $^2E'$ and is degenerate with an additional repulsive surface which is shown as dotted in Figure 3. The dotted neutral surface can also be a route for DR of the low vibrational levels of H_3^+. This degenerate configuration is the well known (Herzberg and Longuet-Higgins, 1963) Jahn-Teller seam and it can be seen in Figure 3 as a ridge running along the lower surface from small r and R out to large r and R. At this ridge, in D_{3h}, the dotted surface is in contact with the lower surface. These wave functions are currently being used in the calculation of the Born-Oppenheimer breakdown couplings between these states.

B. References

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C. Publications Acknowledging NASA Support (March 1, 1995 - May 31, 1997)

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