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Astrochemistry in the Early Universe: Collisional Rates for H on H_2

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ABSTRACT

We present preliminary results of a full quantum calculation of state to state cross sections for H on H_2. These cross sections are calculated for v=0,4 j=0,15 for energies up to 3.0 eV. The cross sections are calculated on the BKMP2 potential surface (Boothroyd et al. 1996) with the ABC scattering code (Skouteris et al. 2000).

1. Introduction

The chemistry of the early universe is dominated by hydrogen. The standard big bang model produces only hydrogen, helium and trace amounts of lithium. These elements must makeup the gas that forms the first compact objects and cooling from these allows these first objects to form. A comprehensive model of the chemistry has been developed in Stancil, Lepp and Dalgarno (1996, 1998, 2002).

As part of that project we started calculations to get improved cooling curves for H_2, we found a large difference in H on H_2 collision rates. There was good agreement within the ground vibrational state, but excited state transitions could differ by orders of magnitude. See figures below.

Our calculations were done using the ABC program by Skoteris, Castillo, and Manolopoulos(2000). We have modified it to use the potential surface of Boothroyd, Keogh, Martin,and Peterson (1996). The ABC program uses the coupled-channel hyperspherical coordinate method to solve the Schrodinger equationfor three nuclei on a single Born-Oppenheimer potential energy surface. The program was run for a grid of energies up to 3.5 eV, so that we can calculate state to state rates for v=0-5, j=0-15.

2. Results

To compare with Sun and Dalgarno (1994) we ran some calculations on the DMBE potential surface (Varandas 1987). The results from the ABC code agree well with the earlier Sun and Dalgarno (1987) results as can be seen in Figure 1.

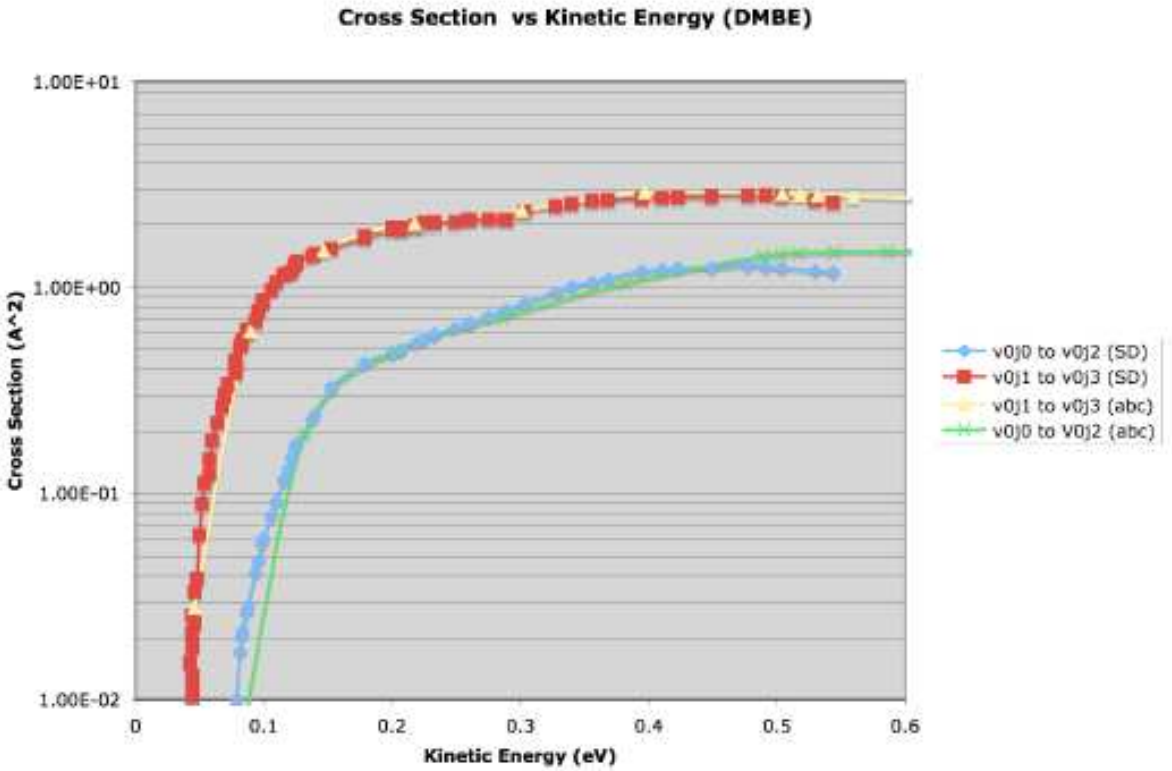

Fig. 1.— The cross section for the lowest two transitions for SD (Sun and Dalgarno 1987) and ABC (this calculation).

We have completed the calculations for the state-state cross sections on the BKMP surface (Boothroyd et al 1996) and will soon publish them (Archer 2006). These will be the first complete study of the state-state rates for H on H_2 for lower levels.

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REFERENCES

Archer, David, 2006 Ph.D Thesis.

A.I. Boothroyd, W.J. Keogh, P.G. Martin and M.R. Peterson, 1996 J. Chem. Phys., 104, 7139.

Stancil, P. C., Lepp, S., & Dalgarno, A. 1996, ApJ, 458, 401

Stancil, P. C., Lepp, S., & Dalgarno, A. 1998, ApJ, 458, 401.

Lepp, S., Stancil, P.C. and Dalgarno, A. 2002 J. Phys. B, 35, R57.

Skouteris, D., Castillo, J. F. and Manolopoulos, D. E. 2000, Comput. Phys. Commun. 133, 128.

Sun, Y. and Dalganro A. 1994 ApJ, 427, 1053.

Varandas, A.J.C., Brown, F.B., Mead, C.A., Truhlar, D.G. and Blaise, N.G. 1987, J Chem. Phys. 90,300.