Calculation of State-specific Rate Coefficients for Dissociation of $H_2(v,j) + H_2(v',j')$

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State-specific rate coefficients for dissociation of H_2 as the result of collisions with H_2 were calculated for all combinations of *(v, j)* with internal energy below 1 eV. Full dimensional quasiclassical trajectories with the chemically accurate BMKP interaction potential [1] were used with a minimum of 80000 trajectories per energy considered. Although preliminary results had indicated dynamic elevation of threshold, restricted dimensionality trajectories were used to verify that the threshold to dissociation was indeed energetic. Additional large batches of trajectories were used to calculate the cross sections near threshold until the desired precision of the rate coefficient was attained. A piecewise linear excitation function was used to calculate the rate coefficient between 600 and 60000 K, bracketing the range of validity for the interaction potential used.

The resulting state-specific rate coefficients, γ, are parametrized [2] as a function of temperature over the range 1000 - 30000 K.

References

[1] A. I. Boothroyd, P. G. Martin, W. J. Keogh, and M. J. Peterson, J. Chem. Phys., 116 (2002) 666.

[2] M. E. Mandy, and P. G. Martin, J. Chem. Phys. 110 (1999) 7811.