

The free energy profiles of two elementary bimolecular reactions as a function of temperature.

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A theoretical study of the free energy profile of the addition reactions between (a) BH_3 and H_2O and (b) Cl_2C and C_2H_4 using ab initio molecular dynamics is presented. Both reaction profiles exhibit a transition state that is only present on the free energy surface due to the loss in entropy. The effect of the temperature is studied to determine the relationship between the temperature and the free energy profile of the reactions.