

Instructions: Answer all questions within the space provided.

Max Marks: 11 (3 + 2 + 2 + 2 + 2)

(1) Following is a potential energy contour corresponding to two degrees of freedom. The six minima are labelled already. Identify and trace the most probable paths by which (a)  $tt$  goes to  $g^+c$ ; (b)  $g^-t$  goes to  $g^-c$ ; (c) Identify one second order saddle point and the corresponding two transition states to which the second order point connects.

(2) State and explain variational theorem.

(3) The Schrodinger equation of  $H_2$  molecule cannot be solved analytically even after using the Born-Oppenheimer approximation. Write the Schrodinger equation and explain.

Ques 4) Write the internal coordinate representation for  $\text{CH}_3\text{-NH}_2$ .



(5) Write the complete Hamiltonian for  $[\text{He-H}]^+$  molecule.