

## REACTION PATH HAMILTONIAN CALCULATION OF TUNNELING SPLITTING IN PROTONATED METHANOL AND METHYLAMINE.

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Both protonated methanol( $\text{CH}_3\text{OH}_2^+$ ) and methylamine( $\text{CH}_3\text{NH}_2$ ) show two interesting large amplitude motion, namely, internal rotation and inversion. The internal rotation spectrum results from the rotation of the  $\text{CH}_3$  moiety against the  $\text{OH}_2$  group in case of protonated methanol and of  $\text{NH}_2$  group in the case of methylamine. The other interesting phenomenon is inversion involving the  $\text{OH}_2$  group and  $\text{NH}_2$  group in the case of protonated methanol and methylamine, respectively. The influence of inversion in methylamine, on bands in the near and middle infrared has been investigated. Microwave and far-IR spectrum of methylamine has been measured and spectral frequency calculations derived from rotation-internal rotation-inversion analysis has been reported. However, in the past, detection of protonated methanol ( $\text{CH}_3\text{OH}_2^+$ ), in interstellar clouds has been impossible due to the lack of both laboratory spectra and calculation.

In this contribution *ab initio* based potential energy surface (PES) and dipole moment surface (DMS) is presented for both protonated methanol and methylamine. The PES and DMS are developed by least squares fitting of *ab initio* energy values computed at CCSD(T)/AVTZ level of theory and dipole moments at MP2/AVTZ level of theory. Internal rotation and inversion transition states and normal-mode frequencies will be reported. One-dimensional tunneling splitting calculations will be reported. Tunneling splittings at higher dimensionality, ro-vibrational states and transition intensities are calculated using reaction path Hamiltonian(RPH) as implemented in MULTIMODE(MM) code. MM treats polyatomic molecules with large-amplitude motion as and one special coordinate which is the large-amplitude vibrational coordinate. Complete integration is performed over reaction path coordinate, and the N-mode MULTIMODE coupling approximation for the evaluation of the matrix elements applies only to the  $3N - 7$  normal coordinates.