

# Study of nonadiabatic effect on dissociation channels of HCNH – the issue of abundance ratio $[\text{HNC}]/[\text{HCN}]$ in upper atmosphere revisited.

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## Abstract

The abundance ratio  $[\text{HNC}]/[\text{HCN}]$  in upper atmosphere is known to vary depending on the various conditions, like the presence of UV radiation, the temperature of the region of abundance, etc. There have been attempts to justify the related observations from kinetic as well as thermodynamic considerations. In the present work we consider the dissociation of HCNH, right after its formation from electron capture of  $\text{HCNH}^+$ , as the primary source of HNC and HCN in upper atmosphere. Few years back, from our group, a study [J.Phys.Chem.A, 2013, 117, 8680-8690] of nonadiabatic effect on low-lying excited states of HCNH was undertaken to understand the formation of HNC. Present study is to explore the nonadiabatic effects on the various dissociation channels of HCNH leading to the formation of HCN and thus to justify the abundance ratio  $[\text{HNC}]/[\text{HCN}]$  in upper atmosphere. We present here the first ever exploration of the presence of conical intersection around the transition state geometries along the intrinsic reaction coordinate for the dissociation of HCNH into HCN and HNC.

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Problem-HCNH-dissociation.docx available at <https://authorea.com/users/488958/articles/572910-study-of-nonadiabatic-effect-on-dissociation-channels-of-hcnh-the-issue-of-abundance-ratio-hnc-hcn-in-upper-atmosphere-revisited>