PROBING ROTATIONALLY EXCITED STATES OF CH_5^+ WITH DIFFUSION MONTE CARLO

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Protonated methane has long proven to be a challenging system for both experimentalists and theoreticians. The essentially flat potential surface comprised of 120 equivalent minima, coupled with a very fluxional molecule, make CH_5^+ a challenging system to study. Using Diffusion Monte Carlo we have had previous success studying vibrationally excited states of CH_5^+. Here we focus on modeling rotationally excited states using Diffusion Monte Carlo. Following our success with H_3O^+ and D_3O^+ we define our rotationally excited states by placing nodes at the zeros in the real rotational eigenstates of a symmetric top. We use this approach to analyze rotationally excited states of CH_5^+ through use of Fixed Node Diffusion Monte Carlo. We use the results of these simulations to analyze the rotation/vibration mixing in rotationally excited states of CH_5^+.