UNDERSTANDING CH_5^+ SPECTROSCOPY FROM A PARTICLE-ON-A-SPHERE MODEL

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Due to the low barrier to H rearrangement in CH_5^+, a good approximation is to separate the angular and radial H coordinates. By fixing R_{CH} at a constant value, the 15 degree-of-freedom problem becomes a more computationally feasible 10 degree-of-freedom problem. The reduced dimensional problem is well suited for capturing the essential low energy, large amplitude bending/rotation dynamics. The "particle-on-a-sphere" (POS) model, which has been shown to provide good experimental agreement in XH_n (n=2-4) systems is extended to accommodate a 5 hydrogen system. Building on past success with the XH_n systems, we use the XH_5 POS model to calculate the patterns of the low J rovibrational spectrum, facilitating the understanding of the jet-cooled CH_5^+ spectrum.