INTERNAL ROTATION IN THE CH_5^+ MOLECULAR ION

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A semirigid bender analysis is performed to calculate the rotation and internal-rotation energy levels of protonated methane in its ground electronic state. The internal rotation is modelled according to a minimum energy pathway fitted through 13 nuclear configurations optimized at the MP2/6-311++G($2df, 2p$) level of *ab initio* theory. The internal rotation coordinate is chosen as the average of the three dihedral angles between the C-H bonds of the CH_3^+ moiety and the somewhat separated H_2 moiety. The shape of the internal rotation potential, and the geometrical changes occurring as the molecule internally rotates, will be discussed, and their effect on the energy levels will be determined. The importance of other large amplitude internal motions will also be considered.