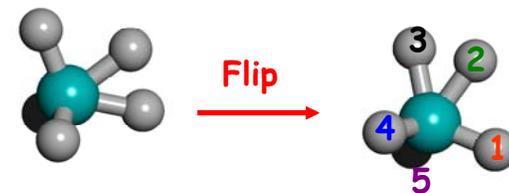
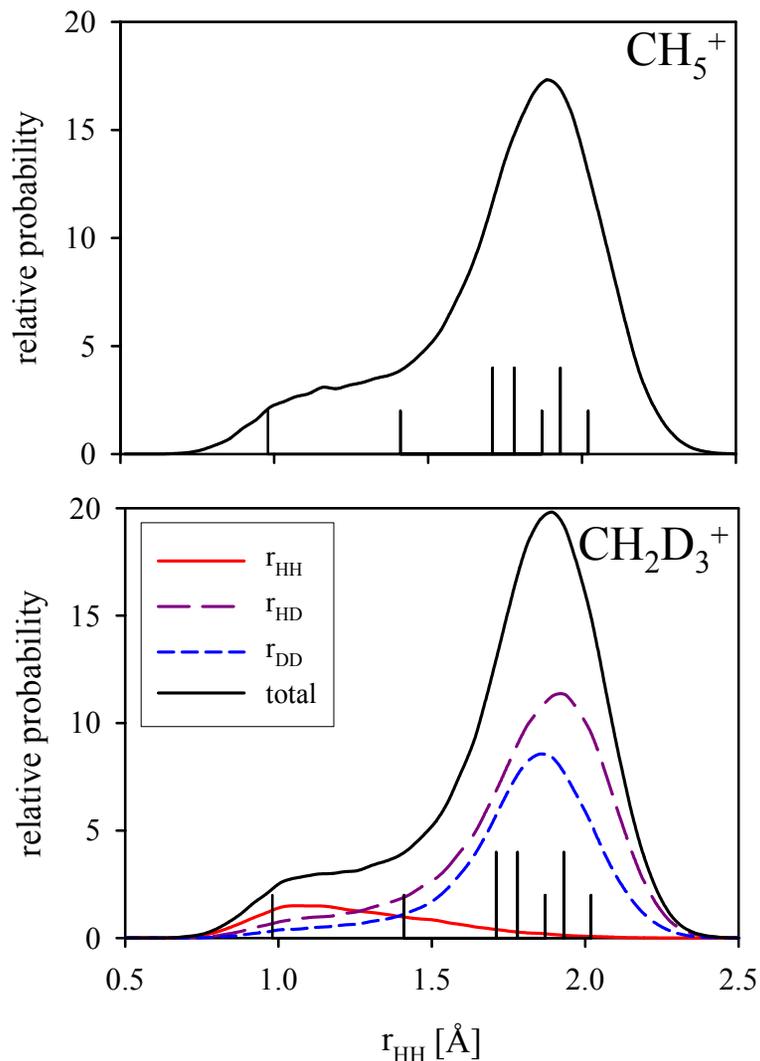


Does CH_5^+ have a Structure?



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Diffusion Monte Carlo studies, carried out on a fully *ab initio* potential energy surface, developed by Joel M. Bowman and his co-workers at Emory University,^a provide answers to the above question as well as implications of the structure to spectroscopy and dynamics of this floppy molecular ion. Even at the zero-point level, CH_5^+ samples all 120 (5!) equivalent minima on the potential surface, and, in the Monte Carlo simulation, the *walkers* move between the minima through the two pathways shown at the top of this page. In spite of this, the distributions at the left display clear evidence of structure. The vertical lines indicate the equilibrium HH distances, while the curves provide projections of a HH distance over the ground state wave function. Partial deuteration breaks the symmetry and, in the case of CH_2D_3^+ , the ion becomes trapped in the $\text{CD}_3^+ \text{-H}_2$ minimum energy structures.

^a A. B. McCoy, B. J. Braams, A. Brown, X. Huang, Z. Jin and J. M. Bowman, *J. Phys. Chem. A*, **2004**, 108.