NATURE OF TORSION-INVERSION COUPLING IN CH_3NH_2, $CH_3OH_2^+$ AND $CH_3CH_2\cdot$

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Two-dimensional torsion-inversion surfaces for methylamine, protonated methanol and ethyl radical were calculated and fit to a function containing a polynomial in the inversion angle(τ) and trigonometric functions of the torsional angle(α). Calculations were done at the B3LYP, MP2, and CCSD(T) levels with the 6-311++G(d,p) and 6-311++G(3df, 2p) basis sets and partial optimization. CH_3NH_2, $CH_3OH_2^+$ and $CH_3CH_2\cdot$ have G_{12} symmetry with 6-equivalent minima which are located by the various calculations at inversion angles 6.5 to 11; 42 to 45.5 and 52.5 to 55 degrees respectively on either side of planar. The three molecules have very different barriers to inversion ranging from no barrier for $CH_3CH_2\cdot$ to 838 cm^{-1} for $CH_3OH_2^+$ to 1837 cm^{-1} for CH_3NH_2. The dominant torsion-inversion coupling term in all cases has the form $\tau cos 3\alpha$.