COUPLING OF THE C-H STRETCH TO LARGE-AMPLITUDE TORSION AND INVERSION MOTIONS: COMPARISON OF $CH_3CH_2^{\cdot}$, $CH_3OH_2^+$ AND CH_3NH_2

RAM S. BHATTA, *Department of Polymer Science and Department of Chemistry, The University of Akron*;
DAVID S. PERRY, *Department of Chemistry, The University of Akron, OH 44325*.

In each of the title molecules, torsional and inversion tunneling occurs between six equivalent minima. Coupling of these degrees of freedom to the CH stretch occurs via variation of the C-H stretching force constants as a function of the torsional (α) and inversion (τ) angles. Maps of the couplings have been computed at the MP2/6-311++G(3df,2p) level. Both the single bond CH stretch force constants and the bilinear couplings between CH bonds are presented as a function of α and τ. Although the torsional barriers differ by more than a factor of 20, the torsion-inversion-vibration coupling patterns are very similar for CH_3NH_2 and $CH_3CH_2^{\cdot}$. On the other hand, the torsion-inversion-vibration coupling in the charged species $CH_3OH_2^+$ is much weaker.