COMPARATIVE TORSION-INVERSION DYNAMICS FOR $CH_3CH_2^{\cdot}$, $CH_3OH_2^{+}$ AND CH_3NH_2

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A general 2-dimensional torsion-inversion Hamiltonian was developed for methylamine, protonated methanol and ethyl radical. The torsion-inversion potential energy surfaces and kinetic parameters were determined from ab initio calculations at CCSD(T)/6-311++G(3df,2p)//MP2/6-311++G(3df,2p). The quantum torsion-inversion dynamics were solved for this Hamiltonian, including the dependence of the reduced masses on the inversion coordinates. The manifolds of torsion-inversion energy levels are calculated for the three molecular species and are compared with the available experimental and theoretical data. The patterns of the tunneling splitings vary as the inversion and torsional barriers go from low to high in the sequence $CH_3CH_2^{\cdot}$, $CH_3OH_2^{+}$ and CH_3NH_2.