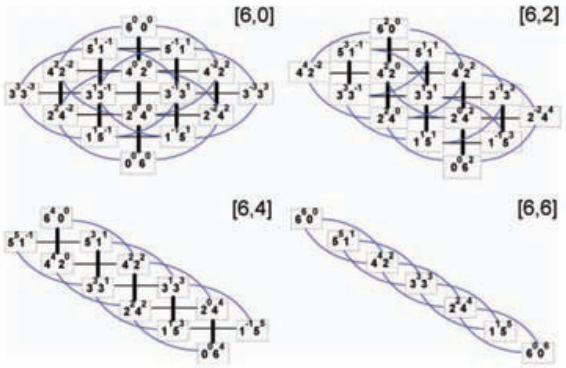
THEORETICAL METHODS AND ALGORITHMS

Critical points bifurcation analysis of high-l bending dynamics in acetylene

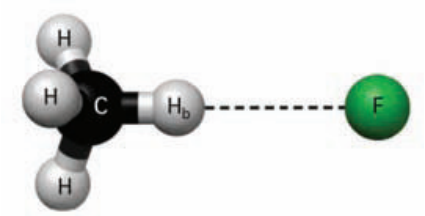
Vivian Tyng and **Michael E. Kellman**

The bending dynamics of acetylene with pure vibrational angular momentum excitation and nonzero quantum number l are analyzed through the method of critical points analysis to find new anharmonic modes born in bifurcations of the low energy normal modes.

J. Chem. Phys. **131**, 244111 (2009)



GAS PHASE DYNAMICS



Accurate *ab initio* potential energy surface, dynamics, and thermochemistry of the $F+CH_4 \rightarrow HF+CH_3$ reaction

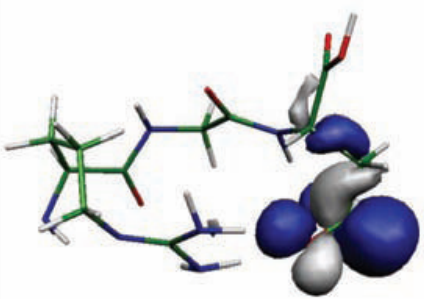
Gábor Czakó, Benjamin C. Shepler, Bastiaan J. Braams, and **Joel M. Bowman**

The reaction dynamics of the gas-phase reaction between a fluorine atom and a methane molecule are studied, and an accurate 12-dimensional potential energy surface (PES) is developed based on 19,384 *ab initio* energy points. Quasiclassical trajectory calculations of the reaction using the new PES are reported.

J. Chem. Phys. **130**, 084301 (2009)

The parent anion of the RGD tripeptide: Photoelectron spectroscopy and quantum chemistry calculations

Xiang Li, Haopeng Wang, Kit H. Bowen, G. Grégoire, F. Lecomte, Jean-Pierre Schermann, and **Charles Desfrançois**



The gas-phase conformation of the intact parent unprotected RGD–peptide anion is investigated using a combination of anion photoelectron spectroscopy and quantum chemistry calculations of its low-energy stable structures.

J. Chem. Phys. **130**, 214301 (2009)