THE MICROWAVE SPECTRUM OF THE TWO-TOP PEPTIDE MIMETIC N-ACETYL-PHENYLALANINE METHYL ESTER

KEVIN O. DOUGLASS, KEVIN M. DAVIS, FRANCIS J. LOVAS, DAVID F. PLUSQUELLIC, *NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY, GAITHERSBURG, MD 20899*; DAVID W. PRATT, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF PITTSBURG, PITTSBURG, PA 15260*; BROOKS H. PATE, *DEPARTMENT OF CHEMISTRY, UNIVERSITY OF VIRGINIA, CHARLOTTESVILLE, VA 22904*.

An on-going project at NIST is to determine the conformational structure of peptide mimetic molecules from analysis of their torsion-rotation spectra.[a] The rotational spectrum of N-acetyl-phenylalanine methyl ester has been recorded using a mini-FTMW spectrometer from 11 - 20 GHz. The peptide mimetic possesses two low barrier methyl tops. the principal axes and ρ - axes frames implemented in the software package, JB95. The rotational constants, methyl top angles and barriers to internal rotation for both tops have been determined. The results will be compared to predictions from quantum chemical calculations at the MP2 and DFT levels and from molecular mechanics (force field) models including CHARMM and Amber. Because the peptide bonds are nearly planar, the methyl top angles provide a direct measure of the Ramachandran angles. These results serve as benchmark data for validation of predictions from classical force field programs often used to model the structure and dynamics of much larger biosystems.

[a] R.J. Lavarich, D.F. Plusquellic, R.D. Suenram, G.T. Fraser, A.R.H. Walker, M.J. Tubergen, J. Chem. Phys. 118, 1253 (2004).