

COMPARATIVE AB-INITIO STUDIES OF HELICAL STRUCTURE OF PERFLUOROCTANOIC ACID (PFOA) AND PERFLUOROCTANE (PFO)

HEENA S. KARANI, SYLVESTRE TWAGIRAYEZU, *Chemistry and Biochemistry, Lamar University, Beaumont, TX, USA.*

As flexible molecules with long fluoroalkyl chain and multiple internal rotations, PFOA and PFO are excellent candidates for studies of molecular helicity and resulting conformational dynamics. Additionally, the exact structure of PFOA, as man-made environmental pollutant, is highly desired for the development of new spectroscopic tools for its detection in environmental samples. We present potential energy landscapes and helical structures of PFOA and PFO that are computed at Density Functional Theory levels with B3LYP-D3BJ/6-311G basis set by scanning dihedral angles and bending angles in steps of 10 degree each. The resulting potential energy surfaces show three equivalent minima for PFO (at 70° , 190° , and 310°) while only two minima (at 120° and 320°) are seen for PFOA. These minima correspond to stable helical conformers as results of maximizing the separation between F-atoms and rotating the carboxylic end terminal (PFOA only). The nature of helical coiling has been further explored by displacing the fluoroalkyl chain away from trans configurations back to the stable helical coiling structures. We notice that a helical angle of 14 degrees is necessary for the helical coiling to be realized and is insensitive to the end terminal. The work to evaluate the exact impact of fluoroalkyl chain on the helical coiling is underway and will be presented this talk.