ROTATIONAL INSIHGTS INTO PRE-REACTIVE INTERMEDIATES OF DIELS-ALDER CYCLOADDITIONS

X. ZHANG, H. WANG X. TIAN, Q. GOU, Department of Chemistry, School of Chemistry and Chemical Engineering, Chongqing University, Daxuecheng South Rd. 55, 401331, Chongqing; J.-U. GRABOW, Institut für Physikalische Chemie and Elektrochemie, Leibniz Universität Hannover, 30167 Hannover, Germany; W. CAMINATI, Dipartimento di Chimica "G. Ciamician", Università di Bologna, Via Selmi 2, I-40126 Bologna, Italy

The Diels-Alder (DA) reaction, with its rich synthetic diversity, has proven to be one of the most powerful protocols for accessing [4+2] cycloaddition to carbo- or heterocycles, and is recognized as one of the cornerstone reactions that both enabled and shaped the modern organic chemistry. In this presentation, taking furan as the diene, acrolein and maleic anhydride as the dienophile, the first stages of their DA reactions have been imaged with rotational spectroscopy, which is an ideal tool to characterize, at the molecular level, the nature of molecular complexes. The results have shown that the pre-reactive molecular complexes are stabilized with pi...pi stacking, which might be attributed to the selectivity as endo- or exo- products of such cycloaddition.