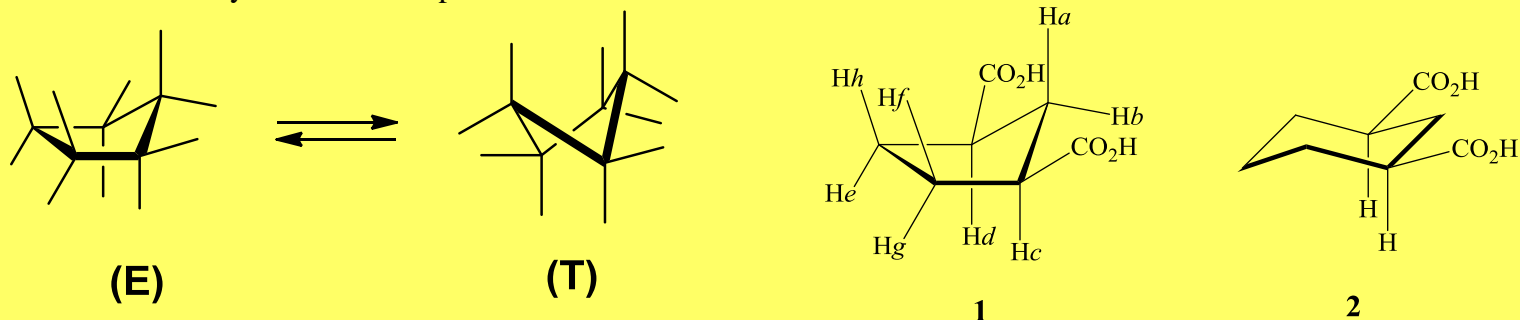
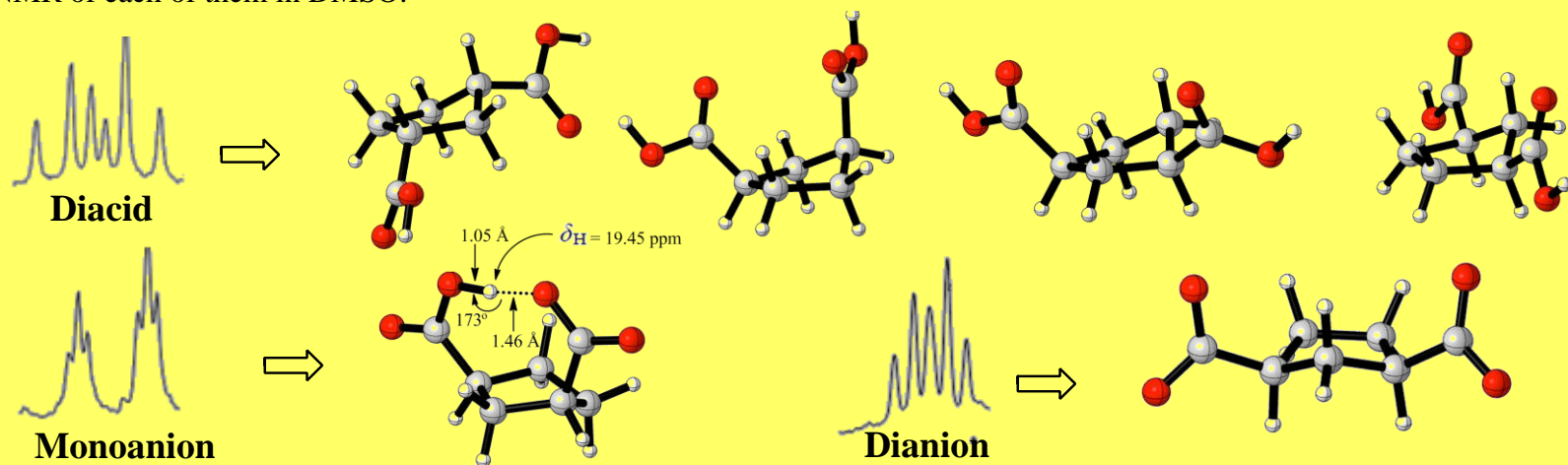


Conformational Preferences of *cis*-1,3-Cyclopentanedicarboxylic Acid and its Salts by ^1H NMR Spectroscopy. Bright U. Emenike, William R. Carroll, John D. Roberts (California Institute of Technology)

Far less published information is available on the possible conformations of substituted cyclopentane rings than for correspondingly substituted cyclohexanes, even though there are natural products that that are cyclopentane or possess the cyclopentane ring as an important element of their structures. In a recent study, Garza, A. J. et al. *J. Am. Chem. Soc.*, **2012**, DOI: 10.1021/ja302133s., we studied the conformations of *cis*-1,3-cyclohexanedicarboxylic acid and its salts and found that the most stable conformations, generally had their carboxyl groups equatorial. In contrast, cyclopentane rings appear to have two main conformations: the envelope **E**, and the twist-boat **T**, which are expected to be easily interconverted, one to the other by what is called pseudorotation.



The question is, can we find discrete conformations for the *cis*-1,3-cyclopentanedicarboxylic acid and its salts or not? So, let us look at the proton NMR of each of them in DMSO.



The amazing thing about the *a,b* proton NMR spectra of **1** is number of peaks that appear, which DFT-calculations suggest come from four different conformations. In striking contrast, the proton spectra of the mono- and dianion of **1** represent single conformations. The monoanion forming an intramolecular hydrogen bond between the carboxyl groups, similar to the monoanion of succinic acid. The dianion of **1** forms a single conformation with diaxial carboxylate groups. It will be interesting to see if other-sized rings do the same.