THE FEASIBILITY OF DETERMINING THE CARBON FRAMEWORK GEOMETRY OF A MOLECULE FROM ANALYSIS OF THE CARBON-13 ISOTOPOLOGUE ROTATIONAL SPECTRA IN NATURAL ABUNDANCE

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One powerful feature of molecular rotational spectroscopy is the ability to obtain quantitative information for the positions of individual atoms in the structure through the analysis of singly-substituted isotopologue spectra. However, because the structural information comes from changes in the moments-of-inertia, the signs of the atom coordinates in the principal axis system are not available. This project explores the ability to obtain the carbon framework geometry of a molecule from isotopologue spectra. The first step of the analysis examines the distributions of carbon-carbon atom distances, C-C-C bond angles, and correlations between the bond angles and bond distances found in molecules. The "rules" for acceptable structures are obtained through the analysis of about 100 optimized structures from quantum chemistry that were available in lab. These rules are then used to find acceptable carbon framework geometries from the 8^{N-1} possible carbon frameworks that come from the sign ambiguity of the substitution coordinates. In the test case of a molecule with 6 carbon atoms, cyclohexene oxide, these rules produced a single (and correct) carbon atom framework from the 32,768 possibilities. For molecules with 12 carbon atoms, a relatively large number of possible carbon atom frameworks are found to be consistent with the structure constraints: about 100,000 out of the 8.6 billion possible geometries. The results of the analysis as a function of molecular mass (number of carbon atoms) and structural characteristics (compact structures compared to structures with long alkyl tails, for example) will be presented. Approaches to assigning quality scores to candidate carbon atom frameworks that meet the structure conditions with the goal of ranking the most likely molecular structures will also be discussed.