NARROWING DOWN THE POSSIBLE GEOMETRIES OF A MOLECULE FROM ISOTOPOLOGUE ROTATIONAL CONSTANTS WITH STRUCTURAL FILTERS

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A computer algorithm is developed to narrow down the list of possible structural geometries of a molecule from the analysis of its isotopologue rotational constants. Based on Kraitchman's equation, the absolute values of the position coordinates of the atoms in a molecule may be obtained from the corresponding isotopologue rotational constants. The algorithm, in attempt to take a step further, narrows down the list of possible combinations of atom positions and bond connections within the molecule. Compared to a previous work by Mayer et al.[a] which focused on carbon atoms, the algorithm extends the application to more atoms including oxygen, nitrogen, etc. More molecular geometry filters are integrated in the algorithm as well. Five filters involving interatomic distance, bond type, valence, bond angles, and coplanarity based on VSEPR theory are developed. As a result, the algorithm was able to narrow down the number of possible structures for Aspirin, a molecule with 13 non-hydrogen atoms, from 10^{10} to 110. However, the exact geometry of molecules could not be determined by the algorithm directly, especially when the molecule is large (usually more than five non-hydrogen atoms). In addition, large errors from Kraitchman's equation near the principle axes of the molecule leads to ambiguous results on those atoms. It leads to the belief that our current understanding may be insufficient to resolve the molecular geometry directly from the isotopologue rotational constants.

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[a]Mayer, Kevin J., et al. "The Feasibility of Determining the Carbon Framework Geometry of a Molecule from Analysis of the CARBON-13 Isotopologue Rotational Spectra in Natural Abundance." *74th International Symposium on Molecular Spectroscopy.* 2019.