Beyond NMR Spectroscopy: Solving Challenging Structural Problems in Pharmaceutical Chemistry using Molecular Rotational Spectroscopy

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Molecular rotational spectroscopy has a direct connection to the three-dimensional structure of molecules that makes it especially well-suited to the analysis of isomers in chemistry. Current instruments for rotational spectroscopy offer high spectral resolution and high dynamic range that make it possible to perform quantitative chemical analysis in a complex sample matrix. In the past two years, we have collaborated with several pharmaceutical chemistry groups to assess the potential of molecular rotational spectroscopy to address unmet needs in analytical chemistry. Many of these challenges are related to stereoisomer analysis for molecules with multiple chiral centers. Examples of diastereomer and enantiomer analysis in pharmaceutical production, including methods for rapid stereoisomer monitoring for emerging flow chemistry production techniques will be presented. Application of rotational spectroscopy to the analysis of regioisomers direct from reaction flask mixtures will also be described. Finally, the unique capabilities of rotational spectroscopy for isotopologue and isotopomer analysis of deuterated active pharmaceutical ingredients will be presented.