ENANTIOMER IDENTIFICATION IN CHIRAL MIXTURES WITH BROADBAND MICROWAVE SPECTROSCOPY

V. ALVIN SHUBERT, DAVID SCHMITZ, CHRIS MEDCRAFT, CoCoMol, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany; DAVID PATTERSON, JOHN M. DOYLE, Department of Physics, Harvard University, Cambridge, MA, USA; MELANIE SCHNELL, CoCoMol, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany.

In nature and as products of chemical syntheses, chiral molecules often exist in mixtures with other chiral molecules. The analysis of these complex mixtures to identify the components, determine which enantiomers are present, and to measure the enantiomeric excesses (ee) is still one of the challenging but very important tasks of analytical chemistry. These analyses are required at every step of modern drug development, from candidate searches to production and regulation.

We present here a new method of identifying individual enantiomers in mixtures of chiral molecules in the gas phase.\textsuperscript{a,\textit{b}} It is based on broadband rotational spectroscopy and employs a sum or difference frequency generation three-wave mixing process that involves a closed cycle of three rotational transitions. The phase of the acquired signal bares the signature of the enantiomer (see figure), as it depends upon the combined quantity, $\mu_a\mu_b\mu_c$, which is of opposite sign between members of an enantiomeric pair. Furthermore, because the signal amplitude is proportional to the ee, this technique allows for both determining which enantiomer is in excess and by how much. The high resolution of our technique allows us to perform molecule specific measurements of mixtures of chiral molecules with $\mu_a\mu_b\mu_c \neq 0$, even when the molecules are very similar (e.g., conformational isomers). We introduce the technique and present results on the analysis of mixtures of the terpenes, carvone, menthone, and carvomenthenol.
