

MOLECULAR CHIRALITY: ENANTIOMER DIFFERENTIATION BY HIGH-RESOLUTION SPECTROSCOPY

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I have demonstrated that triple resonance performed on a three-rotational-level system of a chiral molecule of C_1 symmetry exhibits signals opposite in phase for different enantiomers, thereby making enantiomer differentiation possible by microwave spectroscopy^a. This prediction was realized by Patterson et al. on 1,2-propanediol and 1,3-butanediol^b. We thus now add a powerful method: microwave spectroscopy to the study of chiral molecules, for which hitherto only the measurement of optical rotation has been employed. Although microwave spectroscopy is applied to molecules in the gaseous phase, it is unprecedentedly superior to the traditional method: polarimeter in resolution, accuracy, sensitivity, and so on, and I anticipate a new fascinating research area to be opened in the field of molecular chirality. More versatile and efficient systems should be invented and developed for microwave spectroscopy, in order to cope well with new applications expected for this method

For C_2 and C_n ($n \geq 3$) chiral molecules, the three-rotational-level systems treated above for C_1 molecules are no more available within one vibronic state. It should, however, be pointed out that, if we take into account an excited vibronic state in addition to the ground state, for example, we may encounter many three-level systems. Namely, either one rotational transition in the ground state is combined with two vibronic transitions, or such a rotational transition in an excited state may be connected through two vibronic transitions to a rotational level in the ground state manifold.

The racemization obviously plays a crucial role in the study of molecular chirality. However, like many other terms employed in chemistry, this important process has been “defined” only in a vague way, in other words, it includes many kinds of processes, which are not well classified on a molecular basis. I shall mention an attempt to obviate these shortcomings in the definition of racemization and also to clarify the implicit assumptions made in Hund’s paradox^c.

^aE. Hirota, 3rd Molecular Science Symposium, Nagoya, September 2009, E. Hirota, Proc. Jpn. Acad. Ser. B, 88, 120 (2012).

^bD. Patterson, M. Schnell and J. M. Doyle, Nature 497, 475 (2013), D. Patterson and J. M. Doyle, Phys. Rev. Lett. 111, 023008 (2013).

^cF. Hund, Z. Phys. 43, 805 (1927).