LINE SHIFTS IN ROTATIONAL SPECTRA OF POLYATOMIC CHIRAL MOLECULES CAUSED BY THE PARITY VIOLATING ELECTROWEAK INTERACTION

J. STOHNER, *ZHAW Zürich University for Applied Sciences, ICBC, Reidbach T, CH 8820 Wädenswil, Switzerland, sthj@zhaw.ch.*; M. QUACK, *ETH Zürich, Physical Chemistry, CH 8093 Zürich, Switzerland.*

Are findings in high-energy physics of any importance in molecular spectroscopy ? The answer is clearly 'yes'. Energies of enantiomers were considered as exactly equal in an achiral environment, e.g. the gas phase. Today, however, it is well known that this is not valid. The violation of mirror-image symmetry (suggested theoretically and confirmed experimentally in 1956/57)[a] was established in the field of nuclear, high-energy, and atomic physics since then, and it is also the cause for a non-zero energy difference between enantiomers. We expect today that the violation of mirror-image symmetry (parity violation) influences chemistry of chiral molecules as well as their spectroscopy.[b] Progress has been made in the quantitative theoretical prediction of possible spectroscopic signatures of molecular parity violation. The experimental confirmation of parity violation in chiral molecules is, however, still open. Theoretical studies are helpful for the planning and important for a detailed analysis of rovibrational and tunneling spectra of chiral molecules.

We report results on frequency shifts in rotational, vibrational and tunneling spectra of some selected chiral molecules which are studied in our group.[c] If time permits, we shall also discuss critically some recent claims of experimental observations of molecular parity violation in condensed phase systems.[d]

---

[a] T. D. Lee, C. N. Yang, Phys. Rev., **104**, 254 (1956); C. S. Wu, E. Ambler, R. W. Hayward, D. D. Hoppes, R. P. Hudson, Phys. Rev., **105**, 1413 (1957)

[b] M. Quack, Angew. Chem. Intl. Ed., **28**, 571 (1989); Angew. Chem. Intl. Ed., **41**, 4618 (2002); M. Quack, J. Stohner, Chimia, **59**, 530 (2005); M. Quack, J. Stohner, M. Willeke, Ann Rev. Phys. Chem. **59**, 741 (2008)

[c] M. Quack, J. Stohner, Phys. Rev. Lett., **84**, 3807 (2000); M. Quack, J. Stohner, J. Chem. Phys., **119**, 11228 (2003); J. Stohner, Int. J. Mass Spectrometry **233**, 385 (2004); M. Gottselig, M. Quack, J. Stohner, M. Willeke, Int. J. Mass Spectrometry **233**, 373 (2004); R. Berger, G. Laubender, M. Quack, A. Sieben, J. Stohner, M. Willeke, Angew. Chem. Intl. Ed., **44**, 3623 (2005)

[d] J. Stohner, M. Quack, to be published