High resolution spectroscopy, parity violation and quantum tunneling dynamics in chiral molecules of astrophysical and general interest

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The quantum dynamics of chiral molecules were central to the discovery of tunneling shortly after the development of quantum mechanics in the form of the Heisenberg equations of motion and the Schrödinger equation[a,b,c] . Later in the 20th century they were again crucial in understanding the fundamental role of parity violation for stereochemistry and in introducing electroweak quantum chemistry [d,e,f]. In the 21st century chiral molecules may become the key to the discovery of extraterrestrial life by using small chiral molecules as tracers for homochirality in astrophysical spectroscopy. In the lecture we shall start with a short historical and conceptual introduction and then report about recent work of our group in Zurich including in particular work supported in the recent years by COST COSY. After an effort of 40 years we are close to finally measuring the parity violating energy difference between the enantiomers of chiral molecules, which has been well studied by theory but so far not yet observed in any experiment [d,e,f]. Major current efforts concern the understanding of the complex high resolution spectroscopy and quantum dynamics of chiral molecules and isotopic chirality as governed by the interplay of rotation, vibration, tunneling, and parity violation which is important both for the design of the experiment for detecting molecular parity violation and also for astrophysical spectroscopy (See [f,g,h,i]. www.ir.ETHz.CH and references therein)

References:

[a] Heisenberg, W. ; Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen. Z. Physik , 1925, 33, 879-893.

[b] Schrödinger, E ; Quantisierung als Eigenwertproblem . Ann. d. Physik. 1926, 79, 361-376, 489-527, 734-756,80,437-450, 81, 109-139

[c] Hund, F.; Zur Deutung von Molekülspektren. Z.Physik.,1927, 43, 742-764,788-804,805-826

[d] Quack, M. ; On the measurement of the parity violating energy difference between enantiomers. Chem. Phys. Lett., 1986, 132, 147-153.

[e] Bakasov. A., Ha, T. K., Quack, M. ; Ab initio calculations of molecular energies including parity violating interactions. J.Chem Phys. .,1998, 109, 7263-7285.

[f] Quack, M. , Seyfang, G.,Wichmann, G., Perspectives on parity violation in chiral molecules. Chem. Science., 2022, 13, 10598-10643. (see also M. Quack COST-COSYmeeting Madrid 2026)

[g] Albert, S., Chen, Z., Keppler, K. Wichmann, G., Quack, M., Stohner, J., Schurig V., Trapp, O; High resolution infrared spectroscopy of monodeutero-oxirane (c-C_2H_3DO) and analysis of two fundamentals between 820 and 850 cm^{-1} , Phys. Chem. Chem. Phys. (PCCP)2025, **27**, 14240 – 14253 (2025)

[h] Wichmann, G., Albert,S., Lerch, P., Keppler, K., Quack, M., High-resolution GHz and THz (FTIR) spectroscopy and quantum dynamics of tunneling in aniline Mol. Phys. **000,** e2593929 (2025) DOI: 10.1080/00268976.2025.2593929

[i] Chen, Z., Albert, S., Keppler, K. Wichmann, G., Quack, M., Schurig V., Trapp, O; Isotopic chirality and high-resolution gigahertz and terahertz spectroscopy of trans-2,3-dideuterooxirane(tcCHDCHDO) Phys. Chem. Chem. Phys. (PCCP)2026, **28**, 751- 763 (2026), DOI: 10.1039/d5cp03143e