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High Resolution Spectroscopy and Molecular Chirality: Symmetries and primary processes between less than yoctoseconds and more than days

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Molecular quantum dynamics, the primary processes of molecules in motion, provide the foundation of all chemical processes, covering combustion as an early and still today important use of chemistry by mankind, the chemistry of planetary atmospheres and of interstellar space, of large scale industrial syntheses, catalysis, and also of the microscopic biomolecular processes in the chemistry of life, notably also biomolecular homochirality, its persistence and evolution [1-3]. Spectroscopy with either high frequency or with high time resolution, possibly also with an uncertainty principle limited combination of both, provides the most powerful experimental techniques to study such processes and we shall start by summarizing the experimental and theoretical approaches developed by our group, which allow for studying primary processes over time scales ranging from yoctoseconds to much more than days [3-4]. We shall then focus on our recent results concerning the quantum dynamics of tunnelling, nuclear spin symmetry and parity violation in chiral molecules obtained by our approach to derive molecular quantum dynamics from high resolution spectroscopy[4-7]. We shall discuss the fundamental theoretical understanding of such primary processes within and going beyond quantum chemical kinetics on multidimensional Born Oppenheimer hypersurfaces[7-9] and even going beyond quantum electrodynamics based on the electromagnetic force only[1,6,7]. Indeed, in chiral molecules the electroweak force is essential in understanding the quantum dynamics of stereochemistry and tunneling. Symmetry and asymmetry are the unifying theoretical concepts for a fundamental understanding of molecular primary processes [3-7]. Examples include hydrogen fluoride clusters as prototypes for potentials and dynamics of hydrogen bonds [9], as well as other systems with parity and nuclear spin symmetry conservation and violation, molecular tunneling and tunneling switching phenomena notably also in chiral molecules [1-3,10] and isotopically chiral molecules important for astrophysical observation[11] and the chemistry of the homochirality of life[1,2,12]. We shall also include examples such as quasiadiabatic channel above barrier tunnelling [3,7]. We shall conclude with a brief report on current progress towards the observation of the theoretically predicted, new process of parity change with time due to parity violation in isolated chiral molecules [1,12]. For background reading see notably our reviews and books[1-7].

[1] M. Quack, G. Seyfang, G. Wichmann, Adv.Quantum Chem.Phys. 2020, 81, 51-104 and Chem. Science 2022, 13, 10598-10643.
[2] M. Quack, Adv. Chem. Phys. 2015, 157, 249
[3] M. Quack, Bunsen-Magazin, 2022, 24, 238-246, M. Quack, lecture at Trieste2024
[4] M. Quack, Molecular femtosecond quantum dynamics between less than yoctoseconds and more than days: Experiment and theory, chapter 27 in 'Femtosecond Chemistry', J. Manz, L.Woeste eds. VCH publishers, Weinheim 1995, pp 781-818.
[5] M. Quack, Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy, in Handbook of High Resolution Spectroscopy, Vol. 1, Chap. 18. (Eds.: M. Quack, F. Merkt), Wiley, Chichester, New York, 2011, pp. 659-722.
[6] M. Quack, Frontiers in Spectroscopy,Faraday Discussion 2011, 150, 533-565.
[7] R. Marquardt and M. Quack, eds., Molecular Spectroscopy and Quantum Dynamics, Elsevier, Amsterdam, 2021, chapter 7 on tunnelling by M. Quack and G. Seyfang

[8] C.Fabri, R. Marquardt, A. Csaszar, M. Quack, J.Chem. Phys, 2019, 150, 014102.
[9] H. Hollenstein, M. Hippler, G. Seyfang, M. Quack, Mol. Phys. 2024, 122, e2341106 DOI 10.1080/00268976.2024.2341106 (1-15) and references therein
[10] G.Wichmann, G.Seyfang, M. Quack, Mol. Phys. 2021, 119, e1959073.
[11] S. Albert, Z. Chen, S. Albert, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, Phys. Chem .Chem. Phys. (PCCP) 2019, 20,3669 –3675, DOI: 10.1039/c8cp05311a
[12] M. Quack, G. Seyfang, G. Wichmann, Parity Violation in Chiral Molecules: From Theory, towards Spectroscopic Experiment and the Evolution of Biomolecular Homochirality M. Quack, G. Seyfang, G. Wichmann, in 'Chiral Matter', Proceedings of the Nobel Symposium 167, Lidingö (Stockholm) 28June-2 July 2021, pp 209-268; Ed. E. Babaev, D. Kharzeev, M. Larsson, A. Molochkov, V. Zhaunerchyk, World Scientific Publishing Co, Singapore 2023

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