Parity Violation in Chiral Molecules: From Theory towards Spectroscopic Experiment and the Evolution of Biomolecular Homochirality

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In the lecture we shall start with an introductory discussion of three fundamental questions relating physics to molecular quantum dynamics and stereochemistry [1][2-21].

- (i) To what extent are the fundamental symmetries and conservation laws of physics and their violations reflected in molecular quantum dynamics and spectroscopy, in general?
- (ii) How important is parity violation for the quantum dynamics and spectroscopy of chiral molecules, in particular?
- (iii) How important is parity violation for biomolecular homochirality, i.e. the quasi exclusive preference of L-amino acids and D-sugars in the biopolymers of life (proteins and DNA)?

The observation of biomolecular homochirality can be considered as a quasi-fossil of the evolution of life [2, 3], the interpretation of which has been an open question for more than a century [2-5], with numerous related hypotheses, but no definitive answers. We shall briefly discuss the current status and the relation to the other two questions.

The discovery of parity violation led to one of the most striking developments of physics in the 20th century and is a major pillar of the current fundamental theory of high energy physics (the standard model of particle physics, SMPP). For molecular stereochemistry it leads to the surprising prediction of a small energy difference $\Delta_{pv}E_0$ of the ground state energies of the enantiomers of chiral molecules, corresponding to a small reaction enthalpy for the stereomutation between the *R* and *S* enantiomers [6].

$$R = S \qquad \Delta_R H_0^{\circ} = N_A \Delta_{pv} E_0$$

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This reaction enthalpy would be exactly zero by symmetry with exact parity conservation. Theory predicts $\Delta_{pv}E$ to be in the sub-femto eV range, typically, depending on the molecule (say, $\Delta_{pv}E = 100$ aeV corresponding to about $\Delta_R H_0^{e} = 10^{-11}$ Jmol⁻¹). After our finding in 1995 that early theories had predicted values too low by about 2 orders of magnitude for typical benchmark molecules [7, 8], current theories converge on the new higher values (reviewed in [6, 9]). However, successful experimental tests have so far been lacking. We have outlined 3 decades ago, how this small $\Delta_{pv}E$ might by measured by spectroscopic experiment [10], and recent progress indicates that experiment might be successful in the near future [11-14]. We shall discuss the current status of our experiments including alternatives in other groups and the possible consequences for our understanding of molecular and biomolecular chirality. Background reading can be found in [2-21].

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