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Vibrational evidence for chiral recognition phenomena *in vacuo*¹

MARTIN A. SUHM, U. Goettingen

Molecules and molecular conformations which cannot be superimposed on their mirror image are chiral. Chirality or handedness plays an important role throughout the life sciences. When two molecules interact, they can sense their relative handedness, giving rise to spectroscopic signatures of *chiral recognition*. This is often mediated by hydrogen bonds, most versatile and directional intermolecular interactions. If the distinction between the homo- and heteroconfigurational pairs of molecules is large enough, *chiral discrimination*, i.e. differences in abundance may occur. The contact between two flexible, transiently chiral molecules may induce a matching of their handedness, i.e. *chirality synchronization*. Such phenomena are best studied at low temperatures in vacuum isolation, without perturbing interactions [1]. Structural information on the isolated molecular complexes can be obtained by rotational spectroscopy [2], if there is a sufficient dipole moment. Vibrational spectroscopy [3] provides a more universal, but also more coarse-grained access to these phenomena. Our group has reported the first spectroscopic example of chiral recognition between constitutionally identical molecules in the gas phase [4]. We have found a case of chiral discrimination in tetrameric aggregates of methyl lactate, where the relative configuration controls the hydrogen bond topology [5]. In the case of alcohols, we have observed different degrees of chirality synchronization up to a quantitative chirality matching in dimers of trifluoroethanol [6]. These discoveries became possible through the use of a powerful combination of FTIR spectroscopy and high-throughput, pulsed supersonic nozzle expansions into large vacuum chambers [7]. The isolated and elementary character of the investigated molecular assemblies is favourable for quantum chemical treatments [8]. Valuable benchmarks for the modeling of more complex chiral recognition phenomena are thus established.

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¹Spectroscopy and dynamics of molecular coils and aggregates (www.pcg.de)