CHIRALITY RECOGNITION IN CAMPHOR - 1,2-PROPANEDIOL COMPLEXES

CRISTOBAL PEREZ, MARIYAM FATIMA, ANNA KRIN, <u>MELANIE SCHNELL</u>, CoCoMol, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany.

The molecular interactions in complexes involving chiral molecules are of particular interest, because the interactions change in a subtle way upon replacing one of the partners by its mirror image. This is based on the fact that chiral molecules are sensitive probes for other chiral objects and chiral interactions. In this particular case, we will concentrate on molecule-molecule interactions and investigate them with broadband rotational spectroscopy. When two chiral molecules form complexes, the homochiral and heterochiral forms have different structures (and thus rotational constants and spectra) and different energies. They are diastereomers, which can easily be differentiated, for example via molecular spectroscopy. This is often exploited in chemical synthesis for identifying and separating enantiomers. The phenomena involving chirality recognition are relevant in the biosphere, in organic synthesis and in polymer design.

We use chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy to study the structures and the underlying interactions of camphor-1,2-propanediol complexes. This system is also interesting because the complex formation can be expected to be ruled by an interplay between hydrogen bonding to the polar carbonyl group in camphor and dispersion interactions. The spectra are extremely rich because of the high number of conformers for 1,2-propanediol. We started out with racemic mixtures of both camphor and 1,2-propanediol. Using enantiopure samples of different handedness of the two partners nicely simplifies the spectra and guides the assignment. In the talk, we will report on the latest results for this chiral complex.