ROTATIONAL SPECTROSCOPY OF IMINE-BASED MOLECULAR SWITCHES: ISOLATED AND MICRO-SOLVATED

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Imine-based molecular motors and switches[a] have been recently developed, and many of their properties remain largely unexplored. With potential to perform multi-step unidirectional rotations, these systems are an important addition to the existing nano-motor toolbox.[b] Their photochemically-induced switching processes foresee applications in the regulation of chemical reactions, as well as performing mechanical functions. Previous condensed-phase studies show that the energetic balance between isomers of such a molecular switch can be markedly different to that predicted from quantum chemistry calculations.[c] Micro-solvation studies in supersonic jet conditions are thus an appealing route to investigate the origin of these population manoeuvres. Rotational spectroscopy allows us to study the 3D structure and conformational heterogeneities of these systems and their micro-solvated counterparts with great precision, since we can relate the pattern of rotational frequencies to the structure through the moments of inertia.[d] Experiments using chirped-pulse Fourier transform microwave spectroscopy in the 2-8 GHz range are ongoing. Preliminary results of our study will be presented and discussed.

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