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Probing Potential Energy Surfaces with High-Resolution Spectroscopy: From the Universe's Carbon Locker to Molecular Machines

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Light is a powerful tool that, on the one hand, can alter the molecular state and, on the other hand, can be used to probe molecular properties without changing the state. Fundamentals of these interactions are potential energy surfaces (PESs) of molecular ground and electronically excited states. In this thesis we present high-resolution spectroscopic studies on cold and isolated molecules, shedding a light on the topology of their potential energy surfaces.

In chapters 2,3, and 4 we use light to explore the potential energy surface of polycyclic aromatic hydrocarbons-the most wide-spread polyatomic molecules in the universe that are responsible for a series of IR emission bands observed in a variety of astrophysical environment and that take a part in a life cycle of cosmic carbon-by probing the vibrational level structure of their ground state. In these chapters we resent a comprehensive overview of the CH-stretch region of PAHs, discussing the role of anharmonicity in the 3μm region and a correlation between the spectral and structural properties of PAHs as well as the astrophysical implications of these findings.

Light has the power to initiate structural transformations upon photoexcitation in photoactive molecules. In chapters 5 and 6 light is employed to study the response of photoactive molecules or their functional parts that are of relevance in molecular nanotechnology and opto-electronics. In these chapters we explore their excited states, looking at their vibronic level structure, dynamics properties and the pathways for the deactivation of the excited state.