Efficient exploitation of molecular symmetry in variational rotational-vibrational computations and applications to fluxional molecular systems

The main objective of this STSM is the development and implementation of efficient methods for exploiting molecular symmetry in variational rotational-vibrational computations. Our planned research aims at the highly accurate theoretical investigation of the vibrational and rovibrational quantum dynamics of fluxional molecular systems (such as the very intriguing CH_5^+ molecular ion [1]) by carrying out state-of-the-art variational nuclear motion computations. The rationale for this project is provided by the expertise of Prof. Attila G. Császár's research group and the general variational rotational-vibrational GENIUSH program package [2]. Besides method development this STSM will foster exchange of knowledge about the most recent version of the GENIUSH program package developed at ETH Zürich. GENIUSH enables the accurate solution of both the time-independent and time-dependent Schrödinger equations using arbitrary internal coordinates and body-fixed frame embeddings and it has been applied successfully for molecules with 3, 4, 5 and 6 atoms in full and reduced vibrational dimensions. One particularly important study has focused on the rovibrational energy levels and wavefunctions of H_5^+ and found a highly peculiar rovibrational energy level structure [3,4]. The planned methodological developments can potentially contribute to an improved understanding of the spectroscopy and quantum dynamics of CH_5^+ and they can also support an ongoing research project on H_5^+ and its isotopologues.

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