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Potential energy surfaces for hydrocarbon molecules and ions[1]
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Studies of reaction dynamics and molecular spectroscopy rely on the concept of a potential energy surface (PES): the potential energy of the molecule or reaction complex as a function of the configuration of nuclei. In practice such a PES must be available in an analytical form that can be quickly evaluated and that has been fitted to the results of (expensive) electronic structure calculations. We have been constructing potential energy surfaces for hydrocarbon molecules and complexes C_mH_n, $m \leq 4$ and at most 8 atoms total, neutral or once charged, in full dimensionality and with due respect for the invariance under exchange of identical nuclei. The poster will describe our family of surfaces and will highlight applications to the spectroscopy of methane and of the vinyl radical (C_2H_3).

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