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A quantum full dimensional calculation of vibrational levels of CH_5^+

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Abstract

The vibrational levels of CH_5^+ are notoriously difficult to compute because the five protons move almost freely around the carbon center and the dimensionality is high (12-dimensions). We take a divide-and-conquer approach by first solving a 7-dimension bend problem and a 5-dimension stretch problem and then solving the full problem by coupling the lowest wavefunctions of both sub-problems to form a basis whose size is orders of magnitude smaller than that of the primitive basis. Wavefunctions and energies are obtained by diagonalizing the Hamiltonian matrix using the symmetry-adapted Lanczos method. Converged excited vibrational levels are obtained by starting from 1.3×10^{12} primitive basis functions.