

Supporting information

**Matrix product state formulation of the MCTDH theory in
local mode representations for anharmonic potentials**

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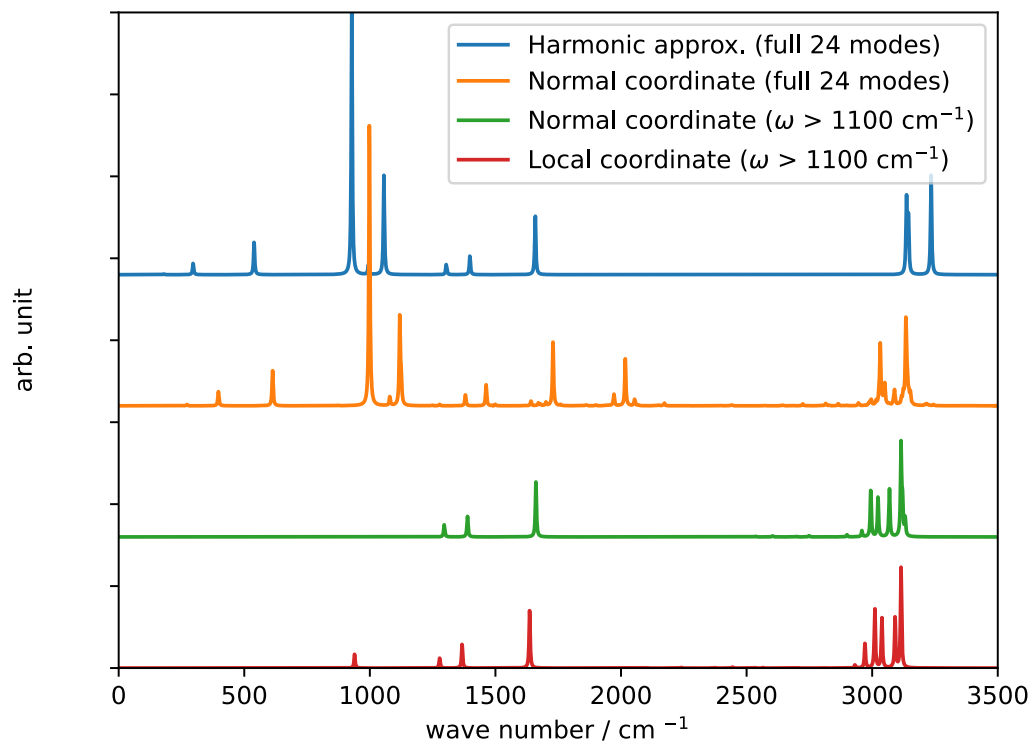


Fig. S1. The calculated IR spectrum of the C₄H₆ molecule. From top to bottom: harmonic potential spanned by all normal modes (blue), grid-based HO DVR + 4th order Taylor 3MR PES spanned by all normal modes and VCI[3]-(4) (orange), 4th order 3MR Taylor PES spanned by normal modes over frequency 1100 cm⁻¹ and VCI[3]-(7) (green), 4th order 3MR Taylor PES spanned by group-localized modes over frequency 1100 cm⁻¹ and VCI[3]-(7) (red). The peaks appear around 2000 cm⁻¹ for the full space calculation (orange) are overtone of the modes around 1000 cm⁻¹ those were truncated in the reduced space calculations (green, red). The peak appears at 900 cm⁻¹ for the reduced space calculations (red) is an artifact of the mode truncation.