

ab initio calculations (64 bit)

RPH 128 bit (new)

RPH 128 bit (old)

Fit to cos/sin-expansion
(variable dimensionality)

Spline interpolation of the data

Calculation of potentials,
frequencies, G-matrix

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Test for correct symmetries

Calculation of quasiadiabatic
channel

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10 dimensional fit to cos
series ('filter')

Solving the Schrödinger
equation on a grid