

MCTDH calculation

Name: NOCl

Hamiltonian:

CH3Quasie_exact
NOCl
CH4_rst

Potential Energy Surface:

☐ on ☒ off

Type of calculation:

- ☒ real - time propagation
☐ imaginary - time propagation
☐ Eigenstate calculation
☐ Thermal flux eigenstate calculation

Integrator:

start time: 0 initialtime step: 1

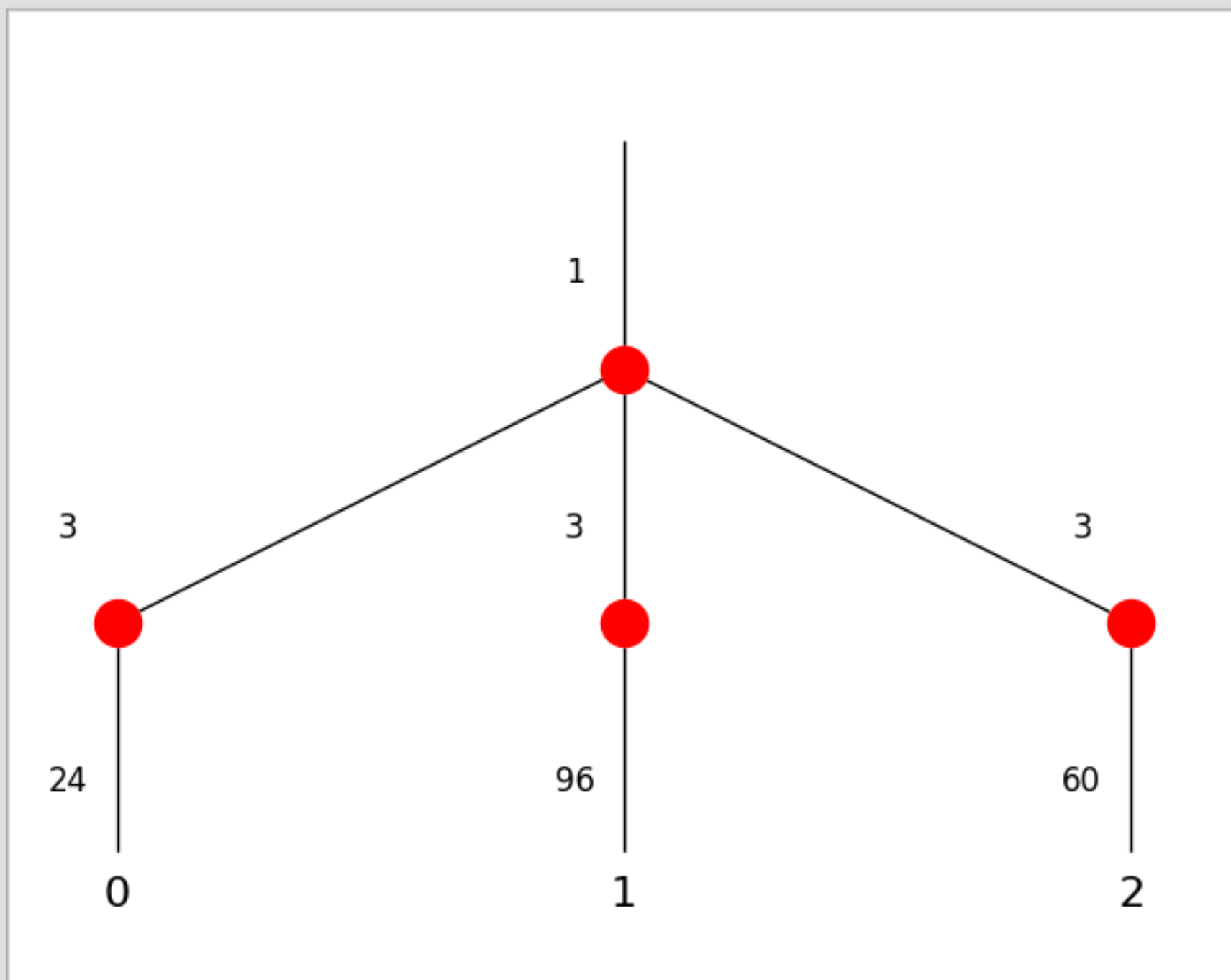
end time: 1985.376 iteration: 100

Node

Mode

1
3 24 0
3 96 1
3

Basis:



Cancel

Save Job

Load...

Start calculation