MCTDH calculation

Name: 10

Hamiltonian: 11

CH3Quasie_exact
NOCl
CH4_rst

Potential Energy Surface:

on off 12

13

PES_HCH4_Zang
PES_CH4
CH3Potential

Type of calculation:

real - time propagation
imaginary - time propagation 14
Eigenstate calculation
Thermal fluxe eigenstate calculation

Integrator: 15

start time: initialtime step:

end time: iteration:

16

Basis: 17

21 18 19 20

Cancel Save Job Load... Start calculation