SINDO 4.0 User's Manual: sindo

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Contents

Acknowledgment

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1 Sindo

1.1 &mol group

- Character(80) :: minfoFile
  The name of the .minfo file, in which the information of molecule is written.
- Integer :: Nat
  The number of atoms
- Real(8), dimension(Nat) :: Mass
  The mass of each atoms (in atomic mass unit)
- Real(8), dimension(3,Nat) :: x
  The reference (equilibrium) geometry (in Angstrom)
- Real(8), dimension(Nfree) :: omega
  The frequencies for the HO basis sets (in cm^{-1})
- Real(8), dimension(Nat*3,Nfree) :: L
  The vibrational displacement vectors

* Note that 'minfoFile' is mutually exclusive from others.

1.2 &sys group

- Integer(8) :: Maxmem
  Maximum size of memory (MB)

1.3 &mrpes group

- Integer :: MR
  Mode representation (MR=1-4)
- Real(8) :: mcs_cutoff
  Cutoff of QFF based on MCS in cm-1 (default = 1.d-04)
- Logical :: au
  The grid data in atomic unit (default = true)
- Character(80) :: mopFile
  The name of the mop file.

1.4 &vib group

- Integer :: Nfree
  Number of degrees of freedom (default = 3Nat - 6)
- Integer :: MR
  Mode representation (MR=1-4)

- Integer, dimension(Nfree) :: vmax
  Number of basis functions for each mode (default=10)
- Integer :: vmaxALL
  Number of basis functions for all modes (default=10)
- Integer :: vmax_base
  same as vmaxALL
- Logical :: vscf, ocvscf, vci, vpt, vqdpt
  invoke vscf/ocvscf/vci/vpt/vqdpt
- Logical :: prpt
  invoke property calculation
- Logical :: readBasis
  read the basis functions from cho.basis

1.5 &states group

- Integer :: Nstate
  Number of states to calculate
- Integer, dimension(Nfree,Nstate) :: target_state
  Labels of the target states
- Logical :: fund
  Compute fundamentals

1.6 &vscf group

- Logical :: state_specific
  State specific VSCF if true (default = .false.)
- Logical :: restart
  Restart from vscf_xxx.wfn (default = .false.)
- Integer :: Maxitr
  Maximum number of iteration (default = 10)
- Real(8) :: Ethresh
  Threshold of convergence (default = 1e-03 cm^{-1})

1.7 &ocvscf group

- Integer :: maxOptIter
  Maximum number of iteration (default = 30)
- Real(8) :: ethresh
  Threshold of the energy (default = 1e-06 cm^{-1})

- Real(8) :: gthresh
  Threshold of the gradient (default = 1e-06 cm^{-1} rad^{-1})
- Integer :: pfit
  Order of the Fourier fitting (default = 2)
- Character(80) :: mopFile
  The name of the mopfile
- Character(80) :: u1File
  The name of the file to write the transformation matrix (default = u1.dat)
- Integer :: icff
  Switch on CFF when icff = 1 and QFF when icff = 0 (default = 0)
- Integer :: iscreen
  Switch off/on pair selection when iscreen=0/1 (default = 1)
- Real(8) :: eta12thresh
  Threshold value for the pair screening (default = 500 cm^{-1})

1.8 &vci group

- Integer :: Nstate
  Number of states to calculate
- Integer :: nCI
  Max CI dimension (cutoff based on the energy)
- Integer(Nfree) :: maxEx
  Max quantum number to excite for each mode
- Integer :: maxExALL
  Max quantum number to excite for all the modes
- Integer :: maxSum
  Max sum of quantum number
- Integer :: nCUP
  Max number of modes to excite
- Logical :: geomAv
  If true, calculate vibrationally averaged geometry
- Logical :: dump
  If true, dump the vci wavefunction to vci-w.wfn
- Real(8) :: printWeight
  Print the configuration with the weight larger than this threshold
- Logical :: readCIbasis
  If true, read CI basis from vci-w.wfn

- Logical :: dumpHmat
  If true, write the VCI hamiltonian matrix

- Logical :: noDiag
  If true, the diagonalization is skipped

1.9 &vpt group

- Integer :: maxSum
  Max sum of quantum number to excite (default = -1)

- Integer :: maxEx
  Max quantum number to excite (default = -1)

- Integer :: nCUP
  Max number of modes to excite (default = MR)

- Real(8) :: thresh_ene
  Threshold energy to avoid divergence (default=1e-04 Hartree)

- Logical :: dump
  Dump the information to vmp-w.wfn

1.10 &vqdpt group

- Integer :: nGen
  The generation of P space (default=3)

- Real(8) :: thresh_p0
  E0 pruning (default=500 cm^{-1})

- Real(8) :: thresh_p1
  VPT based pruning (default=0.1)

- Real(8) :: thresh_p2
  VCI pruning (default=0.05)

- Real(8) :: thresh_p3
  VCI pruning (default=0.9)

- Integer :: pset
  Combine the p-space generated from several target states
  =0 when the target states have an overlap (default)
  =1 when the p-space components have an overlap

- Integer :: maxSum
  Max sum of quantum number to excite (default = -1)

- Integer :: nCUP
  Max number of modes to excite (default = MR)

- Integer :: pqSum
  P/Q interaction scheme
  > 0 prune the interaction when $\lambda_{pq} >$ maxSum (default)
  < 0 full interaction

- Integer :: vqdpt2_loop
  =0 loop over q, then p, p' (default)
  =1 loop over p, then p', q

- Real(8) :: thresh_ene
  Threshold energy to avoid divergence (default=1e-04 Hartree)

- Real(8) :: printWeight
  Print the configuration with the weight larger than this threshold (default=0.001)

- Logical :: dump
  Dump the information to vqdpt-w.wfn (default=true)

1.11 &prpt group

- Logical :: vscfprpt, vciprpt, vptprpt, vqdptprpt
  Invoke property calculation for vscf, vci, vpt, vqpdt wavefuncion

- Integer :: MR
  Mode representation (default = 3)

- Character :: extn(*)
  The extension of the property files

- Integer :: matrix(*)
  = 0 calculate only the average
  > 0 calculate the matrix

- Logical :: infrared
  If true, calculate the IR intensity.

1.12 &prptvci group

- Integer :: Nstate
  The number of states

1.13 &IRspectrum group

- Real(8) :: minOmega, maxOmega
  Min/Max value of the spectrum (default = 100 - 4000 cm^{-1})

- Real(8) :: delOmega
  Interval of the data (default = 1 cm^{-1})

- Real(8) :: fwhm
  Full-width half maximum of the Lorentz function for convolutions (default = 20 cm^{-1})

- Real(8) :: cutoff
  Cutoff of the band (default = -1 km mol^{-1})

2 Interface with Quantum Chemistry Programs

2.1 Gaussian

2.2 Molpro

2.3 ACESII

2.4 QChem

3 Files

References