

User's guide of FSindo

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Contents of Sample Files

Sample files are found in sindo-4.0/doc/FSindo/sample_FSindo

1.water/

VSCF, VCI[3]-(8), VMP2-(4), VQDPT2-(4)

2.ethylene/

VCI[3]-(6), VMP2-(4), VQDPT2-(4)

3.water-hexamer/

nc-VCI[3]-(6), nc-VQDPT2-(4)

3.water-hexamer_oc/

oc-VSCF, oc-VCI[3]-(6), oc-VQDPT2-(4)

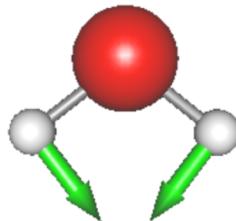
How to run SINDO

```
$ sindo < xxx.inp > xxx.out
```

1. Water

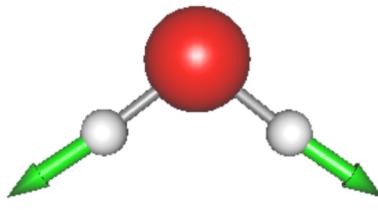
- h2o.minfo

Includes the equilibrium geometry, harmonic frequencies, and vibrational displacement vectors. They can be visualized by JSindo.



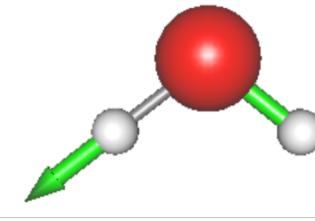
Q1

HOH bending



Q2

Sym. OH stretching



Q3

Asym. OH stretching

- *.pot

Includes the information of grid potential.

eq. q0.pot

1MR q1.pot, q2.pot, q3.pot

2MR q2q1.pot, q3q1.pot, q3q2.pot

3MR q3q2q1.pot

```
B3LYP/cc-pVDZ (11)
# Number of grids and data
 11      1
#   q2          Energy
 -28.05499848  6.7066429978e-02
 -21.28549000  4.3536327557e-02
 -15.49364050  2.5681778470e-02
 -10.14497826  1.2204347140e-02
 -5.02301699  3.3101913787e-03
 -0.00000000  0.0000000000e+00
  5.02301699  4.1200574795e-03
 10.14497826  1.8799126027e-02
 15.49364050  4.9578584037e-02
 21.28549000  1.0751025106e-01
 28.05499848  2.2150954913e-01
q2.pot (END)
```

- vscf.inp

```
#--- [ INPUT PARAMETER ]
&mol minofile='h2o.minfo' /      input minfo file
&sys maxmem=10 /                max memory in MB

#--- [ VIB ]
&vib MR=3 vmaxAll=10 vscf=.t. /
    • MR       : Mode coupling order of the PES
    • vmaxAll : Max num of quanta of HO basis sets for all modes.
    • vscf    : true invokes VSCF.

#--- [ TARGET STATES ]
&states fund=.t. /      Targets all fundamental levels.

#--- [ VSCF ]
&vscf Maxitr=20 Ethresh=1.D-03 /
    • Maxitr   : Max iteration for VSCF
    • Ethresh  : Threshold of convergence in cm-1.
```

- log/vscf.out

```
>> BASIS FUNCTIONS
  MODE :      1      2      3
  MAXV :      10     10     10
  FREQ :  1659.40  3752.61  3853.49
```

```
>> POTENTIAL
[ OPTIONS ]
  MR      =      3
  MCS_CUTOFF = 0.10E-03
  MCS_GRID   = -.10E+01
  POTDIR    = ./
  1MR-PEF          1MR
  o GRID PEF
    MODE= 1, GRID= 11  B3LYP/cc-pVDZ (11)
    MODE= 2, GRID= 11  B3LYP/cc-pVDZ (11)
    MODE= 3, GRID= 11  B3LYP/cc-pVDZ (11)

  2MR-PEF          2MR
  o GRID PEF
    MODE= 2  1, GRID= 11 11  B3LYP/cc-pVDZ (11)
    MODE= 3  1, GRID= 11 11  B3LYP/cc-pVDZ (11)
    MODE= 3  2, GRID= 11 11  B3LYP/cc-pVDZ (11)

  3MR-PEF          3MR
  o GRID PEF
    MODE= 3  2  1, GRID= 11 11 11  B3LYP/cc-pVDZ (11)
```

Setting of HO basis sets. Frequencies are taken from the minfo file.

```
>> STATE 000: ZERO-POINT STATE
  o INITIAL GUESS FROM (CONTRACTED) HARMONIC OSCILLATOR
  -- (ITERATION) ----- (EOLD) ----- (ENEW) ----- (DELTA E) --
    1        4687.67        4589.42      -0.983D+02
    2        4589.42        4586.72      -0.270D+01
    3        4586.72        4586.64      -0.809D-01
    4        4586.64        4586.64      -0.254D-02
    5        4586.64        4586.64      -0.800D-04
  -----
  E(VSCF)= 4586.63552176  Zero-point Energy
```

>> VIRTUAL VSCF ENERGIES

VSCF STATES	TOTAL ENERGY	E-E0
1_1	6184.36878830	1597.73326654
2_1	8220.27988057	3633.64435881
3_1	8388.85466071	3802.21913894

It's a good practice to check if the PES is specified in the way you intended.

Virtual VSCF energies for the fundamental levels.

- vci.inp

```
#--- [ VIB ]
&vib MR=3 vmaxAll=10 vscf=.t. vci=.t. /
    vscf = .t. and vci = .t. invokes VSCF/VCI.
```

```
#--- [ VCI ]
&vci nstate=20 nCUP=3 maxSum=8 /
    • nstate      : Number of states to obtain.
    • nCUP       : Max number of modes to excite.
    • maxSum     : Max sum of quantum numbers to excite.
    * nCUP=3 and maxSum=8 means VCI[3]-(8).
```

- log/vci.out

```
>> VCI OPTIONS

o VCI SPACE SELECTION
  - MAX NUM. OF MODES TO EXCITE : 3
  - MAX SUM OF QUANTUM NUM. : 8
  - MAX EXCITATION OF EACH MODE : 8 8 8

o VCI DIMENSION : 165 Dimension of VCI matrix
o NUM_OF_STATES : 20

> STATE 00000: ZERO-POINT STATE

E(VCI) = 4567.81121 Zero-point energy

Cl coeff.
COEFF. WEIGHT CONFIG.
0.999 0.998 0_0
0.039 0.001 2_1 3_2

> STATE 00001: 1_1 1st excitation of the 1st mode

E(VCI) = 6158.00730 Total energy and
E(VCI)-E0= 1590.19608 excitation energy

Cl coeff.
COEFF. WEIGHT CONFIG.
-0.998 0.996 1_1
-0.038 0.001 1_1 2_1 3_2
```

VCI[3]-(8)

Dimension of VCI matrix

- vmp2.inp

```
#--- [ VIB ]  
&vib MR=3 vmaxAll=10 vscf=.t. vpt=.t. /
```

vscf = .t. and vpt = .t. invokes VMP2.

```
#--- [ VPT ]  
&vpt maxSum=4 /
```

- maxSum : Max sum of quantum numbers to excite.
* maxSum=4 means VMP2-(4).

- log/vmp2.out

```
>> VPT OPTIONS

o VPT WITH ZERO-POINT VSCF REFERENCE (VMP)
  READ VSCF WFN : vscf-000.wfn

o VPT LEVEL:          VMP2-(4)
  NCUP   =    3
  MAXSUM =    4

o THRESH_ENE : 0.100E-03
```

```
o STATE 000: ZERO-POINT STATE

--- Q-SPACE COMPONENTS---
  1-MODE :      0
  2-MODE :     18
  3-MODE :      4
  TOTAL :     22
-----
  E(0th)   =  4509.75410
  E(1st)   =   76.88145
  E(2nd)   = -18.89655
  E(VMP1)  =  4586.63555
  E(VMP2)  =  4567.73900
```

1st and 2nd
order energy

```
o STATE 001: 1_1 1st excitation of
              the 1st mode

--- Q-SPACE COMPONENTS---
  1-MODE :      13
  2-MODE :     24
  3-MODE :      7
  TOTAL :     44
-----
  E(0th)   =  6107.48744
  E(1st)   =   76.87803
  E(2nd)   = -24.52433
  E(VMP1)  =  6184.36547
  E(VMP2)  =  6159.84114
  E(VMP1)-E0 =  1597.72993
  E(VMP2)-E0 =  1592.10214
```

1st and 2nd
order energy

1st and 2nd order
excitation energy

- vqdpt2.inp

```
#--- [ VIB ]
&vib MR=3 vmaxAll=10 vscf=.t. vqdpt=.t. /
    vscf = .t. and vqdpt = .t. invokes VQDPT2.
```

```
&states
fund=.t. All fundamental levels.
```

```
nstate=3
target_state(2,1)=2
target_state(2,2)=1      add (020), (011), (002)
target_state(3,2)=1
target_state(3,3)=2
```

```
/
```

```
#--- [ VPT ]
&vqdpt nGen=3 maxSum=4 /
```

- nGen : Max number of iteration for generating the P space.
- maxSum : Max sum of quantum numbers to excite.

- log/vqdpt2.out

```
>> VQDPT OPTIONS

o VQDPT WITH ZERO-POINT VSCF REFERENCE
READ VSCF WFN : vscf-000.wfn

o P-SPACE CONSTRUCTION
  NGEN =      3
  THRESH_P0 = 0.50E+03
  THRESH_P1 = 0.10E+00
  THRESH_P2 = 0.50E-01
  THRESH_P3 = 0.90E+00
  P SET     =      0

o Q-SPACE CONSTRUCTION
  NCUP =      3
  MAXSUM =     4
```

Parameters for the
P space.

Parameters for the
Q space.

```
o STATE 000: ZERO-POINT STATE

--- Q-SPACE COMPONENTS---
  1-MODE :      0
  2-MODE :     18
  3-MODE :      4
  TOTAL :    22

-----
```

E(0th) =	4509.75410
E(1st) =	76.88145
E(2nd) =	-18.89655

E(VMP1) =	4586.63555
E(VMP2) =	4567.73900

1st and 2nd
order correction

1st and 2nd
order energy

o GROUP 002: 2_1

--- P-SPACE COMPONENTS -----

* 1) 2_1
 2) 1_2

* IS THE TARGET STATE

o Q-SPACE COMPONENTS: 66

(CLOCK) ----> LAST STEP: USER 0.00, SYSTEM 0.00 SECS <----

> STATE 001: 1_2

E(VQDPT2) =	7714.41978
E(VQDPT2)-E0=	3146.68078

COEFF.	WEIGHT	CONFIG.
-0.987	0.975	1_2
-0.159	0.025	2_1

> STATE 002: 2_1

E(VQDPT2) =	8149.29727
E(VQDPT2)-E0=	3581.55827

COEFF.	WEIGHT	CONFIG.
-0.987	0.975	2_1
0.159	0.025	1_2

(CLOCK) ----> LAST STEP: USER 0.00, SYSTEM 0.00 SECS <----

VCI-like output for
the P space.

Quiz

Find the fundamental frequencies of H₂O from the output files, and fill in a table below.

	Harm	VCI[3]-(8)	VMP2-(4)	VQDPT2-(4)	Exp.
1					1595
2					3652
3					3756

2. Ethylene

- eq-mp2dz.minfo
 - Includes the equilibrium geometry, harmonic frequencies, and vibrational displacement vectors. They can be visualized by JSindo.
- prop_no_1.mop
 - Includes the information of QFF

1.1832573615027308000000e-15	1			
2.7040635655127780000000e-03	1	1		
1.1590249883181242000000e-17	1	1	1	
2.2875576159959352000000e-05	1	1	1	1
-2.1030452203654645000000e-16	2			
⋮	⋮	⋮	⋮	⋮

one-body terms:
ci, cii, ci_{iii}, ci_{iiii}

-4.1897357280855250000000e-18	1	2		
-6.3982329963326570000000e-14	1	2	2	
1.8221212840606143000000e-13	1	2	2	2
-1.9301098360709593000000e-15	1	1	2	
2.9510063534107640000000e-05	1	1	2	2
3.2272058841394823000000e-15	1	1	1	2
9.6870281798527820000000e-19	1	3		
3.1255300969821536000000e-13	1	3	3	
⋮	⋮	⋮	⋮	⋮

two-body terms:
cij, c_{ijj}, c_{ijjj}, ci_{ij}, ci_{ijj}, ci_{ijj}

1.4433950673416240000000e-13	1	2	3	
-1.6315521638821910000000e-13	1	2	3	3
3.0819651776043526000000e-13	1	2	2	3
6.1712325565851670000000e-14	1	1	2	3
1.8082830483224921000000e-13	1	2	4	
⋮	⋮	⋮	⋮	⋮

three-body terms:
cijk, c_{ijkk}, c_{ijjk}, ci_{ijk}

-1.7216241284537538000000e-12	1	2	3	4
-6.9604367079630600000000e-13	1	2	3	5
6.2074884931908150000000e-13	1	2	4	5

four-body terms: cijkl

- vci.inp, vmp2.inp, vqdpt2.inp
- Input for QFF

```
#--- [ MRPES ]
&mrpes mopFile='prop_no_1.mop' mcs_cutoff=-1.0D-03 /
```

- **mopFile** : Name of a QFF file.
- **mcs_cutoff** : Cut-off threshold for coupling terms based on MCS.

- Input for VCI, VMP2, VQDPT2 is the same as in the case of water.
- Output for QFF

```
>> POTENTIAL
[ OPTIONS ]
    MR      =      3
    MCS_CUTOFF = -.10E-02
    MCS_GRID  = -.10E+01
    POTDIR   = ./
    MOPFILE  = prop_no_1.mop
```

1MR-PEF **1MR**

```
o QFF  MP2/cc-pVDZ
    MODE= 1
    MODE= 2
    MODE= 3
    MODE= 4
    MODE= 5
    MODE= 6
    MODE= 7
    MODE= 8
    MODE= 9
    MODE= 10
    MODE= 11
    MODE= 12
```

2MR-PEF **2MR**

```
o QFF  MP2/cc-pVDZ
    NUMBER OF TERMS= 66
```

3MR-PEF **3MR**

```
o QFF  MP2/cc-pVDZ
    NUMBER OF TERMS= 220
```

Quiz

Find the fundamental frequencies of C₂H₄ from the output files, and fill in a table below.

	Harm	VCI[3]-(8)	VMP2-(4)	VQDPT2-(4)	Exp.
1					826
2					940
3					949
4					1026
5					1222
6					1344
7					1442
8					1625
					1662
9					2989
10					3022
11					3083
12					3105

3. Water Hexamer

- `h2o_6-mp2dz.minfo`
Includes the equilibrium geometry, harmonic frequencies, and vibrational displacement vectors. They can be visualized by JSindo. In this example, we only treat internal vibration of water molecules (i.e., OH stretching and HOH bending modes) neglecting intermolecular modes. We set modes 31 – 40 to active, and others to inactive.
- `prop_no_1.mop`
Includes the information of QFF. This is 4MR-QFF for all 48 modes. (In fact, it is costly to get this QFF.)

- ocvscf.inp

```
#--- [ VIB ]
&vib MR=4 ocvscf=.t. vscf=.f. vci=.f. vpt=.f.
          ocvscf = .t. invokes oc-VSCF.

  vmaxAll = -1      Make all modes inactive.
  vmax(31) = 10
  vmax(32) = 10
  ...
  vmax(48) = 10    } Make 31-48 active.
/
#--- [ OCVSCF ]
&ocvscf mopfile='prop_no_1.mop' /
  • mopFile      : Name of a QFF file.
  * For oc-VSCF, QFF needs to be full 4MR-QFF.
```

- log/ocvscf.out

o ITERATION: 1		E0	ENEW	DELTA-E	GRADIENT
PAIR	NEWANGLE				
31 32	0.0000	26945.3563507561	26945.3563507561	0.6091643683E-11	0.6393220243E-07
31 33	36.0000	26945.3563507561	26945.1959285686	-0.1604221875E+00	0.2958156264E-07
32 33			26945.1851192583	-0.1080931028E-01	0.7312591220E-06
31 34			26945.1851192583	0.0000000000E+00	0.4959187373E-06
32 34	0.0000	26945.1851192583	26945.1851192583	0.0000000000E+00	0.6187666111E-06
33 34	-10.9606	26945.1851192583	26945.1464144267	-0.3870483161E-01	0.7794531368E-07
:					
:					
DELTA E =		68.3470991265			
o ITERATION: 2		E0	ENEW	DELTA-E	GRADIENT
PAIR	NEWANGLE				
31 32	-6.7920	26877.0092516296	26876.9963853861	-0.1286624343E-01	-0.8027253508E-07
31 33	0.0000	26876.9963853861	26876.9963853861	0.0000000000E+00	-0.2670920474E-06
:					
:					
DELTA E =		iteration over Jacobi sweep			
o ITERATION: 3		E0	ENEW	DELTA-E	GRADIENT
PAIR	NEWANGLE				
31 32	0.0000	26876.0402745534	26876.0402745534	0.0000000000E+00	-0.1354575927E-06
31 33	0.0000	26876.0402745534	26876.0402745534	0.0000000000E+00	-0.3132263692E-06
32 33	0.0000	26876.0402745534	26876.0402745534	0.0000000000E+00	0.7074927365E-06
o TRANSFORMATION MATRIX WRITTEN TO : [u1.dat]					
o FORCE CONSTANTS WRITTEN TO : [prop_no_1.mop_ocvscf]					
o NEW COORDINATES WRITTEN TO : [h2o_6-mp2dz_ocvscf.minfo]					

These files are used in subsequent VSCF calculations.

- `ncvci.inp`, `ncvqdpt2.inp`
VCI and VQDPT2 calculations based on normal coordinates.
They read `h2o_6-mp2dz.minfo` and `prop_no_1.mop`.
- `ocvci.inp`, `ocvqdpt2.inp`
VCI and VQDPT2 calculations based on optimized coordinates.
They read `h2o_6-mp2dz_ocvscf.minfo` and `prop_no_1.mop_ocvscf`.

Quiz

Visualize the normal and optimized coordinates of water hexamer, and discuss on their differences.

List of all Options

&mol

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] 'minfoFile' is mutually exclusive from others.

&sys

Integer(8) :: Maxmem

Maximum size of memory (MB)

&mrpes

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.

&vib

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

&states

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

&vscf

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)

&ocvscf

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)

&vci

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 :: readClbasis
 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

&vpt

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

&vqdpt

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  $\lambda_{pq} > \text{maxSum}$  (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)
```

&prpt

```
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.
```

&prptvci

Integer :: Nstate
The number of states

&IRspectrum

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)