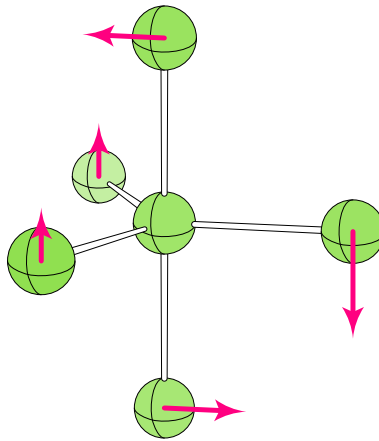


User's Guide of the Program UNIMoVIB

(Ver. 1.2.0)



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1 About UNIMOVIB

UNIMOVIB is a Unified interface for Molecular VIBrational harmonic frequency calculations. The UNIMOVIB programs were originally written by Wenli Zou in FORTRAN 77 during 2014 and 2015 at Southern Methodist University (SMU), Dallas, Texas, within the framework of the LOCALMODE program of the Computational and Theoretical Chemistry Group (CATCO) of SMU. This work was supported by the NSF grants CHE 1152357 and CHE 1464906. Guidance from the late Dr. Dieter Cremer is acknowledged. After being rewritten in Fortran 90 in the spring of 2017, UNIMOVIB has been released as a stand-alone program.

1.1 Features

- Calculate harmonic vibrational frequencies and (optional) I.R. intensities from Hessian, coordinates, and other related data generated by quantum chemistry programs or by the user manually.
Nearly 30 quantum chemistry programs have been supported (see Section 3.1), although some of them may do these calculations much better.
- Analyze point group of geometry and irreducible representations (*irreps.*) of normal modes in full symmetry (for *irreps.*: closed-shell molecule only).
Symmetry analysis is based on the symmetry subroutines from MOPAC 7.1, which is fully in the public domain (at openmopac.net and sourceforge.net).
- Thermochemistry calculation uses the point group in full symmetry, and the results are printed in Gaussian-style (for detailed explanations, see Foresman and Frisch, *Exploring Chemistry With Electronic Structure Methods*, Ed.2, Gaussian Inc., Pittsburgh, PA, **1996**, pp.66).
- Save a MOLDEN file for animation of normal modes.
- Set up isotopic masses, temperature, pressure, scale factor and/or experimental frequencies, and so on.
- Can be used as a third party module for frequency and thermochemistry calculations in a quantum chemistry program, especially when non-Abelian group is not supported therein.

1.2 Symmetry

The point group symmetries supported are listed in Table 1.

Table 1: Available Point Groups.

C_n	$n = 1 \dots 8$
C_s, C_{nv}	$n = 2 \dots 8$
C_i, C_{nh}	$n = 2 \dots 8$
D_n	$n = 2 \dots 8$
D_{nd}	$n = 2 \dots 7$
D_{nh}	$n = 2 \dots 8$
S_n	$n = 4, 6, 8$
Others	$R_3, T, T_d, T_h, O, O_h, I, I_h, C_{\infty v}, D_{\infty h}$

Two point groups will be printed by the program, *i.e.* the molecular point group of “Electronic Wavefunctions” and the molecular point group of “Nuclear & Total Wavefunctions”. The former does not depend on isotopic masses whereas the latter does. The latter point group symmetry should be used to analyze vibrations and do thermochemistry calculations. However, some quantum chemistry programs use the former symmetry by mistake, and therefore the *irreps.* cannot be correctly analyzed and the Gibbs free energy may be wrong. A extreme case is the fullerence $^{12}\text{C}_{59}^{13}\text{C}$, which has I_h symmetry for electronic wavefunctions, but C_1 for nuclear wavefunctions and total wavefunctions. If I_h is used in thermochemistry calculations, the error in the Gibbs free energy will be as large as 2.5 kcal/mol!

2 Compiling and Running

2.1 Compiling the program

```
$ cd $UniMoVib/src  
$ make
```

A Fortran90 compiler is required, which is defined in Makefile.

2.2 Running the program

Double-click the binary program `unimovib.exe`, and type in the name of input file (MS-Windows only),

or

in the terminal, type in

```
$ ./unimovib.exe
```

and then type in the name of input file (if no input file name provided, the default name `job.inp` will be assumed),

or

in the terminal, type in

```
$ ./unimovib.exe -b < input > output
```

In the last way, one can prepare a batch script to perform a series of calculations.

3 Input description

The input options are grouped by namelists, which are ended by \$END. These groups may be given in any order as desired. Before each \$ symbol there should be at least one space.

The input file is case-insensitive except the data file names specified in the \$QCData group (section 3.2).

3.1 \$Contrl group

This group specifies the type of calculation. Keywords:

QCProg="XXXX": XXXX is the name of quantum chemistry program that is used to calculate the molecular Hessian matrix and vibrational frequencies. The following programs are supported:

- Gaussian (default).
- GAMESS (GAMESS-US and GAMESSUS are synonyms).
- Firefly (PCGameess and PC-Gameess are synonyms).
- GAMESS-UK (GAMESSUK is synonym).
- ORCA.
- Molpro.
- QChem (Q-Chem is synonym).
- NWChem.
- CFour.
- Turbomole.
- deMon2k (deMon is synonym).
- PQS.
- OpenMOPAC (MOPAC is synonym). MOPAC 6 and MOPAC 7 are also supported, but the closely related FUJITSU MOPAC 200x (now MO-G in SCIGRESS) has not been tested.
- AMSOL (AMPAC is synonym). AMPAC 2.x is also supported, but the higher versions of AMPAC have not been tested.
- Dalton.
- FHI-AIMS (FHIAIMS and AIMS are synonyms).
- CP2k. The QUICKSTEP module.
- Hyperchem.

- Jaguar. A quantum chemistry module in SCHRÖDINGER SUITE.
- ADF. Only the molecular ADF module was tested.
- MOLDEN, which was generated by a frequency calculation and there should be at least three sections: [FREQ], [FR-COORD], and [FR-NORM-COORD] in it. Through the MOLDEN file, ACES-II, COLUMBUS, DALTON (analytic frequency calculation), MOLCAS, and so on may be supported by the program.
- Crystal. Molecular harmonic frequency is supported and CRYSTAL 14 has been tested.
- Spartan.
- PSI. Only PSI 4 has been tested.
- DMOL3 (DMOL is synonym). Molecular harmonic frequency is supported.
- ACES. Both ACES-II and ACES-III have been tested.
- UniMoVib (ALM is synonym). A plain text file generated by the UNIMOVIB program. See Appendix A.1.

In addition, QCProg="AtomCalc" will do an atomic thermochemistry calculation (see section 3.6).

Isotop: Sets up isotopic masses.

- = 0: (default) all the atomic masses will be read from the data file of frequency calculation; if there was none, then the masses are taken from the library (the most abundant isotopic masses will be used except for several quantum chemistry programs).
- = 1: all the atomic masses will be read from library or the data file of frequency calculation (same as 0), and then the masses of a list of isotopes will be replaced by the values provided after the \$IsoMas group (section 3.3).
- = 2: all the atomic masses are provided after the \$IsoMas group (section 3.3).

IFExp: (.True./.False.) Correct the Hessian matrix using experimental vibrational frequencies which are provided after the \$ExpFrq group (section 3.4). Default: .False.

IFSAVE: (.True./.False.) Save the atomic masses (affected by Isotop), Cartesian coordinates, Hessian matrix (affected by IFExp), and the APT matrix into a plain text data file *.umv. This keyword doesn't work with QCProg="AtomCalc" or "UniMoVib". Default: .False. See Appendix A.1 for the format.

IFMOLDEN: (.True./.False.) Save a MOLDEN file except when QCProg="AtomCalc" or "MOLDEN", which may be opened by the MOLDEN or GABEDIT program to view geometry and normal vibration modes. Default: .False.

IFLOCAL: (.True./.False.) Save a data file for the local mode analysis by LOCALMODES (URL: <https://github.com/catco-smu>). It doesn't work with QCProg="AtomCalc". Default: .False.

3.1.1 Expert keywords

Usually it is not necessary to set up the following keywords in \$Contr1.

QCProg="XYZ": For debugging only.

IFConc: (.True./.False.) Concise output of frequencies or not. Default: .False.

ISyTol = MN: the symmetry tolerance is defined by $M * 10^{N-3}$ where M is always positive and the sign of ISyTol will be assigned to N. So ISyTol = 21 means 0.02 whereas -21 means 0.0002. Default: 10, *i.e.* the tolerance is 0.001.

IFRdNM: (.True./.False.) The normal modes are read directly from the data files specified in the \$QCData group, which may significantly save memory and speed up the calculations since the diagonalization is not performed any more. This keyword doesn't work with Isotop and IExp=.True.. Only QCProg="Gaussian" is supported at present. Default: .False.

IFApprx: (.True./.False.) The force constants (mDyn/Å for stretchings and mDyn·Å/Rad² for angles) and Wilson's B-matrix of internal coordinates will be read from an external data file (specified in the \$QCData group), and then an approximate Hessian matrix will be constructed to calculate vibrational normal frequencies. This keyword doesn't work with IFRdNM=.True.. Default: .False.

3.2 \$QCData group

This group specifies data file(s) enclosed by quotes, where the data (atomic masses, coordinates, APT, and Hessian) are obtained. In general, only one data file is required, which is defined by the option FCHK. However for some programs, multiple data files should be defined separately by the keywords HESS, DDIP, and/or GEOM.

If IFApprx=.True., the data file to construct an approximate Hessian matrix is specified by the keyword BMAT.

- GAUSSIAN: *.fchk. By default, the atomic masses are not included in the fchk file, so the most abundant isotopic masses are assumed, but for GAUSSIAN 09 (and maybe higher versions in the future), one can also use FREQ(SaveNormalModes) instead to save atomic masses automatically. Polarizability derivatives can also be saved by FREQ(Raman) for the calculations of Raman intensity.
- GAMESS: *.dat (by FCHK) + *.out (by GEOM).
- FIREFLY: data file (by FCHK; default name: PUNCH) + *.out (by GEOM).
- GAMESS-UK: *.out file. Use RUNTYPE INFRARED in the frequency calculation to print APT if you are interested in the IR intensities.

- ORCA: *.hess.
- MOLPRO: *.out file. Use the following commands to print Hessian and APT:
`{frequencies,print=1;print,hessian}`
- Q-CHEM: *.fchk. In your Q-CHEM frequency calculation, use GUI=2 to generate the *.fchk file. The atomic masses are not included in the fchk file, so the most abundant isotopic masses are assumed.
- NWCHEM: *.out file (by FCHK) + *.fd_ddipole (by DDIP) + *.hess (by HESS), where DDIP is optional and can be neglected if you are not interested in the IR intensities.
- CFOUR

For analytical frequency (VIB=ANALYTIC): *.out file (by FCHK) + GRD (by GEOM).
For both numerical frequency and analytical frequency: Use the MOLDEN file. However, no IR intensities. See also MOLDEN below.
- TURBOMOLE: *.out file of aoforce (by FCHK; default: aoforce.out) + dipgrad (by DDIP), where DDIP is optional and can be neglected if you are not interested in the IR intensities.
- DEMON2K: *.out file (by FCHK; default: deMon.out). DEMON2K can print Hessian by PRINT DE2.
- PQS: *.coord file (by FCHK) + *.deriv (by DDIP) + *.hess (by HESS), where DDIP is optional and can be neglected if you are not interested in the IR intensities.
- OPENMOPAC: *.out file (by FCHK). Use FORCE DFORCE or FORCE=DFORCE to print Hessian. The averaged isotopic masses are used, which may be not consistent with some very old versions of MOPAC.
- AMSOL: *.out file (by FCHK). Use FORCE DFORCE to print Hessian. The averaged isotopic masses are used, which may be not consistent with some very old versions of AMSOL/AM-PAC.
- DALTON: *.out file (by FCHK). Since DALTON doesn't print nuclear charges and element symbols, the standard element symbols have to be specified in the input file of DALTON's frequency calculation (*ie.*, Mg is okay, but Mg01 and Mgxx don't work).
- FHI-AIMS: masses/*.dat file (by FCHK) + grad_dipole/*.dat (by DDIP) + hessian/*.dat (by HESS), where DDIP is optional and can be neglected if you are not interested in the IR intensities.
- CP2K: the output file of frequency calculation (by FCHK) using the QUICKSTEP module.
- HYPERCHEM: the log file of frequency calculation (by FCHK). HYPERCHEM doesn't generate the log file by default. Before doing a frequency calculation, go to the **File** menu and select **Save log** with print level = 9 to save a log file.
- JAGUAR: the output file of frequency calculation (by FCHK).

- ADF: the formatted TAPE21 or TAPE13 data file (by FCHK). There are some problems in the case of numerical frequency calculation of ADF. See the Known problems section (5).
- MOLDEN: a data file (by FCHK), which contains [FREQ], [FR-COORD], and [FR-NORM-COORD] sections. See the Known problems section (5).
- CRYSTAL: the output file from molecular harmonic frequency calculation (by FCHK).
- SPARTAN: the *.smol archive file (by FCHK). The most abundant isotopic masses are assumed.
- PSI: the output file (by FCHK). In your PSI 4 frequency calculation, use `set print 3` to print Hessian matrix.
- DMOL3: the output file (by FCHK).
- ACES: the output file (by FCHK). But using the MOLDEN file can achieve higher accuracy. See the Known problems section (5).
- UNIMOVIB: an ASCII data file (by FCHK), which was generated by UNIMOVIB with the option `IFSAVE=.TRUE.`, or created manually (see Appendix A.1).
- XYZ: a standard XYZ data file (by FCHK). For debugging only.

See the examples in `$UniMoVib/test`.

3.3 \$IsoMas group

This group is required when `Isotop = 1` or `2`. There is no option in this group. After this group, the isotopic masses are provided.

If `Isotop = 1`, one atom per line, including the atom index and its mass. The program will read isotopic masses until a blank line or the end is encountered. For example,

```
$IsoMas $End
2 15.99491
4 2.01410
```

It means that the masses of the second and the forth atoms are 15.99491 and 2.01410, respectively.

If `Isotop = 2`, all the N atomic masses are defined in free format. For example,

```
$IsoMas $End
12.0 1.0 1.0
1.0
1.0
```

5 atomic masses are defined for CH₄ in the above example.

3.4 \$ExpFrq group

This group is required when IFExp=. True. There is only one option MODE in this group. After this group, the experimental vibrational frequencies are provided.

If MODE = 0 (default), all the N_{Vib} vibrational frequency values, which MUST have been correctly ordered according to the calculated frequencies, are defined in free format. For example,

```
$ExpFrq $End
835.0248 835.3904 926.0930 926.2148
2160.9759
```

If MODE = 1, a list of theoretical frequencies will be replaced by the provided experimental ones. One frequency per line, including the frequency index and its experimental value. The program will read experimental frequencies until a blank line or the end is encountered. For example,

```
$ExpFrq MODE=1 $End
3 926.0930
5 2160.9759
```

3.5 \$Thermo group

This group controls the thermochemistry calculation. Keywords:

Eel: total energy taken from quantum chemistry calculation (in Hartree). Default: 0.

NDeg: degeneracy of the (spin-orbit) electronic state, which affects the entropy and Gibbs free energy. Default: 1.

Temp: temperature (in K). Default: 298.15. If Temp < 0, a series of additional temperatures will also be provided after this group.

Press: pressure (in atm). Default: 1.0. If Press < 0, a series of additional pressures will also be provided after this group.

Scale: frequency scale factor. Default: 1.0. Experimental frequencies defined in the \$ExpFrq group will not be scaled.

PG: specify the name of point group to calculate rotational entropy. It may affect the entropy and Gibbs free energy, so the correct point group name must be provided.

= 0: (default) 2.

= 1: use the isotope independent point group. If isotope leads to lower symmetry, this option may reproduce the results of other quantum chemistry programs, but unfortunately this is not correct.

= 2: use the isotope dependent point group.

= "XXXX": specify the name of point group, which is useful for the high symmetry not supported by the program, for example, "D10h". Don't forget the quotes.

Gibbs free energy may be affected by all of the above keywords except Ee1.

If Temp < 0 or Press < 0, a list of additional temperatures or pressures will be provided. One value per line. The program will read the values until a blank line or the end is encountered. For example,

```
$Thermo Temp=-1 $End
100
200
400
```

In addition to the default temperature 298.15 K, thermochemistry calculations will also be performed at 100, 200, and 400 K in the above example. If both Temp < 0 and Press < 0, two values per line should be provided (a temperature, then a pressure). For example,

```
$Thermo Temp=-1 Press=-1 $End
100 0.5
200 -1
-1 2.0
```

Negative values in the additional data mean the default temperature (298.15 K) or pressure (1.0 atm).

3.6 Atomic thermochemistry calculation

Atomic thermochemistry data can also be calculated using the UNIMOVIB program, which are useful to study some atom related chemical reactions, for example, $CH_3 + H_2 \rightarrow CH_4 + H$. The atomic thermochemistry calculation does not require any data and files from quantum chemistry calculations except the optional total energy. Three groups of keywords may be provided:

\$Contr1 group (section 3.1): qcprog="atomcalc" should be specified.

\$IsoMas group (section 3.3): the atomic mass should be specified (Isotop in the \$Contr1 group is always 2).

\$Thermo group (section 3.5): Ee1, NDeg, Temp, and Press can be specified, which are optional.

The other namelists and keywords do not make sense and will be ignored. See Example 4.1.

4 Examples

4.1 Atomic thermochemistry calculation

example

```
1 Atomic thermochemistry calculation (Ne atom)
2 The total energy was calculated at the HF/STO-3G level
3
4 $contrl
5   qcprog="atomcalc"
6 $end
7
8 $Thermo
9   Eel=-127.8038245 Temp=500 Press=10
10 $end
11
12 $IsoMas $End
13 19.99244
```

4.2 Frequency calculation by GAUSSIAN

example

```
1 a test job
2
3 $contrl
4   qcprog="gaussian"
5 $end
6
7 $qcdata
8   fchk="xef6.fchk"
9 $end
```

4.3 Frequency calculation by MOLPRO

MOLPRO cannot handle non-Abelian point group symmetries, like T_d in CH_4 . Using UNIMOVIB, you can get *irreps.* of normal vibrational modes in full symmetry.

example

```
1 a test job
2
3 $contrl
4   qcprog="molpro"
5 $end
6
7 $qcdata
8   fchk="ch4.out"
9 $end
```

4.4 Calculation of the “experimental” frequencies of HDO

One can estimate frequencies of HDO from experimental frequencies of H_2O .

example

```
1 Step 1.  
2 Save data file using experimental frequencies of H2O.  
3 The normal modes should be calculated at high level of theory.
```

```
4  
5 $contrl  
6   qcprog="cfour"  
7   ifsave=.true.  
8   ifexp=.true.  
9 $end  
10  
11 $qcdata  
12   fchk="h2o.out"  
13   geom="GRD"  
14 $end  
15  
16 $expfrq mode=1 $end  
17 1   1595  
18 2   3657  
19 3   3756   B2
```

example

```
1 Step 2.  
2 Calculate "experimental" frequencies of HDO using the experimental frequencies of H2O.  
3 CCSD(T)/cc-pVTZ frequencies:      1463  2828  3895 cm-1  
4 "experimental" frequencies:      1398  2692  3708 cm-1  
5 real experimental frequencies:    1402  2727  3707 cm-1
```

```
6  
7 $contrl  
8   qcprog="unimovib"  
9   isotop=1  
10 $end  
11  
12 $qcdata  
13   fchk="step1.umv"  
14 $end  
15  
16 $IsoMas $End  
17 2  2.01410
```

5 Known problems

- Open-shell molecule.

Because of (pseudo-)Jahn-Teller effects, maybe the *irreps.* cannot be recognized by the program.

- ADF

For a numerical frequency calculation (for example, by two-component ZORA): if symmetry is used by ADF, and if there are symmetry-equivalent atoms, the IR intensities cannot be calculated correctly since some elements in the APT matrix are missing. The correct values can be obtained from ADF output if you are interested in the IR intensities.

- MOLDEN

1. If there are imaginary frequencies, some program may print positive frequency values by mistake (for example, CFour), then the results will be wrong. So you have to check the imaginary frequencies in the MOLDEN file, and correct them manually if the negative sign is missing.
2. Since there is no isotopic mass information in the MOLDEN file, the most abundant isotopic masses are assumed. If this is not true, however, the results will be totally wrong. So you have to use the most abundant isotopic masses in your frequency calculation to generate a MOLDEN file.

- ACES

Since there is no isotopic mass information in ACES output, the most abundant isotopic masses are assumed. If this is not true, however, the results will be totally wrong. So you have to use the most abundant isotopic masses in your frequency calculation (this is default in ACES) to generate a ACES output file.

A Appendix

A.1 Format of the UniMoVib data file

The UniMoVib data file is an ASCII one in free format.

Format(Ver.1.0.1 2017.10.15)

```
(One title line)
NATM
  (An positive integer)
AMASS
  (NATM number of atomic masses)
ZA
  (NATM number of nuclear charge numbers)
XYZ
  (3*NATM elements of Cartesian coordinates in a.u.;
  Use XYZANG instead if in Angstrom)
FFX
  (3*NATM*3*NATM elements of Hessian matrix;
  Use FFXLT instead for L.T. matrix)
APT
  (3*3*NATM elements of APT data;
  Use NOAPT instead if no APT data provided)
DPR
  (6*3*NATM elements of polarizability derivatives;
  Use DPRSQ instead if in the form of 9*3*NATM;
  Use NODPR instead if no DPR data provided)
```

At present DPR data and Raman intensities are supported only for the .fchk file generated by Gaussian.

A.2 For developers: interface to other QC programs

To support other QC programs which can do harmonic frequency calculation, two interface subroutines should be provided in *interface.f90*.

1. Read or count the number of atoms (NAtm). Dummy atoms are not included. This subroutine is called in subroutine RdNAtm1. Example:

```
1  ! -----
2  ! Read NAtm from XXXX output
3  ! -----
4  subroutine RdNAtmXXXX(ifchk,NAtm,tag,ctmp)
5  implicit real(kind=8) (a-h,o-z)
6  character*100 :: ctmp
7  character*100 :: tag
8  (...)
9  return
10 end
```

2. Read in Cartesian coordinates in *a.u.* (XYZ), atomic nuclear charge number (ZA), atomic or isotopic masses in *a.u.* (AMass; optional), Cartesian force constant matrix in *a.u.* (FFx; a mass-unweighted square matrix), dipole moment gradient (*i.e.* atomic polar tensor; APT) in *a.u.* (APT; optional), and polarizability derivatives in *a.u.* (DPol; optional). This subroutine is called in subroutine RdData1. Example:

```
1  ! -----
2  ! Read data from XXXX output
3  ! -----
4  subroutine RdXXXX(ifchk,tag,ctmp,NAtm,AMass,ZA,XYZ,FFx,APT,DPol)
5  implicit real(kind=8) (a-h,o-z)
6  real(kind=8) :: AMass(NAtm),ZA(NAtm),XYZ(3,NAtm),FFx(3*NAtm,3*NAtm), &
7     APT(3,3*NAtm),DPol(6,3*NAtm)
8  character*100 :: ctmp
9  character*100 :: tag
10 (...)
11 return
12 end
```

3. In addition, add the program name as a new option of QCProg in subroutine RdContrl in *rw.f90*.
4. At last, do not forget to update this manual.

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