# RCD Program – Manual

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# Compilation

Use ./compile.sh [precision] [MPI] [DEBUG]. As an end user, you will most likely need only the first one.

Compile normally (double precision):

./compile.sh OR ./compile.sh 8

Compile for single precision:

./compile.sh 4

Compile for quadruple precision:

./compile.sh 16

Compile for debugging

./compile.sh 8 no DEBUG

Compile for MPI (not implemented yet):

./compile.sh 8 MPI

Compile for MPI and Debugging ():

./compile.sh 8 MPI DEBUG

# Usage

rcd.exe [Gaussian output file OR molecular parameter file] [job file] ([temperature in Kelvin] [pressure HWHM in MHz] [.cat molecular tag])

The program can read molecular quantities (parameters) either from a Gaussian output file or a dedicated molecular parameter file (.rcdmol). The job file specifies the calculation parameters. You can also put in temperature in units of Kelvin and the pressure (Lorentzian) HWHM in MHz.

## Gaussian output file

The program expects these parameters in the Gaussian output: rotational constants, input orientation (geometry), electric dipole moment, g-tensor (referred to as GIAO tensor), charge, SR: spin-rotation interaction tensor. All of these can be calculated by the following keywords in Gaussian NMR(Susceptibility) Output(Pickett). Example:

%chk=XX.chk

%mem=4GB

%nproc=4

#B972/6-311++g\*\* NMR(Susceptibility) Output(Pickett)

iop(2/11=1) 6d 10f nosymm

In our program, the molecular geometry is brought the centre of mass coordinate system. All the molecular parameters are also moved into this system by equations:

[rovnice]

Then moment of inertia tensor is calculated and diagonalized (ie. we calculate the eigenvalues). The eigenvector matrix (rotation matrix in this case) is applied to every molecular parameter. These will be the final molecular parameters used for RCD calculations.

In case you are using a Gaussian output file, simply call the RCD program by:

./rcd.exe /path/to/outfile.out /path/to/jobfile.par

If you want to put in temperature, pressure HWHM and JPL molecular species tag, you would simply do:

./rcd.exe /path/to/outfile.out /path/to/jobfile.par 2 0.5 3003

## Molecular parameter file (.rcdmol)

There are several keywords implemented. Some keywords have options which can also have values. The options are formatted as in a Gaussian input file. For example Keyword(Units=MHz,Hello). The input is case-insensitive.

In case you are using the .rcdmol file, call RCD by:

./rcd.exe /path/to/outfile.rcdmol /path/to/jobfile.par

If you want to put in temperature, pressure HWHM and JPL molecular species tag, you would simply do:

./rcd.exe /path/to/outfile.out /path/to/jobfile.par 2 0.5 3003

### Keywords:

* MASS

The molecular mass in units of amu. Used for the approximate partition function.

* SYMM

The symmetry number of the molecule. Used for the approximate partition function. For example, symmetry number of C2v point group is 2.

* COORDS

The molecular geometry in free format: element x y z

* ABC(Units=GHz)

Rotational constants, by default in GHz. Units value can be substituted with: MHz, cm-1, nm, g.cm2, MC or amu.a2

* DIP(Units=Debye[,REP\_SWITCH,CM\_SHIFT,ROT])

Permanent electric dipole moment, by default in debye, can be substituted with C.m or au.

* G\_TEN([REP\_SWITCH,CM\_SHIFT,ROT])

Molecular g-tensor (GIAO tensor).

* SR\_TEN(Units=GHz[,REP\_SWITCH,CM\_SHIFT,ROT])

Spin-rotation interaction tensor, by default in GHz, can be substituted with GHz. Centre of mass shift for this quantity is not implemented.

### Used options:

* Units

Specify the units of the current molecular quantity (parameter).

* REP\_SWITCH

Switch the axis of THIS quantity according to the molecular representation specified in the .par file. With this option specified, the components correspond to molecular principal axes *a,b,c* and then they are identified with the *x,y,z* molecular axes (switched around) according to the chosen representation (in Arabic numerals 1r,2r,3r,1l,2l,3l). Without this option, the components are assumed to correspond to *x,y,z* and no further operations are done.

* CM\_SHIFT

Shifts this quantity to the centre of mass. Requires the molecular geometry (COORDS) to be specified.

* ROT

Rotates this quantity to the diagonalized moment of inertia system. Requires the molecular geometry (COORDS) to be specified.

## Job file (.par)

Comments are denoted by an exclamation point !. The forward slash signifies several options, only one option can be chosen.

### Keywords:

* CALC\_TYPE

RR/SR

RR stands for rigid rotor (no mixing of angular momenta), SR stands for spin-rotation (**J = N + S** coupling scheme, ie. molecular rotation with one free electron)

* PARTFUN

APPROX/EXACT/number

Partition function. Can be approximated, summed through nearly all transitions or supplied by a decimal point number.

* TEMP

number

Temperature in Kelvin. If the temperature is supplied in the argument, this keyword is ignored.

* GAUSSIAN\_REPAXES

t/f

Identify the components of molecular quantities with *x,y,z* axes. This is recommended to stay *t*.

* HWHM

number

Pressure (Lorentzian) HWHM.

* GRAIN

Number

Distance between two x-points in the spectrum. Note that halving this increases the spectrum file two times!

* MW\_SPECTRUM

t/f

Draw the normal rotational spectrum. Will have the same file size as the RCD spectrum.

* SPECTRAL\_SHAPE

GAU/LOR/VOI

Specify the spectral profile. Gaussian (Doppler broadening), Lorentzian (pressure broadening) or Voigt (Doppler and pressure broadening, NOT IMPLEMENTED YET).

* MOLPAR\_ONLY

t/f

Do not calculate RCD and spectra, only show the final molecular parameters used for RCD calculation.

* J\_START

Non-negative integer

Starting quantum number J.

* J\_END

Non-negative integer

Ending quantum number J.

* REP

1r/2r/3r/1l/2l/3l

Rigid rotor representation. This identifies the principal molecular axes *a,b,c* with molecular axes *x,y,z.*

* SKIP\_TRANS\_NOTINFREQ

t/f

Skip RCD and spectral calculation of transitions not in FREQ\_RANGE.

* SKIP\_TRANS\_LOWPOP

t/f

Skip RCD and spectral calculation of transitions whose population is below LOWPOP\_TOLERANCE.

* LOWPOP\_TOLERANCE

number

Tolerance for low populations.

* FREQ\_RANGE

number

Frequency range used for RCD calculation (if SKIP\_TRANS\_NOTINFREQ is true) and spectral calculation.

* SPIN\_MULT

Non-negative integer

Electron spin multiplicity. Setting this to 2 specifies S=1/2. Used only in spin-rotation calculation. Higher numbers are not yet supported.

* MIN\_DIPSTR

number

Minimum dipole strength shown in the .trn file or spectrum if filtering is enabled. In debye2.

* MIN\_ROTSTR

number

Minimum rotational strength shown in the .trn file or spectrum if filtering is enabled. In debye2.

* MIN\_KUHN

number

Minimum dissymmetry parameter shown in the .trn file if filtering is enabled.

* SPR\_UNITS

cm-1/l.mol-1.cm-1/nm2.mhz

Intensity units in spectrum

* ORDER\_BY

FREQ/QN

Order either by frequency or quantum numbers. Ascending only.

* .molp

Flags (for example 0101110, each digit represents different option, only 0 or 1)

1 – Write this file

* .trn

Flags

1 – Write this file

2 – Show JPL intensity of this transition, uses temperature and partition function

3 – Not in use

4 – Output in decimal point format

5 – Show the top (column description) row

6 – Do not write the transitions with dipole strength, rotational strength or Kuhn parameter lower than MIN\_DIPSTR, MIN\_ROTSTR and MIN\_KUHN

7 – Procedurally write to this file while an RCD calculation is going, overall slower calculation.

8 – Show transitions that have zero dipole strengths or rotational strengths

9 – Differentiate the file naming by spin multiplicity

* .spr

Flags

1 – Write this file

2 – Do not write transitions to the spectrum with dipole strength, rotational strength or Kuhn parameter lower than MIN\_DIPSTR, MIN\_ROTSTR and MIN\_KUHN

3 – Include temperature effects. If 0 the ground state is assumed to have a population of 1 and excited of 0

4 – Differentiate the file naming by temperature and spin multiplicity

* .cat

Flags

1 – Write this file

# Output

## .trn

List of transitions. The columns stand for

1st – Transitions frequency in GHz

2nd – Dipole strength (D) in Debye2

3rd – Rotational strength (R) in Debye2

4th – Kuhn’s dissymmetry parameter (gK, 4R/D)

In case of rigid rotor (no spin interaction):

5th – 7th Excited state quantum numbers J, Ka, Kc

8th – 10th Ground state quantum numbers J, Ka, Kc

In case of spin-rotation interaction:

5th – 8th Excited state quantum numbers N, Ka, Kc, J

9th – 12th Ground state quantum numbers N, Ka, Kc, J

If option #2 for *.trn* is turned on:

Last column – Line intensity in JPL “format”, this is dependent on temperature and partition function

## .spr or .sprMW

RCD (or normal rotational) spectrum file, 1st column is frequency, 2nd is intensity in units chosen in the job file.

## .molp

Molecular parameters as how they are read from Gaussian and as how they are converted into the molecular axes frame.

## .cat

Similar to .trn file but in SPCAT format. In case of RCD, the sign of the intensity is denoted at the last (80th ?) character by plus (+) or minus (-). The Fortran format now is:

(F13.4, F8.4, F8.4, I2, F10.4, I3, I7, I4, 6I2, 6I2,A1)

# References