

Documentation for DPFIT and DPCAT

These programs which use the subroutine DPI.C are used to calculate doublet pi energies and intensities with one nuclear spin using a Hund's case (a).

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Quantum numbers which are used in the files can be given in several formats:

Linear Pi States:					[Q]
$J + 1/2$	$\Omega + 1/2$	λ	v	F	[19]
$J + 1/2$	$\Omega + 1/2$	λ	v	-	[19]
$J + 1/2$	$\Omega + 1/2$	λ	F	-	[8]
$J + 1/2$	$\Omega + 1/2$	λ	-	-	[8]

The field QNFMT in *cat* file can be regarded as having 3 sub-fields: QFMT = Q*100 + H*10 + NQN, in which NQN is the number of quanta per state, H is a binary code the existence of half integer quanta for F, and Q is the number in square brackets in the table above. The least significant bit of H refers to the F quantum number and is 1 if F is half integer. The quantum number λ has a sign for the inversion parity, for e levels the parity is $(-1)^{J+1/2}$, while for f levels the parity is opposite.

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FORMAT of the *lin* file:

line 1-NLINE [12I3,freeform]: QN,FREQ,ERR,WT

QN = 12 integer field of quantum numbers. Interpreted in a multiple I3 format as the quantum numbers for the line (upper quanta first, followed immediately by lower quanta). Unused fields can be used for annotation. The entire field is printed in file.fit

FREQ = frequency in MHz or wavenumbers

ERR = experimental error. Minus sign means that the frequency and error are in units of wavenumbers. FREQ and ERR will be converted internally to units of MHz.

WT = relative weight of line within a blend (normalized to unity by program)

notes: If an end-of-file is encountered before all the lines are read in, NLINE is set to the number read to that point. If successive lines have the same frequency, the lines will be treated as a blend and derivatives will be averaged using WT/ERR. Any lines with format errors will be ignored.

The freeform input begins in column 37 and extends to the end of the line. See the notes at the end of the next section for more on the freeform input.

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FORMAT of the .par file and .var files:

line 1: title

line 2 [freeform]: NPAR, NLINE, NITR, NXPAR, THRESH , ERRTST,FRAC, CAL

NPAR = maximum number of parameters

NLINE = maximum number of lines

NITR = maximum number of iterations

NXPAR = number of parameters to exclude from end of list when fitting special lines (see notes)

THRESH = initial Marquardt-Levenburg parameter

ERRTST = maximum [(obs-calc)/error]

FRAC = fractional importance of variance

CAL = scaling for infrared line frequencies (only NPAR used by CALCAT)

Option information on line 3: SPIND, NVIB

SPIND = degeneracy of nuclear spin

NVIB = number of vibrations

Parameter lines [freeform]: IDPAR, PAR, ERPAR / LABEL

where IDPAR is a parameter identifier, PAR is the parameter value, ERPAR is the parameter uncertainty, LABEL is a parameter label (10 characters are used) that is delimited by /. If the sign of IDPAR is negative, DPFIT constrains the ratio of this parameter to the previous parameter to a fixed value during the fit.

If $NVIB > 1$, $IDPAR = IV + 100 * IDPAR0$, where IV is the vibrational or electronic quantum number. If $NVIB = 1$, $IDPAR = IDPAR0$. There are no matrix elements defined connecting the vibrational states.

PARAMETER identifiers (IDPAR0) are:

IDPAR0	Parameter
1	A
2	A_J
3	A_H
4	$B + q / 2$
5	D
6	H
7	p
8	q
9	p_D
10	q_D
11	$\chi_1 = 0.5 * [a - (b+c) / 2]$
12	$\chi_2 = d / 2$
13	$\chi_3 = 1.5 * [a + (b+c) / 2]$
14	χ_4
15	χ_5
16	χ_6
17	χ_7
18	χ_8
19	χ_9

20	$\zeta_1 = \text{eq}Q_1 \text{ for } \Omega = 1/2$
21	$\zeta_2 = \text{eq}Q_1 \text{ for } \Omega = 3/2$
22	$\zeta_3 = -eQq_2 / 2$
23	ζ_4
24	ζ_5
25	ζ_6
26	ζ_7
27	γ

line (n+1)-end [8F10.6]: ((V(i,j),j=1,i) ,i=1,NPAR)

V = Choleski decomposition of the correlation matrix, optional for file.par
(The index *i* is the index for the parameter.)

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FORMAT for the *int* file:

line 1: title

line 2 [freeform]: FLAGS,TAG,QROT,FBGN,FEND,STR0,STR1,FQLIM,TEMP

FLAGS = IRFLG*1000+OUTFLG*100+STRFLG*10+EGYFLG

IRFLG = 1 if constants are in wavenumbers

IRFLG = 0 if constants are in MHz

OUTFLG = 0 for short form *file.out*

STRFLG = 1 to enable *file.str* output

STRFLG = 2 to enable *file.str* output and print separate entries for each dipole

EGYFLG 0 to enable *file.egy* energy listing

EGYFLG= 2,4 to enable *file.egy* derivative listing

EGYFLG = 3,4 to enable *file.egy* eigenvector listing

EGYFLG 4 to dump Hamiltonian with no diagonalization

TAG = catalog species tag (integer)

QROT = partition function for TEMP

FBGN = beginning integer F quantum (round up)

FEND = ending integer F quantum (round up)

STR0,STR1 = log strength cutoffs

FQLIM = frequency limit in GHz

TEMP = temperature for intensity calculation in degrees K (default is 300K)

line 3-end [freeform]: IDIP,DIPOLE

IDIP is coded in decimal digit form according to the format V2*100+ V1

DIPOLE = dipole value

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FORMAT of *cat* output file:

[F13.4,2F8.4,I2,F10.4,I3,I7,I4,12I2]:

FREQ,ERR,LGINT,DR,ELO,GUP,TAG,QNFMT,QN

FREQ = Frequency of the line

ERR = Estimated or experimental error (999.9999 indicates error is larger)

LGINT = Base 10 logarithm of the integrated intensity in units of nm²
MHz

DR = Degrees of freedom in the rotational partition function (0 for atoms,
2 for linear molecules, and 3 for nonlinear molecules)

ELO = Lower state energy in wavenumbers

GUP = Upper state degeneracy

TAG = Species tag or molecular identifier. A negative value flags that the
line frequency has been measured in the laboratory. The absolute value of

TAG is then the species tag (as given in line 2 of file.int above) and ERR is the reported experimental error.

QNFMT = Identifies the format of the quantum numbers given in the field QN.

QN(12)= Quantum numbers coded according to QNFMT. Upper state quanta start in character 1. Lower state quanta start in character 14. Unused quanta are blank, quanta whose magnitude is larger than 99 or smaller than -9 are shown with alphabetic characters or **. Quanta between -10 and -19 are shown as a0 through a9. Similarly, -20 is b0, etc., up to -259, which is shown as z9. Quanta between 100 and 109 are shown as A0 through A9. Similarly, 110 is B0, etc., up to 359, which is shown as Z9.

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Format of *str* output file:

[F15.4,E15.6,I5,1X,24A,I5]: FREQ,DIPOLE,QNFMT,QN,ITEM

FREQ = Frequency of the line

DIPOLE= Reduced matrix element of the transition dipole

QNFMT = Identifies the format of the quantum numbers given in the field QN.

QN(12) = Quantum numbers coded according to QNFMT. Upper state quanta start in character 1. Lower state quanta start in character 14. Unused quanta are blank, quanta whose magnitude is larger than 99 or smaller than -9 are shown with alphabetic characters or **. Quanta between -10 and -19 are shown as a0 through a9. Similarly, -20 is b0, etc., up to -259, which is shown as z9. Quanta between 100 and 109 are shown as A0 through A9. Similarly, 110 is B0, etc., up to 359, which is shown as Z9.

ITEM = identifies number of dipole

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Format of *egy* output file:

energy output [2I5,3F18.6,6I3]: IBLK,INDX,EGY,PMIX,ERR,QN

IBLK = Internal Hamiltonian block number

INDX = Internal index Hamiltonian block

EGY = Energy in wavenumbers

ERR = Expected error of the energy in wavenumbers

PMIX = mixing coefficient

QN(6)= Quantum numbers for the state

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