

Manual for “DVR3D: a program suite for the calculation of rotation-vibration spectra of triatomic molecules”

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1 Program use: Potential, dipole and property subroutines

DVR3DRJZ requires the user to provide the appropriate potential energy surface as a subroutine using the structure:

SUBROUTINE POTV(V,R1,R2,XCOS)

must be supplied. POTV returns the potential V in Hartree for an arbitrary point given by $R1 = r_1$, $R2 = r_2$ (both in Bohr) and $XCOS = \cos \theta$.

DVR3DRJZ includes COMMON /MASS/ XMASS(3),G1,G2,XMASSR(3) where XMASS contains the (vibrational) masses in atomic mass units, $G1=g_1$, $G2=g_2$ and XMASSR contains the rotational masses also in atomic mass units. This enables users to write flexible potential subroutines which allow for changes in coordinates or isotopic substitution.

DIPOLE requires a subroutine defining the dipole surfaces.

SUBROUTINE DIPD(DIPC,R1,R2,XCOS,NU)

must be supplied. DIPD returns the NU^{th} component of the dipole in atomic units ($1 \text{ a.u.} = 2.5417662 \text{ Debye}$) at point $R1 = r_1$, $R2 = r_2$ (both in Bohr) and $XCOS = \cos \theta$ where $NU = 0$ corresponds to μ_z and $NU = 1$ μ_x .

DIPOLE3 includes COMMON /MASS/ XMASS(3),G1,G2,ZEMBDED,ZBISC where XMASS contains the (vibrational) masses, $G1=g_1$, $G2=g_2$, ZEMBDED is the axis embedding parameter defined below and ZBISC=.TRUE. for the bisector embedding case ($IDIA=-2$, $JROT > 0$ and $ZPERP = .FALSE.$) and

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.FALSE. otherwise. This enables users to write dipole subroutines which allow for changes in coordinates, embeddings or isotopic substitution.

XPECT3 requires a subroutine defining the properties for which expectation values are requested.

SUBROUTINE PROPS(PROP,R1,R2,XCOS,N)

must be supplied. PROPS returns the N properties required in array PROP for an arbitrary point given by $R1 = r_1$, $R2 = r_2$ (both in Bohr) and $XCOS = \cos \theta$.

Like DIPOLE3, XPECT3 includes COMMON /MASS/ XMASS(3),G1,G2,ZEMBED,ZBISC where the variables are as defined above.

2 Input for DVR3DRJZ

DVR3DRJZ requires 9 lines of user input for all runs. Lines giving data not required or for which the defaults [given below in parenthesis] are sufficient should be left blank.

Line 1: NAMELIST /PRT/

ZPHAM[F] = T requests printing of the Hamiltonian matrix.
 ZPRAD[F] = T requests printing of the radial matrix elements.
 ZP1D [F] = T requests printing of the results of 1D calculations.
 ZP2D [F] = T requests printing of the results of 2D calculations.
 ZPMIN[F] = T requests only minimal printing.
 ZPVEC[F] = T requests printing of the eigenvectors.
 ZLMAT[F] = T requests printing of the L -matrix.
 ZCUT[F] = T final dimension selected using an energy cut-off given by EMAX2.
 = F final dimension determined by MAX3D (MAX3D2).
 ZROT[T] = T DVR3DRJZ to perform first step in a two-step variational calculation.
 = F Rotational excitation calculation with Coriolis coupling neglected.
 ZPERP[F] = F z axis embedded in plane.
 = T z axis embedded perpendicular to molecular plane.
 ZEMBED[T] Used only if $J > 0$, ZBISC = F and ZPERP = F,.
 = T z axis embedded along r_2 ;
 = F z axis embedded along r_1 .
 ZLIN [F] = T forces suppression of functions at last DVR point
 (ZBISC = T or ZPERP=T only).
 ZMORS1[T] = T use Morse oscillator-like functions for r_1 coordinate;
 = F use spherical oscillator functions (IDIA > 0 only).
 ZMORS2[T] = T use Morse oscillator-like functions for r_2 coordinate;
 = F use spherical oscillator functions (IDIA > 0 only).
 ZLADD[T] = T NALF kept constant as k increases,
 = F NALF decreases with k (=f has a bug),
 (used if ZROT = T only).

ZTWOD[F] = T perform 2D calculation only at specified grid point.
 ZVEC[F] = T store the eigenvectors from all the parts of the calculation (1D,2D and 3D) on stream IOUT2. Further information relating to this (arrays IV1 and IV2) is stored on stream IOUT1.
 ZALL[F] = T requests **no** truncation of the intermediate solution.
 ZTHETA[T] = T let θ be first in the order of solution;
 = F let θ be last in the order of solution;
 (used if IDIA > -2 only).
 ZR2R1[T] = T let r_2 come before r_1 in the order of solution;
 = F let r_1 come before r_2 in the order of solution;
 (used if IDIA > -2 only).
 ZTRAN[F] = T perform the transformation of the solution coefficients to the expression for the wavefunction amplitudes at the grid points, eq (29).
 Store the data on stream IWAVE.
 ZTRAN = T automatically sets ZVEC = T if IDIA > -2.
 ZQUAD2[T] = T use the DVR quadrature approximation for the integrals of the r_2^{-2} matrix, and hence make its DVR transformation diagonal.
 = F evaluate the r_2^{-2} integrals fully and perform the DVR transformation on them, only implemented for ZMORS2 = F and for ZTHETA = T.
 ZDIAG[T] = F do not do final diagonalisation, instead the final Hamiltonian matrix is written on units IDIAG1[20] and IDIAG2[21].
 For further details see the source code.
 ZPFUN[F] = T eigenvalues concatenated on stream ILEV.
 Warning, the first eigenvalues on this file must be for JROT=0, IPAR=0.
 ZPSEG[F] = T Activates the *recordtype=segmented* option in the unformatted write/read records in the program.
 ILEV[14] output stream for eigenvalue data (formatted).
 IEIGS1[7] stream for eigenvalues of the 1D solutions.
 IVECS1[3] stream for eigenvectors of the 1D solutions.
 IEIGS2[2] stream for eigenvalues of the 2D solutions.
 IVECS2[4] stream for eigenvectors of the 2D solutions.
 IVINT[17] scratch file used for storing intermediate vectors in building the final Hamiltonian.
 IBAND[15] scratch file used for storing bands of the final Hamiltonian.
 INTVEC[16] scratch file for intermediate storage of the 2D vectors.
 IOUT1[24] stream for arrays IV1 and IV2, which record the sizes of the truncated vectors.
 Used when ZVEC = T.
 IOUT2[25] stream for the 1D, 2D and 3D vectors for use when ZVEC = T.
 IWAVE[26] stores the wavefunction amplitudes at the grid points when ZTRAN = T.

Line 2: NCOORD (I5)

NCOORD[3] the number of vibrational coordinates of the problem:
 = 2 for an atom – rigid diatom system,
 = 3 for a full triatomic.

**Line 3: NPNT2,JROT,NEVAL,NALF,MAX2D,MAX3D,IDIA,
KMIN,NPNT1,IPAR,MAX3D2(11I5)**

NPNT2 number of DVR points in r_2 from Gauss-(associated) Laguerre quadrature.
JROT[0] total angular momentum quantum number of the system, J .
NEVAL[10] number of eigenvalues and eigenvectors required.
NALF number of DVR points in θ from Gauss-(associated) Legendre quadrature.
MAX2D maximum dimension of the largest intermediate 2D Hamiltonian,
 (ignored if IDIA = -2).
MAX3D maximum dimension of the final Hamiltonian.
 If ZCUT = F, it is the actual number of functions selected,
 if ZCUT = T, MAX3D must be \geq than the number of functions selected
 using EMAX2.
IDIA = 1 for scattering coordinates with a heteronuclear diatomic,
 = 2 for scattering coordinates with a homonuclear diatomic.
 = -1 for Radau coordinates with a heteronuclear diatomic,
 = -2 for Radau coordinates with a homonuclear diatomic.
KMIN[0] = k for JROT > 0 and ZROT = F,
 = (1 - p) for JROT > 0 and ZROT = T.
 Note:
 For IDIA > 0, KMIN must be 1 in DVR3DRJ if KMIN = 2 in ROTLEV3.
 For ZBISC = T, setting KMIN=2 performs $p = 0$ and 1 calculations.
 For ZPERP = T and ZROT = T, use KMIN = 1.
NPNT1 number of DVR points in r_1 from Gauss-(associated) Laguerre quadrature,
 (ignored if IDIA = -2).
IPAR[0] parity of basis for the AB₂ molecule (ie | IDIA | = 2) case:
 IPAR=0 for even parity and = 1 for odd.
MAX3D2[MAX3D] maximum dimension of odd parity final Hamiltonians.
 (IDIA = -2, ZROT=T only).

Line 4: TITLE (9A8)

A 72 character title.

Line 5: FIXCOS (F20.0)

If ZTWOD = T, FIXCOS is the fixed value of $\cos \theta$ for the run.

If ZTWOD = F, this line is read but ignored.

Line 6: (XMASS(I),I=1,3) (3F20.0)

XMASS(I) contains the (vibrational) mass of atom I in atomic mass units.

Line 7: (XMASSR(I),I=1,3) (3F20.0)

XMASSR(I) contains the rotational mass of atom I in atomic mass units.

If XMASSR(1) is not set, XMASSR is set equal to XMASS.

Line 8: EMAX1, EMAX2 (2F20.0)

EMAX1 is the first cut-off energy in cm^{-1} with the same energy zero as the potential. This determines the truncation of the 1D solutions ($\text{IDIA} > -2$ only).
 EMAX2 is the second cut-off energy in cm^{-1} with the same energy zero as the potential. This controls the truncation of the 2D solutions (ie. the size of the final basis). If $\text{ZCUT} = \text{F}$ it is ignored and the size of the final Hamiltonian is MAX3D.

Line 9: RE1,DISS1,WE1 (3F20.0)

If $\text{NCOORD} = 2$, RE1 is the fixed diatomic bondlength, DISS1 and WE1 ignored.

If $\text{NCOORD} = 3$, $\text{RE1} = r_e$, $\text{DISS1} = D_e$ and $\text{WE1} = \omega_e$

are Morse parameters for the r_1 coordinate when $\text{ZMORS1} = \text{T}$, and are spherical oscillator parameters when $\text{ZMORS1} = \text{F}$.

Line 10: RE2,DISS2,WE2 (3F20.0)

If $\text{ZMORS2} = \text{T}$, $\text{RE2} = r_e$, $\text{DISS2} = D_e$ and $\text{WE2} = \omega_e$

are Morse parameters for the r_2 coordinate.

If $\text{ZMORS2} = \text{F}$, RE2 is ignored; $\text{DISS2} = \alpha$ and $\text{WE2} = \omega_e$

are spherical oscillator parameters for the r_2 coordinate.

If $\text{IDIA} = -2$ line read but ignored.

Line 11: EZERO [0.0] (F20.0)

The ground state of the system in cm^{-1} relative to the energy zero.

Optional and only read when $\text{IDIA} = \pm 2$, $\text{IPAR} = 1$ and $\text{JROT} = 0$.

2.1 Input for ROTLEV3

Most of the data for ROTLEV3, which must have been prepared previously by DVR3DRJZ run with $\text{IDIA} > -2$, is read from stream IWAVE. 3 or 4 lines of data are read.

Line 1: NAMELIST/PRT/

TOLER[0.0D0] tolerance for convergence of the eigenvalues by F02FJF [?],

zero gives machine accuracy, 1×10^{-4} is usually sufficient for most applications.

(Ignored if $\text{ZDCORE} = \text{T}$.)

ZPVEC[F] = T requests printing of the eigenvectors.

THRESH[0.1d0] threshold for printing eigenvector coefficients,

zero requests the full vector (only used if $\text{ZPVEC} = \text{T}$).

ZPHAM[F] = T requests printing of the Hamiltonian matrix.

ZPTRA[F] = T requests printing of the transformed vectors.

IWAVE[26] stream for input data from DVR3DRJZ (unformatted).

IVEC[4] scratch file for the transformed input vectors (unformatted).

JVEC[3] stream for first set of eigenvalue/vector output (unformatted).
 JVEC2[2] stream for second set of eigenvalue/vector output (unformatted), KMIN=2 only.
 ZTRAN[F] = T eigenvectors transformed back to original basis.
 ZVEC[F] = T eigenvalue and eigenvector data to be written to disk file.
 (= T forced if ZTRAN = T).
 KVEC[8] stream for first set of transformed eigenvector output (unformatted).
 KVEC2[9] stream for second set of transformed eigenvector output (unformatted),
 KMIN=2 only.
 ISCR[1] stream for scratch file storing Hamiltonian matrix (unformatted).
 JSCR[7] stream for scratch file storing DVR3DRJZ vectors transformed to an FBR in θ
 (unformatted). Used only if ZTRAN = T.
 IRES[0] restart flag:
 = 0 normal run.
 = 1 full restart.
 = 2 restart second diagonalisation only (for KMIN = 2 only).
 = -1 perform vector transformation only (stream JVEC must be supplied).
 ZPFUN[F] = T eigenvalues concatenated on stream ILEV. The first eigenvalues
 on this file must (with $J = 0$, j even) be already present.
 ILEV[14] stream for eigenvalue data (formatted).
 ZDIAG[T] = F do not diagonalise the Hamiltonian matrix.
 ZDCORE[F] = T diagonalisation performed in core using BLAS routine dsyev,
 = F diagonalisation performed iteratively using NAG Routine F02FJF.
 ZPSEG[F] = T Activates the *recordtype=segmented* option in the unformatted write/read
 records in the program.

Line 2: NVIB,NEVAL,KMIN,IBASS,NEVAL2 (5I5)

NVIB number of vibrational levels from DVR3DRJZ for each k to be read,
 and perhaps selected from, in the second variational step.
 NEVAL[10] the number of eigenvalues required for the first set.
 KMIN[0] = 0, f or $p = 1$ parity calculation.
 = 1, e or $p = 0$ parity calculation.
 = 2, do both e and f parity calculation.
 IBASS[0] = 0 or $> NVIB*(JROT+KMIN)$, use all the vibrational levels.
 Otherwise, select IBASS levels with the lowest energy.
 NEVAL2[NEVAL] the number of eigenvalues required for the second set.

Line 3: TITLE (9A8)

A 72 character title.

Line 4: EZERO [0.0] (F20.0)

Optional. The ground state of the system in cm^{-1} relative to the energy zero.

2.2 Input for ROTLEV3B

Most of the data for ROTLEV3B, which must have been prepared previously by DVR3DRJZ run with IDIA = -2, is read from streams IVEC and IVEC2. 3 or 4 lines of data are read.

Line 1: NAMELIST/PRT/

TOLER[0.0D0] tolerance for convergence of the eigenvalues by F02FJF [?],
zero gives machine accuracy, 1×10^{-4} is usually sufficient for most applications.
(Ignored if ZDCORE = T.)

ZPVEC[F] = T requests printing of the eigenvectors.

THRESH[0.1d0] threshold for printing eigenvector coefficients,
zero requests the full vector (only used if ZPVEC = T).

ZPHAM[F] = T requests printing of the Hamiltonian matrix.

ZPTRA[F] = T requests printing of the transformed vectors.

IVEC[26] stream for input data from DVR3DRJZ (unformatted).

IVEC2[4] second stream for input data from DVR3DRJZ (unformatted);
this file is simply a copy of that on stream IVEC.

ZVEC[F] = T eigenvalue and eigenvector data to be written to disk file.
(= T forced if ZTRAN = T).

JVEC[3] stream for first set of eigenvalue/vector output (unformatted).

JVEC2[2] stream for second set of eigenvalue/vector output (unformatted), KMIN=2 only.

ZTRAN[F] = T eigenvector transformed back to original basis.

ZVEC[F] = T eigenvalue and eigenvector data to be written to disk file.
(= T forced if ZTRAN = T).

KVEC[8] stream for first set of transformed eigenvector output (unformatted).

KVEC2[9] stream for second set of transformed eigenvector output (unformatted),
KMIN=2 only.

ISCR[1] stream for scratch file storing array OFFDG (unformatted).

IRES[0] restart flag:
= 0 normal run.
= 1 full restart.
= 2 restart second diagonalisation only (for KMIN = 2 only).
= -1 perform vector transformation only (stream JVEC must be supplied).

ZPFUN[F] = T eigenvalues concatenated on stream ILEV. The first eigenvalues
on this file must (with $J = 0$, j even) be already present.

ILEV[14] stream for eigenvalue data (formatted).

ZDIAG[T] = F do not diagonalise the Hamiltonian matrix.

ZDCORE[F] = T diagonalisation performed in core using BLAS routine dsyev,
= F diagonalisation performed iteratively using NAG Routine F02FJF.

Line 2: NVIB,NEVAL,KMIN,IBASS,NEVAL2,NPNT (5I5)

NVIB number of vibrational levels from DVR3DRJZ for each k to be read,
 and perhaps selected from, in the second variational step.
 NEVAL[10] the number of eigenvalues required for the first set.
 KMIN[0] = 0, f or $p = 1$ parity calculation.
 = 1, e or $p = 0$ parity calculation.
 = 2, do both e and f parity calculation.
 IBASS[0] = 0 or $> NVIB*(JROT+KMIN)$, use all the vibrational levels.
 Otherwise, select IBASS levels with the lowest energy.
 NEVAL2[NEVAL] the number of eigenvalues required for the second set.
 NPNT[NALF] number of quadrature points for angular integrals.

Line 3: TITLE (9A8)

A 72 character title.

Line 4: EZERO [0.0] (F20.0)

Optional. The ground state of the system in cm^{-1} relative to the energy zero.

2.3 Input for ROTLEV3Z

Most of the data for ROTLEV3Z, which must have been prepared previously by DVR3DRJZ run with IDIA = -2, is read from streams IVEC and IVEC2. The program also uses six scratch files which are associated with streams 1, 11, 60, 61, 70, 80 and 81. 4 or 5 lines of data are read.

Line 1: NAMELIST/PRT/

ZPVEC[F] = T requests printing of the eigenvectors.
 IVEC[26] stream for input data from DVR3DRJZ run with IPAR = 0 (unformatted).
 IVEC2[27] stream for input data from DVR3DRJZ run with IPAR = 1 (unformatted);
 ZVEC[F] = T eigenvalue and eigenvector data to be written to disk file.
 (= T forced if ZTRAN = T).
 JVEC[3] stream for eigenvalues and untransformed vectors (unformatted).
 ZTRAN[F] = T eigenvector transformed back to original basis.
 ZPTRA[F] = T requests printing of the transformed vectors.
 ZVEC[F] = T eigenvalue and eigenvector data to be written to disk file.
 (= T forced if ZTRAN = T).
 KVEC[8] stream for eigenvalues and FBR transformed eigenvector output (unformatted).
 KVEC2[9] stream for eigenvalues and DVR eigenvector output (unformatted).
 ZPFUN[F] = T eigenvalues concatenated on stream ILEV. The first eigenvalues
 on this file must (with $J = 0$, j even) be already present.

ILEV[14] stream for eigenvalue data (formatted).
 ZDIAG[T] = F do not diagonalise the Hamiltonian matrix.
 ZDIAG[F] = T selects the basis elements according to energy considerations.

Line 2: NVIB,NEVAL,KPAR,IBASS,IQPAR,NPNT (6I5)

NVIB number of vibrational levels from DVR3DRJZ for each k to be read,
 and perhaps selected from, in the second variational step.
 NEVAL[10] the number of eigenvalues required for the first set.
 KPAR = 0, for k even calculation,
 = 1, for k odd calculation.
 IBASS[0] = 0 or $> NVIB*(JROT+1)$, use all the vibrational levels.
 Otherwise, select IBASS levels with the lowest energy.
 IQPAR parity of basis set, ie 0 or 1.
 NPNT[NALF] number of quadrature points for angular integrals.

Line 3: TITLE (9A8)

A 72 character title.

Line 4: CUT-OFF [0.0] (F20.0)

The basis elements used to build the rotational Hamiltonian are selected according to energy considerations; that is all levels with 3D energy less than the cut-off are included in the Hamiltonian.

Line 4: EZERO [0.0] (F20.0)

Optional. The ground state of the system in cm^{-1} relative to the energy zero.

3 Input for DIPOLE3

DIPOLE3 takes most of its input from the output streams IWAVE (from DVR3DRJZ) or KVEC and KVEC2 (from ROTLEV3 or ROTLEV3B). It has the option to produce output files for SPECTRA [?] to calculate simulated spectra at a given temperature. Input and output on streams IKET, IBRA and ITRA are in atomic units. The data printed at the end of DIPOLE is given in wavenumbers, Debye for the transition dipoles and s^{-1} for the Einstein A coefficients.

The DIPD subroutine in this case of ZUVVIS=T should contain respective components of the transition dipole moment surface between two different electronic states. Input wavefunctions (KVEC and KVEC2) should be provided from separate ROTLEV calculations for the lower and the upper electronic state.

The user must supply the following three lines of input

Line 1: NAMELIST/PRT/

ZPRINT[F] = T supplies extra print out for debugging purposes.
ZTRA[T] = T writes data for SPECTRA to stream ITRA.
ZSTART[F] = T initiates the output file for the data for SPECTRA.
 = F writes data to the end of existing file on stream ITRA.
IKET[11] input stream from DVR3DRJZ/ROTLEV3/ROTLEV3B for the ket (unformatted).
IBRA[12] input stream for the bra (unformatted).
ITRA[13] output stream to SPECTRA (if ZTRA= T) (unformatted).
ZUVVIS[F] = T performs transitions between different electronic states (Born-Oppenheimer
 approximation).
 = F runs the ro-vibrational version of DVR3D.
ZPSEG[F] = T Activates the *recordtype=segmented* option in the unformatted write/read
 records in the program.

Line 2: TITLE (9A8)

A 72 character title.

Line 3: NPOT, NV1, NV2, IBASE1, IBASE2 (5I5)

NPOT number of Gauss-Legendre quadrature points.
NV1[all] number of ket eigenfunctions considered.
NV2[all] number of bra eigenfunctions considered.
IBASE1[0] number of lowest ket eigenfunctions skipped.
IBASE2[0] number of lowest bra eigenfunctions skipped.

Line 4: EZERO, EZEROU, TE (F20.0)

EZERO [0.0] The ground state of the system in cm^{-1} relative to the energy zero. If ZUVVIS=T,
 it is the zero point energy of the lower electronic state [cm^{-1}]
EZEROU if ZUVVIS=T, zero point energy of the upper electronic state [cm^{-1}]
TE if ZUVVIS=T, it is the vertical excitation energy (Te) between the lower and the
 upper electronic state [cm^{-1}]

4 Input for SPECTRA

SPECTRA takes most of its input from stream ITRA generated by DIPOLE.
Data for generating partition functions may optionally be provided by DVR3DRJZ
and one of the ROTLEV programs via stream ILEV. The user must supply 5

(4 if ZSPE=.FALSE.) lines of input.

Line 1: NAMELIST/PRT/

ZOUT[F] = T, print sorted transition frequencies and line strengths.
ZOUT is set automatically to T if ZSPE=F.
ZSORT[T] = T sort transition data and write it to stream ISPE.
= F sorted transition data is to be read from stream ISPE.
ZSPE[T] = F if the program is to stop after sorting only.
ZPFUN[T] = T calculate the partition function from data on stream ILEV;
= F the partition function is not calculated but set to value Q read in.
ZPSEG[F] = T Activates the *recordtype=segmented* option in the unformatted write/read records in the program.
ITRA[13] input stream transitions file from DIPOLE3 (unformatted).
ILEV[14] formatted input stream with energy levels for the partition function.
The first eigenenergy on ILEV must be the ground state ie J=0, (IPAR=0).
This is the zero energy of the problem if ZPFUN=T.
ISPE[15] stream for the sorted transitions (unformatted).
ITEM[16] scratch file (unformatted).

The following are only used if ZSORT = T.

WSMIN[0.0d0] minimum transition frequency in cm^{-1} for which data sorted.
WSMAX[1.0d6] maximum transition frequency in cm^{-1} for which data sorted.
EMIN[-1.0d27] minimum value of energy of lower state, E", in cm^{-1} for which data sorted.
EMAX[+1.0d27] maximum value of energy of lower state, E", in cm^{-1} for which data sorted.
JMAX[all] maximum value of J", the angular momentum of the lower state,
for which data sorted.
SMIN[0.0] minimum linestrength (in D^2) for which data sorted.
GZ[0.0] ground state energy in cm^{-1} .

Line 2: TITLE (9A8)

A 72 character title.

Line 3: GE, GO (2D10.0)

GE[1.0d0] nuclear-spin times symmetry-degeneracy factors for
AB₂ molecule (ie | IDIA | = 2) for the even (IPAR=0).
GO[1.0d0] nuclear-spin times symmetry-degeneracy factors for homonuclear
AB₂ molecule (ie | IDIA | = 2) for the odd (IPAR=1).

Line 4: TEMP, XMIN, WMIN, WMAX, DWL,Q (6F10.0)

TEMP temperature in K.
XMIN lowest relative intensity printed.
WMIN[0.0] minimum transition frequency required in cm^{-1} .

WMAX[all] maximum transition frequency required in cm^{-1} .
 DWL[0.0] profile half width, in cm^{-1} or μm depending on ZFREQ, used if ZPROF = T and ZDOP = F.
 Q[1.0] value of the partition function, only used if ZPFUN = F.

Line 5: NAMELIST/SPE/

EMIN1[-1.0d27] minimum value of energy of lower state, E'' , in cm^{-1} for which data printed.
 EMAX1[+1.0d27] maximum value of energy of lower state, E'' , in cm^{-1} for which data printed.
 EMIN2[-1.0d27] minimum value of energy of upper state, E' , in cm^{-1} for which data printed.
 EMAX2[+1.0d27] maximum value of energy of upper state, E' , in cm^{-1} for which data printed.
 JMAX[all] maximum value of J'' , the lower state angular momentum, for which data printed.
 ZEMIT[F] = F calculates integrated absorption coefficient.
 = T calculates emissivities.
 ZPLOT[F] = T writes computed spectrum to stream IPLOT.
 IPLOT[20] output stream for formatted file containing spectral data.
 ZPROF[F] = T gives spectrum at NPOINTS points with Gaussian line profiles;
 only used with ZPLOT = T, when results are on stream IPLOT.
 = F generates stick spectrum.
 NPOINTS[3000] number of points at which spectrum is stored if ZPROF = T.
 ZDOP[F] = T use thermal Doppler half width for spectral profile.
 XMOLM[18.0] molecular mass in amu. Only used if ZDOP=T.
 ZENE[F] = T write assignments with lines to IPLOT.
 = F only line position and intensity to IPLOT
 Only used if ZPROF = F.
 IDAT[19] Scratch file used to construct profiles (formatted),
 used if ZPROF = T and ZPLOT = T.
 ZLIST[F] = T write transition data to linelist file on stream ILIST.
 ILIST[36] output stream for formatted linelist if ZLIST=T.
 PRTPR[0.1d0] relative intensity threshold for printing results.
 TINTE[1.0D-15] absolute intensity threshold for printing results.
 ZFREQ[T] = T, stream IPLOT contains wavenumber (cm^{-1}) as first column.
 = F, stream IPLOT contains wavelength (μm) as first column.
 ZEINST[F] = T, stream IPLOT contains spin weighted Einstein A coefficient
 as second column. In this case ZEMIT = T. is forced.
 = F, stream IPLOT contains intensity as second column.

5 Input for XPECT3

XPECT3 requires wavefunctions as generated by DVR3DRJZ on unit IWAVE (ZPERP=F only), or ROTLEV3/ROTELEV3B on units KVEC or KVEC2. An additional four lines of standard input are required:

Line 1: NAMELIST/PRT/

ZPRINT[F] = T supplies extra print out for debugging purposes.
ZTRA[T] = T writes property data to stream ITRA.
ZFORM[F] = T use formatted writes to stream ITRA.
ZFIT[F] = T potential energy fit being performed
= F standard expectation value run.
ZSTART[F] = T initiates the output file ITRA;
= F writes data to the end of existing file on stream ITRA.
(Only used if ZFIT = F.)
IKET[11] input stream from DVR3DRJZ/ROTLEV3/ROTLEV3B (unformatted).
ITRA[12] output stream for properties (if ZTRA= T).
ITRA0[28] derivatives computed by XPECT3 for ground state.
(Only used if ZFIT = T.)

Line 2: TITLE (9A8)

A 72 character title.

Line 3: LPOT, NPROPIN, NPRT, NV1 (5I5)

LPOT number of Gauss-Legendre quadrature points.
(Ignored if $J = 0$).
NPROPIN[1] number of properties to be considered.
NPRT [NPROPIN] total possible number of properties.
NV1[all] number of eigenfunctions considered.

Line 4: (IPROP(I), I =1, NPROPIN) (20I5)

Pointers to the properties in array IPROP to be considered. Default is 1,2,...,NPROPIN.
Values must be unique and in the range 1 to NPRT.