INPUT PARAMETERS

Definitions of input parameters on fort.1

Throughout this documentation, much use is made of the SIGN of an input parameter.
This is to be able to signify, with a single datum, several variants relating to
the facility highlighted. In cases where a particular value of the datum is
required (for example the value of J, input as JMAX), the modulus of the input
parameter is to be assumed. The sign of the input datum indicates how this
parameter is to be used. For example, JMAX>0 is the prompt for a full vibration-
rotation analysis, whereas JMAX<0 indicates that the less complete adiabatic
rotation procedure is to be adopted. In both cases the calculation is to be
performed for values of the total angular momentum quantum number J = |JMAX|. If,
however, no specific value of the input datum is indicated or implied, the values
of +1, 0 ,-1 will always be sufficient. Cases where this is not so will be clearly
indicated in the documentation. Input is in free-format unless otherwise stated.

```
C******************************************************************************
C**TITLE
C-------
C**
C**TITLE:  Any suitable title...maximum 80 characters

C******************************************************************************
C**NATOM,NSTAT,CONV,ICOUPL,ICOUPC,ISCFCI,IWHICH,IDISC,NROTTR,JMAX,MCHECK,INORM
C----------------------------------------------------------------------------
C**
C**NATOM:   Number of atoms (number of Normal Coordinates NMODE=3N-6, unless
C**         facility NROTTR is used - see below)
C**NSTAT:   Number of SCF states required
C**         NSTAT>0: Input NSTAT specific SCF states depending on NDEF (below)
C**         NSTAT<0: Program generates -NSTAT SCF states in increasing energy
C**CONV:    Convergence threshold for SCF states in cm-1
C**ICOUPL:  Number of modes coupled in potential integration (1,2,3,4,5,6)
C**         ICOUPL>0: use REAL*8 grid
C**         ICOUPL<0: use REAL*4 grid (half the disc storage as REAL*8)
C**ICOUPC:  Number of modes coupled in coriolis integration (1,2,3,4)
C**         ICOUPC>0: use REAL*8 grid
C**         ICOUPC<0: use REAL*4 grid (half the disc storage as REAL*8)
C**         Note: ICOUPC can NOT be greater than ICOUPL
C**ISCFCI:  Number of final CI energies required (if positive) for VSCF-CI or
C**         VCI (see ICI below)
C**         ISCFCI>0: SCF + CI calculation
C**         ISCFCI=0: SCF only
C**         ISCFCI<0: Terminates after preliminary checks (see MCHECK,INORM,
C**         IREACT, MOLPRO below)
C**IWHICH:  Type of input potential
C**         IWHICH=0: Conventional Normal coordinate force field...Normal mode
```

```
C**          analysis and force field are assumed to be supplied by user
C**          IWHICH>0: Internal coordinate (global) potential
C**          IWHICH<0: Normal coordinate potential from fitted potential
C**                    if MOLPRO>0
C**          IWHICH<0: Normal coordinate potential from user-supplied routine
C**                    if MOLPRO=0
C**          IWHICH<0: Normal coordinate potential from interpolated potential
C**                    if MOLPRO<0
C**IDISC:   IDISC=0: Write potential and coriolis grid values to disc
C**          IDISC>0: Assumes grid values already on disc
C**          Rigid-rotor energies written to (61),(62),(63),(64) for
C**          ICOUPC=1,2,3,4
C**          Potential written to units (71),(72),(73),(74),(75),(76) for
C**          ICOUPL=1,2,3,4,5,6
C**          Coriolis (vibration) written to units (81),(82),(83),(84) for
C**          ICOUPC=1,2,3,4
C**          Coriolis (rotation) written to units (91),(92),(93),(94) for
C**          ICOUPC=1,2,3,4
C**NROTTR:  Number of rotational and translational degrees of freedom to be
C**          included in 'vibrational' modes
C**          (number of modes = NMODE=3*NATOM-6+NROTTR)
C**JMAX:    Total angular momentum quantum number
C**          JMAX>0: perform exact Whitehead-Handy if ICI < 0 (below)
C**          JMAX<0: perform adiabatic rotation if ICI < 0 (below)
C**          For VSCF only (ISCFCI = 0) or VSCF-CI (ICI > 0) perform adiabatic
C**          rotation
C**MCHECK:  MCHECK=0: Use input coordinate system as principal axis system
C**          MCHECK>0: Transform equilibrium geometry to principal axis system,
C**          and calculate rotational constants. Program continues with geometry
C**          in principal axis system (terminate if ISCFCI < 0)
C**          MCHECK<0: Finds minimum of potential (terminate if ISCFCI < 0)
C**INORM:   INORM=0: Do not perform Normal mode analysis
C**          INORM>0: Perform Normal mode analysis with internal coordinate
C**          (minimum) potential (IWHICH=1) (terminate if ISCFCI < 0)
C**          INORM<0: Perform Normal mode analysis with internal coordinate
C**          (saddle point) potential (IWHICH=1) (terminate if ISCFCI < 0)
C**
C**          Important note:  Normal modes are ordered in increasing energy.

C********************************************************************************
C**ICI,NMAX,CUT,EVLJ0,NVALR,KSTEP,IPRINT,MATSIZ,IREACT,MOLPRO,MOLINC
C-------------------------------------------------------------------
C**
C**ICI:     CI basis definition
C**          ICI>0: Number of specific VSCF states in VSCF-CI calculation
C**          ICI<0: -ICI quanta in each mode in VCI calculation (if NMAX.GE.0):
C**NMAX:    NMAX>0: Maximum sum of quanta in VCI basis
C**          NMAX=0: Unrestricted sum of quanta
C**          NMAX<0: Maximum number coupled modes in basis ... maximum -5
C**          (see MAXSUM, MAXBAS below)
```

```
C**CUT:     Cutoff energy (cm-1) for CI printout
C**EVLJ0:   Reference energy (cm-1) for J>0 CI calculations.  In general, this
C**         will be the zero point energy for J=0, which is printed at the end
C**         of the output for J=0.  This value will depend on the value of the
C**         user's potential at the minimum.  The user may wish to scale his
C**         potential such that the value at the minimum is zero, in which case
C**         the value printed for J=0 is the true zero point energy in cm-1
C**         If the reference geometry (see X0 below) is not at the potential
C**         minimum, the true zero-point energy can only be determined if the
C**         potential at the reference geometry is defined to be zero, in this
C**         case the zero-point energy will be the value printed for J=0,
C**         scaled by the energy difference between that at the reference
C**         geometry and that at the true minimum.
C**NVALR:   Number of rovibrational levels required
C**KSTEP:   Increment between successive K (0 to 2*J+1)
C**         For KSTEP = 0, only one K-diagonal step is carried out, for Ka = 0
C**IPRINT:  Level of output
C**         IPRINT=3: Print everything
C**         IPRINT=2: Omit rotation matrix element output if J>0
C**         IPRINT=1: Omit SCF output, and K-diagonal output if J>0
C**         IPRINT=0: Omit integration grid and normal coordinate output
C**         IPRINT>0: Print full details of Reaction Path; print ONE (largest)
C**         CI coefficient
C**         IPRINT=0: Print ONE (largest) CI coefficient
C**         IPRINT<0: Print -IPRINT largest CI coefficients
C**MATSIZ:  Generate VCI or VSCF matrix size
C**         MATSIZ=0: Normal run
C**         MATSIZ>0: Calculate current size of VCI matrix and terminate
C**                   Calculate (energy-based) VSCF states and terminate
C**IREACT:  Mode number of floppy mode for reaction path hamiltonian
C**         IREACT=0: Normal run
C**         IREACT=mode: Actual (curvilinear) mode in reaction path
C**         If IREACT>0: terminate after 'Normal mode' analysis if ISCFCI < 0
C**         If IREACT<0: denotes 'abinitio' algorithm - terminate after
C**         'Normal mode' analysis if ISCFCI < 0
C**MOLPRO:  Link stage with abinitio package (such as MOLPRO)
C**         MOLPRO=0: Normal run
C**         MOLPRO=1: Produce MOLPRO file for 1-dim Gauss grids using input
C**                   harmonic (omega) force field (IWHICH=0)
C**         MOLPRO=2: Fit 1-dim energies from MOLPRO=1 to 'full' or 'even'
C**                   polynomials depending on ISYM(I)
C**         MOLPRO=3: Generate 2-dim HEG grids using input fitted Gauss V(Q)
C**                   force field (IWHICH=0)
C**         MOLPRO=4: Fit 2-dim energies from MOLPRO=3
C**         MOLPRO=5: Generate 3-dim HEG grids using input fitted HEG V(Q1,Q2)
C**                   force field (IWHICH=0)
C**         MOLPRO=6: Fit 3-dim energies from MOLPRO=5
C**         MOLPRO=7: Generate 4-D HEG grids using input fitted HEG V(Q1,Q2,Q3)
C**                   force field (IWHICH=0)
C**         MOLPRO=8: Fit 4-dim energies from MOLPRO=7
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C**          MOLPRO=9: Generate 5-D HEG grids using input fitted HEG
C**                    V(Q1,Q2,Q3,Q4) force field (IWHICH=0)
C**          MOLPRO=10: Fit 5-dim energies from MOLPRO=9
C****************************************************************************
C**                    To produce grids from (and fits of) global potential,
C**                    set IWHICH>0 (internal coordinates) for above steps
C****************************************************************************
C**          If MOLPRO>0: Fit potentials (terminate if ISCFCI < 0)
C**          If MOLPRO<0: Interpolate potentials (terminate if ISCFCI < 0)
C****************************************************************************
C**                    To calculate vibrational energies using fitted potential
C**                    in normal coordinates Y = gamma.Q set IWHICH<0, MOLPRO>0
C**                    (see XTANPM below)
C**                    To calculate vibrational energies using interpolated
C**                    potential in normal coordinates Q set IWHICH<0, MOLPRO<0
C**                    To calculate vibrational energies using independently
C**                    generated potential in normal coordinates Y = gamma.Q or
C**                    Q set IWHICH<0, MOLPRO=0 (see USER.DOC)
C****************************************************************************
C**MOLINC:  HEG increment used in fits (1 OR 2 = all or alternate, respectively)

C****************************************************************************
C**XTANPM(NMODE)
C---------------
C**
C**Omit data for this input if not fitting potentials (MOLPRO = 0)
C**AND not using fitted potentials (IWHICH = 0 or IWHICH > 0)
C**
C**XTANPM(I), I = 1,NMODE
C**          For fitted potentials, the coordinate tanh(gamma.Q) is used.
C**          XTANPM sets the asymptotic value of the Gauss coordinates
C**          QMAX(MODE) such that GAMMA(MODE)*QMAX(MODE) = XTANPM(MODE)

C****************************************************************************
C**XMODQ(NMODE)
C---------------
C**
C**Scaling factor of HEG points Q for potential
C**
C**XMODQ(I), I = 1,NMODE
C**          Scaling factor XMODQ(I) for mode Q(I)

C****************************************************************************
C**NCONT,NVAL1,NVAL2
C-------------------
C**
C**Omit data for this input if SCF only (ISCFCI.LE.0)
C**Omit data for this input if VSCF-CI (ICI > 0)
C**Omit data for this input if unrestricted VCI (NMAX = 0)
C**Omit data for this input if restricted VCI (NMAX > 0)
```

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C**
C**NCONT:
C**         If ICI<0: NCONT is number of contraction schemes (Maximum 2)
C**         NCONT=+2:  Complete algorithm for 2 contraction schemes
C**         NCONT=-2: Simplified algorithm for 2 contraction schemes
C**         NCONT=+1 and NCONT=-1 both refer to the original (single-scheme)
C**         algorithm
C**NVAL1,NVAL2:
C**         If ICI<0: NVAL1,NVAL2 are maximum number of contracted functions
C**         from schemes 1 and 2 required in complete algorithm
C**         NVAL1:  Number of functions required from contraction scheme 1
C**         NVAL2:  Number of functions required from contraction scheme 2
C**         NVALn>0:  Do all symmetries for contraction scheme 'n'
C**         NVALn<0:  Do specific symmetries for contraction scheme 'n'
C**
C**         (Currently internal use only for NCONT > 0......use NCONT = -1 or
C**         NCONT = -2)


C*******************************************************************************
C**ICONT(NCONT), JCONT(NCONT,ICONT(NCONT)), NCOUPL, NCOUPC
C-----------------------------------------
C**
C**Omit data for this input if SCF only (ISCFCI = 0)
C**Omit data for this input if preliminary checks (ISCFCI < 0)
C**Omit data for this input if VSCF-CI (ICI > 0)
C**Omit data for this input if unrestricted VCI (NMAX = 0)
C**Omit data for this input if restricted VCI (NMAX > 0)
C**
C**ICONT(I), (JCONT(I,J),J=1,ICONT(I)), NCOUPL, NCOUPC
C**
C**         Input one record for each contraction scheme I=1,NCONT
C**ICONT:   Number of modes in contraction scheme NCONT
C**JCONT:   Actual modes in contraction scheme NCONT
C**NCOUPL:  Potential coupling for scheme NCONT
C**NCOUPC:  Coriolis coupling for scheme NCONT


C*******************************************************************************
C**MAXSUM(-NMAX,NCONT)
C--------------------
C**
C**Omit data for this input if SCF only (ISCFCI = 0)
C**Omit data for this input if preliminary checks (ISCFCI < 0)
C**Omit data for this input if VSCF-CI (ICI > 0)
C**Omit data for this input if unrestricted VCI (NMAX = 0)
C**Omit data for this input if restricted VCI (NMAX > 0)
C**
C**(MAXSUM(I,K),I=1,-NMAX)
C**
C**         Input one record for each contraction scheme K=1,NCONT
C**MAXSUM:  Maximum sum quanta in M-mode basis ... restricted only
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C**           Input single record of -NMAX integers (maximum 5)
C**           for each contraction scheme K
C**
C**           MAXSUM(M,-NMAX) are defined as follows:
C**           MAXSUM(1,K) is maximum sum quanta in one-mode basis sets
C**           MAXSUM(2,K) is maximum sum quanta in two-mode basis sets
C**           MAXSUM(3,K) is maximum sum quanta in three-mode basis sets
C**           MAXSUM(4,K) is maximum sum quanta in four-mode basis sets
C**           MAXSUM(5,K) is maximum sum quanta in five-mode basis sets


C****************************************************************************
C**MAXBAS(NMODE,-NMAX)
C---------------------
C**
C**Omit data for this input if SCF only (ISCFCI = 0)
C**Omit data for this input if preliminary checks (ISCFCI < 0)
C**Omit data for this input if VSCF-CI (ICI > 0)
C**Omit data for this input if unrestricted VCI (NMAX = 0)
C**Omit data for this input if restricted VCI (NMAX > 0)
C**
C**(MAXBAS(M,I),M=1,NMODE)
C**
C**           Input one record for each I-mode basis I=1,-NMAX
C**MAXBAS:  Defines selective quanta in VCI basis
C**           Input -NMAX records (maximum 5) of NMODE integers
C**
C**           MAXBAS(M,1) is maximum quanta for mode M in one-mode basis sets
C**           MAXBAS(M,2) is maximum quanta for mode M in two-mode basis sets
C**           MAXBAS(M,3) is maximum quanta for mode M in three-mode basis sets
C**           MAXBAS(M,4) is maximum quanta for mode M in four-mode basis sets
C**           MAXBAS(M,5) is maximum quanta for mode M in five-mode basis sets


C****************************************************************************
C**MODINT(NMODE)
C---------------
C**
C**(MODINT(M),M=1,NMODE)
C**
C**MODINT:    Integration factor (1 or 2) for NMODE modes
C**MODINT=1:  Mode is totally symmetric (A₁g)
C**MODINT=2:  Mode is antisymmetric (B₂g,B₁g,A₂g,A₁u,B₂u,B₁u,A₂u)


C****************************************************************************
C**MEFF(NMODE,2)
C-------------
C**
C**(MEFF(M,I),M=1,NMODE,I=1,2)
C**
C**MEFF:      Corresponding mode forming effective 1-dim potential for
C**           current mode.
```

```
C**MEFF(M,1)=N  An effective 1-dim potential for mode M will be generated in
C**             order to define the 1-dim basis. The effective potential will
C**             be with respect to mode N
C**MEFF(M,2)=K  The effective potential of mode M will also be with respect to
C**             mode K


C******************************************************************************
C**NCYCLE,TOLLAN,LANMAX,IGIV,LAN20,LANCUT,TOLCUT,LANCYC,TOLMAT,LANINC
C-------------------------------
C**
C**NCYCLE:  Number of Lanczos cycles (Lanczos ignored if NCYCLE=0)
C**          NCYCLE>0: use LANCZA (less memory usage - more disc)
C**          NCYCLE<0: use LANCZB (more memory usage - less disc)
C**TOLLAN:  Tolerance for Lanczos eigenvalues
C**LANMAX:  Maximum order of half-matrix used to build Lanczos matrix
C**LGIV:    LGIV=0: Use QL algorithm in Lanczos
C**         LGIV>0: Use GIVENS in Lanczos
C**LAN20:   (Obsolete) Size below which uses single disc file fort.20
C**         If size exceeds LAN20, disc output spread over 5 discs to
C**         avoid Linux 2GB problem
C**         LAN20>0: create all Lanczos files and continue
C**         LAN20<0: restart Lanczos diagonalization using previous files
C**
C**         NB Restart for single VCI symmetry block only.....
C**         .....job with LAN20 > 0 can be `killed' once message:
C**         `Calculating Lanczos' is reached.
C**LANCUT:  LANCUT>0: number of 1 & 2 dim functions to keep
C**         LANCUT<0: stop after set-up (single symmetry only)
C**TOLCUT:  Tolerance for perturbation test
C**         TOLCUT>0: 1 & 2 dim perturbation basis
C**         TOLCUT<0: 1,2 & 3 dim perturbation basis
C**LANCYC:  Size of inner matrix (cf ISCFCI)
C**TOLMAT:  Tolerance below which matrix element = 0 exactly
C**LANINC:  No. of increments for final matrix C' if PT


C******************************************************************************
C**NVSYM,NWSYM,ISYM
C-------------
C**
C**NVSYM:   Number of vibrational symmetry species (1 or 2 or 4 or 8)
C**NWSYM:   Number of mode symmetry species
C**         For no symmetry NVSYM=NWSYM=1 (C1)...can be used for molecules of
C**         any symmetry
C**         For four-atom or larger $C_s$ molecules NVSYM=NWSYM=2 (A',A")
C**         For triatomic $C_{2v}$ molecules NVSYM=NWSYM=2 ($A_1,B_2$)
C**         For four-atom $C_{2v}$ molecules NVSYM=4 ($A_1,B_2,B_1,A_2$),
C**         NWSYM=3 ($A_1,B_2,B_1$)
C**         For larger molecules, where reduction of symmetry to $C_{2v}$ is possible
C**         NVSYM=4 ($A_1,B_2,B_1,A_2$), NWSYM=4 ($A_1,B_2,B_1,A_2$)
C**         Where there is a centre of symmetry, $C_{2v}$ is converted to pseudo D2h
```

```
C**            NVSYM=8 (A_{1g},B_{2g},B_{1g},A_{2g}; A_{1u},B_{2u},B_{1u},A_{2u}), NWSYM=1 -> 8
C**ISYMPG:  Point Group indicator (default setting ISYMPG=0), including:
C**            C_1, C_s or C_2, C_{2v} or D_2 or C_{2h}, D_{2h}

C******************************************************************************
C**NSYM(NWSYM),ISYM(NWSYM,NSYM(NWSYM))    (order of NWSYM:  A_1,B_2,B_1,A_2)
C----------------------------------------------------------------------
C**
C**NSYM(I), (ISYM(I,J),J=1,NSYM(I))
C**
C**            Input one record for each mode symmetry I=1,NWSYM
C**            For triatomic C_{2v} molecules, NWSYM=1 corresponds to A_1,
C**            NWSYM=2 corresponds to B_2
C**            For four-atom C_{2v} molecules, NWSYM=1 corresponds to A_1,
C**            NWSYM=2 corresponds to B_2, NWSYM=3 corresponds to B_1
C**            etc.
C**            For D_{2h} molecules, NWSYM=1 -> 4 are 'g'; NWSYM=5 -> 8 are 'u'
C**            The user must know the symmetry of the Normal modes which are
C**            ordered either in increasing energy (see INORM=1),
C**            or according to the user's convention (see INORM=0)
C**
C**NSYM:    Number of modes of current (NWSYM) symmetry
C**ISYM:    NSYM specific modes of current (NWSYM) symmetry
C**
C**            For example, in the case of H2O, there are 2 mode vibrations
C**            of A1 symmetry (modes 1 and 2, say) corresponding to NWSYM=1.
C**            There is a single mode vibration of B2 symmetry (mode 3, say)
C**            corresponding to NWSYM=2.
C**            Hence for NWSYM=1 (totally symmetric), the input required is:
C**            NSYM=2,  ISYM(I)=1 2
C**            For I=2, the input required is:
C**            NSYM=1,  ISYM(I)=3

C******************************************************************************
C**MVSYM,MWSYM(MVSYM)    (order of MWSYM:  A_1,B_2,B_1,A_2)
C------------------------------------------------------
C**
C**MVSYM,(MWSYM(I),I=1,MVSYM)
C**
C**MVSYM:    Single integer corresponding to the number of actual vibrational
C**            (JMAX=0) or rovibrational (JMAX>0) symmetry species required
C**MWSYM:    MVSYM integers corresponding to the Specific vibrational (JMAX=0)
C**            or rovibrational (JMAX>0) symmetry species required
C**
C**            For J = 0 get vibrational energies of specified symmetry.
C**            For J > 0 all vibrational symmetries are included in K-blocks, but
C**            final rovibrational calculations are done for symmetries specified.
C**
C**Note:    For a triatomic molecule, the number of possible rovibrational
C**            species is twice the number of possible vibrational species
```

```
C*****************************************************************************
C**MXDIP(3)      (Irreducible representations of dipole components)
C----------------------------------------------------------------
C**
C**(MXDIP(I),I=1,3)
C**
C**MXDIP(1): I.R. of molecule-fixed X component of dipole
C**MXDIP(2): I.R. of molecule-fixed Y component of dipole
C**MXDIP(3): I.R. of molecule-fixed Z component of dipole
C**
C**Note:      I.R. are given according to standard MM convention
C**           C₁:  A=1; C₂: A=1,B=2; Cₛ: A'=1,A"=2; C₂ᵥ: A₁=1,B₂=2,B₁=3,A₂=4
C**           D₂:  A=1,B₃=2,B₂=3,B₁=4; C₂ₕ: Aₘ=1,Bₘ=2,Aᵤ=3,Bᵤ=4
C**           D₂ₕ: A₁ₘ=1,B₂ₘ=2,B₁ₘ=3,A₂ₘ=4,A₁ᵤ=5,B₂ᵤ=6,B₁ᵤ=7,A₂ᵤ=8
C**
C*****************************************************************************
C**MX(3)       (Relationships between symmetry axes and principle axes)
C----------------------------------------------------------------
C**
C**(MX(I),I=1,3)
C**
C**MX(1): Symmetry axis (x,y,z) corresponding to principal X-axis
C**MX(2): Symmetry axis (x,y,z) corresponding to principal Y-axis
C**MX(3): Symmetry axis (x,y,z) corresponding to principal Z-axis
C**
C**Note:      Throughout, we will refer to principal axes as X,Y,Z
C**                       we will refer to symmetry axes as x,y,z
C**
C**
C*****************************************************************************
C**MXROT(3)      (Irreducible representations of Rx, Ry, Rz)
C**              (Some Group Tables refer to Jx, Jy, Jz)
C----------------------------------------------------------------
C**
C**(MXROT(I),I=1,3)
C**
C**MXROT(1): I.R. of rotation about symmetry x-axis (Rx)
C**MXROT(2): I.R. of rotation about symmetry y-axis (Ry)
C**MXROT(3): I.R. of rotation about symmetry z-axis (Rz)
C**
C**Note:      I.R. are given according to standard MM convention
C**           C₁:  A=1; C₂: A=1,B=2; Cₛ: A'=1,A"=2; C₂ᵥ: A₁=1,B₂=2,B₁=3,A₂=4
C**           D₂:  A=1,B₃=2,B₂=3,B₁=4; C₂ₕ: Aₘ=1,Bₘ=2,Aᵤ=3,Bᵤ=4
C**           D₂ₕ: A₁ₘ=1,B₂ₘ=2,B₁ₘ=3,A₂ₘ=4,A₁ᵤ=5,B₂ᵤ=6,B₁ᵤ=7,A₂ᵤ=8
C**
C*****************************************************************************
C**
C**ISYMT
C**
```

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C**ISYMT:   I.R. of sin(M.tau/2).   For use only with MM-RPH.
C**         ISYMT=1 if MM-SR

C******************************************************************************
C**LDUMP,MDUMP,IDUMP
C-------------------
C**
C**Omit data for this input if SCF only (ISCFCI = 0)
C**Omit data for this input if preliminary checks (ISCFCI < 0)
C**Omit data for this input if VSCF-CI (ICI > 0)
C**
C**LDUMP:   Restart parameter for property functions
C**         Currently the following seven properties are supported:
C**         LDUMP=1: input dipole functions and evaluate J=0 matrix elements
C**         LDUMP=2: expectation values of Q
C**         LDUMP=3: expectation values of Q^2
C**         LDUMP=4: wavefunction plots
C**         LDUMP=5: user-defined property
C**         LDUMP=6: F-C factors (assumes 2 electronic states)
C**         LDUMP=7: P,Q,R-branch intensities
C**         LDUMP=8: Raman Spectrum
C**         LDUMP=9: Partition Functions
C**         LDUMP<0: Redraw spectrum using previous files...
C**         ...LDUMP=-7 (IR), LDUMP=-8 (Raman)
C**MDUMP:   Number of (central) grid points used to generate Eckart frame
C**         MDUMP>0: program continues with VCI
C**         MDUMP<0: program halts after generating required points
C**         (obsolete)
C**IDUMP:   Number of J=0 VCI functions written to disc (ICI < 0)
C**         LDUMP=0: IDUMP consecutive functions for each symmetry
C**OBSOLETE
C********* LDUMP<0: NDUMP(IABS(IDUMP)) specific functions for each symmetry
C**OBSOLETE

C******************************************************************************
C**NDUMP(-IDUMP,NVSYM)
C--------------------
C**
C**(NDUMP(I,NVSYM),I=1,-IDUMP)
C**
C**         Input only if IDUMP < 0
C**         Input NVSYM records of -IDUMP function numbers
C**NDUMP:   -IDUMP specific functions for symmetry species NVSYM to dump to disc
C**         Function numbers are those given in the J=0 output on fort.2

C******************************************************************************
C**NBF(NMODE),MBF(NMODE),NVF(NMODE),MVF(NMODE)
C--------------------------------
C**
C**         Input NMODE records of three integers
```

```
C**NBF(K):   Number of quanta in harmonic-oscillator basis for mode K
C**MBF(K):   Number of Gauss Hermite integration points for mode K
C**NVF(K):   Number of quanta of contracted numerical functions for mode K
C**MVF(K):   Number of HEG integration points for mode K, cannot exceed NBF(K)
C**Note:       For VCI (ICI < 0) NVF(K) will be overwritten by -ICI or by the
C**            maximum quantum within MAXBAS, depending on the setting of NMAX


C*****************************************************************************
C**SYMBOL(NATOM)
C--------------
C**
C**(SYMBOL(I),I=1,NATOM)
C**
C**SYMBOL:  Nuclear Atomic Symbol (H for hydrogen, etc.) in A2 FORMAT


C*****************************************************************************
C**SCF STATE DEFINITIONS (SEE ORIGINAL DEFINITION BY JEKSKI)
C------
C**
C**Read data for this input ONLY if NSTAT > 0
C**          NSTAT>0 and NDEF<0:
C**          Input NSTAT records ISTAT(NSTAT,NMODE) corresponding to NSTAT
C**          specific SCF state definitions (see Jelski et al in
C**          J. Comput. Chem., 17, 1645 (1996)).
C**
C**          NSTAT>0 and NDEF=0 or NDEF>0:
C**          Input NSTAT records N1 N2 where N1 are the number of quanta for
C**          mode N2
C**          All remaining modes will take on NDEF quanta (see Jelski et al)
C**
C**          NSTAT<0:
C**          Input NOTHING. In this case NDEF is a dummy parameter.
C**          It is recommended that NSTAT<0 is set for all VCI calculations
C**          (see ICI -ve above)


C*****************************************************************************
C**NPOT
C------
C**
C**Read data for this input ONLY for Normal Coordinate Potential (IWHICH=0)
C**NPOT:    Number of user-supplied Normal coordinate force field terms
C**         IPOT,JPOT,CPOT (below).


C*****************************************************************************
C**IPOT(NPOT),JPOT(NPOT),CPOT(NPOT)
C---------------------------------
C**
C**Read data for this input EITHER for Normal Coordinate Potential (IWHICH=0)
C**OR for definition of NMODE values of user-supplied values of omega (INORM=0)
C**          Normal coordinate force field, defined by:
```

```
C**          Jelski et al in J. Comput. Chem., 17, 1645 (1996).
C**          A maximum of 6 coupled modes is allowed.
C**IPOT:     (first 6 integers): defines the Normal mode(s) involved.
C**JPOT:     (second 6 integers): defines the number of quanta in the
C**          corresponding mode(s)
C**CPOT:     defines the potential contribution F(ijkl..) in hartrees
C**
C**These parameters are input under the following conditions:
C**IWHICH=0: Input NPOT terms IPOT,JPOT,CPOT where the first NMODE terms are the
C**          NMODE harmonic force constants F(ii)
C**IWHICH>0: Input NMODE terms corresponding to the NMODE harmonic force
C**          constants F(ii) if INORM=0
C**          Input NOTHING if INORM=1
C**
C**Note:     F(ii) is omega(i) in cm-1

C*******************************************************************************
C**NUCLEAR MASSES XM(NATOM)
C-----------
C**
C**(XM(I),I=1,NATOM)
C**XM:        Nuclear masses (U). Carbon is 12.0

C*******************************************************************************
C**EQUILIBRIUM CARTESIAN COORDINATES X0(NATOM,3)
C-------------
C**
C**(X0(NATOM,I),I=1,3)
C**X0:        Input NATOM records of reference structure x,y,z coordinates in bohr

C*******************************************************************************
C**NORMAL COORDINATE DISPLACEMENTS XL(NATOM,NMODE,3)
C-------------------
C**
C**Omit data for this input for automatic evaluation of Normal Coordinates
C**(INORM>0 or INORM<0)
C**
C**XL(NATOM,NMODE,I),   I=1,3
C**          Mass-weighted Normal Coordinate displacement vectors
C**XL:        Input NMODE groups of NATOM records of x,y,z mass-weighted Normal
C**          Coordinate displacements (INORM=0)

C*******************************************************************************
C**MAXCHK(ICOUPL)
C---------------
C**
C**(MAXCHK(M),M=1,ICOUPL)
C**
C**MAXCHK:    Inspection of M-mode grids for spurious maxima
C**          MAXCHK(M)=0:  Do nothing
```

```
C**             MAXCHK(M)=+N:  Report maxima found for mode N at M-mode
C**             MAXCHK(M)=-N:  Attempt correction for mode IABS(N) at M-mode

C*******************************************************************************
C**OUTPUT VIBRATION FILE
C----------------------
C**
C**File name to store vibrational wavefunction if the user chooses to write them
C**to disk with IDUMP>0

C*******************************************************************************
C**OUTPUT ROTATIONAL FILE
C----------------------
C**
C**File name to store ro-vib wavefunction (JMAX>0) if the user chooses to write
C**them to disk with IDUMP>0
```