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
```

```
C**         or 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
C**         mode 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 (# of modes=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
C**         geometry 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 ro-vibrational 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 'ab initio' algorithm - terminate after
C**       'Normal mode' analysis if ISCFCI < 0
C**MOLPRO: Link stage with ab initio 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
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**
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```
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**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)
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))
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))
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***********************************************************************
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
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)
C-----------------------------------------------------------------------
C**
C**(MEFF(M),M=1,NMODE)
C**
C**MEFF:      Corresponding mode forming effective 1-dim potential for
C**           current mode.
C**MEFF(M)=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*==========================================================================
C**NCYCLE,TOLLAN,LANMAX,IGIV,LAN20
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:   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*==========================================================================
C**NVSYM,NWSYM
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 Cs molecules NVSYM=NWSYM=2 (A',A")
C**        For triatomic C2v molecules NVSYM=NWSYM=2 (A1,B2)
C**        For four-atom C2v molecules NVSYM=4 (A1,B2,B1,A2),
C**        NWSYM=3 (A1,B2,B1)
C**        For larger molecules, where reduction of symmetry to C2v is possible
C**        NVSYM=4 (A1,B2,B1,A2), NWSYM=4 (A1,B2,B1,A2)
C**        Where there is a centre of symmetry, C2v is converted to pseudo D2h
C**        NVSYM=8 (A1g,B2g,B1g,A2g; A1u,B2u,B1u,A2u), NWSYM=1 -> 8
```

```
C*********************************************************************
C**NSYM(NWSYM),ISYM(NWSYM,NSYM(NWSYM))   (order of NWSYM:  A1,B2,B1,A2)
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 C2v molecules, NWSYM=1 corresponds to A1,
C**       NWSYM=2 corresponds to B2
C**       For four-atom C2V molecules, NWSYM=1 corresponds to A1,
C**       NWSYM=2 corresponds to B2, NWSYM=3 corresponds to B1, etc.
C**       For D2h 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: NSYM=1,  ISYM(I)=3

C*********************************************************************
C**MVSYM,MWSYM(MVSYM)    (order of MWSYM:  A1,B2,B1,A2)
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**IDUMP,MDUMP,LDUMP
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**IDUMP:  Number of J=0 VCI functions written to disc (ICI < 0)
C**        IDUMP>0: IDUMP consecutive functions for each symmetry
C**        IDUMP<0: NDUMP(IABS(IDUMP)) specific functions for each symmetry
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**LDUMP:  Restart parameter for property fuunctions
C**        Currently the following single property is supported:
C**        LDUMP=1: input dipole functions and evaluate J=0 matrix elements


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)
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**        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*************************************************************************
C**NDEF
C-------------------------------------------------------------------------
C**
C**        SCF state definition
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 J. Comput.
C**        Chem., 17, 1645 (1996)).
C**
C**        NSTAT>0 and NDEF=0 or NDEF>0:
C**        Input NSTAT-1 records N1 N2 where N1 are the number of quanta for
C**        mode N2. All remaining modes take on NDEF quanta (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 above)
C**


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*********************************************************************
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*********************************************************************
C**XM(NATOM)
C---------------------------------------------------------------------
C**
C**(XM(I),I=1,NATOM)
C**XM:     Nuclear masses (U)
C**


C*********************************************************************
C**X0(NATOM,3)
C-------------
C**
C**(X0(NATOM,I),I=1,3)
C**X0:     Input NATOM records of reference structure x,y,z coordinates
C**Note:    In atomic unit
C**
```

```
C*********************************************************************
C**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*********************************************************************
C**USER-DEFINED POTENTIAL
C** At this point, control passes to the user to input any data he requires
C** in the routine USERIN (see USER.DOC)
C**
```