## Supplementary Material

This document contains Supplementary Material associated with the paper "**LEVEL**: A Computer Program for Solving the Radial Schrödinger Equation for Bound and Quasibound Levels", submitted to the *Journal of Quantitative Spectroscopy and Radiative Transfer* in February 2016. It consists of the six Appendices enumerated below. Note that Equation and Reference numbering appearing herein refer to the equation and reference numbering in the Journal Article.

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## Appendix A. Structure of the Input Data File

All of the READ statements for inputting data to the program, and the associated logical structure, are listed here. Appendix B then provides a detailed description of the nature of and/or options associated with each of the input variables.

```
#1       READ(5,*,END=999) IAN1, IMN1, IAN2, IMN2, CHARGE, NUMPOT
#2       IF(CHARGE.NE.0) READ(5,*) hCHARGE1, hCHARGE2
#3a      IF(IAN1.LE.0) READ(5,*) NAME1, MASS1
#3b      IF(IAN2.LE.0) READ(5,*) NAME2, MASS2
#4       READ(5,*) TITL
#5       READ(5,*) RH, RMIN, RMAX, EPS
         DO  IPOT= 1, NUMPOT
#6           READ(5,*) NTP, LPPOT, OMEGA, VLIM
             IF(NTP.GT.0) THEN
#7               READ(5,*) NUSE, IR2, ILR, NCN, CNN
#8               READ(5,*) RFACT, EFACT, VSHIFT
#9               READ(5,*) (XI(I), YI(I), I= 1,NTP)
               ELSE
#10               READ(5,*) IPOTL, QPAR, PPAR, Nbeta, APSE, IBOB
#11              READ(5,*) DSCM, REQ, Rref
                 IF(IPOTL.GE.4) THEN
#12                  READ(5,*) NCMM, rhoAB, sVSR2, IDSTT
                     DO i= 1,NCMM
#13                      READ(5,*) MMLR(i),CMM(i)
                         ENDDO
                     ENDIF
                 IF(NVARB.GT.0) THEN
                     IF((IPOTL.EQ.4).AND.(APSE.GT.0)) THEN
                         DO i= 1, NVARB
```

```
#14a                         READ(5,*) XPARM(I), PARM(I)
                             ENDDO
                       ELSE
#14b                     READ(5,*) (PARM(I), I=1,NVARB)
                      ENDIF
                     ENDIF
                IF(IBOB.GT.0) THEN
#15                  READ(5,*) MN1R, MN2R, qAD, pAD, NU1, NU2, qNA, NT1, NT2
#16                  IF(NU1.GE.0) READ(5,*) (U1(I), I=0,NU1)
#17                  IF(NU1.GE.0) READ(5,*) U1INF
#18                  IF(NU2.GE.0) READ(5,*) (U2(I), I=0,NU2)
#19                  IF(NU2.GE.0) READ(5,*) U2INF
#20                  IF(NT1.GE.0) READ(5,*) (T1(I), I=0,NT1)
#21                  IF(NT1.GE.0) READ(5,*) T1INF
#22                  IF(NT2.GE.0) READ(5,*) (T2(I), I=0,NT2)
#23                  IF(NT2.GE.0) READ(5,*) T2INF
                     ENDIF
              ENDIF
            ENDDO
#24     READ(5,*) NLEV1, AUTO1, LCDC, LXPCT, NJM, JDJR, IWR, LPRWF
        NLEV= MAX(1,NLEV1)
#25a    IF(AUTO1.GT.0) READ(5,*) (IV(I), IJ(I), I= 1,NLEV)
#25b    IF(AUTO1.LE.0) READ(5,*) (IV(I), IJ(I), GV(I), I= 1,NLEV)
        IF((LXPCT.NE.0).AND.(LXPCT.NE.-1)) THEN
#26         READ(5,*) MORDR, IRFN, DREF
#27         IF((IABS(IRFN).LE.9).AND.(MORDR.GE.0)) READ(5,*) (DM(J), J= 0,MORDR)
            IF(IRFN.GE.10) THEN
#28             READ(5,*) NRFN, RFLIM
#29             READ(5,*) NUSEF, ILRF, NCNF, CNNF
#30             READ(5,*) RFACTF, MFACTF
#31             READ(5,*) (XIF(I), YIF(I), I= 1,IRFN)
               ENDIF
            ENDIF
        IF(IABS(LXPCT).GE.3) THEN
#32         READ(5,*) NLEV2, AUTO2, J2DL, J2DU, J2DD
#33a        IF(AUTO2.GT.0) READ(5,*) (IV2(I),I= 1,NLEV2)
#33b        IF(AUTO2.LE.0) READ(5,*) (IV2(I),GV(I),I= 1,NLEV2)
          ENDIF
```

## Appendix B. Definitions and Description of Input Data File

Read integers identifying the molecule or system.

#1. `READ(5,*) IAN1, IMN1, IAN2, IMN2, CHARGE, NUMPOT`

**IAN1 & IAN2 :** integer atomic numbers of the atoms/particles #1 and 2 forming the molecule. If both are positive and $\leq 109$, atomic masses from the tabulation in subroutine MASSES are used to generate the reduced mass of the system. If either is $< 0$ or $> 109$ the mass of that non-standard particle will be input via READ #3. Setting `IAN`$i = 0$ selects masses of proton, deuteron or triteron for mass numbers `IMN`$i = 1 - 3$, respectively.

**IMN1 & IMN2 :** integer mass numbers of the atoms/particles #1 and 2 forming the molecule. For a normal stable atomic isotope, its mass is taken from the tabulation in subroutine MASSES; if its value lies outside the range for the normal stable isotopes of that atom, the abundance-averaged atomic mass will be used.

**CHARGE :** ± integer for the total charge on the molecule. Normally causes the reduced mass of a molecular ion to be defined as the 'charge-modified' reduced mass of Eq. (2) [5].

**NUMPOT :** the number of potentials considered: `NUMPOT` $= 1$ for calculations involving only a single potential function; `NUMPOT` $= 2$ to input and generate two different potentials and calculate matrix elements coupling their levels.

#2 `If(CHARGE` $\neq 0)$ `READ(5,*) CHARGE1, CHARGE2`

`CHARGE1 & CHARGE2`: the integer number of $m_e/2$ masses to be added to or subtracted from the normal masses of atoms #1 and #2 prior to calculation of a conventional 2-body reduced mass for each isotopologue [42, 68]. If `CHARGE1 = CHARGE2 = 0`, use Watson's charged-modified reduced mass for all species. Otherwise, necessarily, $^1/_2$`(CHARGE1 + CHARGE2) = CHARGE`.

In the special case in which `IAN1` and/or `IAN2` is either $\leq 0$ or $> 109$, read in a two-character alphanumeric name for that particle and its mass (in amu). This facilitates the treatment of model systems or exotic species such as muonium or positronium "molecules".

#3.a `IF(IAN1.LE.0) READ(5,*) NAME1, MASS1`
#3.b `IF(IAN2.LE.0) READ(5,*) NAME2, MASS2`

**NAME1 & NAME2 :** a two-character alphanumeric name for the (1 or 2) particle whose mass is being read, enclosed in single quotes, as in ′mu′.

**MASS1 & MASS2 :** the masses of particles 1 and 2, in amu.

Read a text title or description for the calculation.

#4. `READ(5,510) (TITL(I),I= 1,20)`

**TITL :** a title or output header for the calculation, consisting of up to 78 characters on a single line, enclosed between single quotes: e.g., ′title of problem′.

Read real numbers defining the mesh and range of the numerical integration (all in Å), and the eigenvalue convergence criterion to be used (in cm$^{-1}$).

#5 `READ(5,*) RH, RMIN, RMAX, EPS`

**RH :** the numerical integration mesh size; see discussion associated with Eq. (3) in § 2.1.

**RMIN & RMAX :** the inner and outer limits, respectively, of the range of numerical integration (see § 2.1). Plausible zero$^{th}$ order estimates would be `RMIN` ≈ 0.6×(potential inner wall position) and `RMAX` fairly large (say 40 Å). Internally `RMAX` is set to the smaller of: this read-in value, or the largest distance allowed by `RMIN`, `RH` and the array dimension `NDIMR` (see § 3).

**EPS :** the eigenvalue convergence parameter used by SCHRQ (in $\mathrm{cm}^{-1}$). To ensure that appropriately accurate expectation values or matrix elements are generated, it should normally be set *ca.* 2 orders of magnitude smaller than the eigenvalue precision actually required.

Some combination of the next 18 READ statements defines the potential energy function. A particular case always starts with READ #6, but then uses *either* READs #7–9 for numerical interpolation over a set of input turning points, *or* (some of) READ s #10–23 for the case of an analytic potential function.

#6. `READ(5,*) NTP, LPPOT, OMEGA, VLIM`

**NTP :** an integer that is set $\leq 0$ to generate an analytic potential using POTGEN, in which case the program skips READ s #7–9 and goes directly to READ #10. If `NTP` > 0 , it is the number of turning points to be input via READ #9.

**LPPOT :** controls printing of the potential array (normally set = 0 to have no printing). If `LPPOT` > 0 , write the potential and its first 2 derivatives-by-differences to standard output (Channel–6) at every `LPPOT`$^{th}$ mesh point; it is sometimes useful to do this when troubleshooting. Setting `LPPOT` < 0 writes the resulting potential in condensed format to Channel–8 at every |`LPPOT`|$^{th}$ mesh point; this is useful if one wants to employ this calculated potential as input for a plotting program.

**OMEGA :** the (integer) projection of the electronic orbital angular momentum onto the molecular axis for this state. It causes the reduced centrifugal potential to become $[J(J+1) - \mathtt{OMEGA}^2]\hbar^2/(2\mu r^2)$ . Setting `OMEGA` ≥ 99 will cause the centrifugal potential to have the form $[J^2 - 1/4]\hbar^2/(2\mu r^2)$ that is appropriate for rotation constrained to a plane.

**VLIM :** the absolute energy (in $\mathrm{cm}^{-1}$) of the potential asymptote. This value sets the absolute energy scale for the calculations. For power-series (GPEF- or Dunham-type) potentials (`IPOTL` = 2), it specifies the energy at the potential function minimum, where $r = r_e$ .

For a pointwise potential we must specify how the interpolation is to be done, and since `RMAX` usually lies outside the range of the input turning points, we also must specify how the potential is to be represented in that large–$r$ extrapolation region.

#7. `READ(5,*) NUSE, IR2, ILR, NCN, CNN`

**NUSE :** specifies how the interpolation is to be done. If `NUSE` > 0 , use `NUSE`–point piecewise polynomials; if `NUSE` ≤ 0 , perform cubic spline interpolation. For highly precise and smooth input points, such as those generated from an RKR calculation, `NUSE` = 8, 10 or 12 is often most appropriate; for less precise or less dense points, such as those from *ab initio* calculations, low-order piecewise polynomials (`NUSE` = 4) or a spline (`NUSE` ≤ 0) is normally best.

**IR2 :** for very steep repulsive potential walls, better interpolation is often attained by interpolating over $r^2 \times V(r)$, rather than over $V(r)$ itself; setting integer $\texttt{IR2} > 0$ causes this to be done (normally recommended). A comparison between results obtained with this option turned on *vs.* off provides an indication of the magnitude of ‘interpolation noise’ uncertainties in the final results.

**ILR :** specifies how to extrapolate from the outermost read-in turning points to `RMAX`. For a long extrapolation, one of $\texttt{ILR} = -1$, 0 or 1 is often most appropriate; however, if the outer turning points extend moderately close to the dissociation limit (at `VLIM`), one should set $\texttt{ILR} \geq 2$, specify the theoretically appropriate value of `NCN` ($\geq 1$), and if it is available, also input an estimate of `CNN` (see below).

For $\texttt{ILR} < 0$, fit the last 3 points to: $V(r) = \texttt{VLIM} - A \times \exp[-b(r - r_o)^2]$

For $\texttt{ILR} = 0$, fit the last 3 points to: $V(r) = \texttt{VLIM} - A \times r^p \times \exp[-b\,r]$ .

For $\texttt{ILR} = 1$, fit the last 2 points to: $V(r) = \texttt{VLIM} - A/r^B$ .

For $\texttt{ILR} = 2$ or 3, respectively, fit the outermost 2 or 3 points to a sum of 2 or 3 inverse-power terms, with powers differing by 2: $V(r) = \texttt{VLIM} - \sum_{m=0}^{\texttt{ILR}-1} C_{\texttt{NCN}+2m}/r^{\texttt{NCN}+2m}$ .

For $\texttt{ILR} \geq 4$, fit outermost `ILR` turning points to a sum of `ILR` inverse-power terms, with powers differing by 1: $V(r) = \texttt{VLIM} - \sum_{m=0}^{\texttt{ILR}-1} C_{\texttt{NCN}+m}/r^{\texttt{NCN}+m}$ .

**NCN :** For inverse-power potential extrapolation with $\texttt{ILR} \geq 2$, `NCN` ($> 0$) specifies the limiting inverse-power behaviour: $V(r) \propto \texttt{VLIM} - \texttt{CNN}/r^{\texttt{NCN}}$. Otherwise (for $\texttt{ILR} \leq 1$), it is a dummy input variable.

**CNN :** For inverse-power potential extrapolation with $\texttt{ILR} \geq 2$, setting $\texttt{CNN} \neq 0$ causes the leading inverse-power coefficient to be fixed at the read-in value $\texttt{CNN} = C_{\texttt{NCN}}$ [cm$^{-1}$ Å$^{\texttt{NCN}}$] rather than to be determined from a fit to the outermost turning points.

The input turning points may come from *ab initio* or RKR calculations, and their energies may need to be shifted to make them consistent with the value of `VLIM` input through READ #6, and they may also need also need to have their units converted to those employed in the program (Å and cm$^{-1}$).

#8. `READ(5,*) RFACT, EFACT, VSHIFT`

**RFACT & EFACT :** multiplicative factors required to convert units of the `NTP` input turning point distances `XI`($i$) and energies `YI`($i$) to Å and cm$^{-1}$, respectively. If no conversion is required, set these factors at `1.0D+0`.

**VSHIFT :** an energy shift (in cm$^{-1}$) to be added to the input potential point energies to make them consistent with the user-specified asymptote energy `VLIM`. It addresses the fact that the input *ab initio* or RKR turning points may be expressed relative to a different energy zero.

Read in the actual turning points.

#9. `READ(5,*) (XI(I), YI(I), I= 1,NTP)`

**XI($i$) & YI($i$) :** are the (distance, energy) input turning points defining the potential function.

If the input potential is defined by an analytic function (i.e., when $\texttt{NTP} \leq 0$), use subroutine POTGEN, which reads parameters *via* some or all of READs #10–23. For a user-supplied POTGEN function, no input parameters are read here, and its calling sequence must match that expected by subroutine PREPOT (see the discussion of § 2.6.9). The variable `NVARB`, which specifies the number of parameters being read in through READ #14, is determined internally, as specified below.

#10. `READ(5,*) IPOTL, QPAR, PPAR, Nbeta, APSE, IBOB`

**IPOTL** is an integer specifying the type of analytic function used for the potential.

$\texttt{IPOTL} = 1$: generates a Lennard-Jones($m = \texttt{QPAR}, n = \texttt{PPAR}$) potential energy function using Eq. (12). In this case `APSE` and `Nbeta` are dummy variables, and $\texttt{NVARB} = 0$.

$\texttt{IPOTL} = 2$: uses Eq. (13) to generate a GPEF power series potential of order $N_\beta = \texttt{Nbeta}$ using Seto's [27] form of the Šurkus [26] expansion variable $z = z(r) = (r^{\texttt{QPAR}} - r_e{}^{\texttt{QPAR}})/(a_S\, r^{\texttt{QPAR}} + b_S\, r_e{}^{\texttt{QPAR}})$, with $\beta_0$ defined by the input value of `DSCM`, $\texttt{PARM}(i) = \beta_i$ for $i = 1$ to `Nbeta`, $a_S = \texttt{PARM}(\texttt{Nbeta} + 1)$ and $b_S = (\texttt{Nbeta} + 2)$. *Note* that the Šurkus case of $\texttt{QPAR} < 0$ is accommodated by Seto's identity [27]: $z(-\texttt{QPAR}, a_S, b_S) = z(\texttt{QPAR}, -b_S, -a_S)$. For this case $\texttt{NVARB} = \texttt{Nbeta} + 2$, while `QPAR`, `APSE` and `NCMM` are dummy variables.

- Dunham expansions are generated by setting $\texttt{QPAR} = 1$, $\alpha_S = 0.0$ and $b_S = 1.0$.
- SPF expansions are generated by setting $\texttt{QPAR} = 1$, $\alpha_S = 1.0$ and $b_S = 0.0$.
- Ogilvie–Tipping expansions are generated by setting $\texttt{QPAR} = 1$, $\alpha_S = b_S = 0.5$.
- A harmonic oscillator potential is obtained by setting $\texttt{QPAR} = 1$, $\texttt{Nbeta} = 0$, $a_S = 0.0$ and $b_S = 1.0$, and the harmonic force constant is $k = 2\,\texttt{DSCM}/\texttt{REQ}^2$.
- All of these polynomial-type potentials have an undefined (or at best, indirectly-defined) asymptote, so parameter `VLIM` defines the potential energy minimum.
- If $\texttt{QPAR} = 0$, the potential is generated as an order–`Nbeta` polynomial in $r$ whose constant coefficient is set as $c_0 = \texttt{VLIM}$ and $\texttt{NVARB} = \texttt{Nbeta}$.

$\texttt{IPOTL} = 3$: generates the Morse or EMO potential of Eq. (15), in which $\mathfrak{D}_e = \texttt{DSCM}$, $r_e = \texttt{REQ}$, and the expansion-variable of Eq. (17) is defined by the positive integer $q = \texttt{QPAR}$, while the expansion coefficients are $\texttt{PARM}(i) = \beta_{i-1}$ for $i = 1$ to $\texttt{NVARB} = (\texttt{Nbeta} + 1)$. In this case `PPAR` and `APSE` are dummy variables. Setting $\texttt{Nbeta} = 0$ ($\texttt{NVARB} = 1$) yields the ordinary Morse potential.

If $\texttt{QPAR} \leq 0$, generate the 4–parameter Morse-like potential of Hua Wei [36], $V(r) = \mathfrak{D}_e \left([1 - e^{-b\,(r-r_e)}]/[1 - C\, e^{-b\,(r-r_e)}]\right)^2$ in which $b = \texttt{PARM}(1)$ and $C = \texttt{PARM}(2)$. In this case $\texttt{NVARB} = 2$ while `QPAR`, `APSE` and `Nbeta` are dummy variables.

$\texttt{IPOTL} = 4$: generates an MLR potential from Eqs. (19–20) [33, 34, 37], in which $\mathfrak{D}_e \equiv \texttt{DSCM}$, $r_e \equiv \texttt{REQ}$, and the potential tail $u_{\rm LR}(r)$ is defined either by Eq. (20) or by one of the coupled-state matrix eigenvalues discussed at the end of § 2.6.4.

For $\texttt{APSE} \leq 0$, the exponent coefficient in Eq. (19) is represented by the constrained polynomial expansion of Eq. (23), in which positive integers $\texttt{QPAR} = q$ and $\texttt{PPAR} = p$ are the powers defining its two radial variables, and the upper bound on the summation is $N_\beta = \texttt{Nbeta}$, while the exponent expansion coefficients are $\texttt{PARM}(i) = \beta_{i-1}$ for $i = 1$ to $\texttt{NVARB} = (\texttt{Nbeta} + 1)$.

For `APSE` $> 0$, the exponent coefficient in Eq. (19) is represented by the natural cubic spline of Eq. (24) passing through `Nbeta` points at distances defined by the set of input $y_q^{\rm ref}$ values, whose ordinate values $\beta_i = \texttt{PARM}(i)$ for $i = 1$ to `Nbeta` define the potential function shape.

`IPOTL` $= 5$: generates the DELR potential of Eqs. (28−30) [11], in which $\mathfrak{D}_e \equiv \texttt{DSCM}$, $r_e \equiv \texttt{REQ}$, the power defining the expansion variable $y_q^{\rm ref}(r)$ is $\texttt{QPAR} = q$, and the exponent coefficient $\beta(r)$ is the simple power-series expansion of Eq. (16) in $y_q^{\rm ref}(r)$ with expansion coefficients $\texttt{PARM}(i) = \beta_{i-1}$ for $i = 1$ to $(\texttt{NVARB} = \texttt{Nbeta} + 1)$. The additive long-range tail function $u_{\rm LR}(r)$ is defined either by Eq. (20) or by one of the diagonalizations mentioned at the end of § 2.6.4 (see Reads #12 and 13), and `PPAR` is a dummy parameter.

`IPOTL` $= 6$: generates a generalized HFD-type potential from Eq. (31), with $A_{\rm HFD}$ and $\beta_1$ defined (internally) by the input values of $\mathfrak{D}_e \equiv \texttt{DSCM}$, $r_e \equiv \texttt{REQ}$, and the attractive inverse-power-sum tail, while the parameters defining the damping function $D_{\rm HFD}(r)$ are read in as $\texttt{PARM}(i) = \alpha_i$ for $i = 1 - 3$, and the other exponent coefficients are $\beta_2 = \texttt{PARM}(4)$ and $\gamma = \texttt{PARM}(5)$. For this case, the inverse-power long-range coefficients $C_m$ (in units cm$^{-1}\cdot$Å$^m$) are input through Read #13, and $\texttt{Nbeta} = \texttt{NVARB} = 5$, while `PPAR`, `QPAR` and `APSE` are all dummy parameters.

`IPOTL` $= 7$: generates a generalized Tang-Toennies-type potential from Eq. (33), with the attractive term $u_{\rm LR}(r)$ defined by Reads #12 and 13, and the repulsive term parameters $\{\beta_i\}$ read in as $\texttt{PARM}(i)$ for $i = 1$ to $\texttt{NVARB} = \texttt{Nbeta} = 9$. The reported values of the well depth $\mathfrak{D}_e$ and equilibrium distance $r_e$ are read in as `DSCM` and `REQ`, respectively, and the code compares them with the actual energy and position of the potential minimum as defined by the $\{\beta_i\}$ and $\{C_m\}$ input parameters. For this case, `PPAR`, `QPAR`, and `APSE` are dummy parameters.

`IPOTL` $= 8$: generates a 'Hannover Polynomial Potential' (HPP) [58] from Eq. (34), a power series of order `Nbeta` in the variable $\xi = (r - r_m)/(r + b\, r_m)$, with coefficients $\beta_i = \texttt{PARM}(i+1)$ for $i = 0$ to `Nbeta`, in which $b = \texttt{PARM}(\texttt{Nbeta} + 2)$. The well depth $\mathfrak{D}_e$ is read as `DSCM`, and the reference distance $r_m$ (which for $a_1 \neq 0$ is *not* identical to $r_e$) is read in as `REQ`. For $r < r_{\rm inn} \equiv \texttt{PARM}(\texttt{Nbeta}{+}3)$ the potential is extrapolated inward by smoothly attaching the function $A\, e^{-\alpha(r - r_{\rm inn})}$ at distance $r_{\rm inn}$. For $r > r_{\rm out} \equiv (\texttt{Nbeta} + 4)$ the potential is extrapolated outward continuously as the sum of `NCMM` inverse-power terms defined by Reads #12 and 13, with the (internal) inclusion of an additional term $C_{m_{\rm L}}/r^{m_{\rm L}}$ with $m_{\rm L} = [\texttt{MMLR}(\texttt{NCMM}) + 2]$, whose coefficient $C_{m_{\rm L}}$ is defined (internally) to attach this long-range tail continuously to the polynomial at $r = r_{\rm out}$. For this model, `QPAR`, `PPAR` and `APSE` are dummy parameters, and $\texttt{NVARB} = (\texttt{Nbeta} + 4)$.

**QPAR, PPAR, Nbeta and APSE:** integers used to characterize specific potential forms (see above).

**IBOB:** an integer to specify whether (for `IBOB` $> 0$) or not (for `IBOB` $\leq 0$) atomic-mass-dependent Born-Oppenheimer breakdown correction terms are to be included in the potential energy function $V(r)$, and/or in the centrifugal $\{\, [J(J+1) - \Omega^2]\hbar^2/(2\mu r^2)\, \}$ potential (see § 2.7).

#11. `READ(5,*) DSCM, REQ, Rref`
#12. `IF(IPOTL.GE.4) READ(5,*) NCMM, rhoAB, sVSR2, IDSTT`
#13. `IF(IPOTL.GE.4) READ(5,*) (MMLR(I), CMM(I), I= 1,NCMM)`

**DSCM :** normally (except for the `IPOTL` $= 2$ case) the potential well depth $\mathfrak{D}_e$ in $\mathrm{cm}^{-1}$.

**REQ :** normally (except for the `IPOTL` $= 8$ case, in which it defines $r_m$) the equilibrium distance $r_e$ in Å.

**Rref :** the reference distance in the definition of the exponent expansion radial variable of Eqs. (17) and (23). If the input value is $\leq 0.0$, the code sets $r_{\mathrm{ref}} = r_e$.

**NCMM :** the number of inverse-power long-range terms to be incorporated into $u_{\mathrm{LR}}(r)$ via Eq. (20), or to be used to define the elements of the $2 \times 2$ or $3 \times 3$ matrices whose eigenvalues define $u_{\mathrm{LR}}(r)$ for $nS + nP$ alkali homo-dimers [33, 49–51, 69].

For the $2 \times 2$ alkali-homodimer ($\mathrm{X}_2$) cases, set `NCMM` $= 7$ with `MMLR`$(1) = 0$ or $-1$ and `MMLR`$(i > 1) =$ 3, 3, 6, 6, 8, 8, while the input values of `CmVAL`$(i)$ are $A_{\mathrm{so}}$, $C_3^{\Sigma}$, $C_3^{\Pi}$, $C_6^{\Sigma}$, $C_6^{\Pi}$, $C_8^{\Sigma}$ and $C_8^{\Pi}$ for $i = 1 - 7$, respectively, and

- For the $A\,^1\Sigma_u^+$ state of $\mathrm{X}_2$, set `MMLR(1)= 0` to select the lower root of the $2 \times 2$ determinant.
- For the $b\,^3\Pi_u$ state of $\mathrm{X}_2$, set `MMLR(1)= -1` to select the upper root of the $2 \times 2$ determinant.

For the $3 \times 3$ alkali-homodimer cases, set `NCMM` $= 10$ with `MMLR`$(1) = -2$ or $-3$ or $-4$, and `MMLR`$(i > 1) =$ 3, 3, 3, 6, 6, 6, 8, 8, 8, while `CmVAL`$(i) = A_{\mathrm{so}}$, $C_3^{\Sigma}$, $C_3^{1\Pi}$, $C_3^{3\Pi}$, $C_6^{\Sigma}$, $C_6^{1\Pi}$, $C_6^{3\Pi}$, $C_8^{\Sigma}$, $C_8^{1\Pi}$ and $C_8^{3\Pi}$, respectively, and:

- For the $1\,^3\Sigma_g^+$ state of $\mathrm{X}_2$, set `MMLR(2)= -2` to select the lowest root of the $3 \times 3$ determinant [49, 50].
- For the $B\,^1\Pi_u$ state of $\mathrm{X}_2$, set `MMLR(2)= -3` to select the middle root of the $3 \times 3$ determinant.
- set `MMLR(2)= -4` to select the highest root of the $3 \times 3$ determinant.

**rhoAB :** selects whether (`rhoAB` $> 0$) or not (`rhoAB` $\leq 0$) damping functions are to be used with the inverse-power long-range terms. If `rhoAB` $> 0$, it is the value of the system-dependent range-scaling parameter of $\rho$ of Eqs. (25) and (26).

**sVSR2 :** when damping functions are used, integer `sVSR2` is twice the value of the very-short-range power parameter '$s$' of Eqs. (25)-(27), (`sVSR2` $\equiv 2\,s$). For the generalized Tang-Toennies functions of Eq. (26), its allowed values are -4 -2, 0, 2, or 4, while for the generalized Douketis-type functions of Eq. (25), its allowed values are -4, -3, -2, -1, or 0.

**IDSTT :** an integer specifying the form of the damping function, for `rhoAB` $> 0$ :

- `IDSTT` $> 0$ invokes use of the Douketis-type damping functions of Eq. (25).
- `IDSTT` $\leq 0$ specifies use of the Tang-Toennies-type damping functions of Eq. (26).

#14 a. `IF((IPOTL.EQ.4).AND.(APSE.GT.0)) READ(5,*) (XPARM(I), PARM(I), I=1,NVARB)`

**XPARM($i$) & PPARM($i$)** : the `NVARB` values of the distance coordinate $y_q^{\mathrm{ref}}(r_i)$ and of the associated exponent coefficient $\beta(r_i)$ defining the cubic spline used to represent the MLR exponent coefficient function $\beta(r)$ when `APSE` $> 0$. Read them in, one pair per line.

#14 b. `IF((NVARB.GE.0).AND.(APSE.LE.0)) READ(5,*) (PARM(I), I=1,NVARB)`

**PPARM($i$) :** are the `NVARB` parameters characterizing the potential functions described above for all cases *other* than an MLR with `APSE` $> 0$. For example, the $\beta_i$ parameters of Eqs. (13), (23), (33) or (34), or the coefficients $\beta_i$ of the exponent polynomials defining the EMO or DELR potentials.

If atomic-mass-dependent Born-Oppenheimer breakdown (BOB) terms are to be incorporated into the potential energy and/or centrifugal potential functions ( `IBOB` $> 0$ ), use Reads #15 and two or more (as needed) of #16–23. These BOB functions have the forms defined by Eqs. (35) and (36). If a given type of correction function is to be omitted, the associated expansion order (e.g., `NU1`, `NU2`, `NT1` or `NT2`) should be set $< 0$, in which case the associated parameter Read statements (from among #16–23) are omitted, while if no BOB corrections are considered (`IBOB` $\leq 0$), omit all of Reads #15–23.

#15. `READ(5,*) MN1R, MN2R, QAD, PAD, NU1, NU2, QNA, NT1, NT2`

**MN1R & MN2R :** The integer mass numbers of the *reference* isotopes of atoms 1 and 2 , respectively, whose masses $M_a^{\rm ref}$ appear in Eqs. (35) and (36) [70].

**NU1 & NU2 :** For atoms $a = 1$ and 2 (or $A$ and $B$), these are the orders $N_{\rm ad}^a$ of the polynomial expansions of Eq. (35). If either of them is set $< 0$ , neglect the corresponding pair from among Reads #16 − 19.

**NTA & NTB :** For atoms $a = 1$ and 2 (or $A$ and $B$), these are the orders $N_{\rm na}^a$ of the polynomial expansions of Eq. (36). If either of them is set $< 0$ , neglect the corresponding pair from among Reads #20 − 23.

**QAD , PAD & QNA :** positive integers $q_{\rm ad}$ , $p_{\rm ad}$ , and $q_{\rm na}$ , respectively, define the variables $y_p^{r_e}(r)$ and $y_q^{r_e}(r)$ in the expressions for the potential energy and centrifugal BOB functions of Eqs. (35) and (36). One should normally set `PAD` $\equiv p_{\rm ad} > m_{\rm Last} \equiv$ `MMLR(NCMM)` . Note that if `PAD` $= 0$ and `U`$a$`INF` $= 0$ , the adiabatic potential correction function is collapsed to a simple power series in $y_q(r)$.

For cases in which `IBOB` $> 0$ ,

#16. `IF(NU1.GE.0) READ(5,*) (U1(i), i= 0,NU1)`
#17. `IF(NU1.GE.0) READ(5,*) U1INF`
#18. `IF(NU2.GE.0) READ(5,*) (U2(i), i= 0,NU2)`
#19. `IF(NU2.GE.0) READ(5,*) U2INF`
#20. `IF(NT1.GE.0) READ(5,*) (T1(i), i= 0,NT1)`
#21. `IF(NT1.GE.0) READ(5,*) T1INF`
#22. `IF(NT2.GE.0) READ(5,*) (T2(i), i= 0,NT2)`
#23. `IF(NT2.GE.0) READ(5,*) T2INF`

**U$a$($i$) and U$a$INF :** For $a = 1$ or 2, they are, respectively, the `REAL*8` expansion parameters and limiting asymptotic values defining the 'adiabatic' potential correction functions of Eq. (35): `U`$a(i) = {u_i}^a$ and `U`$a$`INF` $= u_\infty^a$ , all have units cm$^{-1}$.

**T$a$($i$) and T$a$INF :** For $a = 1$ or 2, they are, respectively, the `REAL*8` expansion parameters and limiting asymptotic values defining the 'non-adiabatic' centrifugal potential energy correction functions of Eq. (36). All of `T`$a(i) = {t_i}^a$ and `T`$a$`INF` $= t_\infty^a$ are dimensionless.

For a calculation involving only a single potential energy curve ( `NUMPOT` $= 1$ in Read #1), the code now proceeds directly to Read #24. However, if `NUMPOT` $= 2$ , it first first repeats Reads #6–23 to input the second potential function.

Now read the parameters controlling which levels (of Potential-1) are to be calculated, and what expectation values and or matrix elements are to be calculated (if any).

#24. `READ(5,*) NLEV1, AUTO1, LCDC, LXPCT, NJM, JDJR, IWR, LPRWF`

**NLEV1 :** • if $> 0$ , integer `NLEV1` is the number of vibrational or vibrotational levels to be calculated. Their quantum number specifications are then input via Read #25.

• if $\leq 0$ , the program automatically finds all vibrational levels from $v = 0 - |$`NLEV1`$|$ associated with the rotational quantum number read in as `IJ`(1) (see below). If the input value of `NLEV` is very large and negative, the program will (attempt to) find *all* possible vibrational levels associated with the specified $J =$ `IJ`(1).

**AUTO1 :** integer `AUTO1` $> 0$ (normal option) causes the program to (attempt to) generate automatically realistic trial eigenvalues for all desired levels, so that only their quantum number labels need be input via (Read #25a). If this fails, setting `AUTO1` $\leq 0$ will allow/require a trial energy `GV`$(i)$ to be input (via Read #25b) for each specified level using the `NLEV1` $> 0$ option.

**LCDC :** If `LCDC` $> 0$ , calculate the inertial rotational constant $B_v$ and the first 6 centrifugal distortion constants $\{-D_v, H_v, L_v, M_v, N_v, \,\&\, O_v\}$ for all of the levels specified by `NLEV1`. These results are also written in a compact format to Channel-9.

**LXPCT :** An integer controlling which expectation values/matrix elements are to be calculated. For `LXPCT` $= 0$ , no expectation values or matrix elements are calculated (in which case Read s #26–31 are omitted).

• *Even* values of $|$`LXPCT`$| \neq 0$ cause the results to be written in compact form to Channels–7 or 8 (as appropriate, see below), as well as to Channel-6;

• *Odd* values of `LXPCT` yield only Channel–6 output, while *negative* values of `LXPCT` cause most of the (relatively wordy) output to Channel–6 to be suppressed.

`LXPCT` $= -1$ causes the eigenvalues and (if appropriate) quasibound level widths to be written compactly to Channel–7, and no expectation values or matrix elements are calculated (so Read s #$26 - 31$ are omitted).

`LXPCT` $= 1$, 2 or $-2$ causes calculation of expectation values of the kinetic energy and of positive powers of the distance variable specified by Read #26 plus either #27 or #$28 - 31$ (as appropriate, see below). Write results to Channel–6 if `LXPCT` $= 1$ or 2; also write them (compactly) to Channel–7 if `LXPCT` $= 2$ , and write them only (compactly) to Channel–8 if `LXPCT` $= -2$.

$|$`LXPCT`$| \geq 3$ invokes the calculation of matrix elements coupling levels of Potential-1 to each other (if `NUMPOT` $= 1$) or to levels of Potential-2 (if `NUMPOT` $= 2$), as specified by Reads #27 and 28. Write results to Channel–6 if `LXPCT` $> 0$ and (compactly) to Channel–8 if `LXPCT` $= \pm 4$ .

$|$`LXPCT`$| \geq 5$ also causes the component radial moments comprising the overall matrix elements to be written to Channel–7, while still writing the overall matrix elements for selection-rule allowed transitions to Channel–8. For `LXPCT` $= \pm 6$ write *only* the radial moment components, and omit the output to Channel–8.

**NJM & JDJR:** if (integer) `NJM` $> 0$, then for each (vibrational) level generated by the `NLEV1` specification, automatically calculate eigenvalues (and if appropriate, expectation values and matrix elements) for all rotational sublevels $J$ ranging from the input-specified (see below) $J = \texttt{IJ}(i)$ to a maximum of $J = \texttt{NJM}$ (or until that vibrational level energy predissociates above the potential barrier), with $J$ increasing in steps of `JDJR`. e.g., to determine automatically *all* possible rotational levels, set $\texttt{JDJR} = 1$, $\texttt{IJ}(i) = 0$ (or more strictly $= |\Omega|$) and `NJM` very large (e.g., $\texttt{NJM} = 999$).

**IWR:** an integer controlling the printout of diagnostics and calculation details inside subroutine SCHRQ.

- If $\texttt{IWR} \neq 0$ print warning and error messages inside SCHRQ, as appropriate. Unless one is troubleshooting, normally set $\texttt{IWR} = -1$.
- If $\texttt{IWR} \geq 1$ also print final eigenvalue and node count for every level determined.
- If $\texttt{IWR} \geq 2$ also print end-of-range wave function amplitudes.
- If $\texttt{IWR} \geq 3$ also print intermediate trial eigenvalues as the iterative convergence proceeds.

**LPRWF:** • If `LPRWF` $> 0$ write to Channel–6 the wavefunction of each specified level at every $\{\texttt{LPRWF}\}^{th}$ mesh point.

- If `LPRWF` $< 0$ write wavefunction of each specified level compactly to Channel–10, at every $|\texttt{LPRWF}|^{th}$ mesh point.
- If $\texttt{LPRWF} = 0$, no wavefunction printout.

**SINNER & INNOD1:** parameters to facilitate finding inner *vs.* outer wells of a double well potential if `IAUTO1` $> 0$ fails, or to facilitate treating a precisely symmetric potential. These parameters may be added to READ #24 by making small modifications to Lines #411–423 of the code.

Read quantum numbers specifying which vibration-rotation levels (of Potential-1) are to be determined.

#25 a. `IF(AUTO1.GT.0) READ(5,*) (IV(`$i$`),IJ(`$i$`),`$i$`= 1,`$max$`{1,|NLEV1|})`

#25 b. `IF(AUTO1.LE.0) READ(5,*) (IV(`$i$`),IJ(`$i$`),GV(`$i$`),`$i$`= 1,`$max$`{1,|NLEV1|})`

**IV($i$) & IJ($i$):** • For `NLEV1` $> 0$ these are the vibrational $[\,v = \texttt{IV}(i)\,]$ and rotational $[\,J = \texttt{IJ}(i)\,]$ quantum numbers of the levels to be determined; if $\texttt{NJM} > \texttt{IJ}(i)$ the program also automatically calculates rotational levels for that $v = \texttt{IV}(i)$ with $J = \texttt{IJ}(i)$ to `NJM` in steps of `JDJR`.

- For `NLEV1` $\leq 0$, read one $\{\texttt{IV}(i), \texttt{IJ}(i)\}$ pair. The value of $\texttt{IV}(1)$ is ignored, but $J = \texttt{IJ}(1)$ is the rotational quantum number for which all vibrational levels up to $v = |\texttt{NLEV1}|$ are to be determined.

**GV($i$):** If `AUTO1` $\leq 0$, READ #25b is used in place of #25a, and $\texttt{GV}(i)$ is the trial energy read in for each level $v = \texttt{IV}(i)$, $J = \texttt{IJ}(i)$. This option presumes `NLEV1` $> 0$.

If expectation values or matrix elements are to be calculated (i.e., if LXPCT$\neq 0$ or $-1$), READs #$26 - 31$ specify the desired arguments. However, if $\texttt{LXPCT} = 0$ or $-1$, the data input for this case is now finished.

#26. `READ(5,*) MORDR, IRFN, DREF`

**MORDR :** an integer specifying the highest power of the chosen radial function or distance coordinate `RFN`$(r)$ for which expectation values or matrix elements are to be calculated (see Eq. (8)). The current program version is dimensioned for `MORDR` $\leq 20$ . To calculate only Franck-Condon factors (when $|$`LXPCT`$| \geq 3$), set `MORDR` $= -1$ .

**IRFN & DREF :** integer and real variables, respectively, specifying the definition of the radial function or distance coordinate `RFN`$(r)$.

- If `IRFN` $\leq -10$ , `RFN` is generated by user-supplied code inserted at Lines #565-586 of the main program. In this case `DREF` is a dummy variable, and READs #27-31 are omitted.
- If `IRFN` $= -4$ , then `RFN`$(r) = r$ and the matrix element operator is a polynomial in $r$, of order `MORDR`, and having coefficients `DM`$(i)$, that pre-multiplies the derivative operator $^{d}/_{dr}$ that acts on the wavefunction for 'Potential–2' (inserted for Bob Field).
- If `IRFN` $= -3$ , `RFN`$(r) = 1/r^3$ .
- If `IRFN` $= -2$ , `RFN`$(r) = 1/r^2$ .
- If `IRFN` $= -1$ , use a Dunham-type expansion coordinate `RFN`$(r) = (r - \texttt{DREF})/\texttt{DREF}$ .
- If `IRFN` $= 0$ , the function `RFN`$(r) = r$ , the distance coordinate itself.
- If `IRFN` $= 1 - 9$ , use the Šurkus-type variable `RFN`$(r) = y_p^{\texttt{DREF}}(r) = (r^p - \texttt{DREF}^{\,p})/(r^p + \texttt{DREF}^{\,p})$ , with $p =$ `IRFN` .

For `IRFN` $= -1$ or $1 - 9$ , a positive (real) input value of `DREF` specifies it as the reference distance $r =$ `DREF` ; for these cases, normally set `DREF` $= r_e$ . However, if the input value of `DREF` $\leq 0.0$ , the program internally (iteratively) determines a value of `DREF` such that the expectation value of `RFN`$(r)$ is identically zero for the first vibration-rotation level considered.

If `IRFN` $\geq 10$ , `RFN`$(r)$ is a function defined by reading in and interpolating over (and extrapolating beyond) input values of some known radial function (e.g., a dipole or transition moment function). This reading and interpolation/extrapolation is performed by the same subroutine package PREPOT used to treat a numerical input potential (see READs #6–9). In this case `DREF` is a dummy variable, READ #27 is omitted, and the code internally sets `MORDR` $= 1$, `DM(0)` $= 0.0$ and `DM(1)` $= 1.0$ .

#27. `IF(DABS(IRFN).LE.9) READ(5,*) (DM(J), J= 0,MORDR)`

**DM(j) :** Coefficients of the power series in `RFN`$(r)$ defining the argument of the overall expectation values or matrix elements: $M(r) = \sum_{j=0}^{\texttt{MORDR}} \texttt{DM}(j) \times \texttt{RFN}(r)^j$ .

If the expectation value or matrix element radial function argument is to be defined by interpolating over and extrapolating beyond a set of read-in points (`IRFN` $\geq 10$), use the same read sequence, options and procedures employed for treating a numerical input potential. Most input parameters here have definitions essentially equivalent to those associated with READ #6–9.

#28. `READ(5,*) NRFN, RFLIM`
#29. `READ(5,*) NUSEF, ILRF, NCNF, CNNF`
#30. `READ(5,*) RFACTF, MFACTF`
#31. `READ(5,*) (XIF(I), YIF(I), I= 1,NRFN)`

**NRFN :** Is the number of known function values $\{$`XIF`$(i)$, `YIF`$(i)\}$ to be read in,

**RFLIM :** Is the limiting asymptotic value imposed when extrapolating beyond the range of the input values, and

**NUSEF :** Specifies how the interpolation is to be performed, while **ILRF**, **NCNF** and **CNNF** define the manner in which it extrapolates to large $r$ (see comments for READ #7).

**RFACTF & MFACTF :** Convert units of input distances `XIF`$(i)$ and ordinates `YIF`$(i)$, respectively, to Å and whatever units are required for the expectation value/matrix element argument $M(r)$ (debye, for a dipole or transition moment function).

For matrix element calculations ( $|\texttt{LXPCT}| \geq 3$ ), couple each level of Potential-1, generated as specified by READ s #24 and 25, to all rotation levels of the `NLEV2` vibrational levels $v = \texttt{IV2}(i)$ allowed by the rotational selection rules $\Delta J = \texttt{J2DL}$ to `J2DU` in steps of `J2DD` (e.g., for $P$ and $R$ transitions: $\texttt{J2DL} = -1$ , $\texttt{J2DU} = +1$ $\texttt{J2DD} = +2$ ). If $\texttt{NUMPOT} = 2$ these are levels of Potential-2 and no constraints are imposed, but if $\texttt{NUMPOT} = 1$ the matrix elements couple levels of Potential-1 to one another, and to avoid redundancy the program considers only emission from (rotational sublevels of) these `NLEV2` vibrational levels into *lower* ($v''$, $J''$) levels generated as per READ s #32 & 33. Integer $\texttt{AUTO2} > 0$ causes **LEVEL** to generate trial eigenvalues automatically for all desired levels (preferred option), so only their vibrational quantum number labels need be input (READ #33a). If this fails, setting $\texttt{AUTO2} \leq 0$ will require a trial pure vibrational energy `GV2`$(i)$ to be read in (READ #33b) for each specified level.

#32. `READ(5,*) NLEV2, AUTO2, J2DL, J2DU, J2DD`
#33 a. `IF(NLEV2.GT.0) READ(5,*) (IV2(I), I= 1,NLEV2)`
#33 b. `IF(NLEV2.GT.0) READ(5,*) (IV2(I), GV2(I), I= 1,NLEV2)`

## Appendix C : Illustrative Cases and Sample Input and Output Files

The running time for this program depends entirely upon the complexity of the calculation being performed and the type of computer being used; CPU requirements may range from a fraction of a second to a couple of minutes. This Appendix presents three sets of sample data files and the resulting output for representative cases illustrating some of the types of problems to which the program may be applied. The sets of sample input data files described below are available as a plain ASCII text file in the Supplementary Material associated with this paper. Note that entries after the "%" sign on each line of those input data files are comments identifying the variables, and are ignored by the program.

### Appendix C 1 : Input/Output for LJ(12,6) PECs and a double minimum potential

The first three cases considered in this subsection are based on use of a simple Lennard-Jones(12,6) potential and serve to provided an introduction to the types of calculations that may be performed, and illustrates the nature of the resulting output. The fourth case is introduced to illustrate the ability of **LEVEL** to locate specified eigenvalues of a double-minimum potential. On a decade-old SGI UNIX workstation, the 4 examples of **Case 1** require 0.125 *s* of CPU time.

**Case 1 :** This data file consists of five separate data sets that illustrate a variety of the capabilities of the program, including the fact that it can treat several independent problems in a single run by simply putting the input data for several cases into the same file, one after the other.

(a) For a Lennard-Jones(12,6) potential, find all the vibrational levels, and calculate the associated values of the centrifugal distortion constants. This is a model system with fictitious particle masses, so those masses and the chosen particle names ′L1′ and ′J2′ are input by READ #3.

(b) For the same simple model Lennard-Jones(12,6) potential of Case 1 (a), calculate all possible infrared matrix elements involving levels with $v \leq 2$ and $J(upper) \leq 1$ .

(c) For the same model Lennard-Jones(12,6) potential of Case 1a (a), locate all (four) vibrational levels of the centrifugally-distorted potential associated with $J = 18$ . This demonstrates that the procedure for automatically finding all vibrational levels works for a potential with a barrier (here, centrifugal in origin) protruding above its dissociation limit. This example invokes the highest print level inside SCHRQ (by setting `IWR` $= 3$ , see READ #24) in order to illustrate the progress of the iterative eigenvalue convergence procedure. In this case convergence details for each level are presented twice (though only one iteration is required the second time) because of a quirk of the internal program logic.

(d) To illustrate the ability to determine the eigenvalues of a double-minimum potential, find the eigenvalues for vibrational levels $v = 56 - 80$ of an *ab initio* potential for the $^3\Pi_g$ state of $Cl_2$ [71], and calculate expectation values of various powers of $r$. The lowest of these levels lies in the region in which all levels belong to the deeper outer well, while the highest lies above the barrier separating the two wells. The output expectation values show that as the energy increases, the region of maximum wave function amplitude hops back and forth between the two wells. This case illustrates the ability of the program, and in particular, its automatic level-finder subroutine `ALF`, to find arbitrary levels of a double minimum potential automatically.

```
 -1 0  -1 0   0   1                % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
 'L1' 30.34373256D0                % NAME1 MASS1
 'J2' 30.34373256D0                % NAME2 MASS2
'Case 1.a: For a model L.J.(12,6) get all vib. levels and their CDCs'
 0.0020  0.6  20.  1.d-6           % RH RMIN RMAX EPS
 0  0  0  0.D0                     % NTP LPPOT IOMEG VLIM
 1  12 6  0  0  0                  % IPOTL PPAR QPAR APSE Nbeta IBOB
  1000.d0   1.d0  1.d0             % DSCM REQ Rref
-999  1  1  -1  0 1  -1 0          % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR
LPRWF
  0 0                              % IV(1) IJ(1)

 -1 30  -1 30   0   1              % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
 'L1' 30.34373256D0                % NAME1 MASS1
 'J2' 30.34373256D0                % NAME2 MASS2
'Case 1.b: For same model L.J.(12,6) get radial matrix elements for v < 3'
 0.0020  0.6  20.   1.d-6          % RH RMIN RMAX EPS
 0  0  0  0.D0                     % NTP LPPOT IOMEG VLIM
 1  12 6  0  0  0                  % IPOTL PPAR QPAR APSE Nbeta IBOB
  1000.d0   1.d0  1.d0             % DSCM REQ Rref
-2  1  0  5  1 1  -1 0             % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR
LPRWF
  0 0                              % IV(1) IJ(1)
 4 -1  1.D0                        % MORDR IRFN RREF
 1.d0  -0.2d0 0.03d0 -0.004d0 0.0005d0  % {DM(j)}
 3  1  -1 +1 2                     % NLEV2 AUTO2 J2DL J2DU J2DD
  0  1  2                          % IV2(1) IV2(2) IV2(3)


 -1 0  -1 0   0   1                % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
 'L1' 30.34373256D0                % NAME1 MASS1
 'J2' 30.34373256D0                % NAME2 MASS2
'Case 1.c: For the same L.J.(12,6), find levels of potential with a barrier'
 0.0020  0.6  20.  1.d-6           % RH RMIN RMAX EPS
 0  0  0  0.D0                     % NTP LPPOT IOMEG VLIM
 1  12 6  0  0  0                  % IPOTL PPAR QPAR APSE Nbeta IBOB
  1000.d0   1.d0  1.d0             % DSCM REQ Rref
-999  1  0  -1  0 1   3  0         % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR
LPRWF
  0 18                             % IV(1) IJ(1)


17 35  17 35   0   1               % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
'Case 1.d:  Levels of a pointwise double-minimum potential for 3(PI)g Cl2'
 0.001  1.6  10.   1.d-06          % RH RMIN RMAX EPS
 29  0  0  95440.D0                % NTP LPPOT IOMEG VLIM
 0 0  2  1  0.D5                   % NUSE IR2 ILR NCN CNN
 0.5291772108D0  8065.5444D0  0.d0   % RFACT EFACT VSHIFT
  3.34 10.608 3.40 9.683  3.43 9.221  3.49 8.758
  3.57 8.295  3.66 8.132  3.76 8.051  3.86 8.132  3.94 8.268
  4.03 8.350  4.17 8.595  4.26 8.704  4.31 8.758  4.46 8.432
  4.56 8.134  4.66 7.887  4.80 7.615  4.91 7.425  5.00 7.343
  5.17 7.125  5.37 6.962  5.51 6.908  5.66 6.880  5.80 6.908
  5.94 6.989  6.00 7.044  6.20 7.125  6.40 7.261  6.60 7.425
 22  1  0  1  0 1   -1 0           % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR
LPRWF
  56 0  57 0  58 0  59 0  60 0  61 0  62 0  63 0  64 0  65 0  66 0  67  0
  68 0  69 0  70 0  72 0  72 0  73 0  74 0  75 0  76 0  77 0  78 0  80 0
 3  0  0.D0                        % MORDR IRFN RREF
  1.d0  -2.d-1  3.d-2  -4.d-3       % {DM(j)}
```

## *Standard Channel-6 output for Introductory Illustrative Cases* $1(a) - 1(d)$

```
Case 1.a: For a model L.J.(12,6) get all vib. levels and their CDCs
================================================================================
 Generate   ZMU= 15.17186628000(u)   &   BZ= 8.999999997D-01((1/cm-1)(1/Ang**2))
          from atomic masses:  30.34373256000  &   30.34373256000(u)
 Integrate from  RMIN=  0.600  to  RMAX=  20.00  with mesh  RH= 0.002000(Angst)

 Potential #1 for L1(  0)-J2(  0)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=     0.00000(cm-1)

 Lennard-Jones(12, 6) potential with   De=  1000.000(cm-1)   Re =  1.000000(A)
 ----------------------------------------------------------------------------
 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN
 Eigenvalue convergence criterion is   EPS= 1.0D-06(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition
 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2
 For  J=  0, seek the first 400 levels of Potential-1   with   VLIM=     0.000
 ALF finds the highest calculated level is  E(v=  6)= -7.7249284D-01

 E(v=  0, J=  0)=  -811.519   Bv=  1.0540426  -Dv= -4.1381D-05   Hv= -6.5120D-09
           Lv= -1.9007D-12   Mv= -7.2230D-16   Nv= -3.1926D-19   Ov= -1.5585D-22
 E(v=  1, J=  0)=  -507.170   Bv=  0.9332450  -Dv= -6.0794D-05   Hv= -1.4820D-08
           Lv= -6.5533D-12   Mv= -3.7208D-15   Nv= -2.4359D-18   Ov= -1.7523D-21
 E(v=  2, J=  0)=  -287.838   Bv=  0.8013476  -Dv= -9.2177D-05   Hv= -3.5187D-08
           Lv= -2.3947D-11   Mv= -2.0879D-14   Nv= -2.1041D-17   Ov= -2.3384D-20
 E(v=  3, J=  0)=  -141.503   Bv=  0.6566553  -Dv= -1.4627D-04   Hv= -9.2303D-08
           Lv= -1.0432D-10   Mv= -1.5291D-13   Nv= -2.6179D-16   Ov= -4.9802D-19
 E(v=  4, J=  0)=   -54.890   Bv=  0.4974391  -Dv= -2.4978D-04   Hv= -2.9569D-07
           Lv= -6.5212D-10   Mv= -1.9135D-12   Nv= -6.6507D-15   Ov= -2.5885D-17
 E(v=  5, J=  0)=   -13.337   Bv=  0.3221808  -Dv= -4.9470D-04   Hv= -1.4933D-06
           Lv= -9.1824D-09   Mv= -7.7465D-11   Nv= -7.8195D-13   Ov= -8.8619D-15
 E(v=  6, J=  0)=-.772493      Bv=  0.1290036  -Dv= -1.6478D-03   Hv= -3.8715D-05
           Lv= -2.0424D-06   Mv= -1.4479D-07   Nv= -1.1986D-08   Ov= -1.0942D-09

 Find   7 Potential-1 vibrational levels with  J=  0
     v     E(v)        v     E(v)        v     E(v)        v     E(v)
    --------------    --------------    --------------    --------------
     0   -811.5192     2   -287.8379     4    -54.8902     6     -0.7725
     1   -507.1696     3   -141.5034     5    -13.3368
 An  n=12  N-D theory extrapolation from  v=   5 &   6  implies   vD =   6.439
 ===============================================================================
```

```
Case 1.b: For same model L.J.(12,6) get radial matrix elements for v < 3
================================================================================
 Generate   ZMU= 15.17186628000(u)   &   BZ= 8.999999997D-01((1/cm-1)(1/Ang**2))
          from atomic masses:  30.34373256000  &   30.34373256000(u)
 Integrate from  RMIN=  0.600  to  RMAX=  20.00  with mesh  RH= 0.002000(Angst)

 Potential #1 for L1( 30)-J2( 30)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=     0.00000(cm-1)

 Lennard-Jones(12, 6) potential with   De=  1000.000(cm-1)   Re =  1.000000(A)
 ----------------------------------------------------------------------------
 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN
 Eigenvalue convergence criterion is   EPS= 1.0D-06(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition
 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2
 For  J=  0, seek the first   3 levels of Potential-1   with   VLIM=     0.000
   and automatically increment  J  in steps of  1 to a maximum value of   1

 Matrix element argument expansion variable is:    X = (r - DREF)/DREF
     where reference length is held fixed at   DREF = 1.0000000000(Angstroms)
 Coefficients of expansion for radial matrix element/expectation value argument:
       1.000000D+00 -2.000000D-01  3.000000D-02 -4.000000D-03  5.000000D-04

 Using the rotational selection rule:  delta(J)= -1 to 1 with increment 2
   calculate matrix elements for coupling to the   3 vibrational levels of
   Potential-2:   v =   0   1   2
 Coupling   E(v=  0, J=  1)=   -809.4112   to   E(v=  0, J=  0)=   -811.5192
     Moment matrix elements:   <X** 0>=  0.9999997392   <X** 1>=  0.0315663983
      <X** 2>=  0.0043724231   <X** 3>=  0.0004274505   <X** 4>=  0.0000681864
 FCF= 1.0000D+00   <M>= 9.93816D-01   d(E)=     -2.11   A(Einst)= 9.6706D-07 s-1
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 For vibrational level  v =  0   of Potential-1
   J      E         J      E         J      E         J      E         J      E
 -------------  --------------  --------------  --------------  --------------
   0   -811.519    1   -809.411
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  1, J=  0)=   -507.1696   to   E(v=  0, J=  1)=   -809.4112
     Moment matrix elements:   <X** 0>=  0.0007038706   <X** 1>=  0.0555644965
      <X** 2>=  0.0061799007   <X** 3>=  0.0011668795   <X** 4>=  0.0002051809
 FCF= 4.9543D-07   <M>=-1.02282D-02   d(E)=   -302.24   A(Einst)= 9.0586D-04 s-1
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  1, J=  1)=   -505.3034   to   E(v=  0, J=  0)=   -811.5192
     Moment matrix elements:   <X** 0>= -0.0007036644   <X** 1>=  0.0554599642
      <X** 2>=  0.0061672593   <X** 3>=  0.0011650604   <X** 4>=  0.0002048749
 FCF= 4.9514D-07   <M>=-1.16152D-02   d(E)=   -306.22   A(Einst)= 4.0496D-04 s-1
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  1, J=  1)=   -505.3034   to   E(v=  0, J=  2)=   -805.1964
```

```
     Moment matrix elements:   <X** 0>=  0.0014096830   <X** 1>=  0.0556429498
      <X** 2>=  0.0062065908   <X** 3>=  0.0011721096   <X** 4>=  0.0002064159
 FCF= 1.9872D-06   <M>=-9.53729D-03   d(E)=   -299.89   A(Einst)= 5.1293D-04 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  1, J=  1)=   -505.3034   to   E(v=  1, J=  0)=   -507.1696
     Moment matrix elements:   <X** 0>=  0.9999989173   <X** 1>=  0.1072309514
      <X** 2>=  0.0227481313   <X** 3>=  0.0044941830   <X** 4>=  0.0010331538
 FCF= 1.0000D+00   <M>= 9.79218D-01   d(E)=     -1.87   A(Einst)= 6.5155D-07 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 For vibrational level  v =  1   of Potential-1
   J      E         J      E         J      E         J      E         J      E
 --------------  --------------  --------------  --------------  --------------
   0   -507.170    1   -505.303
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  2, J=  0)=   -287.8379   to   E(v=  0, J=  1)=   -809.4112
     Moment matrix elements:   <X** 0>= -0.0001445686   <X** 1>= -0.0146868141
      <X** 2>=  0.0021494006   <X** 3>=  0.0006270858   <X** 4>=  0.0002038462
 FCF= 2.0900D-08   <M>= 2.85487D-03   d(E)=   -521.57   A(Einst)= 3.6268D-04 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  2, J=  0)=   -287.8379   to   E(v=  1, J=  1)=   -505.3034
     Moment matrix elements:   <X** 0>=  0.0012364336   <X** 1>=  0.0838602021
      <X** 2>=  0.0215270661   <X** 3>=  0.0065378301   <X** 4>=  0.0019424342
 FCF= 1.5288D-06   <M>=-1.49150D-02   d(E)=   -217.47   A(Einst)= 7.1749D-04 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  2, J=  1)=   -286.2356   to   E(v=  0, J=  0)=   -811.5192
     Moment matrix elements:   <X** 0>=  0.0001452962   <X** 1>= -0.0147714152
      <X** 2>=  0.0021295981   <X** 3>=  0.0006226650   <X** 4>=  0.0002028174
 FCF= 2.1111D-08   <M>= 3.16108D-03   d(E)=   -525.28   A(Einst)= 1.5140D-04 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  2, J=  1)=   -286.2356   to   E(v=  0, J=  2)=   -805.1964
     Moment matrix elements:   <X** 0>= -0.0002889435   <X** 1>= -0.0146592358
      <X** 2>=  0.0021551720   <X** 3>=  0.0006307829   <X** 4>=  0.0002051064
 FCF= 8.3488D-08   <M>= 2.70514D-03   d(E)=   -518.96   A(Einst)= 2.1384D-04 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  2, J=  1)=   -286.2356   to   E(v=  1, J=  0)=   -507.1696
     Moment matrix elements:   <X** 0>= -0.0012355622   <X** 1>=  0.0834456954
      <X** 2>=  0.0214393061   <X** 3>=  0.0065170119   <X** 4>=  0.0019370216
 FCF= 1.5266D-06   <M>=-1.73066D-02   d(E)=   -220.93   A(Einst)= 3.3767D-04 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  2, J=  1)=   -286.2356   to   E(v=  1, J=  2)=   -501.5723
     Moment matrix elements:   <X** 0>=  0.0024778195   <X** 1>=  0.0841137737
      <X** 2>=  0.0216303217   <X** 3>=  0.0065743346   <X** 4>=  0.0019558701
 FCF= 6.1396D-06   <M>=-1.37213D-02   d(E)=   -215.34   A(Einst)= 3.9306D-04 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
 Coupling   E(v=  2, J=  1)=   -286.2356   to   E(v=  2, J=  0)=   -287.8379
     Moment matrix elements:   <X** 0>=  0.9999970447   <X** 1>=  0.2089561346
      <X** 2>=  0.0661950523   <X** 3>=  0.0214010286   <X** 4>=  0.0074711130
 FCF= 9.9999D-01   <M>= 9.60110D-01   d(E)=     -1.60   A(Einst)= 3.9644D-07 s-1
 ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 For vibrational level  v =  2   of Potential-1
   J      E         J      E         J      E         J      E         J      E
 --------------  --------------  --------------  --------------  --------------
   0   -287.838    1   -286.236
 +++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

 Find   3 Potential-1 vibrational levels with  J=  0
     v     E(v)        v     E(v)        v     E(v)        v     E(v)
    --------------    --------------    --------------    --------------
     0   -811.5192     1   -507.1696     2   -287.8379
 An  n=12  N-D theory extrapolation from  v=   1 &   2  implies   vD =   5.757
 ==============================================================================


Case 1.c: For the same L.J.(12,6), find levels of potential with a barrier
===============================================================================
 Generate   ZMU= 15.17186628000(u)   &   BZ= 8.999999997D-01((1/cm-1)(1/Ang**2))
          from atomic masses:  30.34373256000  &   30.34373256000(u)
 Integrate from  RMIN=  0.600  to  RMAX=  20.00  with mesh  RH= 0.002000(Angst)

 Potential #1 for L1(  0)-J2(  0)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=     0.00000(cm-1)

 Lennard-Jones(12, 6) potential with   De=  1000.000(cm-1)   Re =  1.000000(A)
 ----------------------------------------------------------------------------
 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN

 Eigenvalue convergence criterion is   EPS= 1.0D-06(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2
 For  J= 18, seek the first 400 levels of Potential-1   with   VLIM=     0.000

 Solve for  v=  0   J= 18   ETRIAL= -4.6535526D+02  INNER= 0   WF(1st) WF(NEND)
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 ------------------------------------------------------------------------------
  1 -4.6535526D+02  9.86D+00    258    1.11  8.3D-27  2.5D-13    2.54    1  178
  2 -4.5549824D+02 -6.65D-01    260    1.12  1.0D-26  3.6D-13    2.54    1  177
  3 -4.5616312D+02 -4.08D-03    260    1.12  9.9D-27  3.5D-13    2.54    1  177
  4 -4.5616720D+02 -1.53D-07    260    1.12  9.9D-27  3.5D-13    2.54    1  177
 ------------------------------------------------------------------------------
E(v=  0,J= 18)=  -456.1672   4 Iter  R(M)=  1.12  WF(NBEG=   52)/WF(M)= 9.9D-27
                                    INNER= 0     WF(NEND=   799)/WF(M)= 3.5D-13
Single well  ICOR= 0:  E(v=  0,J= 18)=   -456.17  v(SC)=   0.002  dGdv= 308.355
                                       (vD-v)=    4.0487   E(next)= -1.9930D+02

 Solve for  v=  1   J= 18   ETRIAL= -1.9929905D+02  INNER= 0   WF(1st) WF(NEND)
```

```
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 -------------------------------------------------------------------------------
  1 -1.9929905D+02  3.65D+00    330    1.26 -1.9D-26  3.6D-13    3.23    1  164
  2 -1.9565349D+02 -1.62D-01    331    1.26 -2.1D-26  4.5D-13    3.23    1  164
  3 -1.9581525D+02 -3.75D-04    331    1.26 -2.1D-26  4.5D-13    3.23    1  164
  4 -1.9581563D+02 -2.25D-09    331    1.26 -2.1D-26  4.5D-13    3.23    1  164
 -------------------------------------------------------------------------------
E(v=  1,J= 18)=  -195.8156   4 Iter  R(M)=  1.26  WF(NBEG=   51)/WF(M)=-2.1D-26
                                    INNER= 0     WF(NEND=  1066)/WF(M)= 4.5D-13
Single well  ICOR= 0:  E(v=  1,J= 18)=   -195.82  v(SC)=   1.003  dGdv= 213.103
                                       (vD-v)=    2.9262   E(next)= -3.1232D+01

 Solve for  v=  2   J= 18   ETRIAL= -3.1232480D+01  INNER= 0   WF(1st) WF(NEND)
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 -------------------------------------------------------------------------------
  1 -3.1232480D+01  5.23D+00    418    1.43  2.3D-26  7.1D-13    5.09    1  158
  2 -2.6003756D+01 -4.39D-01    423    1.44  2.9D-26  6.8D-13    5.30    1  158
  3 -2.6442466D+01 -4.69D-03    422    1.44  2.8D-26  6.1D-13    5.30    1  158
  4 -2.6447160D+01 -5.09D-07    422    1.44  2.8D-26  6.1D-13    5.30    1  158
 -------------------------------------------------------------------------------
E(v=  2,J= 18)=   -26.4472   4 Iter  R(M)=  1.44  WF(NBEG=   50)/WF(M)= 2.8D-26
                                    INNER= 0     WF(NEND=  1780)/WF(M)= 6.1D-13
Single well  ICOR= 0:  E(v=  2,J= 18)=    -26.45  v(SC)=   2.002  dGdv= 126.808
                                       (vD-v)=    1.7121   E(next)=  5.2997D+01

 Solve for  v=  3   J= 18   ETRIAL=  5.2996575D+01  INNER= 0   WF(1st) WF(NEND)
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 -------------------------------------------------------------------------------
  1  5.2996575D+01  6.26D+00    562    1.72 -1.6D-26  1.6D-01    2.49    1  156
  2  5.9253832D+01 -7.10D-01    600    1.80 -2.5D-26  4.1D-01    2.27    1  156
  3  5.8543620D+01 -4.68D-02    594    1.79 -2.3D-26  3.8D-01    2.29    1  156
  4  5.8496786D+01 -1.39D-03    594    1.79 -2.3D-26  3.7D-01    2.30    1  156
  5  5.8495398D+01 -4.63D-05    594    1.79 -2.3D-26  3.7D-01    2.30    1  156
  6  5.8495352D+01 -1.54D-06    594    1.79 -2.3D-26  3.7D-01    2.30    1  156
  7  5.8495350D+01 -5.12D-08    594    1.79 -2.3D-26  3.7D-01    2.30    1  156
 -------------------------------------------------------------------------------
E(v=  3,J= 18)=    58.4954   7 Iter  R(M)=  1.79  WF(NBEG=   51)/WF(M)=-2.3D-26
                                    INNER= 0     WF(NEND=   849)/WF(M)= 3.7D-01
   Lifetime= 5.035D-12(s)   Width= 1.054D+00   dG/dv=  41.60   V(max)=    64.01
Single well  ICOR= 0:  E(v=  3,J= 18)=     58.50  v(SC)=   2.983  dGdv=  44.289
                                       (vD-v)=    0.2492   E(next)=  1.3932D+01
          Find highest level of this potential is   E(v=  3)=  5.8495350075D+01
 ALF finds the highest calculated level is  E(v=  3)=  5.8495350D+01

 Solve for  v=  0   J= 18   ETRIAL= -4.5616720D+02  INNER= 0   WF(1st) WF(NEND)
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 -------------------------------------------------------------------------------
  1 -4.5616720D+02 -1.53D-07    260    1.12  9.9D-27  3.5D-13    2.54    1  177
 -------------------------------------------------------------------------------
E(v=  0,J= 18)=  -456.1672   1 Iter  R(M)=  1.12  WF(NBEG=   52)/WF(M)= 9.9D-27
                                    INNER= 0     WF(NEND=   799)/WF(M)= 3.5D-13
 Solve for  v=  1   J= 18   ETRIAL= -1.9581563D+02  INNER= 0   WF(1st) WF(NEND)
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 -------------------------------------------------------------------------------
  1 -1.9581563D+02 -2.25D-09    331    1.26 -2.1D-26  4.5D-13    3.23    1  164
 -------------------------------------------------------------------------------
E(v=  1,J= 18)=  -195.8156   1 Iter  R(M)=  1.26  WF(NBEG=   51)/WF(M)=-2.1D-26
                                    INNER= 0     WF(NEND=  1066)/WF(M)= 4.5D-13
 Solve for  v=  2   J= 18   ETRIAL= -2.6447160D+01  INNER= 0   WF(1st) WF(NEND)
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 -------------------------------------------------------------------------------
  1 -2.6447160D+01 -5.09D-07    422    1.44  2.8D-26  7.2D-13    5.27    1  158
 -------------------------------------------------------------------------------
E(v=  2,J= 18)=   -26.4472   1 Iter  R(M)=  1.44  WF(NBEG=   50)/WF(M)= 2.8D-26
                                    INNER= 0     WF(NEND=  1780)/WF(M)= 7.2D-13
 Solve for  v=  3   J= 18   ETRIAL=  5.8495350D+01  INNER= 0   WF(1st) WF(NEND)
 ITER    ETRIAL        D(E)      M    R(M)   /WF(M)   /WF(M)   R(NEND) NBEG ITP1
 -------------------------------------------------------------------------------
  1  5.8495350D+01 -5.12D-08    594    1.79 -2.3D-26  3.7D-01    2.30    1  156
 -------------------------------------------------------------------------------
E(v=  3,J= 18)=    58.4954   1 Iter  R(M)=  1.79  WF(NBEG=   51)/WF(M)=-2.3D-26
                                    INNER= 0     WF(NEND=   849)/WF(M)= 3.7D-01
   Lifetime= 5.035D-12(s)   Width= 1.054D+00   dG/dv=  41.60   V(max)=    64.01

 Find   4 Potential-1 vibrational levels with  J= 18
     v     E(v)           v     E(v)           v     E(v)           v     E(v)
    --------------    --------------    --------------    --------------
     0   -456.1672        1   -195.8156        2    -26.4472        3     58.4954
 ===============================================================================


Case 1.d:  Levels of a pointwise double-minimum potential for 3(PI)g Cl2
================================================================================
 Generate   ZMU= 17.48442634000(u)   &   BZ= 1.037181808D+00((1/cm-1)(1/Ang**2))
          from atomic masses:  34.96885268000  &   34.96885268000(u)
 Integrate from  RMIN=  1.600  to  RMAX=  10.00  with mesh  RH= 0.001000(Angst)

 Potential #1 for Cl( 35)-Cl( 35)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)= 95440.00000(cm-1)
 Perform cubic spline interpolation over the   29 input points
 To make input points Y(i) consistent with  Y(lim),  add  Y(shift)=      0.0000
 Scale input points:  (distance)* 5.291772108D-01  &  (energy)* 8.065544400D+03
            to get required internal units  [Angstroms & cm-1 for potentials]
      r(i)         Y(i)         r(i)           Y(i)        r(i)         Y(i)
   ----------------------   ----------------------   ----------------------
    3.340000  10.60800000     4.170000   8.59500000     5.370000   6.96200000
    3.400000   9.68300000     4.260000   8.70400000     5.510000   6.90800000
    3.430000   9.22100000     4.310000   8.75800000     5.660000   6.88000000
    3.490000   8.75800000     4.460000   8.43200000     5.800000   6.90800000
```

```
   3.570000   8.29500000    4.560000   8.13400000    5.940000   6.98900000
   3.660000   8.13200000    4.660000   7.88700000    6.000000   7.04400000
   3.760000   8.05100000    4.800000   7.61500000    6.200000   7.12500000
   3.860000   8.13200000    4.910000   7.42500000    6.400000   7.26100000
   3.940000   8.26800000    5.000000   7.34300000    6.600000   7.42500000
   4.030000   8.35000000    5.170000   7.12500000
-----------------------------------------------------------------------------
Extrapolate to   X .le. 1.7992  with
  Y= -5091495.587  +5.609801D+06 * exp(-4.542065D-02*X)
Extrapolate to  X .GE.  3.3867  using
  Y=  95440.0000 - [ 1.128770D+05/X**1 +1.377826D+05/X**3]
-----------------------------------------------------------------------------
Calculate properties of the single potential described above
Potential-1 uses inner boundary condition of  zero value  at  RMIN

Eigenvalue convergence criterion is   EPS= 1.0D-06(cm-1)
Airy function at 3-rd turning point is quasibound outer boundary condition

Since state-1 has (projected) electronic angular momentum  OMEGA= 0
        eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

Solve for the  22 vibration-rotation levels of Potential-1:
  (v,J) =  ( 56,  0)  ( 57,  0)  ( 58,  0)  ( 59,  0)  ( 60,  0)  ( 61,  0)
           ( 62,  0)  ( 63,  0)  ( 64,  0)  ( 65,  0)  ( 66,  0)  ( 67,  0)
           ( 68,  0)  ( 69,  0)  ( 70,  0)  ( 72,  0)  ( 72,  0)  ( 73,  0)
           ( 74,  0)  ( 75,  0)  ( 76,  0)  ( 77,  0)
Matrix element arguments are powers of the distance  r (in Angstroms)
Coefficients of expansion for radial matrix element/expectation value argument:
      1.000000D+00 -2.000000D-01  3.000000D-02 -4.000000D-03
Find  2  potential minima:   Vmin=   64929.256   55490.947
              at mesh points   R =    1.99400    2.99500
Find  2  potential maxima:   Vmax=   70645.436   84014.515
              at mesh points   R =    2.28400   10.00000
E(v= 56, J=  0)=  68214.438   <M(r)>=  0.4721236994        <KE>=   4580.196
          <X** 1>=   3.63045127   <X** 2>=  13.66002892   <X** 3>=  52.89672853
--------------------------------------------------------------------------------
E(v= 57, J=  0)=  68387.998   <M(r)>=  0.4695211055        <KE>=   4617.063
          <X** 1>=   3.64732349   <X** 2>=  13.79516352   <X** 3>=  53.71727533
--------------------------------------------------------------------------------
E(v= 58, J=  0)=  68476.426   <M(r)>=  0.6824612177        <KE>=   1651.393
          <X** 1>=   2.04384519   <X** 2>=   4.18845602   <X** 3>=   8.60585634
--------------------------------------------------------------------------------
E(v= 59, J=  0)=  68559.695   <M(r)>=  0.4669189761        <KE>=   4652.829
          <X** 1>=   3.66408683   <X** 2>=  13.93033264   <X** 3>=  54.54340917
--------------------------------------------------------------------------------
E(v= 60, J=  0)=  68729.539   <M(r)>=  0.4643045290        <KE>=   4686.656
          <X** 1>=   3.68083020   <X** 2>=  14.06617696   <X** 3>=  55.37868492
--------------------------------------------------------------------------------
E(v= 61, J=  0)=  68897.547   <M(r)>=  0.4617011736        <KE>=   4718.810
          <X** 1>=   3.69738156   <X** 2>=  14.20154715   <X** 3>=  56.21723207
--------------------------------------------------------------------------------
E(v= 62, J=  0)=  69063.700   <M(r)>=  0.4591313914        <KE>=   4749.186
          <X** 1>=   3.71357576   <X** 2>=  14.33535705   <X** 3>=  57.05354180
--------------------------------------------------------------------------------
E(v= 63, J=  0)=  69214.948   <M(r)>=  0.6781183397        <KE>=   1985.878
          <X** 1>=   2.07712475   <X** 2>=   4.36259568   <X** 3>=   9.33364510
--------------------------------------------------------------------------------
E(v= 64, J=  0)=  69228.156   <M(r)>=  0.4588457942        <KE>=   4751.128
          <X** 1>=   3.71260668   <X** 2>=  14.36531493   <X** 3>=  57.39807961
--------------------------------------------------------------------------------
E(v= 65, J=  0)=  69390.488   <M(r)>=  0.4540380379        <KE>=   4803.188
          <X** 1>=   3.74528392   <X** 2>=  14.60094615   <X** 3>=  58.73339038
--------------------------------------------------------------------------------
E(v= 66, J=  0)=  69551.030   <M(r)>=  0.4516314964        <KE>=   4825.287
          <X** 1>=   3.75994565   <X** 2>=  14.72704336   <X** 3>=  59.54766857
--------------------------------------------------------------------------------
E(v= 67, J=  0)=  69709.530   <M(r)>=  0.4496202586        <KE>=   4837.877
          <X** 1>=   3.77158473   <X** 2>=  14.83463802   <X** 3>=  60.27548393
--------------------------------------------------------------------------------
E(v= 68, J=  0)=  69864.123   <M(r)>=  0.4631813287        <KE>=   4633.896
          <X** 1>=   3.66813651   <X** 2>=  14.22170337   <X** 3>=  57.46061741
--------------------------------------------------------------------------------
E(v= 69, J=  0)=  69900.180   <M(r)>=  0.6579325788        <KE>=   2352.457
          <X** 1>=   2.22764740   <X** 2>=   5.25807538   <X** 3>=  13.57005061
--------------------------------------------------------------------------------
E(v= 70, J=  0)=  70022.038   <M(r)>=  0.4464976859        <KE>=   4867.346
          <X** 1>=   3.78784876   <X** 2>=  15.00980661   <X** 3>=  61.55668989
--------------------------------------------------------------------------------
E(v= 72, J=  0)=  70321.487   <M(r)>=  0.4485338715        <KE>=   4776.940
          <X** 1>=   3.76631221   <X** 2>=  14.93793365   <X** 3>=  61.58542409
--------------------------------------------------------------------------------
E(v= 72, J=  0)=  70321.487   <M(r)>=  0.4485338715        <KE>=   4776.940
          <X** 1>=   3.76631221   <X** 2>=  14.93793365   <X** 3>=  61.58542409
--------------------------------------------------------------------------------
E(v= 73, J=  0)=  70453.823   <M(r)>=  0.5032628690        <KE>=   4057.676
          <X** 1>=   3.36247828   <X** 2>=  12.39895889   <X** 3>=  49.05256070
--------------------------------------------------------------------------------
E(v= 74, J=  0)=  70524.503   <M(r)>=  0.5646387149        <KE>=   3567.119
          <X** 1>=   2.91080360   <X** 2>=   9.57364570   <X** 3>=  35.10248406
--------------------------------------------------------------------------------
E(v= 75, J=  0)=  70634.089   <M(r)>=  0.4560303262        <KE>=   4812.997
          <X** 1>=   3.70350160   <X** 2>=  14.63177900   <X** 3>=  60.55568119
--------------------------------------------------------------------------------
E(v= 76, J=  0)=  70771.143   <M(r)>=  0.4453926382        <KE>=   4880.577
          <X** 1>=   3.77812257   <X** 2>=  15.13371060   <X** 3>=  63.24854142
--------------------------------------------------------------------------------
E(v= 77, J=  0)=  70905.689   <M(r)>=  0.4521314033        <KE>=   4783.371
          <X** 1>=   3.72580681   <X** 2>=  14.82855323   <X** 3>=  61.89095769
--------------------------------------------------------------------------------
================================================================================
```

## Appendix C 2 : Input/Output files for Several Families of Analytic Potentials

**Case 2 .** Illustrative input data files are presented for eigenvalue calculations using a number of the analytic potential energy functions supported by the code, as described in § 2.6. Performing this set of seven calculations required 1.60 s of CPU on a decade-old Silicon Graphics UNIX server.

(a) To illustrate an application to an **Extended Morse Oscillator (EMO)** potential and the inclusion of BOB correction terms, this case presents a calculation of the eigenvalues of $^{109}$AgD from the ‘EMO$_3$(7)’ potential determined in Ref. [72] from a combined-isotopologue analysis that treated $^{107}$AgH as the ‘reference isotopologue’.

(b) To illustrate use of a standard **P**olynomial-**E**xponent **Morse/Long-Range (PE-MLR)** potential form, and incorporation of Born-Oppenheimer breakdown (BOB) contributions to the radial and centrifugal potentials, this case is a calculation of properties of levels of the ground state of $^{24}$MgD using the analytic **PE-MLR potential** and BOB correction functions determined from a combined isotopologue analysis of data for the MgH system in which $^{24}$MgH was the “reference isotopologue” (see Ref. [73]). Note that in such cases, calculation of the rotational constants is based on a centrifugal potential that includes the BOB correction function of Eq. (36).

(c) To illustrate use of a **S**pline-**E**xponent **Morse/Long-Range (SE-MLR)** potential form, this case calculates the band constants for all levels of the ground $X\,^1\Sigma^+$ state of NaH using parameter values generated from the example of Appendix C.3 of Ref. [44].

(d) This is an example of a calculation performed using the **D**ouble-**E**xponential **L**ong-**R**ange (**DELR**) potential form that was introduced in Ref. [11]. This is not precisely the same **DELR** functional form reported there, since our current model for this function no longer allows the exponent polynomial to have different orders for $r \leq r_e$ and $r > r_e$ . However, it provides an equally good representation of the data for emission into the $B\,^1\Pi_u$ state of Li$_2$.

(e) This calculation is performed using the “**X-expansion or HPP” polynomial potential** for the $X\,^1\Sigma_g^+$ state of Ca$_2$ reported by Allard *et al.* [74]. Note that the fact that the 18-digit polynomial expansion coefficients reported in Ref. [74] are rounded to (approximately) 13 digits by our program appears to have no significant effect on the results.

(f) This calculation for the ground $X\,^1\Sigma^+$ state of $^{20}$Xe$^{84}$Kr is performed using the **generalized HFD function** reported by Aziz *et al.* [75].

(g) This calculation for the ground $X\,^1\Sigma^+$ state of $^{40}$Ar$_2$ using the **generalized Tang-Toennies type function** reported by Jaeger *et al.* [76].

```
 47 109  1 2   0  1                  % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
’Case 2.a: EMO potential for {109}AgD w. BOB corrn [JCP 123, 204304(2005)]’
 0.0010  0.8  30.0  1.d-6            % RH RMIN RMAX EPS
 0  0  0    19250.d0   0.d0          % NTP LPPOT OMEGA VLM
 3  3 3  7  0  1                     % IPOTL QPAR PPAR Nbeta APSE IBOB
 19250.d0 1.6179162d0  0.d0          % DSCM REQ Rref
  1.54358095D+00 3.73860D-02 1.66424D-01 9.8030D-02 1.7089D-01 6.0200D-02
  1.4000D-01 2.2400D-01
 107 1  3 3 -1 3  3 -1 2             % MN1R MN2R qAD pAD NU1 NU2 qNA NT1 NT2
 0.0D+0 1.175D+01 1.756D+01 -1.270D+01  % UA2(0) UA2(1) ...
```

```
 0.0D+0                                 % U2INF
 0.0D+0 1.5D-04 9.3D-04              % TA2(0) TA2(1) ...
 0.0D+0                              % T2INF
-99  1  2  -1  0 1  -1  0            % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRWF
  0 0                                % IV(1) IJ(1)

 12 24  1 2  0  1                    % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
'Case 2.b: PE-MLR fx for MgD w. BOB corrn: from JPCA 117, 13373 (2013)'
 0.0005d0  0.50 99.d0  1.d-05        % RH RMIN RMAX EPS
 0  0  0  0.0d0                      % NTP LPPOT IOMEG VLIM
 4  4 5  12 -1  1                    % IPOTL QPAR PPAR Nbeta APSE IBOB
 11104.25d0  1.7296854D0  2.74d0     % DSCM REQ Rref
 3 0.81 -2  1                        % NCMM rhoAB IVSR IDSTT
 6 2.77550D+05
 8 3.45490D+06
10 4.61400D+07                       % MMLR CMM
  1.170475460D+00 1.08015790D+00 2.67329710D+00  2.483590D+00
  7.401300000D-01 1.91470000D-01 6.03830000D-01 -2.48730D+00
 -7.665300000D+00 -5.7310000D+00 2.83900000D+00  6.05400D+00
  2.400000000D+00                    % PARM(i=0,13)
 24 1  4 6  3 13  4 -1 7             % MN1R MN2R qAD pAD NU1 NU2 qNA NT1 NT2
  1.310D+00 4.180D+00 2.670D+00 4.0D+00  % U1i(i)
 0.0D+0                              % U2INF
  -1.5183D+01 3.7524D+01 -1.1607D+01 3.2200D+01 6.0570D+01 2.2950D+02
 -1.5610D+03 -2.0130D+03 1.2530D+04 5.3600D+03 -4.9740D+04 1.0500D+04
  7.110D+04 -4.70D+04                % U2i(i)
 0.0D+0                              % U2INF
  0.0D+00 7.266D-04 2.70D-04 9.110D-04 2.970D-03 -1.90D-03 -7.20D-03
  2.30D-02                           % T2i(i)
 0.0D+0                              % T2INF
-99  1  1  -1 0 1  1  0   0          % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRWF
  0 0                                % IV(1) IJ(1)

11 23 1 1 0 1                        % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
'Case 2.c: SE-MLR potential for NaH X^1Sigma^+: see betaFIT paper in JQSRT'
0.001d0 0.4d0 50.d0 5.d-08           % RH RMIN RMAX EPS
0 -0 0  0.d0                         % NTP LPPOT IOMEG VLIM
4 3 6 16 16 0                        % IPOTL PPAR QPAR APSE Nbeta IBOB
15793.4d0 1.88681084d0 3.6d0         % DSCM REQ Rref
 3 0.69 -2 1                         % NCMM rhoAB IVSR IDSTT
6 3.57502D+05
8 5.41796D+06
10 1.12920D+8                        % (MMLR(I) CMM(I) I= 1,NCMM)
  -1.0000000    -1.4436321033D-03
  -0.9300000     5.5253175808D-02
  -0.8700000     5.2283859294D-02
  -0.8100000     4.4152720636D-02
  -0.7900000     4.1302296514D-02
  -0.6300000     3.2224967101D-02
  -0.4800000     3.7117729038D-02
  -0.3200000     6.2549013369D-02
  -0.1600000     1.2724804641D-01
   0.0000000     2.5944401578D-01
   0.1500000     4.6902225016D-01
   0.3100000     7.9765582107D-01
   0.4700000     1.2594053426D+00
   0.6300000     1.9422405193D+00
   0.7900000     2.7670029551D+00
   1.0000000     3.0169976694D+00
-99  1  1  -1 0 1  1  0   0          % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRWF
```

```
  0 0                                % IV(1) IJ(1)

 3 7  3 7  0   1                     % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
'Case 2.d: DELR(8) for Li2(B) [see JCP 119, 7398 (2003)]'
 0.005 1.5  60.    1.d-8             % RH RMIN RMAX EPS
-1  0 1 0.d0                         % NTP LPPOT IOMEG VLIM
 5  3 3  8 -1  1                     % IPOTL PPAR QPAR APSE Nbeta IBOB
 2986.600d0 2.935961d0  3.6d0        % DSCM REQ Rref
 4 0.54d0  -0  1                     % NCMM rhoAB IVSR IDSTT
 3 -1.788d5                          % MMCM(1) CMM(1)
 6 6.97586d6                         % MMCM(2) CMM(2)
 8 1.378d8                           % MMCM(3) CMM(3)
 10 3.445d9                          % MMCM(4) CMM(4)
 1.0585149D+00 3.70878D-01 2.77660D-01 1.1109D-01 -1.3076D-01 -2.805D-01
-8.69D-02      3.29D-01    1.61D-01
  7 7  3  3  2  2  3  -1 -1          % MN1R MN2R pAD qAD NU1 NU2 QNA NT1 NT2
  2.52D-01 -3.29D+00 1.40D+00        % U1(0) U1(1)
  1.05578d0                          % U1INF
  2.52D-01 -3.29D+00 1.40D+00        % U2(0) U2(1)
  1.05578d0                          % U2INF
 -99 1  2   0   0  1  -1  0          % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRWF
  0  0                               % IV(i) IJ(i)

 20 40  20 40  0   1                 % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
'Case 2.e: "Tiemann-type" potential for Ca2(X) [Phys.Rev. A66, 042503(2002)'
 0.0005  3.0  80.   1.d-08           % RH RMIN RMAX EPS
 -1  0  0  1102.096077d0             % NTP LPPOT IOMEG VLIM
 8 1 1  20 -1   0                    % IPOTL PPAR QPAR APSE Nbeta IBOB
 1102.096077d0 4.277277d0   0.d0     % DSCM REQ  Rref
  2  0.d0  -2  1                     % NCMM rhoAB IVSR IDSTT
  6 -1.074d7                         % MMLR(1) CMM(1)
  8 -2.4505d8                        % MMLR(2) CMM(2)
  0.00042747d0
 -0.25408309276477307 7d01  0.37961100260114922 1d04  0.38207030202249524 1d03
```

```
 -0.254083092764773077d01  0.379611002601149221d04  0.382070302022495241d03
 -0.274390396954679318d04 -0.322736334190800926d04  0.363113805693018548d03
  0.634370542189755270d04 -0.740151835960846893d04 -0.190738913003729067d05
  0.542347392433017594d05  0.440392304373011066d05 -0.155387944954526116d06
 -0.836628381353236182d05  0.213831067083156871d06  0.155922449222826835d06
 -0.156260872999483137d06 -0.146711120959219668d06  0.277542999772230869d05
  0.712908015579339117d05 -0.126115550408998979d04
 -0.5929d0      3.66d0  10.d0        %  b  R{inn}  R{out}
 -99 1  2  0  0 1  -1  0             % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRWF
  0  0                               % IV(i) IJ(i)

 10 20  36 84  0   1                 % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
'Case 2.f: Barrow-Aziz HFD-B(6,8,10,12) for {20}Ne{84}Xe [JCP 91, 6348 (1989)]'
 0.001  1.5   29.   1.d-08           % RH RMIN RMAX EPS
 -1 00  0     0.d0  49.75d0          % NTP LPPOT IOMEG VLIM
 6  0 0  5 0  0                      % IPOTL PPAR QPAR APSE Nbeta IBOB
 51.5750d0   3.861d0  0.d0           % DSCM REQ Rref
 4  0.d0  -2  1                      % NCMM rhoAB IVSR IDSTT
  6 1.892088392d5                    % MMLR(1) CMM(1)
  8 1.032416239d6                    % MMLR(2) CMM(2)
 10 9.939199461d6                    % MMLR(3) CMM(3)
 12 1.693237609d8                    % MMLR(4) CMM(4)
 1.d0  3.872583d0  2.d0  0.1324d0  0.d0   % alpha_i (i=1-3),beta2,gamma
 -99 1 2  0  0 1  -1  0              % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRW
 0  0                                % IV(i) IJ(i)

 10 20  36 84  0   1                 % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
```

```
'Case 2.g:  Generalized Tang-Toennies PEC for Ar2 [Jaeger Mol.Phys. 107, 2181]'
 0.001  1.5   29.   1.d-08           % RH RMIN RMAX EPS
 -1 00  0     0.d0  49.75d0          % NTP LPPOT IOMEG VLIM
 7  0 0  9 0  0                      % IPOTL PPAR QPAR Nbeta APSE IBOB
 99.4734d0   3.762d0  0.d0           % DSCM REQ Rref
 6  4.02517211d0  +2  0              % NCMM rhoAB IVSR IDSTT
  6 3.077697440d+05                  % MMLR(1) CMM(1)
  8 2.270731967d+06                  % MMLR(2) CMM(2)
 10 1.707398322d+07                  % MMLR(3) CMM(3)
 12 1.308376851d+08                  % MMLR(4) CMM(4)
 14 1.021785836d+09                  % MMLR(5) CMM(5)
 16 8.132347553d+09                  % MMLR(6) CMM(6)
   2.98337630d0
   0.097120881d0
  -2.75206827d-1
   1.01489050d0
 3.206404873d+07  0.d0  0.d0  0.d0  0.d0   % \beta1 - \beta9
 -99 1 2  0  0 1  -1  0              % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRW
 0  0                                % IV(i) IJ(i)
```

### *Standard Channel-6 output for Introductory Illustrative Cases* $2(a) - 2(g)$

```
Case 2.a: EMO potential for {109}AgD w. BOB corrn [JCP 123, 204304(2005)]
===========================================================================
 Generate   ZMU=  1.97752904306(u)   &   BZ= 1.173076605D-01((1/cm-1)(1/Ang**2))
         from atomic masses: 108.90475530000  &    2.01410177812(u)
 Integrate from  RMIN=  0.800  to  RMAX=  30.00  with mesh  RH= 0.001000(Angst)

 Potential #1 for Ag(109)- D(  2)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)= 19250.00000(cm-1)

 BOB adiabatic potential correction for atom-2  of mass   2.01410177812
   consists of mass factor  [1- MASS(  1 H)/MASS(  2 H)]  multiplying all of:
     u1INF=   0.000000  times  y3= [(r**3 - Re**3)/(r**3 + Re**3)]  plus
       [1 - y3]  times an order  3 polynomial in
       y3=[(r**3 - Re**3)/(r**3 + Re**3)]  with the   4 coefficients:
     0.000000000D+00  1.175000000D+01  1.756000000D+01 -1.270000000D+01

 BOB centrifugal correction for atom-2  of mass   2.01410177812
   consists of mass factor  [MASS(  1 H)/MASS(  2 H)]  multiplying all of:
     q2INF=  0.000000000D+00 times  y3= [(r**3 - Re**3)/(r**3 + Re**3)]
   plus [1 - y3] times an order  2 polynomial in y3(r) with the  3 coefficients:
     0.000000000D+00  1.500000000D-04  9.300000000D-04

 EMO_3 Potential with   De= 19250.0000    Re= 1.61791620   Rref= 1.61791620
   Exponent coeft: order- 7 power series in  y=(r**3 - Rref**3)/(r**3 + Rref**3)
   with  8 coefficients:   1.543580950D+00  3.738600000D-02  1.664240000D-01
         9.803000000D-02  1.708900000D-01  6.020000000D-02  1.400000000D-01
         2.240000000D-01
 ------------------------------------------------------------------------

 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN
 Eigenvalue convergence criterion is   EPS= 1.0D-06(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2
 For  J=  0, seek the first 100 levels of Potential-1   with   VLIM= 19250.000

 ALF finds the highest calculated level is  E(v= 25)=  1.9244508D+04

 E(v=  0, J=  0)=   621.527   Bv=  3.2205459  -Dv= -8.7936D-05   Hv=  1.3523D-09
           Lv= -3.8730D-14   Mv=  2.8933D-19   Nv= -2.8833D-23   Ov= -1.2833D-27
 E(v=  1, J=  0)=  1837.802   Bv=  3.1483027  -Dv= -8.7227D-05   Hv=  1.2955D-09
           Lv= -3.9617D-14   Mv=  8.9664D-20   Nv= -3.7762D-23   Ov= -1.4750D-27
 E(v=  2, J=  0)=  3019.707   Bv=  3.0762265  -Dv= -8.6598D-05   Hv=  1.2322D-09
           Lv= -4.1154D-14   Mv= -1.2066D-19   Nv= -5.3964D-23   Ov= -2.2640D-27
 E(v=  3, J=  0)=  4167.280   Bv=  3.0042163  -Dv= -8.6064D-05   Hv=  1.1614D-09
           Lv= -4.3541D-14   Mv= -3.8002D-19   Nv= -7.8139D-23   Ov= -3.7304D-27
 E(v=  4, J=  0)=  5280.497   Bv=  2.9321578  -Dv= -8.5642D-05   Hv=  1.0814D-09
           Lv= -4.7039D-14   Mv= -7.2433D-19   Nv= -1.1204D-22   Ov= -6.1362D-27
 E(v=  5, J=  0)=  6359.267   Bv=  2.8599186  -Dv= -8.5352D-05   Hv=  9.8985D-10
           Lv= -5.1964D-14   Mv= -1.1935D-18   Nv= -1.5921D-22   Ov= -9.9956D-27
 E(v=  6, J=  0)=  7403.421   Bv=  2.7873437  -Dv= -8.5219D-05   Hv=  8.8331D-10
           Lv= -5.8715D-14   Mv= -1.8395D-18   Nv= -2.2594D-22   Ov= -1.6211D-26
 E(v=  7, J=  0)=  8412.700   Bv=  2.7142503  -Dv= -8.5273D-05   Hv=  7.5763D-10
           Lv= -6.7817D-14   Mv= -2.7376D-18   Nv= -3.2294D-22   Ov= -2.6337D-26
 E(v=  8, J=  0)=  9386.744   Bv=  2.6404234  -Dv= -8.5549D-05   Hv=  6.0753D-10
           Lv= -7.9999D-14   Mv= -4.0023D-18   Nv= -4.6800D-22   Ov= -4.3071D-26
 E(v=  9, J=  0)= 10325.075   Bv=  2.5656104  -Dv= -8.6092D-05   Hv=  4.2622D-10
           Lv= -9.6308D-14   Mv= -5.8127D-18   Nv= -6.9092D-22   Ov= -7.1230D-26
```

```
 E(v= 10, J=  0)= 11227.083   Bv=  2.4895158  -Dv= -8.6955D-05   Hv=  2.0474D-10
           Lv= -1.1829D-13   Mv= -8.4541D-18   Nv= -1.0426D-21   Ov= -1.1967D-25
 E(v= 11, J=  0)= 12092.012   Bv=  2.4117931  -Dv= -8.8203D-05   Hv= -6.9065D-11
           Lv= -1.4829D-13   Mv= -1.2391D-17   Nv= -1.6122D-21   Ov= -2.0531D-25
 E(v= 12, J=  0)= 12918.934   Bv=  2.3320360  -Dv= -8.9920D-05   Hv= -4.1216D-10
           Lv= -1.8994D-13   Mv= -1.8402D-17   Nv= -2.5624D-21   Ov= -3.6175D-25
 E(v= 13, J=  0)= 13706.737   Bv=  2.2497650  -Dv= -9.2210D-05   Hv= -8.4892D-10
           Lv= -2.4898D-13   Mv= -2.7830D-17   Nv= -4.2008D-21   Ov= -6.5890D-25
 E(v= 14, J=  0)= 14454.090   Bv=  2.1644091  -Dv= -9.5214D-05   Hv= -1.4153D-09
           Lv= -3.3481D-13   Mv= -4.3090D-17   Nv= -7.1385D-21   Ov= -1.2503D-24
 E(v= 15, J=  0)= 15159.423   Bv=  2.0752796  -Dv= -9.9120D-05   Hv= -2.1663D-09
           Lv= -4.6337D-13   Mv= -6.8730D-17   Nv= -1.2658D-20   Ov= -2.4951D-24
 E(v= 16, J=  0)= 15820.880   Bv=  1.9815321  -Dv= -1.0419D-04   Hv= -3.1883D-09
           Lv= -6.6291D-13   Mv= -1.1381D-16   Nv= -2.3634D-20   Ov= -5.2999D-24
 E(v= 17, J=  0)= 16436.280   Bv=  1.8821097  -Dv= -1.1081D-04   Hv= -4.6243D-09
           Lv= -9.8634D-13   Mv= -1.9764D-16   Nv= -4.7051D-20   Ov= -1.2176D-23
 E(v= 18, J=  0)= 17003.044   Bv=  1.7756548  -Dv= -1.1955D-04   Hv= -6.7223D-09
           Lv= -1.5397D-12   Mv= -3.6498D-16   Nv= -1.0165D-19   Ov= -3.0940D-23
 E(v= 19, J=  0)= 17518.114   Bv=  1.6603681  -Dv= -1.3130D-04   Hv= -9.9432D-09
           Lv= -2.5552D-12   Mv= -7.3137D-16   Nv= -2.4462D-19   Ov= -8.9823D-23
 E(v= 20, J=  0)= 17977.832   Bv=  1.5337691  -Dv= -1.4758D-04   Hv= -1.5222D-08
           Lv= -4.6021D-12   Mv= -1.6407D-15   Nv= -6.8287D-19   Ov= -3.1333D-22
 E(v= 21, J=  0)= 18377.770   Bv=  1.3922564  -Dv= -1.7116D-04   Hv= -2.4701D-08
           Lv= -9.3190D-12   Mv= -4.3405D-15   Nv= -2.3671D-18   Ov= -1.4293D-21
 E(v= 22, J=  0)= 18712.468   Bv=  1.2302153  -Dv= -2.0777D-04   Hv= -4.4238D-08
           Lv= -2.2676D-11   Mv= -1.4927D-14   Nv= -1.1578D-17   Ov= -9.9942D-21
 E(v= 23, J=  0)= 18975.036   Bv=  1.0378809  -Dv= -2.7179D-04   Hv= -9.5322D-08
           Lv= -7.6990D-11   Mv= -8.2964D-14   Nv= -1.0641D-16   Ov= -1.5297D-19
 E(v= 24, J=  0)= 19156.482   Bv=  0.7945156  -Dv= -4.1659D-04   Hv= -3.2127D-07
           Lv= -5.8062D-10   Mv= -1.4623D-12   Nv= -4.4539D-15   Ov= -1.5359D-17
 E(v= 25, J=  0)= 19244.508   Bv=  0.4195501  -Dv= -1.4775D-03   Hv= -1.4620D-05
           Lv= -3.4825D-07   Mv= -1.1158D-08   Nv= -4.1855D-10   Ov= -1.7371D-11

 Find  26 Potential-1 vibrational levels with  J=  0
     v     E(v)       v     E(v)       v     E(v)       v     E(v)
    --------------    --------------    --------------    --------------
     0    621.5267     7   8412.7004    14  14454.0900    21  18377.7702
     1   1837.8022     8   9386.7439    15  15159.4225    22  18712.4681
     2   3019.7070     9  10325.0747    16  15820.8804    23  18975.0358
     3   4167.2795    10  11227.0834    17  16436.2800    24  19156.4822
     4   5280.4968    11  12092.0119    18  17003.0435    25  19244.5078
     5   6359.2672    12  12918.9344    19  17518.1136
     6   7403.4212    13  13706.7365    20  17977.8324

 An  n=99  N-D theory extrapolation from  v=  24 &  25  implies   vD =  25.332
 ===============================================================================


Case 2.b: PE-MLR fx for MgD w. BOB corrn: from JPCA 117, 13373 (2013)
================================================================================
 Generate   ZMU=  1.85807333140(u)   &   BZ= 1.102215091D-01((1/cm-1)(1/Ang**2))
          from atomic masses:  23.98504169800  &    2.01410177812(u)
 Integrate from  RMIN=  0.500  to  RMAX=  99.00  with mesh  RH= 0.000500(Angst)

 Potential #1 for Mg( 24)- D(  2)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=     0.00000(cm-1)

 BOB adiabatic potential correction for atom-1  of mass  23.98504169800
   consists of mass factor  [1- MASS( 24Mg)/MASS( 24Mg)]  multiplying all of:
     u1INF=   0.000000  times  y6= [(r**6 - Re**6)/(r**6 + Re**6)]  plus
       [1 - y6]  times an order  3 polynomial in
       y4=[(r**4 - Re**4)/(r**4 + Re**4)]  with the   4 coefficients:
     1.310000000D+00  4.180000000D+00  2.670000000D+00  4.000000000D+00

 BOB adiabatic potential correction for atom-2  of mass   2.01410177812
   consists of mass factor  [1- MASS(  1 H)/MASS(  2 H)]  multiplying all of:
     u1INF=   0.000000  times  y6= [(r**6 - Re**6)/(r**6 + Re**6)]  plus
       [1 - y6]  times an order 13 polynomial in
       y4=[(r**4 - Re**4)/(r**4 + Re**4)]  with the  14 coefficients:
    -1.518300000D+01  3.752400000D+01 -1.160700000D+01  3.220000000D+01
     6.057000000D+01  2.295000000D+02 -1.561000000D+03 -2.013000000D+03
     1.253000000D+04  5.360000000D+03 -4.974000000D+04  1.050000000D+04
     7.110000000D+04 -4.700000000D+04

 BOB centrifugal correction for atom-2  of mass   2.01410177812
   consists of mass factor  [MASS(  1 H)/MASS(  2 H)]  multiplying all of:
     q2INF=  0.000000000D+00 times  y4= [(r**4 - Re**4)/(r**4 + Re**4)]
   plus [1 - y4] times an order  7 polynomial in y4(r) with the  8 coefficients:
     0.000000000D+00  7.266000000D-04  2.700000000D-04  9.110000000D-04
     2.970000000D-03 -1.900000000D-03 -7.200000000D-03  2.300000000D-02

 uLR inverse-power terms incorporate DS-type damping with   rhoAB= 0.810000
        defined to give very short-range  Dm(r)*Cm/r^m  behaviour   r^{-2/2}
        Dm(r)= [1 - exp(- 3.30(rhoAB*r)/m - 0.423(rhoAB*r)^2/sqrt{m})]^{m -2/2}
 uLR(r) has   3 inverse-power terms:    C6 =  2.77550000D+05
                                        C8 =  3.45490000D+06
                                        C10=  4.61400000D+07

 MLR(q=4, p=5) Potential with:   De=11104.2500[cm-1]    Re=  1.72968540[A]
  with PE-MLR exponent coefft:  beta(r)= beta{INF}*y5 + [1-y5]*Sum{beta_i*y4^i}
      exponent power series of order 12 in a variable in which   Rref= 2.74000
      with 13 coefficients:  1.170475460D+00  1.080157900D+00  2.673297100D+00
            2.483590000D+00  7.401300000D-01  1.914700000D-01  6.038300000D-01
           -2.487300000D+00 -7.665300000D+00 -5.731000000D+00  2.839000000D+00
            6.054000000D+00  2.400000000D+00
    Generate   betaINF=  2.046201180015  from uLR(Re)= 2.8698906226D+03
 ----------------------------------------------------------------------------
```

```
 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN

 Eigenvalue convergence criterion is   EPS= 1.0D-05(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

 For  J=  0, seek the first 100 levels of Potential-1   with   VLIM=     0.000

E(v=  0,J=  0)=-10576.9713
E(v=  1,J=  0)= -9531.1273
E(v=  2,J=  0)= -8517.5782
E(v=  3,J=  0)= -7537.4551
E(v=  4,J=  0)= -6592.2479
E(v=  5,J=  0)= -5683.9300
E(v=  6,J=  0)= -4815.1134
E(v=  7,J=  0)= -3989.2702
E(v=  8,J=  0)= -3211.0590
E(v=  9,J=  0)= -2486.8045
E(v= 10,J=  0)= -1825.1989
E(v= 11,J=  0)= -1238.3300
E(v= 12,J=  0)=  -743.1449
E(v= 13,J=  0)=  -363.0851
E(v= 14,J=  0)=  -126.0360
E(v= 15,J=  0)=   -30.5770
E(v= 16,J=  0)=    -2.7309
          Find highest level of this potential is   E(v= 16)= -2.7309323395D+00
 ALF finds the highest calculated level is  E(v= 16)= -2.7309323D+00

E(v=  0,J=  0)=-10576.9713
 E(v=  0, J=  0)=-10576.971   Bv=  3.0009468   -Dv= -9.6194D-05   Hv=  2.0891D-09
           Lv= -1.0297D-13   Mv=  1.8787D-18   Nv= -2.8462D-22   Ov= -3.9837D-27
E(v=  1,J=  0)= -9531.1273
 E(v=  1, J=  0)= -9531.127   Bv=  2.9333876   -Dv= -9.6337D-05   Hv=  1.9600D-09
           Lv= -1.1534D-13   Mv=  6.7506D-19   Nv= -4.0035D-22   Ov= -1.8539D-26
E(v=  2,J=  0)= -8517.5782
 E(v=  2, J=  0)= -8517.578   Bv=  2.8643763   -Dv= -9.6828D-05   Hv=  1.7810D-09
           Lv= -1.3369D-13   Mv= -1.4522D-18   Nv= -7.1077D-22   Ov= -4.9236D-26
E(v=  3,J=  0)= -7537.4551
 E(v=  3, J=  0)= -7537.455   Bv=  2.7933659   -Dv= -9.7786D-05   Hv=  1.5280D-09
           Lv= -1.6404D-13   Mv= -5.2122D-18   Nv= -1.2423D-21   Ov= -1.3838D-25
E(v=  4,J=  0)= -6592.2479
 E(v=  4, J=  0)= -6592.248   Bv=  2.7196297   -Dv= -9.9396D-05   Hv=  1.1631D-09
           Lv= -2.1360D-13   Mv= -1.2452D-17   Nv= -2.3423D-21   Ov= -3.4728D-25
E(v=  5,J=  0)= -5683.9300
 E(v=  5, J=  0)= -5683.930   Bv=  2.6421849   -Dv= -1.0193D-04   Hv=  6.2174D-10
           Lv= -2.9701D-13   Mv= -2.6867D-17   Nv= -4.8363D-21   Ov= -8.5123D-25
E(v=  6,J=  0)= -4815.1134
 E(v=  6, J=  0)= -4815.113   Bv=  2.5596786   -Dv= -1.0579D-04   Hv= -2.0991D-10
           Lv= -4.4425D-13   Mv= -5.6382D-17   Nv= -1.0793D-20   Ov= -2.1867D-24
E(v=  7,J=  0)= -3989.2702
 E(v=  7, J=  0)= -3989.270   Bv=  2.4701994   -Dv= -1.1164D-04   Hv= -1.5383D-09
           Lv= -7.1777D-13   Mv= -1.1988D-16   Nv= -2.6016D-20   Ov= -6.1356D-24
E(v=  8,J=  0)= -3211.0590
 E(v=  8, J=  0)= -3211.059   Bv=  2.3709745   -Dv= -1.2055D-04   Hv= -3.7550D-09
           Lv= -1.2572D-12   Mv= -2.6769D-16   Nv= -6.8839D-20   Ov= -1.9375D-23
E(v=  9,J=  0)= -2486.8045
 E(v=  9, J=  0)= -2486.804   Bv=  2.2578703   -Dv= -1.3439D-04   Hv= -7.6602D-09
           Lv= -2.4088D-12   Mv= -6.5150D-16   Nv= -2.0617D-19   Ov= -7.1509D-23
E(v= 10,J=  0)= -1825.1989
 E(v= 10, J=  0)= -1825.199   Bv=  2.1245297   -Dv= -1.5657D-04   Hv= -1.5062D-08
           Lv= -5.1513D-12   Mv= -1.8077D-15   Nv= -7.3449D-19   Ov= -3.2785D-22
E(v= 11,J=  0)= -1238.3300
 E(v= 11, J=  0)= -1238.330   Bv=  1.9607791   -Dv= -1.9391D-04   Hv= -3.0630D-08
           Lv= -1.2783D-11   Mv= -6.1094D-15   Nv= -3.3875D-18   Ov= -2.0746D-21
E(v= 12,J=  0)=  -743.1449
 E(v= 12, J=  0)=  -743.145   Bv=  1.7495212   -Dv= -2.6164D-04   Hv= -6.8835D-08
           Lv= -3.9679D-11   Mv= -2.8259D-14   Nv= -2.3600D-17   Ov= -2.1938D-20
E(v= 13,J=  0)=  -363.0851
 E(v= 13, J=  0)=  -363.085   Bv=  1.4609104   -Dv= -3.9887D-04   Hv= -1.8763D-07
           Lv= -1.7762D-10   Mv= -2.2062D-13   Nv= -3.2568D-16   Ov= -5.3844D-19
E(v= 14,J=  0)=  -126.0360
 E(v= 14, J=  0)=  -126.036   Bv=  1.0524948   -Dv= -6.9579D-04   Hv= -6.2944D-07
           Lv= -1.1429D-09   Mv= -2.8624D-12   Nv= -8.7147D-15   Ov= -3.0196D-17
E(v= 15,J=  0)=   -30.5770
 E(v= 15, J=  0)=   -30.577   Bv=  0.6130777   -Dv= -9.3162D-04   Hv= -1.4581D-06
           Lv= -7.8253D-09   Mv= -5.6840D-11   Nv= -4.6701D-13   Ov= -4.2484D-15
E(v= 16,J=  0)=    -2.7309
 E(v= 16, J=  0)=    -2.731   Bv=  0.2852832   -Dv= -2.1746D-03   Hv= -2.9685D-05
           Lv= -9.2968D-07   Mv= -3.9645D-08   Nv= -1.9920D-09   Ov= -1.1090D-10

 Find  17 Potential-1 vibrational levels with  J=  0
     v     E(v)        v     E(v)        v     E(v)        v     E(v)
    --------------    --------------    --------------    --------------
     0 -10576.9713     5  -5683.9300    10  -1825.1989    15    -30.5770
     1  -9531.1273     6  -4815.1134    11  -1238.3300    16     -2.7309
     2  -8517.5782     7  -3989.2702    12   -743.1449
     3  -7537.4551     8  -3211.0590    13   -363.0851
     4  -6592.2479     9  -2486.8045    14   -126.0360

 An  n= 6  N-D theory extrapolation from  v=  15 &  16  implies   vD =  16.808
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Case 2.c: SE-MLR potential for NaH X^1Sigma^+: see betaFIT paper in JQSRT
================================================================================
```

```
 Generate   ZMU=  0.96549948567(u)   &   BZ= 5.727374080D-02((1/cm-1)(1/Ang**2))
          from atomic masses:  22.98976928200  &    1.00782503223(u)
 Integrate from  RMIN=  0.400  to  RMAX=  50.00  with mesh  RH= 0.001000(Angst)

 Potential #1 for Na( 23)- H(  1)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=     0.00000(cm-1)

 uLR inverse-power terms incorporate DS-type damping with   rhoAB= 0.690000
        defined to give very short-range  Dm(r)*Cm/r^m  behaviour   r^{-2/2}
        Dm(r)= [1 - exp(- 3.30(rhoAB*r)/m - 0.423(rhoAB*r)^2/sqrt{m})]^{m -2/2}
 uLR(r) has   3 inverse-power terms:    C6 =  3.57502000D+05
                                        C8 =  5.41796000D+06
                                        C10=  1.12920000D+08

 MLR(q=3, p=6) Potential with:   De=15793.4000[cm-1]    Re=  1.88681084[A]
   with SE-MLR exponent coefft   beta(r)=
                      y6^{eq} *{Spline through the 16 function values} beta_i =
           -0.14436321D-02  0.55253176D-01  0.52283859D-01  0.44152721D-01
            0.41302297D-01  0.32224967D-01  0.37117729D-01  0.62549013D-01
            0.12724805D+00  0.25944402D+00  0.46902225D+00  0.79765582D+00
            0.12594053D+01  0.19422405D+01  0.27670030D+01  0.30169977D+01
     at distances defined by y_3(r; RREF) =
            0.36000000D+01 -0.10000000D+01 -0.93000000D+00 -0.87000000D+00
           -0.81000000D+00 -0.79000000D+00 -0.63000000D+00 -0.48000000D+00
           -0.32000000D+00 -0.16000000D+00  0.00000000D+00  0.15000000D+00
            0.31000000D+00  0.47000000D+00  0.63000000D+00  0.79000000D+00
            0.10000000D+01
    Generate   betaINF=  2.992811377060  from uLR(Re)= 1.5839598324D+03
 ----------------------------------------------------------------------------

 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN

 Eigenvalue convergence criterion is   EPS= 5.0D-08(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

 For  J=  0, seek the first 100 levels of Potential-1   with   VLIM=     0.000

E(v=  0,J=  0)=-15205.1139
E(v=  1,J=  0)=-14059.9108
E(v=  2,J=  0)=-12954.1908
E(v=  3,J=  0)=-11887.6945
E(v=  4,J=  0)=-10859.4081
E(v=  5,J=  0)= -9868.5071
E(v=  6,J=  0)= -8914.4586
E(v=  7,J=  0)= -7997.0494
E(v=  8,J=  0)= -7116.3661
E(v=  9,J=  0)= -6272.7065
E(v= 10,J=  0)= -5466.5854
E(v= 11,J=  0)= -4698.9715
E(v= 12,J=  0)= -3971.4345
E(v= 13,J=  0)= -3286.1933
E(v= 14,J=  0)= -2646.3120
E(v= 15,J=  0)= -2055.9614
E(v= 16,J=  0)= -1520.8021
E(v= 17,J=  0)= -1048.1654
E(v= 18,J=  0)=  -647.3388
E(v= 19,J=  0)=  -330.1624
E(v= 20,J=  0)=  -111.1142
E(v= 21,J=  0)=    -7.5824
          Find highest level of this potential is   E(v= 21)= -7.5824289234D+00
 ALF finds the highest calculated level is  E(v= 21)= -7.5824289D+00

E(v=  0,J=  0)=-15205.1139
 E(v=  0, J=  0)=-15205.114   Bv=  4.8331668  -Dv= -3.3310D-04   Hv=  1.9277D-08
           Lv= -1.6555D-12   Mv=  2.2203D-16   Nv= -3.9992D-20   Ov=  2.4754D-24
E(v=  1,J=  0)=-14059.9108
 E(v=  1, J=  0)=-14059.911   Bv=  4.6941582  -Dv= -3.2844D-04   Hv=  2.0000D-08
           Lv= -2.1257D-12   Mv=  2.1432D-16   Nv=  2.6476D-20   Ov= -7.9004D-24
E(v=  2,J=  0)=-12954.1908
 E(v=  2, J=  0)=-12954.191   Bv=  4.5586852  -Dv= -3.2535D-04   Hv=  2.0353D-08
           Lv= -1.7867D-12   Mv=  5.5906D-17   Nv= -3.3163D-20   Ov=  3.7621D-23
E(v=  3,J=  0)=-11887.6945
 E(v=  3, J=  0)=-11887.695   Bv=  4.4257375  -Dv= -3.2148D-04   Hv=  1.9969D-08
           Lv= -1.7212D-12   Mv=  2.0411D-16   Nv= -1.6028D-19   Ov=  6.3876D-23
E(v=  4,J=  0)=-10859.4081
 E(v=  4, J=  0)=-10859.408   Bv=  4.2945424  -Dv= -3.1731D-04   Hv=  1.9479D-08
           Lv= -2.1157D-12   Mv=  6.0713D-16   Nv= -2.2889D-19   Ov= -1.4273D-23
E(v=  5,J=  0)= -9868.5071
 E(v=  5, J=  0)= -9868.507   Bv=  4.1645485  -Dv= -3.1354D-04   Hv=  1.9600D-08
           Lv= -2.9019D-12   Mv=  7.0236D-16   Nv= -1.0183D-19   Ov= -1.4209D-23
E(v=  6,J=  0)= -8914.4586
 E(v=  6, J=  0)= -8914.459   Bv=  4.0355776  -Dv= -3.1085D-04   Hv=  1.9839D-08
           Lv= -3.5138D-12   Mv=  7.0500D-16   Nv= -1.0195D-19   Ov=  4.0625D-23
E(v=  7,J=  0)= -7997.0494
 E(v=  7, J=  0)= -7997.049   Bv=  3.9071118  -Dv= -3.0945D-04   Hv=  1.9995D-08
           Lv= -3.9581D-12   Mv=  8.2102D-16   Nv= -1.4751D-19   Ov= -9.2558D-24
E(v=  8,J=  0)= -7116.3661
 E(v=  8, J=  0)= -7116.366   Bv=  3.7784456  -Dv= -3.0925D-04   Hv=  2.0222D-08
           Lv= -4.4146D-12   Mv=  7.4436D-16   Nv= -1.8574D-19   Ov= -5.6741D-23
E(v=  9,J=  0)= -6272.7065
 E(v=  9, J=  0)= -6272.707   Bv=  3.6489419  -Dv= -3.1027D-04   Hv=  2.0001D-08
           Lv= -5.2227D-12   Mv=  5.8585D-16   Nv=  2.6970D-20   Ov= -1.3817D-22
```

```
E(v= 10,J=  0)= -5466.5854
 E(v= 10, J=  0)= -5466.585   Bv=  3.5175361  -Dv= -3.1331D-04   Hv=  1.8882D-08
           Lv= -5.9354D-12   Mv=  3.9491D-16   Nv=  2.8319D-19   Ov= -1.0225D-22
E(v= 11,J=  0)= -4698.9715
 E(v= 11, J=  0)= -4698.971   Bv=  3.3824634  -Dv= -3.1910D-04   Hv=  1.7026D-08
           Lv= -6.2479D-12   Mv= -1.7939D-16   Nv= -8.7693D-20   Ov=  2.1916D-22
E(v= 12,J=  0)= -3971.4345
 E(v= 12, J=  0)= -3971.434   Bv=  3.2416371  -Dv= -3.2807D-04   Hv=  1.3791D-08
           Lv= -7.1829D-12   Mv= -5.2298D-16   Nv= -2.1715D-19   Ov=  2.1104D-22
E(v= 13,J=  0)= -3286.1933
 E(v= 13, J=  0)= -3286.193   Bv=  3.0923821  -Dv= -3.4152D-04   Hv=  8.6767D-09
           Lv= -8.6163D-12   Mv= -1.2237D-15   Nv= -1.1067D-18   Ov=  2.0155D-22
E(v= 14,J=  0)= -2646.3120
 E(v= 14, J=  0)= -2646.312   Bv=  2.9311694  -Dv= -3.6133D-04   Hv=  2.8620D-10
           Lv= -1.2034D-11   Mv= -2.1016D-15   Nv= -1.2972D-18   Ov= -3.4999D-22
E(v= 15,J=  0)= -2055.9614
 E(v= 15, J=  0)= -2055.961   Bv=  2.7530085  -Dv= -3.9095D-04   Hv= -1.2843D-08
           Lv= -1.7209D-11   Mv= -4.1249D-15   Nv= -2.7177D-18   Ov= -1.2986D-21
E(v= 16,J=  0)= -1520.8021
 E(v= 16, J=  0)= -1520.802   Bv=  2.5512339  -Dv= -4.3431D-04   Hv= -3.2942D-08
           Lv= -2.7298D-11   Mv= -1.1300D-14   Nv= -8.9361D-18   Ov= -5.2467D-21
E(v= 17,J=  0)= -1048.1654
 E(v= 17, J=  0)= -1048.165   Bv=  2.3174627  -Dv= -4.9839D-04   Hv= -6.9505D-08
           Lv= -5.3828D-11   Mv= -3.1131D-14   Nv= -2.3355D-17   Ov= -2.1422D-20
E(v= 18,J=  0)=  -647.3388
 E(v= 18, J=  0)=  -647.339   Bv=  2.0391708  -Dv= -5.9924D-04   Hv= -1.4274D-07
           Lv= -1.2066D-10   Mv= -1.0524D-13   Nv= -1.1615D-16   Ov= -1.4195D-19
E(v= 19,J=  0)=  -330.1624
 E(v= 19, J=  0)=  -330.162   Bv=  1.6970822  -Dv= -7.6935D-04   Hv= -3.2068D-07
           Lv= -3.8549D-10   Mv= -5.9131D-13   Nv= -1.0961D-15   Ov= -2.2057D-18
E(v= 20,J=  0)=  -111.1142
 E(v= 20, J=  0)=  -111.114   Bv=  1.2568292  -Dv= -1.1313D-03   Hv= -1.0898D-06
           Lv= -2.7861D-09   Mv= -9.8299D-12   Nv= -4.2384D-14   Ov= -2.0574D-16
E(v= 21,J=  0)=    -7.5824
 E(v= 21, J=  0)=    -7.582   Bv=  0.6000757  -Dv= -3.2026D-03   Hv= -2.9845D-05
           Lv= -7.0675D-07   Mv= -2.2843D-08   Nv= -8.6687D-10   Ov= -3.6386D-11

 Find  22 Potential-1 vibrational levels with  J=  0
     v     E(v)       v     E(v)       v     E(v)        v     E(v)
    --------------    --------------    --------------    --------------
     0 -15205.1139     6  -8914.4586    12  -3971.4345    18   -647.3388
     1 -14059.9108     7  -7997.0494    13  -3286.1933    19   -330.1624
     2 -12954.1908     8  -7116.3661    14  -2646.3120    20   -111.1142
     3 -11887.6945     9  -6272.7065    15  -2055.9614    21     -7.5824
     4 -10859.4081    10  -5466.5854    16  -1520.8021
     5  -9868.5071    11  -4698.9715    17  -1048.1654

 An  n= 6  N-D theory extrapolation from  v=  20 &  21  implies   vD =  21.691
 ===============================================================================
```

```
Case 2.d: DELR(8) for Li2(B) [see JCP 119, 7398 (2003)]
================================================================================
 Generate   ZMU=  3.50800171850(u)   &   BZ= 2.080957930D-01((1/cm-1)(1/Ang**2))
          from atomic masses:   7.01600343700  &    7.01600343700(u)
 Integrate from  RMIN=  1.500  to  RMAX=  60.00  with mesh  RH= 0.005000(Angst)

 Potential #1 for Li(  7)-Li(  7)
 ================================
 State has  OMEGA= 1   and energy asymptote:   Y(lim)=     0.00000(cm-1)

 BOB adiabatic potential correction for atom-1  of mass   7.01600343700
   consists of mass factor  [1- MASS(  7Li)/MASS(  7Li)]  multiplying all of:
     u1INF=   1.055780  times  y3= [(r**3 - Re**3)/(r**3 + Re**3)]  plus
       [1 - y3]  times an order  2 polynomial in
       y3=[(r**3 - Re**3)/(r**3 + Re**3)]  with the   3 coefficients:
     2.520000000D-01 -3.290000000D+00  1.400000000D+00

 BOB adiabatic potential correction for atom-2  of mass   7.01600343700
   consists of mass factor  [1- MASS(  7Li)/MASS(  7Li)]  multiplying all of:
     u1INF=   1.055780  times  y3= [(r**3 - Re**3)/(r**3 + Re**3)]  plus
       [1 - y3]  times an order  2 polynomial in
       y3=[(r**3 - Re**3)/(r**3 + Re**3)]  with the   3 coefficients:
     2.520000000D-01 -3.290000000D+00  1.400000000D+00

 uLR inverse-power terms incorporate DS-type damping with   rhoAB= 0.540000
        defined to give very short-range  Dm(r)*Cm/r^m  behaviour   r^{ 0/2}
        Dm(r)= [1 - exp(- 3.95(rhoAB*r)/m - 0.390(rhoAB*r)^2/sqrt{m})]^{m +0/2}
 uLR(r) has   4 inverse-power terms:    C3 = -1.78800000D+05
                                        C6 =  6.97586000D+06
                                        C 8=  1.37800000D+08
                                        C10=  3.44500000D+09

 DELR(q= 3) Potential with   De=  2986.6000[cm-1]   Re= 2.93596100[A]   where
   exponent coefft. has power series order   8
      with polynomial coefficients          1.05851490D+00   3.70878000D-01
           2.77660000D-01   1.11090000D-01  -1.30760000D-01  -2.80500000D-01
          -8.69000000D-02   3.29000000D-01   1.61000000D-01
      where the radial variable   y_3= (r**3 - Rref**3)/(r**3 + Rref**3)
          is defined w.r.t.   Rref= 3.60000000
   Generate A(DELR)=  3.595299321D+03   B(DELR)=  8.493929499D+03
      from uLR defined by 4 inverse-power terms
 ----------------------------------------------------------------------------

 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN

 Eigenvalue convergence criterion is   EPS= 1.0D-08(cm-1)
```

```
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 1
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 1]/r**2

 For  J=  0, seek the first 100 levels of Potential-1   with   VLIM=     0.000

 Case 2.d: DELR(8) for Li2(B) [see JCP 119, 7398 (2003)]                               for Li(  7)-Li(  7)
 =====================================================================================================================================
 Although  OMEGA=   1, these band constants obtained for  [J(J+1) - OMEGA^2] = 0
 =====================================================================================================================================
   v     J       E           Bv            -Dv              Hv              Lv              Mv              Nv              Ov
 =====================================================================================================================================
 ALF finds the highest calculated level is  E(v= 17)=  4.7570998D+02

 E(v=  0, J=  0)= -2852.038   Bv=  0.5532317  -Dv= -9.4985D-06   Hv=  1.2218D-10
           Lv= -4.4026D-15   Mv=  7.3145D-20   Nv= -5.4567D-24   Ov=  8.8161D-29
 E(v=  1, J=  0)= -2587.420   Bv=  0.5445462  -Dv= -9.6053D-06   Hv=  1.1744D-10
           Lv= -4.8761D-15   Mv=  6.7107D-20   Nv= -7.2329D-24   Ov=  4.7341D-29
 E(v=  2, J=  0)= -2329.158   Bv=  0.5355791  -Dv= -9.7359D-06   Hv=  1.1133D-10
           Lv= -5.4803D-15   Mv=  5.1407D-20   Nv= -9.6568D-24   Ov= -4.6601D-29
 E(v=  3, J=  0)= -2077.485   Bv=  0.5262880  -Dv= -9.8948D-06   Hv=  1.0327D-10
           Lv= -6.2617D-15   Mv=  2.1592D-20   Nv= -1.3222D-23   Ov= -2.4070D-28
 E(v=  4, J=  0)= -1832.661   Bv=  0.5166217  -Dv= -1.0088D-05   Hv=  9.2527D-11
           Lv= -7.2904D-15   Mv= -3.0040D-20   Nv= -1.8801D-23   Ov= -6.2656D-28
 E(v=  5, J=  0)= -1594.986   Bv=  0.5065187  -Dv= -1.0323D-05   Hv=  7.8113D-11
           Lv= -8.6766D-15   Mv= -1.1683D-19   Nv= -2.7998D-23   Ov= -1.3898D-27
 E(v=  6, J=  0)= -1364.801   Bv=  0.4959047  -Dv= -1.0610D-05   Hv=  5.8653D-11
           Lv= -1.0597D-14   Mv= -2.6233D-19   Nv= -4.3886D-23   Ov= -2.9237D-27
 E(v=  7, J=  0)= -1142.500   Bv=  0.4846894  -Dv= -1.0963D-05   Hv=  3.2132D-11
           Lv= -1.3345D-14   Mv= -5.0959D-19   Nv= -7.2654D-23   Ov= -6.1073D-27
 E(v=  8, J=  0)=  -928.539   Bv=  0.4727617  -Dv= -1.1399D-05   Hv= -4.5249D-12
           Lv= -1.7424D-14   Mv= -9.4086D-19   Nv= -1.2748D-22   Ov= -1.3033D-26
 E(v=  9, J=  0)=  -723.447   Bv=  0.4599828  -Dv= -1.1945D-05   Hv= -5.6223D-11
           Lv= -2.3747D-14   Mv= -1.7227D-18   Nv= -2.3841D-22   Ov= -2.9080D-26
 E(v= 10, J=  0)=  -527.850   Bv=  0.4461745  -Dv= -1.2638D-05   Hv= -1.3120D-10
           Lv= -3.4054D-14   Mv= -3.2179D-18   Nv= -4.8005D-22   Ov= -6.9492D-26
 E(v= 11, J=  0)=  -342.490   Bv=  0.4311013  -Dv= -1.3538D-05   Hv= -2.4417D-10
           Lv= -5.1946D-14   Mv= -6.2925D-18   Nv= -1.0587D-21   Ov= -1.8317D-25
 E(v= 12, J=  0)=  -168.266   Bv=  0.4144372  -Dv= -1.4741D-05   Hv= -4.2372D-10
           Lv= -8.5655D-14   Mv= -1.3284D-17   Nv= -2.6332D-21   Ov= -5.5532D-25
 E(v= 13, J=  0)=    -6.299   Bv=  0.3957050  -Dv= -1.6421D-05   Hv= -7.3179D-10
           Lv= -1.5682D-13   Mv= -3.1668D-17   Nv= -7.7763D-21   Ov= -2.0724D-24
 E(v= 14, J=  0)=   141.959   Bv=  0.3741416  -Dv= -1.8929D-05   Hv= -1.3267D-09
           Lv= -3.3549D-13   Mv= -9.2290D-17   Nv= -3.0123D-20   Ov= -1.0817D-23
 E(v= 15, J=  0)=   274.497   Bv=  0.3483528  -Dv= -2.3134D-05   Hv= -2.7377D-09
           Lv= -9.4309D-13   Mv= -3.9285D-16   Nv= -1.9411D-19   Ov= -1.0754D-22
 ** CAUTION ** Comparison tests for Hv, Lv & Mv give:  2.1D-06  2.5D-05  8.4D-05
 E(v= 16, J=  0)=   388.152   Bv=  0.3150520  -Dv= -3.2224D-05   Hv= -8.1442D-09
           Lv= -5.4382D-12   Mv= -5.3802D-15   Nv= -7.9291D-18   Ov= -1.7009D-20
 ** CAUTION ** Comparison tests for Hv, Lv & Mv give:  1.4D-03  2.8D-03  4.5D-03
 E(v= 17, J=  0)=   475.710   Bv=  0.2568926  -Dv= -8.5613D-05   Hv= -9.0170D-08
           Lv= -8.5881D-11   Mv=  9.5157D-14   Nv=  6.8551D-16   Ov=  1.5784D-18

 Find  18 Potential-1 vibrational levels with  J=  0
     v     E(v)        v     E(v)        v     E(v)         v     E(v)
    --------------    --------------    --------------    --------------
     0  -2852.0385     5  -1594.9861    10   -527.8503    15    274.4971
     1  -2587.4196     6  -1364.8012    11   -342.4898    16    388.1516
     2  -2329.1579     7  -1142.5003    12   -168.2661    17    475.7100
     3  -2077.4845     8   -928.5388    13     -6.2994
     4  -1832.6611     9   -723.4475    14    141.9588
 =====================================================================================


Case 2.e: "Tiemann-type" potential for Ca2(X) [Phys.Rev. A66, 042503(2002)
======================================================================================
 Generate   ZMU= 19.98129543200(u)   &   BZ= 1.185296888D+00((1/cm-1)(1/Ang**2))
           from atomic masses:  39.96259086400  &   39.96259086400(u)
 Integrate from  RMIN=  3.000  to  RMAX=  103.00  with mesh  RH= 0.000500(Angst)

 Potential #1 for Ca( 40)-Ca( 40)
 ==================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=  1102.09608(cm-1)
 uLR(r) inverse-power terms inlude NO individual-term damping
 uLR(r) has   2 inverse-power terms:    C6 = -1.07400000D+07
                                        C8 = -2.45050000D+08
 Tiemann-type potential with   De=  1102.0961   Rm= 4.277277   is a power series
           in  (r - Re)/(r  -0.59290*Re) of order 20  with the 21 coefficients:
  0.42747000D-03 -0.25408309D+01  0.37961100D+04  0.38207030D+03 -0.27439040D+04
 -0.32273633D+04  0.36311381D+03  0.63437054D+04 -0.74015184D+04 -0.19073891D+05
  0.54234739D+05  0.44039230D+05 -0.15538794D+06 -0.83662838D+05  0.21383107D+06
  0.15592245D+06 -0.15626087D+06 -0.14671112D+06  0.27754300D+05  0.71290802D+05
 -0.12611555D+04
 where for  r < Rinn= 3.6600   V=   +950.7477 +4.305315D+00/R**12
  and  for  r > Rout= 10.000   V= VLIM  -1.074000D+07/r** 6
                                        -2.450500D+08/r** 8
                                        -1.169444D+10/r**10
 ---------------------------------------------------------------------------------

 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN

 Eigenvalue convergence criterion is   EPS= 1.0D-08(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

 For  J=  0, seek the first 100 levels of Potential-1   with   VLIM=  1102.096
```

```
 ** CAUTION ** For  J=  0  E= 1.102096D+03  WF(NEND)/WF(Max)= 5.7D-01 > 1.0D-09
    & initialization quality test  1.2D-01 > 1.D-3   so RMAX may be too small
 ALF finds the highest calculated level is  E(v= 40)=  1.1020959D+03

 E(v=  0, J=  0)=    32.204   Bv=  0.0457401  -Dv= -9.4654D-08   Hv= -3.3305D-13
           Lv= -3.3246D-18   Mv= -4.0622D-23   Nv= -5.6827D-28   Ov= -8.5755D-33
 E(v=  1, J=  0)=    95.054   Bv=  0.0450062  -Dv= -9.8341D-08   Hv= -3.7684D-13
           Lv= -3.9526D-18   Mv= -5.0319D-23   Nv= -7.5985D-28   Ov= -1.2498D-32
 E(v=  2, J=  0)=   155.798   Bv=  0.0442590  -Dv= -1.0221D-07   Hv= -4.2344D-13
           Lv= -4.7010D-18   Mv= -6.3142D-23   Nv= -9.9740D-28   Ov= -1.7691D-32
 E(v=  3, J=  0)=   214.445   Bv=  0.0434991  -Dv= -1.0630D-07   Hv= -4.7409D-13
           Lv= -5.5623D-18   Mv= -7.9639D-23   Nv= -1.3062D-27   Ov= -2.4535D-32
 E(v=  4, J=  0)=   271.006   Bv=  0.0427269  -Dv= -1.1060D-07   Hv= -5.3001D-13
           Lv= -6.5442D-18   Mv= -1.0030D-22   Nv= -1.7194D-27   Ov= -3.3662D-32
 E(v=  5, J=  0)=   325.494   Bv=  0.0419425  -Dv= -1.1515D-07   Hv= -5.9239D-13
           Lv= -7.6705D-18   Mv= -1.2566D-22   Nv= -2.2786D-27   Ov= -4.6134D-32
 E(v=  6, J=  0)=   377.924   Bv=  0.0411461  -Dv= -1.1994D-07   Hv= -6.6232D-13
           Lv= -8.9811D-18   Mv= -1.5651D-22   Nv= -3.0327D-27   Ov= -6.3729D-32
 E(v=  7, J=  0)=   428.311   Bv=  0.0403376  -Dv= -1.2499D-07   Hv= -7.4089D-13
           Lv= -1.0532D-17   Mv= -1.9417D-22   Nv= -4.0386D-27   Ov= -8.9291D-32
 E(v=  8, J=  0)=   476.674   Bv=  0.0395169  -Dv= -1.3032D-07   Hv= -8.2923D-13
           Lv= -1.2392D-17   Mv= -2.4081D-22   Nv= -5.3626D-27   Ov= -1.2710D-31
 .............................................................................
 .................... omit 44 lines ..........................................
 .............................................................................
 E(v= 31, J=  0)=  1079.635   Bv=  0.0154215  -Dv= -6.7120D-07   Hv= -5.1856D-11
           Lv= -7.9288D-15   Mv= -1.6245D-18   Nv= -3.8921D-22   Ov= -1.0265D-25
 E(v= 32, J=  0)=  1086.072   Bv=  0.0139305  -Dv= -7.7955D-07   Hv= -7.5399D-11
           Lv= -1.4677D-14   Mv= -3.7909D-18   Nv= -1.1253D-21   Ov= -3.6457D-25
 E(v= 33, J=  0)=  1091.201   Bv=  0.0123769  -Dv= -9.2059D-07   Hv= -1.1401D-10
           Lv= -2.8196D-14   Mv= -9.2413D-18   Nv= -3.6481D-21   Ov= -1.6459D-24
 E(v= 34, J=  0)=  1095.127   Bv=  0.0107672  -Dv= -1.1012D-06   Hv= -1.7891D-10
           Lv= -6.1402D-14   Mv= -2.8932D-17   Nv= -1.5615D-20   Ov= -9.1350D-24
 E(v= 35, J=  0)=  1097.986   Bv=  0.0091176  -Dv= -1.3486D-06   Hv= -3.1207D-10
           Lv= -1.5448D-13   Mv= -1.0323D-16   Nv= -8.1857D-20   Ov= -7.1549D-23
 E(v= 36, J=  0)=  1099.934   Bv=  0.0074345  -Dv= -1.7140D-06   Hv= -6.1272D-10
           Lv= -4.7939D-13   Mv= -5.0339D-16   Nv= -6.2338D-19   Ov= -8.5943D-22
 E(v= 37, J=  0)= 1101.14      Bv=  0.0057239  -Dv= -2.3165D-06   Hv= -1.4545D-09
           Lv= -2.0275D-12   Mv= -3.8107D-15   Nv= -8.4656D-18   Ov= -2.0996D-20
 E(v= 38, J=  0)= 1101.79      Bv=  0.0039883  -Dv= -3.5003D-06   Hv= -4.8270D-09
           Lv= -1.4991D-11   Mv= -6.3394D-14   Nv= -3.1918D-16   Ov= -1.8021D-18
 E(v= 39, J=  0)= 1102.05      Bv=  0.0022213  -Dv= -6.8558D-06   Hv= -3.4745D-08
           Lv= -4.0813D-10   Mv= -6.6059D-12   Nv= -1.2744D-13   Ov= -2.7477D-15
 ** CAUTION ** For  J=  0  E= 1.102096D+03  WF(NEND)/WF(Max)= 5.7D-01 > 1.0D-09
    & initialization quality test  1.2D-01 > 1.D-3   so RMAX may be too small
 ** CAUTION ** CDJOEL orthogonality tests OV01,OV02 & OV03:  4.4D+01 -2.9D+00  4.4D-02
 ** CAUTION ** Comparison tests for Hv, Lv & Mv give:  4.8D-01  1.5D+00  2.5D+00
 E(v= 40, J=  0)= 1102.10      Bv=  0.0003267  -Dv= -1.9045D-05   Hv=  3.3129D-07
           Lv=  1.4042D-07   Mv= -1.1500D-08   Nv= -1.7039D-09   Ov=  1.7270D-10

 Find  41 Potential-1 vibrational levels with  J=  0
     v     E(v)         v     E(v)         v     E(v)         v     E(v)
    --------------    --------------    --------------    --------------
     0     32.2039     11    609.8189     22    953.1705     33   1091.2007
     1     95.0542     12    650.2901     23    973.7409     34   1095.1269
     2    155.7982     13    688.8432     24    992.6240     35   1097.9858
     3    214.4453     14    725.5009     25   1009.8399     36   1099.9340
     4    271.0063     15    760.2858     26   1025.4107     37   1101.1416
     5    325.4942     16    793.2205     27   1039.3608     38   1101.7856
     6    377.9236     17    824.3270     28   1051.7191     39   1102.0451
     7    428.3109     18    853.6268     29   1062.5203     40   1102.0959
     8    476.6741     19    881.1410     30   1071.8076
     9    523.0327     20    906.8899     31   1079.6353
    10    567.4071     21    930.8932     32   1086.0717

 An  n= 6  N-D theory extrapolation from  v=  39 &  40  implies   vD =  40.176
 ===============================================================================


Case 2.f: Barrow-Aziz HFD-B(6,8,10,12) for {20}Ne{84}Xe [JCP 91, 6348 (1989)]
================================================================================
 Generate   ZMU= 16.14564021596(u)   &   BZ= 9.577645835D-01((1/cm-1)(1/Ang**2))
          from atomic masses:  19.99244017620  &   83.91149772800(u)
 Integrate from  RMIN=  1.500  to  RMAX=  29.00  with mesh  RH= 0.001000(Angst)

 Potential #1 for Ne( 20)-Kr( 84)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=     0.00000(cm-1)
 uLR(r) inverse-power terms inlude NO individual-term damping
 uLR(r) has   4 inverse-power terms:    C6 =  1.89208839D+05
                                        C8 =  1.03241624D+06
                                        C10=  9.93919946D+06
                                        C12=  1.69323761D+08
               and overall damping function:
                    D(r)= exp[ -1.000000*( 3.87258300/r -1.0)** 2.00]
 Potential is Generalized HFD-ABC  with   radial power   gamma= 0.000000
   De=   51.5750[cm-1]   Re= 3.861000[Ang.],   with  exponential-term factors:     beta1= 2.85717137   beta= 0.13240000   and A(pre-
 ----------------------------------------------------------------------------
 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN

 Eigenvalue convergence criterion is   EPS= 1.0D-08(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
        eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

 For  J=  0, seek the first 100 levels of Potential-1   with   VLIM=     0.000

 For J=  0  ETRY=     0.0032 > VMAX=    -0.0003  find onee turn point:  R=  3.46
```

```
 *** CAUTION for  v=999  J=  0  SCHRQ doesn't converge by  ITER=30  DE=-6.40D-05

 *** SCHRQ FAILS in ALF when searching for  v=  5 J=  0   with   EO=   -0.000
     Check range and/or contact R.J. Le Roy [leroy@uwaterloo.ca]
 E(v=  0, J=  0)=   -39.839   Bv=  0.0662725  -Dv= -2.7537D-06   Hv= -4.9208D-10
           Lv= -1.7301D-13   Mv= -7.9564D-17   Nv= -4.2802D-20   Ov= -2.5532D-23
 E(v=  1, J=  0)=   -21.463   Bv=  0.0578380  -Dv= -4.6900D-06   Hv= -1.5922D-09
           Lv= -1.0039D-12   Mv= -8.0955D-16   Nv= -7.5504D-19   Ov= -7.7801D-22
 E(v=  2, J=  0)=    -9.445   Bv=  0.0475245  -Dv= -8.9746D-06   Hv= -6.0767D-09
           Lv= -7.3617D-12   Mv= -1.1521D-14   Nv= -2.1084D-17   Ov= -4.2986D-20
 E(v=  3, J=  0)=    -2.941   Bv=  0.0348686  -Dv= -1.9514D-05   Hv= -3.0794D-08
           Lv= -9.0233D-11   Mv= -3.5340D-13   Nv= -1.6458D-15   Ov= -8.6004D-18
 E(v=  4, J=  0)=-.426588      Bv=  0.0198498  -Dv= -5.4842D-05   Hv= -3.4307D-07
           Lv= -4.4460D-09   Mv= -7.8830D-11   Nv= -1.6610D-12   Ov= -3.9046D-14

 Find   5 Potential-1 vibrational levels with  J=  0
     v     E(v)         v     E(v)         v     E(v)         v     E(v)
    --------------    --------------    --------------    --------------
     0    -39.8395      2    -9.4449      4    -0.4266
     1    -21.4627      3    -2.9410

 An  n= 6  N-D theory extrapolation from  v=   3 &   4  implies   vD =   5.107
 ================================================================================


Case 2.g:  Generalized Tang-Toennies PEC for Ar2 [Jaeger Mol.Phys. 107, 2181]
=================================================================================
 Generate   ZMU= 16.14564021596(u)   &   BZ= 9.577645835D-01((1/cm-1)(1/Ang**2))
          from atomic masses:  19.99244017620  &   83.91149772800(u)
 Integrate from  RMIN=  1.500  to  RMAX=  29.00  with mesh  RH= 0.001000(Angst)

 Potential #1 for Ne( 20)-Kr( 84)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)=     0.00000(cm-1)

 uLR inverse-power terms incorporate TT-type damping with   rhoAB= 4.0251721100
        defined to give very short-range  Dm(r)*Cm/r^m  behaviour   r^{ 1}
        Dm(r)= [1 - exp(-bTT*r)*SUM{(bTT*r)^k/k!}]   where   bTT= rhoAB
 uLR(r) has   6 inverse-power terms:    C6 =  3.07769744D+05
                                        C8 =  2.27073197D+06
                                        C10=  1.70739832D+07
                                        C12=  1.30837685D+08
                                        C14=  1.02178584D+09
                                        C16=  8.13234755D+09

 Generalized Tang-Tonnies Potential function with exponent function
 - {{ +2.98337630000*r +0.09712088100*r^2 -0.27520682700/r +1.01489050000/r^2}}
 and pre-exp factor:
   {{+3.20640487D+07 +0.00000000D+00*r +0.00000000D+00/r +0.00000000D+00*r^2
                     +0.00000000D+00*r^3}}

          Input    DSCM=   99.4734   REQ= 3.762000
          Actual   DSCM=   99.4756   REQ= 3.761825
 -----------------------------------------------------------------------------

 Calculate properties of the single potential described above
 Potential-1 uses inner boundary condition of  zero value  at  RMIN

 Eigenvalue convergence criterion is   EPS= 1.0D-08(cm-1)
 Airy function at 3-rd turning point is quasibound outer boundary condition

 Since state-1 has (projected) electronic angular momentum  OMEGA= 0
         eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

 For  J=  0, seek the first 100 levels of Potential-1   with   VLIM=     0.000

 ** CAUTION ** For  J=  0  E=-1.531965D-03  WF(NEND)/WF(Max)= 7.8D-01 > 1.0D-09
    & initialization quality test  1.7D+00 > 1.D-3   so RMAX may be too small
 ALF finds the highest calculated level is  E(v=  7)= -1.5319646D-03

 E(v=  0, J=  0)=   -83.056   Bv=  0.0709971  -Dv= -1.5817D-06   Hv= -1.3654D-10
           Lv= -2.3775D-14   Mv= -5.4168D-18   Nv= -1.4376D-21   Ov= -4.2174D-25
 E(v=  1, J=  0)=   -55.113   Bv=  0.0649167  -Dv= -2.2323D-06   Hv= -3.0495D-10
           Lv= -8.0158D-14   Mv= -2.7074D-17   Nv= -1.0537D-20   Ov= -4.5027D-24
 E(v=  2, J=  0)=   -33.559   Bv=  0.0579472  -Dv= -3.3313D-06   Hv= -7.2758D-10
           Lv= -2.9172D-13   Mv= -1.4903D-16   Nv= -8.7685D-20   Ov= -5.6762D-23
 E(v=  3, J=  0)=   -18.081   Bv=  0.0498513  -Dv= -5.3022D-06   Hv= -1.9203D-09
           Lv= -1.2440D-12   Mv= -1.0337D-15   Nv= -9.9732D-19   Ov= -1.0659D-21
 E(v=  4, J=  0)=    -8.097   Bv=  0.0404110  -Dv= -9.0846D-06   Hv= -5.9100D-09
           Lv= -6.9579D-12   Mv= -1.0733D-14   Nv= -1.9480D-17   Ov= -3.9467D-20
 E(v=  5, J=  0)=    -2.654   Bv=  0.0295445  -Dv= -1.7235D-05   Hv= -2.4255D-08
           Lv= -6.5523D-11   Mv= -2.3848D-13   Nv= -1.0333D-15   Ov= -5.0240D-18
 E(v=  6, J=  0)=-.442120      Bv=  0.0172872  -Dv= -4.1499D-05   Hv= -2.0780D-07
           Lv= -2.1990D-09   Mv= -3.1958D-11   Nv= -5.5340D-13   Ov= -1.0713D-14
 ** CAUTION ** For  J=  0  E=-1.531965D-03  WF(NEND)/WF(Max)= 7.8D-01 > 1.0D-09
    & initialization quality test  1.7D+00 > 1.D-3   so RMAX may be too small
 ** CAUTION ** CDJOEL orthogonality tests OV01,OV02 & OV03:  1.6D+01 -2.3D+00 -1.4D-01
 ** CAUTION ** Comparison tests for Hv, Lv & Mv give:  1.4D+00  1.6D+00  9.7D+00
 E(v=  7, J=  0)=-.153196E-02  Bv=  0.0031793  -Dv= -7.2632D-05   Hv=  7.7691D-07
           Lv=  4.6342D-07   Mv= -5.2140D-08   Nv= -1.6843D-09   Ov=  6.1002D-10

 Find   8 Potential-1 vibrational levels with  J=  0
     v     E(v)         v     E(v)         v     E(v)         v     E(v)
    --------------    --------------    --------------    --------------
     0    -83.0560      2    -33.5594     4    -8.0969      6    -0.4421
     1    -55.1130      3    -18.0807     5    -2.6540      7    -0.0015

 An  n= 6  N-D theory extrapolation from  v=   6 &   7  implies   vD =   7.178
 ================================================================================
```

## Appendix C 3 : Input/Output files for for Illustrative linelist “production run”

**Case 3 .** This is a data set for an illustrative line-list “production run” for the case of two pointwise potentials (`NUMPOT` $= 2$ in Read #1 and `NTP` $> 0$ in Read #6) which generates the predicted transition energies and Einstein emission coefficients for some 267 555 lines in the $B(^3\Pi^+_{0u}) - X(^1\Sigma^+_g)$ spectrum of $\mathrm{Br}_2$ . This case again exploits the capability of the `NLEV1` $< 0$ option for locating automatically the first $|$`NLEV1`$| + 1$ levels of a given potential. It also illustrates a use of the `NJM` $> 0$ option to find many (or all) rotational sublevels for each $v$ , and of the application of rotational selection rules to calculate transitions between two different electronic states. The input data file is listed in below, followed by parts of the main Channel–6 output and a portion of the associated Channel–8 output file. This calculation of 267 555 matrix elements coupling levels of the two electronic states consumed 23.64 s of CPU time on our decade-old SGI UNIX server.

```
 35 79  35 79  0   2                 % IAN1 IMN1 IAN2 IMN2 CHARGE NUMPOT
'Case 3:  Predict emission for B-X Br2 based on Gerstenkorn (1987) constants'
 0.0015 1.85  15.0   1.d-4           % RH RMIN RMAX EPS
 123  0  0  19742.072d0              % NTP LPPOT IOMEG VLIM
 10 0  4  5 1.8D+05                  % NUSE IR2 ILR NCN CNN
 1.D0 1.D0  15902.4802d0             % RFACT EFACT VSHIFT & B-state turn. pnts.
   2.32483352887883   3834.348717   2.32492725139916   3831.646866
   2.32505070817846   3828.090070   2.32520875281731   3823.540508
   2.32540641247184   3817.856430   2.32564885907544   3810.893306
  .................................................................
  .......... skip 56 lines listing 112 more turning points ........
  .................................................................
   6.87678817820732   3817.856430   7.25492791418183   3823.540508
   7.69918940093639   3828.090070   8.22965127226713   3831.646866
   8.87579778305112   3834.348717

 47  0  0  16056.926D0               % NTP2 LPPOT2 IOMEG2 VLIM2
 10 0  0  6 0.D0                     % NUSE2 IR22 ILR2 NCN2 CNN2
 1.D0 1.D0  0.d0                     % RFACT EFACT VSHIFT2
   2.05649830399176   4483.356304   2.06283295581950   4189.629584
   2.06951602200031   3893.539190   2.07659093472317   3595.104297
  .................................................................
  .......... skip 20 lines listing 36 more turning points .........
  .................................................................
   2.60140908192717   3893.539190   2.61738272682198   4189.629584
   2.63310768612594   4483.356304

-40  1  0  -4  999 1  -1 0           % NLEV1 AUTO1 LCDC LXPCT NJM JDJR IWR LPRWF
  0 0                                % IV(1) IJ(1)
 1  0   1.D0                         % MORDR IRFN RREF
-0.219 0.265                         % DM(0) DM(1)
 15  1  -1 +1 2                      % NLEV2 AUTO2 J2DL J2DU J2DD
 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14  % {IV2(i)}
```

### *Standard Channel-6 output for Illustrative linelist “production run”*

The largest piece of output for this case consists of a listing of the transition frequencies and Einstein $\mathcal{A}$–coefficients for some 267 555 transitions (yielding a line-list of that length) written to Channel–8. A small segment of this output file is presente at the end of this Appendix. Since the associated “standard” output to Channel–6 is also moderately lengthy (some 3221 lines), the listing of it presented below is also considerably truncated. However, this output illustrates some of the (normally not serious) warning messages that may be generated by the program. In particular, for $v' = 34$ , $J' = 100 - 103$ of the truncated listing below, warnings occur for quasibound levels for which `RMAX` is smaller than the outermost turning point at which the program was attempting to apply the Airy function boundary condition (see Section II.B). This warning is printed once each iteration as SCHRQ converges on the associated eigenvalue; as it indicates, in this case the Airy function boundary condition is replaced by use of the WKB wave function initialization of Eq. (4). The second type of warning ("... `so tunneling calculation uses`...") is printed following convergence on the eigenvalue for such a level, as a reminder that the width calculation for this case uses an approximation estimate of the portion of the exponent integral from the end of the range to the actual outermost turning point. However, when this situation arises, the associated tunneling level widths are usually extremely small, and although the resulting predicted width may be slightly in error, the calculated eigenvalue is normally quite accurate.

A different type of problem gives rise to the lines beginning with " `CAUTION for` ..." "`SCHRQ doesn't converge by ...''`, seen here for $v = 34$ , $J = 127$ . This is the highest quasibound level for this $v$; it lies very close to the centrifugal barrier maximum, and after 30 iterations from each of two separate starting points, the Airy function boundary condition was unable to achieve full convergence to `EPS` for this particular level. In spite of this problem, however, the last eigenvalue change of "`DE`= 1.75D-03" $\mathrm{cm}^{-1}$ is considerably smaller than the width (`FWHM` $= 0.90\ \mathrm{cm}^{-1}$) of this tunneling predissociation level, so the lack of full convergence has negligible effect on the true accuracy of the resulting eigenvalue.

Another type of warning message is that seen for $v = 40$ when $J = 93$ ("... "`find onee turn point:` ..."). This message appears when the automatic search for ever higher rotational sublevels goes past the top of the (centrifugal) barrier maximum. In this case the code makes additional tries to place a level marginally below the barrier maximum, an effort that sometimes succeeds, but always eventually fails (as it did for this case).

```
Case 3:  Predict emission for B-X Br2 based on Gerstenkorn (1987) constants
=================================================================================
 Generate   ZMU= 39.45916880000(u)   &   BZ= 2.340730616D+00((1/cm-1)(1/Ang**2))
          from atomic masses:  78.91833760000  &   78.91833760000(u)
 Integrate from  RMIN=  1.850  to  RMAX=  15.00  with mesh  RH= 0.001500(Angst)

 Potential #1 for Br( 79)-Br( 79)
 ================================
 State has  OMEGA= 0   and energy asymptote:   Y(lim)= 19742.07200(cm-1)
 Perform 10-point piecewise polynomial interpolation over  123 input points
 Beyond read-in points extrapolate to limiting asymptotic behaviour:
                   Y(r)  =  Y(lim) - (   0.1800000D+06)/r** 5
 To make input points Y(i) consistent with  Y(lim),  add  Y(shift)=  15902.4802
 Scale input points:  (distance)* 1.000000000D+00  &  (energy)* 1.000000000D+00
             to get required internal units  [Angstroms & cm-1 for potentials]
      r(i)         Y(i)           r(i)         Y(i)          r(i)         Y(i)
   ----------------------   ----------------------   ----------------------
   2.32483353   3834.3487   2.42191370   1696.7527   3.22507343   1821.0440
   2.32492725   3831.6469   2.43001839   1568.5519   3.26089292   1941.3789
 ..........................................................................
 ......................... skip 37 lines of this listing ..................
 ..........................................................................
   2.40751394   1941.3789   3.15509529   1568.5519   8.22965127   3831.6469
   2.41443578   1821.0440   3.18985642   1696.7527   8.87579778   3834.3487
 ----------------------------------------------------------------------------
 Extrapolate to   X .le. 2.3249  with
   Y=    14763.263  +3.552602D+09 * exp(-5.797858D+00*X)
 Function for  X .GE.  8.230  generated by  4-point inverse-power interpolation
   with leading term  1/r**5  relative to dissociation limit   YLIM=  19742.072
   and (dimensionless) leading coefficient fixed as   C5=  180000.00
 ----------------------------------------------------------------------------

 Get matrix elements between levels of Potential-1 (above) & Potential-2 (below)
 ------------------------------------------------------------------------------
 For Potential #2:
 ================
```

```
State has  OMEGA= 0   and energy asymptote:   Y(lim)= 16056.92600(cm-1)
Perform 10-point piecewise polynomial interpolation over   47 input points
To make input points Y(i) consistent with  Y(lim),  add  Y(shift)=      0.0000
Scale input points:  (distance)* 1.000000000D+00  &  (energy)* 1.000000000D+00
            to get required internal units  [Angstroms & cm-1 for potentials]
     r(i)         Y(i)         r(i)         Y(i)         r(i)         Y(i)
  ----------------------   ----------------------   ----------------------
  2.05649830   4483.3563   2.18626063    646.2909   2.42013527    966.1727
  2.06283296   4189.6296   2.19810575    485.5309   2.43259119   1125.2912
  2.06951602   3893.5392   2.21248391    324.2269   2.44438269   1283.8592
  2.07659093   3595.1043   2.22316187    227.1840   2.45563605   1441.8751
  2.08411094   3294.3433   2.23177061    162.3804   2.46644318   1599.3372
  2.09214251   2991.2740   2.24253421     97.4903   2.47687343   1756.2436
  2.10077036   2685.9133   2.25851483     32.5137   2.49680783   2068.3827
  2.11010533   2378.2776   2.28102606      0.0000   2.51575473   2378.2776
  2.12029713   2068.3827   2.30436129     32.5137   2.53392724   2685.9133
  2.13155647   1756.2436   2.32199230     97.4903   2.55147764   2991.2740
  2.13767849   1599.3372   2.33440900    162.3804   2.56851941   3294.3433
  2.14419655   1441.8751   2.34467357    227.1840   2.58514009   3595.1043
  2.15117974   1283.8592   2.35784040    324.2269   2.60140908   3893.5392
  2.15871971   1125.2912   2.37638051    485.5309   2.61738273   4189.6296
  2.16694249    966.1727   2.39240504    646.2909   2.63310769   4483.3563
  2.17602973    806.5054   2.40683303    806.5054
----------------------------------------------------------------------------
Extrapolate to   X .le. 2.0628  with
  Y=    -2292.367  +1.200354D+10 * exp(-6.996051D+00*X)
Function for  X .GE.  2.6174   generated as
  Y=  16056.9260 - ( 1.657906D+06) * r** 22.046446  * exp{-(   9.991684*r)}
----------------------------------------------------------------------------
Potential-1 uses inner boundary condition of  zero value  at  RMIN

Eigenvalue convergence criterion is   EPS= 1.0D-04(cm-1)
Airy function at 3-rd turning point is quasibound outer boundary condition

Since state-1 has (projected) electronic angular momentum  OMEGA= 0
        eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

For  J=  0, seek the first  41 levels of Potential-1   with   VLIM= 19742.072

  and automatically increment  J  in steps of  1 to a maximum value of 999

Matrix element arguments are powers of the distance  r (in Angstroms)
Coefficients of expansion for radial matrix element/expectation value argument:
     -2.190000D-01  2.650000D-01
Potential-2 uses inner boundary condition of  zero value  at  RMIN

Using the rotational selection rule:  delta(J)= -1 to 1 with increment 2
  calculate matrix elements for coupling to the  15 vibrational levels of
  Potential-2:   v =   0   1   2   3   4   5   6   7   8   9  10  11  12  13
                      14

Since state-2 has (projected) electronic angular momentum  OMEGA= 0
        eigenvalue calculations use centrifugal potential  [J*(J+1) - 0]/r**2

...............................................................................
........... skip 2724 lines summarizing results for v= 1-33 ...................
...............................................................................
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
*** For  J=100  E= 19743.24  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=100  E= 19743.22  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=100  E= 19743.22  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)=  99.17  for  R > R(max)=  15.00
*** For  J=101  E= 19748.69  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=101  E= 19748.67  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=101  E= 19748.67  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)= 100.17  for  R > R(max)=  15.00
*** For  J=102  E= 19754.16  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=102  E= 19754.15  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=102  E= 19754.15  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)= 101.18  for  R > R(max)=  15.00
*** For  J=103  E= 19759.66  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=103  E= 19759.65  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J=103  E= 19759.65  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)= 102.19  for  R > R(max)=  15.00
For J=127  ETRY= 19891.7867 > VMAX= 19891.7746  find onee turn point:  R=  2.37
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT=  7, so halve  DE= -3.22D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT=  8, so halve  DE=  1.80D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 10, so halve  DE= -3.51D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 12, so halve  DE= -3.40D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 14, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 16, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 18, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 20, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 22, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 24, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 26, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 28, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 29, so halve  DE=  1.70D-03
*** CAUTION for  v= 34  J=127  SCHRQ doesn't converge by  ITER=30  DE= 1.01D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT=  6, so halve  DE= -3.22D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT=  7, so halve  DE=  1.80D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT=  9, so halve  DE= -3.51D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 11, so halve  DE= -3.40D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 13, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 15, so halve  DE= -3.39D-03
```

```
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 17, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 19, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 21, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 23, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 25, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 27, so halve  DE= -3.39D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 28, so halve  DE=  1.70D-03
** @ J=127  E= 1.99D+04 SCHRQ has cgce prob at  IT= 30, so halve  DE= -3.52D-03
*** CAUTION for  v= -1  J=127  SCHRQ doesn't converge by  ITER=30  DE=-1.76D-03

For vibrational level  v = 34   of Potential-1
  J      E         J       E         J      E         J       E         J      E
--------------   --------------   --------------   --------------   --------------
  0  19443.803   26  19466.021   52  19529.969   78  19632.179  104  19765.173
  1  19443.867   27  19467.723   53  19533.224   79  19636.793  105  19770.719
  2  19443.994   28  19469.486   54  19536.537   80  19641.452  106  19776.284
  3  19444.185   29  19471.312   55  19539.905   81  19646.158  107  19781.868
  4  19444.439   30  19473.198   56  19543.330   82  19650.908  108  19787.469
  5  19444.756   31  19475.147   57  19546.811   83  19655.702  109  19793.083
  6  19445.138   32  19477.157   58  19550.347   84  19660.539  110  19798.709
  7  19445.582   33  19479.228   59  19553.939   85  19665.420  111  19804.345
  8  19446.090   34  19481.360   60  19557.585   86  19670.343  112  19809.988
  9  19446.662   35  19483.553   61  19561.286   87  19675.307  113  19815.634
 10  19447.297   36  19485.806   62  19565.042   88  19680.311  114  19821.282
 11  19447.995   37  19488.120   63  19568.851   89  19685.356  115  19826.927
 12  19448.756   38  19490.495   64  19572.714   90  19690.440  116  19832.565
 13  19449.581   39  19492.930   65  19576.629   91  19695.561  117  19838.191
 14  19450.468   40  19495.425   66  19580.598   92  19700.721  118  19843.802
 15  19451.419   41  19497.979   67  19584.619   93  19705.916  119  19849.390
 16  19452.433   42  19500.594   68  19588.692   94  19711.148  120  19854.948
 17  19453.510   43  19503.267   69  19592.816   95  19716.413  121  19860.467
 18  19454.650   44  19506.000   70  19596.992   96  19721.713  122  19865.936
 19  19455.852   45  19508.792   71  19601.218   97  19727.044  123  19871.337
 20  19457.117   46  19511.643   72  19605.494   98  19732.407  124  19876.643
 21  19458.445   47  19514.552   73  19609.820   99  19737.800  125  19881.820
 22  19459.836   48  19517.520   74  19614.196  100  19743.222  126  19886.844
 23  19461.289   49  19520.546   75  19618.620  101  19748.672
 24  19462.804   50  19523.629   76  19623.092  102  19754.148
 25  19464.381   51  19526.770   77  19627.612  103  19759.649
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
.................................................................................
........... skip 230 lines summarizing results for v= 35-39 .....................
.................................................................................

*** For  J= 74  E= 19742.97  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 74  E= 19742.96  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 74  E= 19742.96  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)=  72.87  for  R > R(max)=  15.00
*** For  J= 75  E= 19746.03  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 75  E= 19746.02  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 75  E= 19746.02  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)=  73.89  for  R > R(max)=  15.00
*** For  J= 76  E= 19749.10  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 76  E= 19749.09  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 76  E= 19749.09  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)=  74.90  for  R > R(max)=  15.00
*** For  J= 77  E= 19752.19  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 77  E= 19752.18  R(3-rd) > RMAX  & E < V(N)  so try WKB B.C. @ RMAX
*** For  J= 77  E= 19752.18  R(3-rd) beyond range so tunneling calculation uses
       pure centrifugal potential with  J(app)=  75.92  for  R > R(max)=  15.00
For J= 93  ETRY= 19800.6818 > VMAX= 19800.4705  find onee turn point:  R=  2.35
For J= 93  ETRY= 19800.6892 > VMAX= 19800.4705  find onee turn point:  R=  2.35
For J= 93  ETRY= 19800.6892 > VMAX= 19800.4705  find onee turn point:  R=  2.35
For J= 93  ETRY= 19800.6892 > VMAX= 19800.4705  find onee turn point:  R=  2.35

For vibrational level  v = 40   of Potential-1
  J      E         J       E         J      E         J       E         J      E
--------------   --------------   --------------   --------------   --------------
  0  19616.873   19  19626.163   38  19652.625   57  19694.708   76  19749.092
  1  19616.922   20  19627.136   39  19654.470   58  19697.304   77  19752.181
  2  19617.020   21  19628.157   40  19656.358   59  19699.935   78  19755.283
  3  19617.168   22  19629.225   41  19658.289   60  19702.600   79  19758.395
  4  19617.364   23  19630.341   42  19660.263   61  19705.297   80  19761.516
  5  19617.609   24  19631.503   43  19662.279   62  19708.027   81  19764.642
  6  19617.904   25  19632.713   44  19664.337   63  19710.788   82  19767.771
  7  19618.247   26  19633.970   45  19666.437   64  19713.579   83  19770.899
  8  19618.639   27  19635.273   46  19668.577   65  19716.401   84  19774.022
  9  19619.081   28  19636.623   47  19670.759   66  19719.250   85  19777.138
 10  19619.571   29  19638.019   48  19672.980   67  19722.128   86  19780.239
 11  19620.109   30  19639.461   49  19675.242   68  19725.033   87  19783.320
 12  19620.697   31  19640.949   50  19677.543   69  19727.963   88  19786.373
 13  19621.333   32  19642.482   51  19679.882   70  19730.918   89  19789.385
 14  19622.017   33  19644.061   52  19682.260   71  19733.896   90  19792.337
 15  19622.750   34  19645.685   53  19684.676   72  19736.896   91  19795.203
 16  19623.531   35  19647.353   54  19687.130   73  19739.918   92  19797.968
 17  19624.360   36  19649.066   55  19689.620   74  19742.958
 18  19625.238   37  19650.824   56  19692.146   75  19746.017
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++

Find  41 Potential-1 vibrational levels with  J=  0
    v     E(v)         v     E(v)         v     E(v)         v     E(v)
   --------------     --------------     --------------     --------------
    0  15985.8099     11  17599.2328     22  18743.5515     33  19404.8742
    1  16150.1163     12  17723.5255     23  18822.9413     34  19443.8033
    2  16311.0672     13  17843.8623     24  18898.2750     35  19479.6566
    3  16468.6043     14  17960.1998     25  18969.6004     36  19512.5503
    4  16622.6712     15  18072.4992     26  19036.9760     37  19542.6009
    5  16773.2113     16  18180.7266     27  19100.4706     38  19569.9259
    6  16920.1678     17  18284.8542     28  19160.1627     39  19594.6434
```

```
    7  17063.4841     18  18384.8610     29  19216.1394     40  19616.8729
    8  17203.1035     19  18480.7338     30  19268.4954
    9  17338.9707     20  18572.4682     31  19317.3318
   10  17471.0312     21  18660.0691     32  19362.7547

 An  n= 5  N-D theory extrapolation from  v=  39 &  40  implies   vD =  59.899
 ==========================================================================
```

## *Standard Channel-8 output for Illustrative linelist “production run”*

```
Case 3:  Predict emission for B-X Br2 based on Gerstenkorn (1987) constants
============================================================
 Note that (v’,J’) & (v",J") strictly label the upper and lower levels, resp.,
      and  E(lower)=E"
 but  E(2)-E(1)  is:  (energy of State-2 level) - (energy of State-1 level)

           Band
 dJ(J")    v’   v"  E(lower)  E(2)-E(1)  A(Einstein)   F-C Factor  <v’j’|M|v"j">
 ------   -------  --------   --------   -----------   -----------   -----------
 P(  1)    0 -  0    162.54  -15823.27  7.51655D-05   3.26301D-10   7.77793D-06
 P(  1)    0 -  1    485.69  -15500.12  1.98479D-03   9.03473D-09   4.12243D-05
 P(  1)    0 -  2    806.67  -15179.14  2.56291D-02   1.22429D-07   1.52860D-04
 P(  1)    0 -  3   1125.45  -14860.36  2.15688D-01   1.08216D-06   4.57792D-04
 P(  1)    0 -  4   1442.03  -14543.78  1.33030D+00   7.01609D-06   1.17424D-03
 P(  1)    0 -  5   1756.40  -14229.41  6.41089D+00   3.55737D-05   2.66365D-03
 P(  1)    0 -  6   2068.54  -13917.27  2.51332D+01   1.46864D-04   5.45245D-03
 P(  1)    0 -  7   2378.43  -13607.38  8.24026D+01   5.07537D-04   1.02119D-02
 P(  1)    0 -  8   2686.06  -13299.75  2.30523D+02   1.49801D-03   1.76763D-02
 P(  1)    0 -  9   2991.42  -12994.39  5.58669D+02   3.83406D-03   2.84933D-02
 P(  1)    0 - 10   3294.49  -12691.32  1.18684D+03   8.61075D-03   4.30264D-02
 P(  1)    0 - 11   3595.25  -12390.56  2.23108D+03   1.71302D-02   6.11533D-02
 P(  1)    0 - 12   3893.69  -12092.12  3.73965D+03   3.04191D-02   8.21222D-02
 P(  1)    0 - 13   4189.78  -11796.03  5.62413D+03   4.85201D-02   1.04526D-01
 ...............................................................................
 ...................... omit 267521 lines .....................................
 ...............................................................................
 R( 91)   40 -  5   2427.17  -17370.80  4.55940D+01   3.22713D-04  -7.46819D-03
 P( 93)   40 -  5   2456.75  -17341.21  4.45961D+01   3.13842D-04  -7.36500D-03
 R( 91)   40 -  6   2736.53  -17061.44  1.63941D+01   1.20264D-04   4.60057D-03
 P( 93)   40 -  6   2765.99  -17031.98  1.74563D+01   1.27340D-04   4.73392D-03
 R( 91)   40 -  7   3043.63  -16754.34  8.11570D+01   6.22525D-04   1.05187D-02
 P( 93)   40 -  7   3072.96  -16725.00  8.14359D+01   6.21159D-04   1.05076D-02
 R( 91)   40 -  8   3348.45  -16449.52  6.05804D+00   4.87388D-05   2.95411D-03
 P( 93)   40 -  8   3377.66  -16420.31  5.45704D+00   4.36756D-05   2.79608D-03
 R( 91)   40 -  9   3650.98  -16146.99  4.46439D+01   3.71936D-04  -8.24583D-03
 P( 93)   40 -  9   3680.06  -16117.91  4.60071D+01   3.81203D-04  -8.34820D-03
 R( 91)   40 - 10   3951.19  -15846.78  4.35551D+01   3.79843D-04  -8.37720D-03
 P( 93)   40 - 10   3980.15  -15817.82  4.27258D+01   3.70610D-04  -8.27501D-03
 R( 91)   40 - 11   4249.08  -15548.89  4.25958D+00   3.84497D-05   2.69541D-03
 P( 93)   40 - 11   4277.91  -15520.06  4.87948D+00   4.38321D-05   2.87733D-03
 R( 91)   40 - 12   4544.62  -15253.35  5.56357D+01   5.28869D-04   1.00258D-02
 P( 93)   40 - 12   4573.32  -15224.64  5.60365D+01   5.29892D-04   1.00359D-02
 R( 91)   40 - 13   4837.80  -14960.17  6.82655D+00   6.82839D-05   3.61565D-03
 P( 93)   40 - 13   4866.37  -14931.60  6.15591D+00   6.12800D-05   3.42476D-03
 R( 91)   40 - 14   5128.60  -14669.37  2.97279D+01   3.08674D-04  -7.77062D-03
 P( 93)   40 - 14   5157.04  -14640.93  3.09159D+01   3.19393D-04  -7.90463D-03
================================================================================
```

## Appendix D : Program Structure

The present section lists the names and outlines the functions of the various subroutines used by **LEVEL**, and indicates their hierarchy. In particular, the level of indentation in this list indicates which subroutines call which others; unless stated otherwise, each subroutine is called exclusively by the immediately preceding routine having one lower level of indentation.

- **LEVEL :** The main program which reads input data and instructions, and calls the potential preparation, eigenfunction determination, and overlap integral routines.
  - **MASSES :** A data subroutine containing accurate atomic masses and other properties of all stable atomic isotopes. For normal cases, its presence obviates the need for a user to look up and type precise particle masses into the input data file. It is lso called by POTGEN to define mass-scaling of BOB functions.
  - **ALF :** For any smooth single-minimum, shelf-state or double-minimum potential, ALF (**A**utomatic **L**evel Finder) uses multiple calls to subroutine SCHRQ (see below) to determine the vibrational energies of all levels from $v = 0$ up to some maximum $v$ specified by its input parameter `KVMAX`. If fewer than the specified number of levels are found, warnings are printed.
    - **SCECOR :** uses first-order semiclassical estimates of $(v + 1/2)$ and $dG(v)/dv$ (see Eqs. (10) and (11), and sometimes more brute force methods, to generate a trial eigenvalue for the 'next' level of interest.
  - **SCHRQ :** Solves the Schrödinger equation to determine the eigenvalue and (unit normalized) eigenfunction of the vibrational level lying closest to the input trial energy.
    - **QBOUND :** For quasibound levels (those lying above the potential asymptote, but behind a potential barrier), applies the Airy function boundary condition at the third turning point to initiate the inward inward integration of the wave function for such levels [8, 9].
    - **WIDTH :** Calculates the tunneling predissociation lifetime or width of a quasibound level [9–11].
      - **LEVQAD :** Called by WIDTH to evaluate the near-turning-point contributions to the semiclassical quadratures over the potential well and the barrier to tunneling which are required for calculating the predissociation rate.
  - **CDJOEL :** Calculates the diatomic molecule centrifugal distortion constants of Eq. (8). The required input is the effective (centrifugally-distorted, if appropriate) radial potential, and the eigenvalue and eigenfunction of the level in question (as calculated by SCHRQ).
  - **LEVXPC :** Calculates the desired diagonal expectation values of powers of the specified distance coordinate or (interpolated) radial function `RFN`$(r)$ (see Read $^{\#}$26 in Appendix B).
  - **MATXEL :** Calculates the desired off-diagonal matrix elements of powers of the specified radial function or distance coordinate, and the radiative lifetime or Einstein emission coefficient $\mathcal{A}$ [s$^{-1}$].
  - **PREPOT :** The subroutine that oversees reading of the parameters defining the potential and generating the required potential array at the `N` distances specified by the input distance array.

**GENINT :** Uses piecewise polynomial or cubic spline functions to interpolate over a set of read-in turning points to yield the potential function array at the equally-spaced radial mesh required by SCHRQ . If necessary, it extrapolates beyond the range of the given points with analytic functions (see options for parameter `ILR` of READ #7).

**PLYINTRP :** Performs piecewise polynomial interpolation on a given array of point, and returns the function value and (if desired) its derivatives at a specified point. It is used by GENINT to interpolate for the potential for cases with `NUSE` $> 0$ . This routine is also used by SPLINT to define the first derivatives at the inner and outer ends of the interpolation region, $R =$ `XI`$(1)$ and `XI(NTP)`, respectively.

**SPLINT :** Calls subroutine SPLINE to generate the $4 \times (\texttt{NTP} - 1)$ coefficients required to define the cubic spline through the `NTP` given turning points, and then uses these coefficients to generate the desired interpolated function values at the specified integration mesh points.

**SPLINE :** Generates the coefficients defining the cubic spline function through the given `NTP` turning points.

**POTGEN :** For the various analytic potential function specified by input parameter `IPOTL` (see READ #10), reads in the parameters defining those functions and generates the desired array of potential function values on the specified radial grid. If BOB correction functions are to be included, also reads in the parameters defining them and incorporates them into the effective adiabatic potential used by `SCHRQ`.

**DAMPF :** Generates the damping functions of Eqs. (25) and (26) utilized in defining the tails of the MLR, DELR and HPP potential energy functions.

**AFdiag :** Performs the $2 \times 2$ or $3 \times 3$ diagonalization used to define the long-range tail of a potential energy function the case or interstate coupling near the $nS{+}nP$ asymptote of a homonuclear alkali dimer [33, 49–51].

**LKoef :** Asen Pashov's subroutine to generate the array of `Nbeta` × `Nbeta` coefficients that define his spline 'basis functions' [45].

**Scalc :** A function subroutine to generate the $S_m(x)$ 'basis functions' used by Pashov to generate values of a spline function.

**ludcmp :** A subroutine used by `LKoef`.