

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.

Appendix A.	Structure of the Input Data File	pp. 1–2
Appendix B.	Definitions and Descriptions of the Input Data File Parameters	pp. 3–13
Appendix C.	Illustrative Cases and Sample Input and Output Files	pp. 14–19
Appendix C.1:	Introductory Illustrative Applications	pp. 14–19
Appendix C.2:	Applications with 7 Types of Analytical Potentials ...	pp. 20–30
Appendix C.3:	Sample pointwise-PEC line-list “production run”	pp. 31–35
Appendix D.	Overview of Program Structure	pp. 36–37

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 ≤ 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 tritron 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: \pm 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 ≤ 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 zeroth order estimates would be $\text{RMIN} \approx 0.6 \times (\text{potential inner wall position})$ 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 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) **READS** #10–23 for the case of an analytic potential function.

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

NTP: an integer that is set ≤ 0 to generate an analytic potential using **POTGEN**, in which case the program skips **READS** #7–9 and goes directly to **READ** #10. If $\text{NTP} > 0$, 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 $\text{LPPOT} > 0$, 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 $\text{LPPOT} < 0$ writes the resulting potential in condensed format to Channel-8 at every $|\text{LPPOT}|^{\text{th}}$ 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 $[J(J+1) - \text{OMEGA}^2]\hbar^2/(2\mu r^2)$. Setting $\text{OMEGA} \geq 99$ 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 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 $\text{NUSE} > 0$, use **NUSE**-point piecewise polynomials; if $\text{NUSE} \leq 0$, perform cubic spline interpolation. For highly precise and smooth input points, such as those generated from an **RKR** calculation, $\text{NUSE} = 8, 10$ or 12 is often most appropriate; for less precise or less dense points, such as those from *ab initio* calculations, low-order piecewise polynomials ($\text{NUSE} = 4$) or a spline ($\text{NUSE} \leq 0$) 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 **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 **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 **ILR** \geq 2, specify the theoretically appropriate value of **NCN** (≥ 1), and if it is available, also input an estimate of **CNN** (see below).

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

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

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

For **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: $V(r) = \text{VLIM} - \sum_{m=0}^{\text{ILR}-1} C_{\text{NCN}+2m}/r^{\text{NCN}+2m}$.

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

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

CNN: For inverse-power potential extrapolation with **ILR** \geq 2, setting **CNN** \neq 0 causes the leading inverse-power coefficient to be fixed at the read-in value **CNN** = C_{NCN} [$\text{cm}^{-1} \text{\AA}^{\text{NCN}}$] 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 to have their units converted to those employed in the program (\AA 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 \AA 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 $\text{NTP} \leq 0$), 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.

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

IPOTL = 2: uses Eq. (13) to generate a GPEF power series potential of order $N_\beta = \text{Nbeta}$ using Seto's [27] form of the Šurkus [26] expansion variable $z = z(r) = (r^{\text{QPAR}} - r_e^{\text{QPAR}})/(a_S r^{\text{QPAR}} + b_S r_e^{\text{QPAR}})$, with β_0 defined by the input value of **DSCM**, $\text{PARM}(i) = \beta_i$ for $i = 1$ to **Nbeta**, $a_S = \text{PARM}(\text{Nbeta} + 1)$ and $b_S = (\text{Nbeta} + 2)$. Note that the Šurkus case of $\text{QPAR} < 0$ is accommodated by Seto's identity [27]: $z(-\text{QPAR}, a_S, b_S) = z(\text{QPAR}, -b_S, -a_S)$. For this case **NVARB** = **Nbeta** + 2, while **QPAR**, **APSE** and **NCMM** are dummy variables.

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

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

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

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

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

For $\text{APSE} > 0$, 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^{ref} values, whose ordinate values $\beta_i = \text{PARM}(i)$ for $i = 1$ to Nbeta define the potential function shape.

IPOTL = 5: generates the DELR potential of Eqs. (28–30) [11], in which $\mathfrak{D}_e \equiv \text{DSCM}$, $r_e \equiv \text{REQ}$, the power defining the expansion variable $y_q^{\text{ref}}(r)$ is $\text{QPAR} = q$, and the exponent coefficient $\beta(r)$ is the simple power-series expansion of Eq. (16) in $y_q^{\text{ref}}(r)$ with expansion coefficients $\text{PARM}(i) = \beta_{i-1}$ for $i = 1$ to $(\text{NVARB} = \text{Nbeta} + 1)$. The additive long-range tail function $u_{\text{LR}}(r)$ 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_{HFD} and β_1 defined (internally) by the input values of $\mathfrak{D}_e \equiv \text{DSCM}$, $r_e \equiv \text{REQ}$, and the attractive inverse-power-sum tail, while the parameters defining the damping function $D_{\text{HFD}}(r)$ are read in as $\text{PARM}(i) = \alpha_i$ for $i = 1 - 3$, and the other exponent coefficients are $\beta_2 = \text{PARM}(4)$ and $\gamma = \text{PARM}(5)$. For this case, the inverse-power long-range coefficients C_m (in units $\text{cm}^{-1} \cdot \text{\AA}^m$) are input through READ #13, and $\text{Nbeta} = \text{NVARB} = 5$, 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 $u_{\text{LR}}(r)$ defined by READS #12 and 13, and the repulsive term parameters $\{\beta_i\}$ read in as $\text{PARM}(i)$ for $i = 1$ to $\text{NVARB} = \text{Nbeta} = 9$. 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 $\beta_i = \text{PARM}(i + 1)$ for $i = 0$ to Nbeta , in which $b = \text{PARM}(\text{Nbeta} + 2)$. 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 $r < r_{\text{inn}} \equiv \text{PARM}(\text{Nbeta} + 3)$ the potential is extrapolated inward by smoothly attaching the function $A e^{-\alpha(r - r_{\text{inn}})}$ at distance r_{inn} . For $r > r_{\text{out}} \equiv (\text{Nbeta} + 4)$ 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 $C_{m_{\text{L}}}/r^{m_{\text{L}}}$ with $m_{\text{L}} = [\text{MMLR}(\text{NCMM}) + 2]$, whose coefficient $C_{m_{\text{L}}}$ is defined (internally) to attach this long-range tail continuously to the polynomial at $r = r_{\text{out}}$. For this model, QPAR , PPAR and APSE are dummy parameters, and $\text{NVARB} = (\text{Nbeta} + 4)$.

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

IBOB: an integer to specify whether (for $\text{IBOB} > 0$) or not (for $\text{IBOB} \leq 0$) 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 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 ≤ 0.0 , the code sets $r_{\text{ref}} = r_e$.

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

For the 2×2 alkali-homodimer (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 $\text{CmVAL}(i)$ are $A_{\text{so}}, C_3^\Sigma, C_3^\Pi, C_6^\Sigma, C_6^\Pi, C_8^\Sigma$ and C_8^Π for $i = 1 - 7$, respectively, and

- For the $A^1\Sigma_u^+$ state of X_2 , set $MMLR(1) = 0$ to select the lower root of the 2×2 determinant.
- For the $b^3\Pi_u$ state of X_2 , set $MMLR(1) = -1$ to select the upper root of the 2×2 determinant.

For the 3×3 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 $\text{CmVAL}(i) = A_{\text{so}}, C_3^\Sigma, C_3^{1\Pi}, C_3^{3\Pi}, C_6^\Sigma, C_6^{1\Pi}, C_6^{3\Pi}, C_8^\Sigma, C_8^{1\Pi}$ and $C_8^{3\Pi}$, respectively, and:

- For the $1^3\Sigma_g^+$ state of X_2 , set $MMLR(2) = -2$ to select the lowest root of the 3×3 determinant [49, 50].
- For the $B^1\Pi_u$ state of X_2 , set $MMLR(2) = -3$ to select the middle root of the 3×3 determinant.
- set $MMLR(2) = -4$ to select the highest root of the 3×3 determinant.

rhoAB: selects whether ($\text{rhoAB} > 0$) or not ($\text{rhoAB} \leq 0$) damping functions are to be used with the inverse-power long-range terms. If $\text{rhoAB} > 0$, it is the value of the system-dependent range-scaling parameter of ρ 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), ($\text{sVSR2} \equiv 2s$). 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 $\text{rhoAB} > 0$:

- $IDSTT > 0$ 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 $y_q^{\text{ref}}(r_i)$ and of the associated exponent coefficient $\beta(r_i)$ defining the cubic spline used to represent the MLR exponent coefficient function $\beta(r)$ when $\text{APSE} > 0$. 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 β_i parameters of Eqs. (13), (23), (33) or (34), or the coefficients β_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^{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_{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_{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_{ad} , p_{ad} , and q_{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 $PAD \equiv p_{\text{ad}} > m_{\text{Last}} \equiv \text{MMLR}(\text{NCMM})$. Note that if $PAD = 0$ and $Ua\text{INF} = 0$, 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

Ua(*i*) and UaINF: 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): $Ua(i) = u_i^a$ and $Ua\text{INF} = u_{\infty}^a$, all have units cm^{-1} .

Ta(*i*) and TaINF: 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 $Ta(i) = t_i^a$ and $Ta\text{INF} = t_{\infty}^a$ are dimensionless.

For a calculation involving only a single potential energy curve ($\text{NUMPOT} = 1$ in READ #1), the code now proceeds directly to READ #24. However, if $\text{NUMPOT} = 2$, it 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 ≤ 0 , the program automatically finds all vibrational levels from $v = 0 - |\text{NLEV1}|$ 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 $J = \text{IJ}(1)$.

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 ≤ 0 will allow/require a trial energy $\text{GV}(i)$ 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 READs #26–31 are omitted).

- *Even* values of $|\text{LXPCT}| \neq 0$ 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 READs #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 .

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

$|\text{LXPCT}| \geq 5$ 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 = ± 6 write *only* the radial moment components, and omit the output to Channel-8.

NJM & JDJR: if (integer) $\text{NJM} > 0$, 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) $J = \text{IJ}(i)$ to a maximum of $J = \text{NJM}$ (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 $\text{JDJR} = 1$, $\text{IJ}(i) = 0$ (or more strictly $= |\Omega|$) and NJM very large (e.g., $\text{NJM} = 999$).

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

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

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

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

SINNER & INNOD1: parameters to facilitate finding inner *vs.* outer wells of a double well potential if $\text{IAUTO1} > 0$ 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 $\text{NLEV1} > 0$ these are the vibrational [$v = \text{IV}(i)$] and rotational [$J = \text{IJ}(i)$] quantum numbers of the levels to be determined; if $\text{NJM} > \text{IJ}(i)$ the program also automatically calculates rotational levels for that $v = \text{IV}(i)$ with $J = \text{IJ}(i)$ to NJM in steps of JDJR.

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

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

If expectation values or matrix elements are to be calculated (i.e., if $\text{LXPCT} \neq 0$ or -1), READS #26 – 31 specify the desired arguments. However, if $\text{LXPCT} = 0$ 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 $\text{RFN}(r)$ for which expectation values or matrix elements are to be calculated (see Eq. (8)). The current program version is dimensioned for $\text{MORDR} \leq 20$. To calculate only Franck-Condon factors (when $|\text{LXPCT}| \geq 3$), set $\text{MORDR} = -1$.

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

- If $\text{IRFN} \leq -10$, 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 $\text{IRFN} = -4$, then $\text{RFN}(r) = r$ and the matrix element operator is a polynomial in r , of order MORDR , and having coefficients $\text{DM}(i)$, that pre-multiplies the derivative operator d/dr that acts on the wavefunction for ‘Potential-2’ (inserted for Bob Field).
- If $\text{IRFN} = -3$, $\text{RFN}(r) = 1/r^3$.
- If $\text{IRFN} = -2$, $\text{RFN}(r) = 1/r^2$.
- If $\text{IRFN} = -1$, use a Dunham-type expansion coordinate $\text{RFN}(r) = (r - \text{DREF})/\text{DREF}$.
- If $\text{IRFN} = 0$, the function $\text{RFN}(r) = r$, the distance coordinate itself.
- If $\text{IRFN} = 1 - 9$, use the Šurkus-type variable $\text{RFN}(r) = y_p^{\text{DREF}}(r) = (r^p - \text{DREF}^p)/(r^p + \text{DREF}^p)$, with $p = \text{IRFN}$.

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

If $\text{IRFN} \geq 10$, $\text{RFN}(r)$ 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 $\text{MORDR} = 1$, $\text{DM}(0) = 0.0$ and $\text{DM}(1) = 1.0$.

#27. $\text{IF}(\text{DABS}(\text{IRFN}).\text{LE}.9) \text{ READ}(5,*) (\text{DM}(\text{J}), \text{J}= 0, \text{MORDR})$

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

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 ($\text{IRFN} \geq 10$), 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. $\text{READ}(5,*) \text{NRFN}, \text{RFLIM}$

#29. $\text{READ}(5,*) \text{NUSEF}, \text{ILRF}, \text{NCNF}, \text{CNNF}$

#30. $\text{READ}(5,*) \text{RFACTF}, \text{MFACTF}$

#31. $\text{READ}(5,*) (\text{XIF}(\text{I}), \text{YIF}(\text{I}), \text{I}= 1, \text{NRFN})$

NRFN: Is the number of known function values $\{\text{XIF}(i), \text{YIF}(i)\}$ 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 ($|\text{LXPCT}| \geq 3$), couple each level of Potential-1, generated as specified by READs #24 and 25, to all rotation levels of the **NLEV2** vibrational levels $v = \text{IV2}(i)$ allowed by the rotational selection rules $\Delta J = \text{J2DL}$ to J2DU in steps of J2DD (e.g., for P and R transitions: $\text{J2DL} = -1$, $\text{J2DU} = +1$, $\text{J2DD} = +2$). If **NUMPOT** = 2 these are levels of Potential-2 and no constraints are imposed, but if **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 READs #32 & 33. Integer **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 **AUTO2** ≤ 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 provide an introduction to the types of calculations that may be performed, and illustrate 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 $J(\text{upper}) \leq 1$.
- (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 EFACCT 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)= -7.72493 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
-----
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
-----
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 ‘EMO₃(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 **Polynomial-Exponent 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 **Spline-Exponent 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 **Double-Exponential Long-Range (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 $^{20}\text{Xe}^{84}\text{Kr}$ is performed using the **generalized HFD function** reported by Aziz *et al.* [75].
- (g) This calculation for the ground $X^1\Sigma^+$ state of $^{40}\text{Ar}_2$ 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 corr: 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
-0.254083092764773077d01 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 LPRWF
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 % \beta_1 - \beta_9
-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 coeff: 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 corr: 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(1H)/MASS(2H)] 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(1H)/MASS(2H)] 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	Bv= 3.0009468	Dv= -9.6194D-05	Hv= 2.0891D-09
E(v= 0, J= 0)=-10576.9713	Mv= 1.8787D-18	Nv= -2.8462D-22	Ov= -3.9837D-27
E(v= 1, J= 0)=-9531.1273	Lv= -1.0297D-13		
E(v= 1, J= 0)=-9531.1273	Bv= 2.9333876	Dv= -9.6337D-05	Hv= 1.9600D-09
E(v= 1, J= 0)=-9531.1273	Mv= 6.7506D-19	Nv= -4.0035D-22	Ov= -1.8539D-26
E(v= 2, J= 0)=-8517.5782	Lv= -1.1534D-13		
E(v= 2, J= 0)=-8517.5782	Bv= 2.8643763	Dv= -9.6828D-05	Hv= 1.7810D-09
E(v= 2, J= 0)=-8517.5782	Mv= -1.4522D-18	Nv= -7.1077D-22	Ov= -4.9236D-26
E(v= 3, J= 0)=-7537.4551	Lv= -1.3369D-13		
E(v= 3, J= 0)=-7537.4551	Bv= 2.7933659	Dv= -9.7786D-05	Hv= 1.5280D-09
E(v= 3, J= 0)=-7537.4551	Mv= -5.2122D-18	Nv= -1.2423D-21	Ov= -1.3838D-25
E(v= 4, J= 0)=-6592.2479	Lv= -1.6404D-13		
E(v= 4, J= 0)=-6592.2479	Bv= 2.7196297	Dv= -9.9396D-05	Hv= 1.1631D-09
E(v= 4, J= 0)=-6592.2479	Mv= -1.2452D-17	Nv= -2.3423D-21	Ov= -3.4728D-25
E(v= 5, J= 0)=-5683.9300	Lv= -2.1360D-13		
E(v= 5, J= 0)=-5683.9300	Bv= 2.6421849	Dv= -1.0193D-04	Hv= 6.2174D-10
E(v= 5, J= 0)=-5683.9300	Mv= -2.6867D-17	Nv= -4.8363D-21	Ov= -8.5123D-25
E(v= 6, J= 0)=-4815.1134	Lv= -2.9701D-13		
E(v= 6, J= 0)=-4815.1134	Bv= 2.5596786	Dv= -1.0579D-04	Hv= -2.0991D-10
E(v= 6, J= 0)=-4815.1134	Mv= -5.6382D-17	Nv= -1.0793D-20	Ov= -2.1867D-24
E(v= 7, J= 0)=-3989.2702	Lv= -4.4425D-13		
E(v= 7, J= 0)=-3989.2702	Bv= 2.4701994	Dv= -1.1164D-04	Hv= -1.5383D-09
E(v= 7, J= 0)=-3989.2702	Mv= -1.1988D-16	Nv= -2.6016D-20	Ov= -6.1356D-24
E(v= 8, J= 0)=-3211.0590	Lv= -7.1777D-13		
E(v= 8, J= 0)=-3211.0590	Bv= 2.3709745	Dv= -1.2055D-04	Hv= -3.7550D-09
E(v= 8, J= 0)=-3211.0590	Mv= -2.6769D-16	Nv= -6.8839D-20	Ov= -1.9375D-23
E(v= 9, J= 0)=-2486.8045	Lv= -1.2572D-12		
E(v= 9, J= 0)=-2486.8045	Bv= 2.2578703	Dv= -1.3439D-04	Hv= -7.6602D-09
E(v= 9, J= 0)=-2486.8045	Mv= -6.5150D-16	Nv= -2.0617D-19	Ov= -7.1509D-23
E(v= 10, J= 0)=-1825.1989	Lv= -2.4088D-12		
E(v= 10, J= 0)=-1825.1989	Bv= 2.1245297	Dv= -1.5657D-04	Hv= -1.5062D-08
E(v= 10, J= 0)=-1825.1989	Mv= -1.8077D-15	Nv= -7.3449D-19	Ov= -3.2785D-22
E(v= 11, J= 0)=-1238.3300	Lv= -5.1513D-12		
E(v= 11, J= 0)=-1238.3300	Bv= 1.9607791	Dv= -1.9391D-04	Hv= -3.0630D-08
E(v= 11, J= 0)=-1238.3300	Mv= -6.1094D-15	Nv= -3.3875D-18	Ov= -2.0746D-21
E(v= 12, J= 0)=-743.1449	Lv= -1.2783D-11		
E(v= 12, J= 0)=-743.1449	Bv= 1.7495212	Dv= -2.6164D-04	Hv= -6.8835D-08
E(v= 12, J= 0)=-743.1449	Mv= -2.8259D-14	Nv= -2.3600D-17	Ov= -2.1938D-20
E(v= 13, J= 0)=-363.0851	Lv= -3.9679D-11		
E(v= 13, J= 0)=-363.0851	Bv= 1.4609104	Dv= -3.9887D-04	Hv= -1.8763D-07
E(v= 13, J= 0)=-363.0851	Mv= -2.2062D-13	Nv= -3.2568D-16	Ov= -5.3844D-19
E(v= 14, J= 0)=-126.0360	Lv= -1.7762D-10		
E(v= 14, J= 0)=-126.0360	Bv= 1.0524948	Dv= -6.9579D-04	Hv= -6.2944D-07
E(v= 14, J= 0)=-126.0360	Mv= -2.8624D-12	Nv= -8.7147D-15	Ov= -3.0196D-17
E(v= 15, J= 0)=-30.5770	Lv= -1.1429D-09		
E(v= 15, J= 0)=-30.5770	Bv= 0.6130777	Dv= -9.3162D-04	Hv= -1.4581D-06
E(v= 15, J= 0)=-30.5770	Mv= -5.6840D-11	Nv= -4.6701D-13	Ov= -4.2484D-15
E(v= 16, J= 0)=-2.7309	Lv= -7.8253D-09		
E(v= 16, J= 0)=-2.7309	Bv= 0.2852832	Dv= -2.1746D-03	Hv= -2.9685D-05
E(v= 16, J= 0)=-2.7309	Mv= -3.9645D-08	Nv= -1.9920D-09	Ov= -1.1090D-10
E(v= 16, J= 0)=-2.7309	Lv= -9.2968D-07		

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

```

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 v	22 Potential-1 E(v)	vibrational v	levels E(v)	with v	J= 0 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 include NO individual-term damping

uLR(r) has 2 inverse-power terms: C6 = -1.0740000D+07

C8 = -2.4505000D+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 0.7129802D+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 ** CDJDEL 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 include 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)= -0.42658 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)= -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)= -1.53196E-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 Br_2 . This case again exploits the capability of the NLEV1 < 0 option for locating automatically the first $|\text{NLEV1}| + 1$ 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**” cm^{-1} is considerably smaller than the width (**FWHM** = 0.90 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	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	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)
0	15985.8099	11	17599.2328	22	18743.5515
1	16150.1163	12	17723.5255	23	18822.9413
2	16311.0672	13	17843.8623	24	18898.2750
3	16468.6043	14	17960.1998	25	18969.6004
4	16622.6712	15	18072.4992	26	19036.9760
5	16773.2113	16	18180.7266	27	19100.4706
6	16920.1678	17	18284.8542	28	19160.1627
				33	19404.8742
				34	19443.8033
				35	19479.6566
				36	19512.5503
				37	19542.6009
				38	19569.9259
				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)

dJ(J'')	Band 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.

MASSSES: 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 also called by POTGEN to define mass-scaling of BOB functions.

ALF: For any smooth single-minimum, shelf-state or double-minimum potential, ALF (Automatic Level 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 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 $\text{NUSE} > 0$. This routine is also used by SPLINT to define the first derivatives at the inner and outer ends of the interpolation region, $R = \text{XI}(1)$ and $\text{XI}(\text{NTP})$, respectively.

SPLINT : Calls subroutine SPLINE to generate the $4 \times (\text{NTP} - 1)$ 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 2×2 or 3×3 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].

LKcoef : Asen Pashov's subroutine to generate the array of $\text{Nbeta} \times \text{Nbeta}$ 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 LKcoef.