Supplementary Data

This document contains Supplementary Material associated with the paper "**RKR1**: A Computer Program Implementing the First-Order RKR Method for Determining Diatomic Molecule Potential Energy Functions", submitted to the *Journal of Quantitative Spectroscopy and Radiative Transfer* in January 2016. It consists of the five 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

The logical structure and read statements that define the Channel–5 input data file describing the system to be treated and provide all necessary system-specific parameters are shown below. 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=99) IAN1, IMN1, IAN2, IMN2, CHARGE, NDEGv, NDEBv
#2a     IF((IAN1.LE.0).OR.(IAN1.GT.109) READ(5,*) NAME1, MASS1
#2b     IF((IAN2.LE.0).OR.(IAN2.GT.109) READ(5,*) NAME2, MASS2
#3      READ(5,*) TITLE
        IF((NDEGv.EQ.0).OR.(NDEGv.EQ.2)) THEN
#4          READ(5,*) LMAXGv
#5          READ(5,*) (YL0(L),L= 1,LMAXGv)
            ENDIF
#6      IF(NDEGv.GE.2) READ(5,*) VS, DVS, DLIM
        IF(NDEGv.GE.1) THEN
#7          READ(5,*) NLR, ITYPE, IZP0, IZQ0, NP0, NQ0, VD, XCN0
#8          IF(NP0.GT.0) READ(5,*) (P0(I),I= 1,NP0)
#9          IF(NQ0.GT.0) READ(5,*) (Q0(I),I= 1,NQ0)
            ENDIF
#10     IF(NDEBv.LT.0) READ(5,*) Req
        IF((NDEBv.EQ.0).OR.(NDEBv.EQ.2)) THEN
#11         READ(5,*) LMAXBv
#12         IF(LMAXBv.GE.0) READ(5,*) (YL1(L),L= 0,LMAXBv)
            ENDIF
        IF(NDEBv.GE.1) THEN
#13         READ(5,*) ITYPB, IZP1, IZQ1, NP1, NQ1, XCN1
#14         IF(NP1.GT.0) READ(5,*) (P1(I),I= 1,NP1)
#15         IF(NQ1.GT.0) READ(5,*) (Q1(I),I= 1,NP1)
            ENDIF
#16     READ(5,*)  Kaiser, NSV, VEXT
        DO  J= 1,NSV
#17         READ(5,*) V1(I), DV(I), V2(I)
            ENDDO
```

Appendix B. Definitions and Descriptions of the Input File Data

Read integers identifying the molecule or system.

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

IAN1 & IAN2 : integer atomic numbers of the atoms/particles #1 & 2 forming the molecule. If both are positive and ≤ 109 , atomic masses from the tabulation in subroutine MASSES will generate the reduced mass of the system. If either is ≤ 0 or > 109 , the mass of that particle must be input via READ statement #2.

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

CHARGE : $\pm$ integer for the total charge on the molecule. Used to generate Watson's charge-modified reduce mass for neutral or ionic molecules:[26] $\mu = \mu_W = M_A\, M_B/(M_A + M_B - m_e \times \mathrm{CHARGE})$.

NDEGv : specifies whether G_v for this state is to be represented: a) by the Dunham expansion of Eq. (9) when NDEGv $= 0$, b) by the NDE expressions of Eqs. (12) and (14) - (16), when NDEGv $= 1$, or c) by the Tellinghuisen-type MXR "mixed" representation of Eq. (18) when NDEGv $= 2$.

NDEBv : specifies whether B_v for this state is to be represented: a) by the Dunham expansion of Eqs. (10) when NDEBv $= 0$, b) by the NDE expressions of Eqs. (13) and (14) - (16), when NDEBv $= 1$, or c) by the Tellinghuisen-type MXR "mixed" representation of Eq. (19) when NDEBv ≥ 2 . If no rotational data are available and a potential is to be generated using a Morse function inner wall (see § 2.5), one should set NDEBv $= -1$. Note that necessarily NDEBv $\leq$ NDEGv .

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

#2.a `IF((IAN1.LE.0).OR.(IAN1.GT.109)) READ(5,*) NAME1, MASS1`

#2.b `IF((IAN2.LE.0).OR.(IAN2.GT.109)) READ(5,*) NAME2, MASS2`

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

MASS1 & MASS2 : the masses (in amu) of the particles.

Read 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′.

#3. `READ(5,*) TITLE`

Representation for the vibrational energies G_v

READ statements #4 − 9 are concerned with the three possible ways of representing G_v: #4 & 5 are used for a pure Dunham function, #7 − 9 for a pure NDE function, and all of #4 − 9 are used for an MXR function.

If Dunham or MXR expansions are used for G_v (NDEGv$=$ 0 or 2), read in the (integer) order of the G_v vibrational polynomials, LMAXGv, and values of the Dunham coefficients $Y_{l,0}$, starting with $l = 1$.

\#4. `READ(5,*) LMAXGv`
\#5. `READ(5,*) (YL0(L), L= 1,LMAXGv)`

If an MXR mixed representation is to be used for G_v (NDEGv$=$ 2), read in the *real number* values of VS $= v_s$, the value of v at which the Dunham/NDE switching function Eq. (17) is centred, and of DVS $= \delta v_s$, the width parameter for that switching function. Because of the sensitivity of the calculation to their values, VS and DVS should be read in floating point "d" format (e.g., $v_s = 55.0\mathrm{d}0$).
For an MXR function, the absolute value of DLIM $\equiv [G(v = v_{\mathfrak{D}}) - G(v = -1/2)]$ must also be specified.

\#6. `READ(5,*) VS, DVS, DLIM`

If an NDE or MXR functions is used for G_v (NDEGv$\geq$ 1), read in parameters characterizing the NDE function that are to be used.

\#7. `READ(5,*) NLR, ITYPE, IZP0, IZQ0, NP0, NQ0, vD, XCN0`

NLR : is the integer power of the asymptotically-dominant inverse-power term in the long-range potential of Eq. (11).

ITYPE : is an integer specifying the type of NDE expression to be used for G_v:
- ITYPE$=$ 1 for an "outer" rational polynomial expansion using Eq. (15) with $\mathcal{S} = 1$.
- ITYPE$=$ 2 for an "inner" rational polynomial expansion using Eq. (15) with $\mathcal{S} = 2n/(n-2)$.
- ITYPE$=$ 3 uses the exponential NDE function of Eq. (16).

IZP0 & IZQ0 : are the values of the integer t specifying the leading term in the polynomial expansions in, respectively, the numerator and denominator of Eq. (15) for ITYPE$=$ 1 or 2, while for ITYPE$=$ 3 IZP0 specifies the power of the leading term in the exponent expansion of Eq. (16) and IZQ0 is a dummy variable.

NP0 & NQ0 : are the (integer) numbers of coefficients in, respectively, the numerator and denominator polynomials of Eq. (15) for ITYPE$=$ 1 or 2, while for ITYPE$=$ 3 NP0 is the number of terms in the exponent polynomial of Eq. (16) and NQ0 is a dummy variable which should be set ≤ 0: NP0$= L + 1 - t$ and NQ0$= M + 1 - t$.

vD : is the non-integer effective vibrational index at dissociation $v_{\mathfrak{D}}$, and should be read in floating point "d" format (e.g., $v_{\mathfrak{D}} = 64.41\mathrm{d}0$).

XCN0 : is the numerical value of the ND-theory coefficient $X_0(n, C_n, \mu)$ of Eq. (14) for $m = 0$.

Now read in the actual values of the NDE expansion coefficients `P0`$(i) = p^0_{i-t+1}$ and `Q0`$(j) = q^0_{j-t+1}$ required to define the particular NDE function.

\#8. `READ(5,*) (P0(i), i=1, NP0)`
\#9. `READ(5,*) (Q0(j), j=1, NQ0)`

Representation for the inertial rotational constants B_v

If no reliable B_v function is available for this state and one wishes to utilize the approach described in § 2.5 to generate an approximate potential, one should have NDEBv $= -1$ and read in here a value of Req $= r_e$ to specify the position of the minimum of the Morse function for this case.

#10. `READ(5,*) Req`

If a Dunham or MXR expansion is used for B_v (NDEBv $= 0$ or 2), read in the order of the B_v vibrational polynomial LMAXBv and the values of the expansion coefficients YL1(l) $= Y_{l,1}$ for $l = 0 -$ LMAXBv .

#11. `READ(5,*) LMAXBv`

#11. `IF(LMAXBv.GE.0) READ(5,*) (YL1(L), L= 0,LMAXBv)`

If an NDE or MXR functions is used for B_v, read the parameters defining the type of NDE function and the values of the associated expansion parameters. The function types and definitions of the parameters are precisely analogous to those for the vibrational case: see description of READs #7 – 9.

#13. `READ(5,*) ITYPB, IZP1, IZQ1, NP1, NQ1, XCN1`

#14. `READ(5,*) (P1(I), I=1, NP1)`

#15. `READ(5,*) (Q1(J), J=1, NQ1)`

Finally, specify the sophistication of the calculation and define the set(s) of v values for which turning points are to be calculated.

#16. `READ(5,*) Kaiser, NSV, VEXT`

Kaiser : is an integer that specifies whether (Kaiser ≥ 1) or not (Kaiser $= 0$) the "Kaiser correction" of § 2.1 is to be applied.

NSV : is an integer specifying the number of different mesh sizes Δv to be used in specifying the set of v values for which turning points are to be calculated.

VEXT : is a real number whose value controls the option that allows the program to correct unphysical behaviour of the upper part of the inner potential wall defined by the input G_v and B_v functions, as described in § 2.4. For VEXT ≤ 0.0, no inner-wall smoothing is performed, but if VEXT > 0.0 , for $v >$ VEXT inner turning points $r_1(v)$ are generated from Eq. (21) using values of the coefficients A, B & C determined by fitting this function to the inner turning points for the three largest v values with $v \leq$ VEXT , while the outer turning points are defined as the sum of these analytic values plus the calculated quantity $2f$.

For each of NSV cases, read in (floating point) variables V1(i), DV(i) & V2(i) to specify the set of v values running from V1(i) to V2(i) in steps of DV(i) $= \Delta v$, at which turning points are to be calculated. If necessary, the program internally corrects the input values of V2(i) to ensure that when NSV > 1 , necessarily V1(i) $\leq$ V2(i+1). A reasonable example would be to set NSV $= 2$ and then to input

$$\{\mathrm{V1(i)},\ \mathrm{DV(i)},\ \mathrm{V2(i)}\} = \{-0.4\mathrm{d0},\ 0.2\mathrm{d0},\ 1.6\mathrm{d0}\} \quad \text{and} \quad \{2.0\mathrm{d0},\ 0.5\mathrm{d0},\ \mathrm{v}_{\max}\} \quad \text{for} \quad \mathrm{i} = 1\ \&\ 2$$

in which $v_{\max}$ is the highest vibrational level for which turning points are desired. It is usually best to set V1(1) ≥ -0.4d0 .

#17. `READ(5,*) V1(i), DV(i), V2(i)`

Appendix C. Illustrative Sample Data Files and Commentary

This section presents sample data files and (truncated) outputs for seven cases, and discusses some features of the results illustrated by the Channel-6 output files. Note that in the sample data files shown below, the "`%`" symbol appearing on most lines after the last parameter associated with that READ statement and any following text are merely comments, and are ignored by the program. It is often convenient to include such comments in the input files to help recall which parameter is which.

C.1 *Cases (i) & (ii): Standard Dunham-Representation Applications*

The first two sample data files shown below are for the common case in which pure Dunham polynomials in $(v+\frac{1}{2})$ are used for both G_v and B_v. The experimental data on which these Dunham polynomials were based stops at $v = 82$, so the turning point calculation also stops there. The input data files for these cases are shown below.

```
 53 127  53 127  0  0 0                % IAN1 IMN1 IAN2 IMN2 CHARGE NDEGv NDEBv
'(i) Dunham Calculation with Gerstenkorn constants for I2(B)    [VEXT = 0]'
 16                                    % LMAXGv
  1.256643430002D+2 -7.475284960242D-01 -5.016833169864D-3  3.788414181699D-4
 -4.983773834286D-5  4.200565944860D-06 -2.462699605029D-7  1.035559345644D-8
 -3.168784847369D-10 7.099055257498D-12 -1.159685360751D-13 1.361205680478D-15
 -1.115309496593D-17 6.046170833273D-20 -1.947198245975D-22 2.820031243526D-25
 15                                    % LMAXBv
  2.900080684844D-2 -1.496203558218D-04 -1.122999681016D-6 -8.598750387065D-9
 -3.993514191186D-9  7.442705931721D-10 -7.729114740147D-11 4.998660579762D-12
 -2.157393379080D-13 6.436910217056D-15 -1.347501253707D-16 1.977227945639D-18
 -1.994896518940D-20 1.320031684314D-22 -5.162433698190D-25 9.047632057664D-28
  0  2  0.d0                           % Kaiser NSV VEXT
  -0.4d0  0.2d0  1.6d0                 %(1) V1 DV V2
   2.0d0  1.0d0  82.d0                 %(2) V1 DV V2
```

```
 53 127  53 127  0  0 0                % IAN1 IMN1 IAN2 IMN2 CHARGE NDEGv NDEBv
'(ii) Dunham Calculation with Gerstenkorn constants for I2(B)    [VEXT = 45]'
 16                                    % LMAXGv
  1.256643430002D+2 -7.475284960242D-01 -5.016833169864D-3  3.788414181699D-4
 -4.983773834286D-5  4.200565944860D-06 -2.462699605029D-7  1.035559345644D-8
 -3.168784847369D-10 7.099055257498D-12 -1.159685360751D-13 1.361205680478D-15
 -1.115309496593D-17 6.046170833273D-20 -1.947198245975D-22 2.820031243526D-25
 15                                    % LMAXBv
  2.900080684844D-2 -1.496203558218D-04 -1.122999681016D-6 -8.598750387065D-9
 -3.993514191186D-9  7.442705931721D-10 -7.729114740147D-11 4.998660579762D-12
 -2.157393379080D-13 6.436910217056D-15 -1.347501253707D-16 1.977227945639D-18
 -1.994896518940D-20 1.320031684314D-22 -5.162433698190D-25 9.047632057664D-28
  0  2  45.d0                          % Kaiser NSV VEXT
  -0.4d0  0.2d0  1.6d0                 %(1) V1 DV V2
   2.0d0  1.0d0  82.d0                 %(2) V1 DV V2
```

Case (i) is a calculation performed with the input value of VEXT$=0$, so that no inner-wall extrapolation is performed. However, the rapid growth of the value of `C`(exp) above $v \sim 45$ and the warning message printed at $v = 63$ shows that the inner-wall unreliability discussed in § 2.4 is a problem here.

Case (ii) repeats exactly the same calculation as Case (i), but with the input value VEXT$=45$, so that for $v > 45$ the inner wall is defined by Eq. (21) and the outer turning points are adjusted accordingly. As shown by the resulting values of `d`(RMIN) in the last column of the output for this case, the resulting inner-wall smoothing requires only very modest displacements of the turning points. The various warning messages " `*** STOP ITERATION:  At  NDIV= ...` " appearing in both output files for $v > 69$ illustrates the type of convergence problem that was discussed at the end of § 2.3. At high v the higher-order terms in Dunham polynomials tend to yield large contributions of alternating sign, and a substantial amount of numerical cancellation occurs when they are combined to give the overall values of G_v, $G_{v'}$ and $B_{v'}$ appearing in the integrands of Eq. (2) and (3). This loss of significant digits introduces "numerical noise" into the calculation, and prevents the specified degree of numerical convergence from being achieved. Precisely the same problem sometimes occurs at low v when using high-order pure NDE functions, because of the high powers of $(v_{\mathfrak{D}} - v)$ involved. This problem usually has nothing to do with the RKR procedure itself, but rather is a precision problem associated with the type of G_v and/or B_v representation being employed. In this case the best way of avoiding this type of problem would be to use MXR representations, as relatively lower-order polynomials would be required for both the Dunham and NDE components of the MXR than for equivalent pure Dunham or NDE functions of equivalent quality, so that the introduction of numerical noise due to cancellation of significant digits would be greatly reduced.

Standard Channel-6 output for Case (i): Dunham-Representation Application with VEXT = 0

```
(i) Dunham Calculation with Gerstenkorn constants for I2(B)    (VEXT = 0)
 ***********************************************************
 RKR potential for  I(127)- I(127)   with   Charge= 0
 Reduced mass   ZMU= 63.45223600000   and constant   C_u/ZMU =  0.265674312975
     from atomic masses: 126.9044720000  &  126.9044720000(u)

 Seek relative quadrature convergence 1.0D-10.  Bisect interval up to  5 times.
     performing 16-point Gaussian quadrature in each segment

 The 16 Dunham  Gv  expansion coefficients are
        1.2566434300D+02 -7.4752849602D-01 -5.0168331699D-03  3.7884141817D-04
       -4.9837738343D-05  4.2005659449D-06 -2.4626996050D-07  1.0355593456D-08
       -3.1687848474D-10  7.0990552575D-12 -1.1596853608D-13  1.3612056805D-15
       -1.1153094966D-17  6.0461708333D-20 -1.9471982460D-22  2.8200312435D-25

 The 16 Dunham  Bv  expansion coefficients are
        2.9000806848D-02 -1.4962035582D-04 -1.1229996810D-06 -8.5987503871D-09
       -3.9935141912D-09  7.4427059317D-10 -7.7291147401D-11  4.9986605798D-12
       -2.1573933791D-13  6.4369102171D-15 -1.3475012537D-16  1.9772279456D-18
       -1.9948965189D-20  1.3200316843D-22 -5.1624336982D-25  9.0476320577D-28

 At  v00= -0.50000   Gv=  0.00000000   dG/dv= 125.6643   (1/2)d2G/dv2= -0.747528
                     Bv=  0.02900081   { ==>   Req= 3.026702550(A) }
                     alpha_e = 0.000149620

 Calculate turning points at the  92 v-values
   -0.40  -0.20   0.00   0.20   0.40   0.60   0.80   1.00   1.20   1.40   1.60
    2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00  10.00  11.00  12.00
   13.00  14.00  15.00  16.00  17.00  18.00  19.00  20.00  21.00  22.00  23.00
   24.00  25.00  26.00  27.00  28.00  29.00  30.00  31.00  32.00  33.00  34.00
   35.00  36.00  37.00  38.00  39.00  40.00  41.00  42.00  43.00  44.00  45.00
   46.00  47.00  48.00  49.00  50.00  51.00  52.00  53.00  54.00  55.00  56.00
   57.00  58.00  59.00  60.00  61.00  62.00  63.00  64.00  65.00  66.00  67.00
   68.00  69.00  70.00  71.00  72.00  73.00  74.00  75.00  76.00  77.00  78.00
   79.00  80.00  81.00  82.00

 Resulting Turning Points:
   v        E(v)     dE(v)/dv       B(v)           Rmin(v)         Rmax(v)   NDIV  tst(f)   tst(g)    C(exp)       d(RMIN)
 *************************************************************************************************************************
 -0.400     12.5590   125.5147   0.0289858336   2.9982686098   3.0564580703   2  2.0D-15  1.9D-15
 -0.200     37.6319   125.2145   0.0289558194   2.9782445947   3.0791322241   2  1.0D-15  1.1D-15
  0.000     62.6447   124.9132   0.0289257146   2.9648301731   3.0952061509   2  8.9D-16  8.9D-16  24.136903
  0.200     87.5971   124.6109   0.0288955185   2.9541434172   3.1085618558   2  8.9D-16  0.0D+00  18.743521
  0.400    112.4890   124.3076   0.0288652304   2.9450561482   3.1203275989   2  2.7D-15  0.0D+00  16.187465
  0.600    137.3201   124.0033   0.0288348494   2.9370523256   3.1310195049   2  5.6D-15  0.0D+00  14.589502
  0.800    162.0902   123.6980   0.0288043746   2.9298446500   3.1409249606   2  3.4D-15  0.0D+00  13.464354
  1.000    186.7992   123.3919   0.0287738052   2.9232537205   3.1502234566   2  1.2D-15  0.0D+00  12.615397
  1.200    211.4469   123.0849   0.0287431401   2.9171586442   3.1590359772   2  1.6D-15  0.0D+00  11.944830
  1.400    236.0331   122.7771   0.0287123783   2.9114733875   3.1674486490   2  4.4D-16  0.0D+00  11.397566
  1.600    260.5577   122.4684   0.0286815190   2.9061341562   3.1755253604   2  5.3D-15  0.0D+00  10.939821
  2.000    309.4212   121.8487   0.0286195034   2.8963088472   3.1908562062   2  6.7D-16  0.0D+00  10.441069
  3.000    430.4899   120.2854   0.0284626875   2.8753680822   3.2257436830   2  1.6D-15  0.0D+00   9.702227
  4.000    549.9855   118.7026   0.0283032399   2.8579347256   3.2573947391   2  3.2D-15  0.0D+00   8.895459
  5.000    667.8885   117.1000   0.0281410524   2.8428708485   3.2869595709   2  1.3D-15  0.0D+00   8.178077
.....................................................................................................................
 ................................ delete 35 lines of intermediate output .................................
.....................................................................................................................
 41.000   3681.1924    47.2736   0.0194400086   2.6537024925   4.3732707113   2  1.9D-14  0.0D+00   5.192286
 42.000   3727.4605    45.2666   0.0190953193   2.6519000717   4.4195058415   2  7.3D-15  0.0D+00   5.224621
```

```
43.000   3771.7343    43.2856   0.0187450476   2.6501912338   4.4675139688   2  2.7D-13  0.0D+00   5.274020
44.000   3814.0412    41.3331   0.0183893231   2.6485727775   4.5174035438   2  2.6D-13  0.0D+00   5.347653
45.000   3854.4110    39.4118   0.0180282757   2.6470416301   4.5692910591   2  5.6D-13  0.0D+00   5.453392
46.000   3892.8760    37.5240   0.0176620329   2.6455948379   4.6233022676   2  7.7D-13  0.0D+00   5.599117
47.000   3929.4709    35.6718   0.0172907158   2.6442295529   4.6795736198   2  8.4D-14  0.0D+00   5.791765
48.000   3964.2321    33.8570   0.0169144365   2.6429430150   4.7382539489   2  2.9D-14  0.0D+00   6.036134
49.000   3997.1980    32.0814   0.0165332948   2.6417325324   4.7995064402   2  7.5D-14  0.0D+00   6.333525
50.000   4028.4084    30.3464   0.0161473763   2.6405954590   4.8635109219   2  7.1D-13  0.0D+00   6.680356
51.000   4057.9046    28.6531   0.0157567507   2.6395291740   4.9304665189   2  2.8D-12  0.0D+00   7.067006
52.000   4085.7289    27.0026   0.0153614704   2.6385310632   5.0005947206   2  3.1D-13  0.0D+00   7.477325
53.000   4111.9244    25.3958   0.0149615706   2.6375985072   5.0741429189   2  1.2D-13  0.0D+00   7.889412
54.000   4136.5351    23.8333   0.0145570694   2.6367288780   5.1513884849   2  2.4D-12  0.0D+00   8.278751
55.000   4159.6059    22.3158   0.0141479701   2.6359195469   5.2326434674   2  7.5D-12  0.0D+00   8.624812
56.000   4181.1819    20.8439   0.0137342632   2.6351679047   5.3182600153   2  1.6D-12  0.0D+00   8.923178
57.000   4201.3091    19.4181   0.0133159311   2.6344713954   5.4086366543   2  2.3D-12  0.0D+00   9.204994
58.000   4220.0337    18.0390   0.0128929531   2.6338275618   5.5042255799   2  3.7D-12  0.0D+00   9.566790
59.000   4237.4027    16.7071   0.0124653122   2.6332340991   5.6055411791   2  2.0D-11  0.0D+00  10.213553
60.000   4253.4639    15.4232   0.0120330036   2.6326889126   5.7131700545   2  3.4D-12  0.0D+00  11.519257
61.000   4268.2654    14.1880   0.0115960442   2.6321901705   5.8277829069   2  1.4D-11  0.0D+00  14.112736
62.000   4281.8564    13.0023   0.0111544832   2.6317363427   5.9501487510   2  4.8D-12  0.0D+00  18.999369
*** CAUTION *** inner wall exponent parameter becomes very large so skip converging it.
63.000   4294.2868    11.8670   0.0107084144   2.6313262135   6.0811520902   2  4.0D-11  0.0D+00  27.731861
64.000   4305.6074    10.7830   0.0102579875   2.6309588552   6.2218138926   2  1.2D-11  0.0D+00  42.727788
65.000   4315.8701     9.7512   0.0098034201   2.6306335500   6.3733175108   2  8.8D-11  0.0D+00  67.687139
66.000   4325.1275     8.7726   0.0093450080   2.6303496491   6.5370411114   2  4.3D-11  0.0D+00 108.374840
67.000   4333.4333     7.8480   0.0088831328   2.6301063604   6.7145988056   4  2.9D-11  0.0D+00 173.796459
68.000   4340.8418     6.9782   0.0084182663   2.6299024668   6.9078935273   2  3.9D-11  0.0D+00 277.904219
69.000   4347.4081     6.1636   0.0079509683   2.6297359826   7.1191861088   4  7.0D-11  0.0D+00 440.777928
*** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 3.4D-10/1.5D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
70.000   4353.1875     5.4046   0.0074818794   2.6296037771   7.3511869483  16  3.4D-10  0.0D+00 684.397740
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 3.9D-10/2.1D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
71.000   4358.2357     4.7012   0.0070117035   2.6295012062   7.6071799085   8  3.9D-10  0.0D+001001.114776
72.000   4362.6083     4.0531   0.0065411828   2.6294218245   7.8911929944   8  4.2D-11  0.0D+001227.526974
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 2.3D-09/4.4D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
73.000   4366.3602     3.4598   0.0060710625   2.6293572585   8.2082387252   8  2.3D-09  0.0D+00 741.232893
74.000   4369.5458     2.9203   0.0056020488   2.6292973289   8.5646609995   2  5.2D-11  0.0D+00***********
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 1.2D-09/5.3D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
75.000   4372.2184     2.4334   0.0051347613   2.6292304946   8.9686492907   8  1.2D-09  0.0D+00***********
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 2.2D-09/1.9D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
76.000   4374.4295     1.9973   0.0046696885   2.6291445031   9.4310262823   8  2.2D-09  0.0D+00***********
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 5.6D-09/3.5D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
77.000   4376.2292     1.6102   0.0042071562   2.6290268957   9.9664981544   8  5.6D-09  0.0D+00***********
*** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 1.8D-08/1.8D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
78.000   4377.6655     1.2700   0.0037473247   2.6288641803  10.5957277894  16  1.8D-08  0.0D+00***********
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 1.0D-08/8.5D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
79.000   4378.7840     0.9744   0.0032902410   2.6286369521  11.3489510560   8  1.0D-08  0.0D+00***********
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 2.2D-08/2.2D-08   tst(g)/(previous)= 0.0D+00/0.0D+00
80.000   4379.6283     0.7211   0.0028359793   2.6283047716  12.2726819021   8  2.2D-08  0.0D+00***********
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 1.0D-08/5.2D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
81.000   4380.2397     0.5082   0.0023849172   2.6277674770  13.4430893263   8  1.0D-08  0.0D+00***********
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 6.6D-08/2.0D-08   tst(g)/(previous)= 0.0D+00/0.0D+00
82.000   4380.6576     0.3339   0.0019382124   2.6267751470  14.9951672938   8  6.6D-08  0.0D+00***********
**************************************************************************************************************************
```

Illustrative Channel-7 'exported' Output for Case (i)

```
(i) Dunham Calculation with Gerstenkorn constants for I2(B)    (VEXT = 0)
NTP=  185   RKR turning points for  mu= 63.4522360000
   2.62677514702682   4380.65760088575
   2.62776747704117   4380.23973483585
   2.62830477159960   4379.62834557798
   2.62863695205478   4378.78403151789
   2.62886418031796   4377.66549364827
   2.62902689567425   4376.22924252643
   2.62914450309652   4374.42952124383
   2.62923049459116   4372.21837854992
   2.62929732892902   4369.54584835785
   2.62935725853759   4366.36020386397
   2.62942182449420   4362.60826201274
   2.62950120618387   4358.23571805973
   2.62960377713792   4353.18749189746
   2.62973598261309   4347.40806998883
   2.62990246679508   4340.84182826540
   2.63010636039545   4333.43332355261
.........................................
........... omit 60 lines .............
.........................................
   2.82954485456883    784.17876660728
   2.84287084849047    667.88846971460
   2.85793472557816    549.98551872415
   2.87536808220588    430.48990122119
   2.89630884723996    309.42123778347
   2.90613415621106    260.55771065056
   2.91147338746386    236.03314370519
   2.91715864419834    211.44692651450
   2.92325372051888    186.79922689459
   2.92984464998390    162.09021653568
   2.93705232558977    137.32007179574
   2.94505614818662    112.48897459509
   2.95414341724933     87.59711342140
   2.96483017314763     62.64468445586
   2.97824459469180     37.63189283144
   2.99826860982315     12.55895403562
```

```
   3.02670255019776      0.00000000000
   3.05645807030235     12.55895403562
   3.07913222410956     37.63189283144
   3.09520615091131     62.64468445586
   3.10856185583827     87.59711342140
   3.12032759886547    112.48897459509
   3.13101950487040    137.32007179574
   3.14092496062325    162.09021653568
   3.15022345657212    186.79922689459
   3.15903597719346    211.44692651450
   3.16744864904584    236.03314370519
   3.17552536044531    260.55771065056
   3.19085620618194    309.42123778347
   3.22574368302320    430.48990122119
   3.25739473907939    549.98551872415
   3.28695957093366    667.88846971460
   3.31508221725534    784.17876660728
   3.34216881736425    898.83593156504
.........................................
........... omit 62 lines .............
.........................................
   7.35118694827326   4353.18749189746
   7.60717990850308   4358.23571805973
   7.89119299441792   4362.60826201274
   8.20823872523806   4366.36020386397
   8.56466099947824   4369.54584835785
   8.96864929073722   4372.21837854992
   9.43102628229367   4374.42952124383
   9.96649815440838   4376.22924252643
  10.59572778944601   4377.66549364827
  11.34895105596528   4378.78403151789
  12.27268190208392   4379.62834557798
  13.44308932634094   4380.23973483585
  14.99516729384480   4380.65760088575
```

Standard Channel-6 output for Case (ii): Dunham-Representation Application with VEXT > 0

```
(ii) Dunham Calculation with Gerstenkorn constants for I2(B)    (VEXT =45)
************************************************************
RKR potential for  I(127)- I(127)   with   Charge= 0
Reduced mass   ZMU= 63.45223600000   and constant   C_u/ZMU =  0.265674312975
    from atomic masses: 126.9044720000  &  126.9044720000(u)

Seek relative quadrature convergence 1.0D-10.   Bisect interval up to  5 times.
    performing 16-point Gaussian quadrature in each segment

The 16 Dunham  Gv  expansion coefficients are
       1.2566434300D+02 -7.4752849602D-01 -5.0168331699D-03  3.7884141817D-04
      -4.9837738343D-05  4.2005659449D-06 -2.4626996050D-07  1.0355593456D-08
      -3.1687848474D-10  7.0990552575D-12 -1.1596853608D-13  1.3612056805D-15
      -1.1153094966D-17  6.0461708333D-20 -1.9471982460D-22  2.8200312435D-25

The 16 Dunham  Bv  expansion coefficients are
       2.9000806848D-02 -1.4962035582D-04 -1.1229996810D-06 -8.5987503871D-09
      -3.9935141912D-09  7.4427059317D-10 -7.7291147401D-11  4.9986605798D-12
      -2.1573933791D-13  6.4369102171D-15 -1.3475012537D-16  1.9772279456D-18
      -1.9948965189D-20  1.3200316843D-22 -5.1624336982D-25  9.0476320577D-28

At  v00= -0.50000   Gv=  0.00000000   dG/dv= 125.6643   (1/2)d2G/dv2= -0.747528
                    Bv=  0.02900081   { ==>   Req= 3.026702550(A) }
                    alpha_e = 0.000149620

Above   v =  45.000   extrapolate inner wall with exponential
        fitted to last 3 points ( & shift  RMAX  accordingly)

Calculate turning points at the  92 v-values
  -0.40  -0.20   0.00   0.20   0.40   0.60   0.80   1.00   1.20   1.40   1.60
   2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00  10.00  11.00  12.00
  13.00  14.00  15.00  16.00  17.00  18.00  19.00  20.00  21.00  22.00  23.00
  24.00  25.00  26.00  27.00  28.00  29.00  30.00  31.00  32.00  33.00  34.00
  35.00  36.00  37.00  38.00  39.00  40.00  41.00  42.00  43.00  44.00  45.00
  46.00  47.00  48.00  49.00  50.00  51.00  52.00  53.00  54.00  55.00  56.00
  57.00  58.00  59.00  60.00  61.00  62.00  63.00  64.00  65.00  66.00  67.00
  68.00  69.00  70.00  71.00  72.00  73.00  74.00  75.00  76.00  77.00  78.00
  79.00  80.00  81.00  82.00

Resulting Turning Points:
    v        E(v)    dE(v)/dv       B(v)           Rmin(v)        Rmax(v)    NDIV  tst(f)   tst(g)    C(exp)       d(RMIN)
*******************************************************************************************************************************
-0.400     12.5590   125.5147   0.0289858336   2.9982686098   3.0564580703   2  2.0D-15  1.9D-15
-0.200     37.6319   125.2145   0.0289558194   2.9782445947   3.0791322241   2  1.0D-15  1.1D-15
 0.000     62.6447   124.9132   0.0289257146   2.9648301731   3.0952061509   2  8.9D-16  8.9D-16  24.136903
 0.200     87.5971   124.6109   0.0288955185   2.9541434172   3.1085618558   2  8.9D-16  7.8D-16  18.743521
 0.400    112.4890   124.3076   0.0288652304   2.9450561482   3.1203275989   2  2.7D-15  2.6D-15  16.187465
 0.600    137.3201   124.0033   0.0288348494   2.9370523256   3.1310195049   2  5.6D-15  5.3D-15  14.589502
 0.800    162.0902   123.6980   0.0288043746   2.9298446500   3.1409249606   2  3.4D-15  3.2D-15  13.464354
 1.000    186.7992   123.3919   0.0287738052   2.9232537205   3.1502234566   2  1.2D-15  2.0D-15  12.615397
 1.200    211.4469   123.0849   0.0287431401   2.9171586442   3.1590359772   2  1.6D-15  1.3D-15  11.944830
 1.400    236.0331   122.7771   0.0287123783   2.9114733875   3.1674486490   2  4.4D-16  6.7D-16  11.397566
 1.600    260.5577   122.4684   0.0286815190   2.9061341562   3.1755253604   2  5.3D-15  5.3D-15  10.939821
 2.000    309.4212   121.8487   0.0286195034   2.8963088472   3.1908562062   2  6.7D-16  1.1D-15  10.441069
 3.000    430.4899   120.2854   0.0284626875   2.8753680822   3.2257436830   2  1.6D-15  1.9D-15   9.702227
 4.000    549.9855   118.7026   0.0283032399   2.8579347256   3.2573947391   2  3.2D-15  2.9D-15   8.895459
 5.000    667.8885   117.1000   0.0281410524   2.8428708485   3.2869595709   2  1.3D-15  1.6D-15   8.178077
```

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...................................................................................................
................................ delete 35 intermediate lines of output ...........................
...................................................................................................
41.000   3681.1924    47.2736   0.0194400086   2.6537024925   4.3732707113   2  1.9D-14  1.4D-14   5.192286
42.000   3727.4605    45.2666   0.0190953193   2.6519000717   4.4195058415   2  7.3D-15  5.9D-15   5.224621
43.000   3771.7343    43.2856   0.0187450476   2.6501912338   4.4675139688   2  2.7D-13  2.3D-13   5.274020
44.000   3814.0412    41.3331   0.0183893231   2.6485727775   4.5174035438   2  2.6D-13  2.2D-13   5.347653
45.000   3854.4110    39.4118   0.0180282757   2.6470416301   4.5692910591   2  5.6D-13  4.6D-13   5.453392
46.000   3892.8760    37.5240   0.0176620329   2.6455945252   4.6233019549   2  7.7D-13  0.0D+00   5.453392  -0.0000003127
47.000   3929.4709    35.6718   0.0172907158   2.6442282999   4.6795723669   2  8.4D-14  0.0D+00   5.453392  -0.0000012529
48.000   3964.2321    33.8570   0.0169144365   2.6429398909   4.7382508248   2  2.9D-14  0.0D+00   5.453392  -0.0000031241
49.000   3997.1980    32.0814   0.0165332948   2.6417263314   4.7995002393   2  7.5D-14  0.0D+00   5.453392  -0.0000062009
50.000   4028.4084    30.3464   0.0161473763   2.6405847486   4.8635002115   2  7.1D-13  0.0D+00   5.453392  -0.0000107104
...................................................................................................
................................ delete 15 intermediate lines of output ...........................
...................................................................................................
66.000   4325.1275     8.7726   0.0093450080   2.6300725431   6.5367640053   2  4.3D-11  0.0D+00   5.453392  -0.0002771061
67.000   4333.4333     7.8480   0.0088831328   2.6297867831   6.7142792283   4  2.9D-11  0.0D+00   5.453392  -0.0003195773
68.000   4340.8418     6.9782   0.0084182663   2.6295322691   6.9075233296   2  3.9D-11  0.0D+00   5.453392  -0.0003701977
69.000   4347.4081     6.1636   0.0079509683   2.6293069854   7.1187571116   4  7.0D-11  0.0D+00   5.453392  -0.0004289972
*** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 3.4D-10/1.5D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
70.000   4353.1875     5.4046   0.0074818794   2.6291089257   7.3506920969  16  3.4D-10  0.0D+00   5.453392  -0.0004948514
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 3.9D-10/2.1D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
71.000   4358.2357     4.7012   0.0070117035   2.6289360989   7.6066148012   8  3.9D-10  0.0D+00   5.453392  -0.0005651073
72.000   4362.6083     4.0531   0.0065411828   2.6287865356   7.8905577055   8  4.2D-11  0.0D+00   5.453392  -0.0006352889
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 2.3D-09/4.4D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
73.000   4366.3602     3.4598   0.0060710625   2.6286582973   8.2075397640   8  2.3D-09  0.0D+00   5.453392  -0.0006989612
74.000   4369.5458     2.9203   0.0056020488   2.6285494849   8.5639131555   2  5.2D-11  0.0D+00   5.453392  -0.0007478440
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 1.2D-09/5.3D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
75.000   4372.2184     2.4334   0.0051347613   2.6284582488   8.9678770450   8  1.2D-09  0.0D+00   5.453392  -0.0007722458
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 2.2D-09/1.9D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
76.000   4374.4295     1.9973   0.0046696885   2.6283827981   9.4302645773   8  2.2D-09  0.0D+00   5.453392  -0.0007617050
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 5.6D-09/3.5D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
77.000   4376.2292     1.6102   0.0042071562   2.6283214092   9.9657926679   8  5.6D-09  0.0D+00   5.453392  -0.0007054865
*** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 1.8D-08/1.8D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
78.000   4377.6655     1.2700   0.0037473247   2.6282724330  10.5951360422  16  1.8D-08  0.0D+00   5.453392  -0.0005917473
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 1.0D-08/8.5D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
79.000   4378.7840     0.9744   0.0032902410   2.6282343000  11.3485484039   8  1.0D-08  0.0D+00   5.453392  -0.0004026521
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 2.2D-08/2.2D-08   tst(g)/(previous)= 0.0D+00/0.0D+00
80.000   4379.6283     0.7211   0.0028359793   2.6282055210  12.2725826515   8  2.2D-08  0.0D+00   5.453392  -0.0000992506
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 1.0D-08/5.2D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
81.000   4380.2397     0.5082   0.0023849172   2.6281846842  13.4435065335   8  1.0D-08  0.0D+00   5.453392   0.0004172072
*** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 6.6D-08/2.0D-08   tst(g)/(previous)= 0.0D+00/0.0D+00
82.000   4380.6576     0.3339   0.0019382124   2.6281704443  14.9965625911   8  6.6D-08  0.0D+00   5.453392   0.0013952972
****************************************************************************************************************

For   v .GE. 45.00  inner wall extrapolated as:   V(R) =   -1000.5387 + 0.90236044D+10*exp(-  5.45339201*R)
****************************************************************************************************************
```

C.2 *Cases (iii) & (iv): Pure* NDE G_v *and* B_v *Function Applications*

The third and fourth data files are based on NDE functions reported for the $1\,^3\Sigma_g^-$ state of Na_2.[52] These two cases again differ only in that one uses VEXT $= 0$ and the other VEXT $= 35$, with the value of VEXT used in Case (iv) having been selected based upon trends in the values of `C(exp)` seen in the output for Case (iii) in Appendix D. The output for Case (iii) shows three different types of warning message associated with inner-wall misbehaviour, but from the output for Case (iv) we see that the turning point adjustments required to give a smooth inner wall are also quite modest for this case, especially relative to the magnitude of the turning point differences `[RMAX(v) - RMIN(v)]`. Note too that in contrast to Cases (i) and (ii), these Na_2 calculations apply the Kaiser correction, so that the lower bound on the integrals in Eqs. (2) and (3) is v00 $= v_{\rm min} = -0.5018267\ldots$.

```
 11 23  11 23  0  1  1                 % IAN1 IMN1 IAN2 IMN2 CHARGE NDEGv NDEBv
'(iii) JCP 111,3494(1999): NDE functions for Na2(1^3Sigma):  VEXT = 0'
 6  1  1 1  3 2   61.41d0  4.4867d-2   % NLR ITYPE IZP0 IZQ0 NP0 NQ0 VD XCN0
 0.436636d0  -3.529d-3  1.54d-5
 4.8d-2  1.366d-2
 3  1 0  7 0  3.0921d-3                % ITYPB IZP1 IZQ1 NP1 NQ1 XCN1
 0.1341d0  -1.6863d-2  9.2d-4  -2.810837d-5  4.924d-7  -4.61952d-9  1.8d-11
 1  2   0.d0                           % Kaiser NSV VEXT
  -0.4d0  0.2d0  1.6d0                 %(1) V1 DV V2
   1.d0   1.0d0 61.d0                  %(2) V1 DV V2

 11 23  11 23  0  1  1                 % IAN1 IMN1 IAN2 IMN2 CHARGE NDEGv NDEBv
'(iv) JCP 111,3494(1999): NDE functions for Na2(1^3Sigma):  VEXT = 35'
 6  1  1 1  3 2   61.41d0  4.4867d-2   % NLR ITYPE IZP0 IZQ0 NP0 NQ0 VD XCN0
 0.436636d0  -3.529d-3  1.54d-5
 4.8d-2  1.366d-2
 3  1 0  7 0  3.0921d-3                % ITYPB IZP1 IZQ1 NP1 NQ1 XCN1
 0.1341d0  -1.6863d-2  9.2d-4  -2.810837d-5  4.924d-7  -4.61952d-9  1.8d-11
 1  2   35.d0                          % Kaiser NSV VEXT
  -0.4d0  0.2d0  1.6d0                 %(1) V1 DV V2
   1.d0   1.0d0 61.d0                  %(2) V1 DV V2
```

Channel-6 Output file for Case (iii): Pure NDE Functions for G_v *and* B_v VEXT $= 0$

```
(iii) JCP 111,3494(1999): NDE functions for Na2(1^3Sigma):  VEXT = 0
**********************************************************************
RKR potential for Na( 23)-Na( 23)   with   Charge= 0
Reduced mass   ZMU= 11.49488464100   and constant   C_u/ZMU =  1.466533134736
    from atomic masses:  22.9897692820  &   22.9897692820(u)

Seek relative quadrature convergence 1.0D-10.   Bisect interval up to  5 times.
    performing 16-point Gaussian quadrature in each segment

NDE for  Gv  is an  (NP= 3/NQ= 2)  OUTER Pade  expansion in  (vD-v)  with
       X0(n=6)= 4.4867000D-02  and leading num. and denom. powers  1  &   1
       vD=   61.410000    D-G(v=-1/2)=   3432.458368
    Numerator coefficients are:  4.366360000000D-01 -3.529000000000D-03
             1.540000000000D-05
    Denominator coefficients :   4.800000000000D-02  1.366000000000D-02

NDE for  Bv  is an  (NP= 7/NQ= 0) Exponential  expansion in  (vD-v)  with
       X1(n=6)= 3.0921000D-03  and leading num. and denom. powers  1  &   0
    Numerator coefficients are:  1.341000000000D-01 -1.686300000000D-02
             9.200000000000D-04 -2.810837000000D-05  4.924000000000D-07
            -4.619520000000D-09  1.800000000000D-11

Calculate   Y00=  0.171244236    v(cor)= -0.0018267047    v(min)= -0.5018267047
    using    we=  93.7441    wexe= 0.451924    Be=  0.118327    ae= 0.00188162
    and corrected effective    De=  3432.629612 (after adding Y00)

At  v00= -0.50183   Gv=  0.00000000   dG/dv=  93.7457   (1/2)d2G/dv2= -0.451924
                    Bv=  0.11833058   { ==>   Req= 3.520444006(A) }
                    alpha_e = 0.001881624

Calculate turning points at the  67 v-values
  -0.40  -0.20   0.00   0.20   0.40   0.60   1.00   2.00   3.00   4.00   5.00
   6.00   7.00   8.00   9.00  10.00  11.00  12.00  13.00  14.00  15.00  16.00
```

```
  17.00  18.00  19.00  20.00  21.00  22.00  23.00  24.00  25.00  26.00  27.00
  28.00  29.00  30.00  31.00  32.00  33.00  34.00  35.00  36.00  37.00  38.00
  39.00  40.00  41.00  42.00  43.00  44.00  45.00  46.00  47.00  48.00  49.00
  50.00  51.00  52.00  53.00  54.00  55.00  56.00  57.00  58.00  59.00  60.00
  61.00

Resulting Turning Points:
    v        E(v)    dE(v)/dv       B(v)          Rmin(v)        Rmax(v)   NDIV  tst(f)   tst(g)    C(exp)       d(RMIN)
************************************************************************************************************************
-0.400      9.5411    93.6537   0.1181411455   3.4433775243   3.6030899681   2  3.7D-12  3.7D-12
-0.200     28.2538    93.4731   0.1177817356   3.3910255732   3.6662176913   2  4.5D-13  4.4D-13
 0.000     46.9304    93.2926   0.1174382433   3.3563299157   3.7114568524   2  5.8D-13  5.8D-13   9.540879
 0.200     65.5709    93.1123   0.1171096782   3.3288990458   3.7492108472   2  5.5D-14  0.0D+00   7.535556
 0.400     84.1753    92.9322   0.1167950997   3.3056943782   3.7825297317   2  7.1D-14  0.0D+00   6.547257
 0.600    102.7438    92.7521   0.1164936143   3.2853252705   3.8128152096   2  1.2D-13  0.0D+00   5.901498
 1.000    139.7727    92.3924   0.1159265724   3.2502928508   3.8671290938   2  7.9D-14  0.0D+00   5.307723
 2.000    231.7160    91.4946   0.1146836989   3.1817426241   3.9811208342   2  4.0D-14  0.0D+00   4.541315
 3.000    322.7622    90.5979   0.1136272512   3.1278016799   4.0774161687   2  3.4D-14  0.0D+00   3.770565
 4.000    412.9118    89.7012   0.1126941968   3.0821210964   4.1632699371   2  4.0D-14  0.0D+00   3.145085
 5.000    502.1641    88.8032   0.1118369435   3.0419589256   4.2421563702   2  4.1D-14  0.0D+00   2.770094
.............................................................................................................
.............................. delete 25 intermediate lines of output ...............................
.............................................................................................................
31.000   2475.5535    60.8194   0.0853376407   2.5748003281   5.8987370706   2  6.6D-15  0.0D+00   2.494313
32.000   2535.6636    59.3943   0.0839351846   2.5660411629   5.9710694085   2  3.0D-15  0.0D+00   2.557118
33.000   2594.3287    57.9291   0.0824882473   2.5576787510   6.0454465171   2  5.3D-15  0.0D+00   2.572445
34.000   2651.5077    56.4219   0.0809967870   2.5496940544   6.1220842278   2  8.9D-16  0.0D+00   2.516015
35.000   2707.1579    54.8708   0.0794609787   2.5420647863   6.2012202048   2  2.4D-15  0.0D+00   2.361046
36.000   2761.2341    53.2737   0.0778809883   2.5347655285   6.2831192628   2  4.1D-15  0.0D+00   2.080646
37.000   2813.6893    51.6284   0.0762566898   2.5277681799   6.3680802034   2  2.2D-15  0.0D+00   1.651688
38.000   2864.4740    49.9324   0.0745873285   2.5210427621   6.4564445628   2  2.2D-16  0.0D+00   1.060115
39.000   2913.5363    48.1832   0.0728711368   2.5145586043   6.5486077891   2  1.6D-15  0.0D+00   0.307079
*** CAUTION ***  Inner potential wall has negative curvature and requires smoothing for   VEXT .ge.  40.00
40.000   2960.8217    46.3779   0.0711049093   2.5082859223   6.6450335476   2  1.7D-15  0.0D+00  -0.585320
41.000   3006.2725    44.5136   0.0692835503   2.5021977994   6.7462721082   2  4.4D-15  0.0D+00  -1.570285
42.000   3049.8281    42.5869   0.0673996069   2.4962725637   6.8529841480   2  2.7D-15  0.0D+00  -2.575856
43.000   3091.4244    40.5943   0.0654428122   2.4904965401   6.9659718637   2  4.9D-15  0.0D+00  -3.507648
44.000   3130.9935    38.5319   0.0633996671   2.4848671285   7.0862201311   2  2.6D-15  0.0D+00  -4.252501
45.000   3168.4635    36.3954   0.0612531062   2.4793961253   7.2149517566   2  2.2D-15  0.0D+00  -4.677874
46.000   3203.7583    34.1806   0.0589823104   2.4741131522   7.3537029134   2  6.7D-16  0.0D+00  -4.618253
47.000   3236.7971    31.8829   0.0565627497   2.4690689932   7.5044281613   2  1.1D-15  0.0D+00  -3.832714
48.000   3267.4950    29.4981   0.0539665741   2.4643385610   7.6696499185   2  1.3D-15  0.0D+00  -1.897550
49.000   3295.7631    27.0227   0.0511634986   2.4600231336   7.8526765723   2  2.2D-16  0.0D+00   2.069065
50.000   3321.5095    24.4547   0.0481223659   2.4562514563   8.0579298257   2  2.2D-16  0.0D+00  10.203665
*** CAUTION *** inner wall exponent parameter becomes very large so skip converging it.
51.000   3344.6420    21.7955   0.0448135876   2.4531793539   8.2914518932   2  1.3D-15  0.0D+00  28.503161
52.000   3365.0721    19.0516   0.0412126675   2.4509877999   8.5617205253   2  5.7D-14  0.0D+00  79.410278
53.000   3382.7221    16.2389   0.0373049516   2.4498802104   8.8810153652   2  2.8D-13  0.0D+00 292.309496
*** WARNING ***  inner wall becomes unstable at    v = 54.00   where  RMIN  turns ourward!
54.000   3397.5369    13.3878   0.0330916168   2.4500815815   9.2678268990   2  1.7D-12  0.0D+00
55.000   3409.5017    10.5499   0.0285966481   2.4518458748   9.7513732918   2  1.1D-11  0.0D+00
56.000   3418.6677     7.8065   0.0238741458   2.4554853140  10.3807554101   2  7.8D-11  0.0D+00
57.000   3425.1846     5.2741   0.0190147352   2.4614486705  11.2455146457   4  7.5D-14  0.0D+00
58.000   3429.3359     3.1019   0.0141491994   2.4705000550  12.5288254702   4  1.5D-12  0.0D+00
59.000   3431.5617     1.4483   0.0094468833   2.4840954640  14.6775186814   8  4.2D-13  0.0D+00
60.000   3432.4448     0.4276   0.0051062558   2.5051465112  19.1825155133   8  1.7D-11  0.0D+00
61.000   3432.6260     0.0272   0.0013357077   2.5396187088  37.5136886427  32  8.5D-11  0.0D+00
************************************************************************************************************************
```

Channel-6 Output file for Case (iv): Pure NDE Functions for G_v *and* B_v VEXT > 0

```
 (iv) JCP 111,3494(1999): NDE functions for Na2(1^3Sigma):  VEXT = 35
************************************************************************
RKR potential for Na( 23)-Na( 23)   with   Charge= 0
Reduced mass   ZMU= 11.49488464100   and constant   C_u/ZMU =  1.466533134736
    from atomic masses:  22.9897692820  &   22.9897692820(u)

Seek relative quadrature convergence 1.0D-10.   Bisect interval up to  5 times.
    performing 16-point Gaussian quadrature in each segment

NDE for  Gv  is an  (NP= 3/NQ= 2)  OUTER Pade  expansion in  (vD-v)  with
       X0(n=6)= 4.4867000D-02  and leading num. and denom. powers  1  &   1
       vD=  61.410000    D-G(v=-1/2)=   3432.458368
    Numerator coefficients are:  4.366360000000D-01 -3.529000000000D-03
             1.540000000000D-05
    Denominator coefficients :   4.800000000000D-02  1.366000000000D-02

NDE for  Bv  is an  (NP= 7/NQ= 0) Exponential  expansion in  (vD-v)  with
       X1(n=6)= 3.0921000D-03  and leading num. and denom. powers  1  &   0
    Numerator coefficients are:  1.341000000000D-01 -1.686300000000D-02
             9.200000000000D-04 -2.810837000000D-05  4.924000000000D-07
            -4.619520000000D-09  1.800000000000D-11

Calculate   Y00=  0.171244236    v(cor)= -0.0018267047    v(min)= -0.5018267047
    using    we=  93.7441    wexe= 0.451924    Be=  0.118327    ae= 0.00188162
    and corrected effective   De=  3432.629612 (after adding Y00)

At  v00= -0.50183   Gv=  0.00000000   dG/dv=  93.7457   (1/2)d2G/dv2= -0.451924
                    Bv=  0.11833058   { ==>   Req= 3.520444006(A) }
                    alpha_e = 0.001881624

Above   v =  35.000   extrapolate inner wall with exponential
        fitted to last 3 points ( & shift  RMAX  accordingly)

Calculate turning points at the  67 v-values
  -0.40  -0.20   0.00   0.20   0.40   0.60   1.00   2.00   3.00   4.00   5.00
```

```
   6.00   7.00   8.00   9.00  10.00  11.00  12.00  13.00  14.00  15.00  16.00
  17.00  18.00  19.00  20.00  21.00  22.00  23.00  24.00  25.00  26.00  27.00
  28.00  29.00  30.00  31.00  32.00  33.00  34.00  35.00  36.00  37.00  38.00
  39.00  40.00  41.00  42.00  43.00  44.00  45.00  46.00  47.00  48.00  49.00
  50.00  51.00  52.00  53.00  54.00  55.00  56.00  57.00  58.00  59.00  60.00
  61.00

Resulting Turning Points:
   v        E(v)      dE(v)/dv       B(v)           Rmin(v)          Rmax(v)     NDIV  tst(f)   tst(g)    C(exp)        d(RMIN)
*************************************************************************************************************************
-0.400      9.5411    93.6537   0.1181411455   3.4433775243   3.6030899681   2  3.7D-12  3.7D-12
-0.200     28.2538    93.4731   0.1177817356   3.3910255732   3.6662176913   2  4.5D-13  4.4D-13
 0.000     46.9304    93.2926   0.1174382433   3.3563299157   3.7114568524   2  5.8D-13  5.8D-13   9.540879
 0.200     65.5709    93.1123   0.1171096782   3.3288990458   3.7492108472   2  5.5D-14  5.1D-14   7.535556
 0.400     84.1753    92.9322   0.1167950997   3.3056943782   3.7825297317   2  7.1D-14  8.5D-14   6.547257
 0.600    102.7438    92.7521   0.1164936143   3.2853252705   3.8128152096   2  1.2D-13  1.3D-13   5.901498
 1.000    139.7727    92.3924   0.1159265724   3.2502928508   3.8671290938   2  7.9D-14  9.1D-14   5.307723
.............................................................................................................
................................. delete 30 intermediate lines of output .................................
.............................................................................................................
32.000   2535.6636    59.3943   0.0839351846   2.5660411629   5.9710694085   2  3.0D-15  2.7D-15   2.557118
33.000   2594.3287    57.9291   0.0824882473   2.5576787510   6.0454465171   2  5.3D-15  5.6D-15   2.572445
34.000   2651.5077    56.4219   0.0809967870   2.5496940544   6.1220842278   2  8.9D-16  2.9D-15   2.516015
35.000   2707.1579    54.8708   0.0794609787   2.5420647863   6.2012202048   2  2.4D-15  4.9D-15   2.361046
36.000   2761.2341    53.2737   0.0778809883   2.5347806574   6.2831343917   2  4.1D-15  0.0D+00   2.361046    0.0000151289
37.000   2813.6893    51.6284   0.0762566898   2.5278325976   6.3681446211   2  2.2D-15  0.0D+00   2.361046    0.0000644177
38.000   2864.4740    49.9324   0.0745873285   2.5212126821   6.4566144827   2  2.2D-16  0.0D+00   2.361046    0.0001699200
39.000   2913.5363    48.1832   0.0728711368   2.5149140717   6.5489632565   2  1.6D-15  0.0D+00   2.361046    0.0003554675
40.000   2960.8217    46.3779   0.0711049093   2.5089309666   6.6456785919   2  1.7D-15  0.0D+00   2.361046    0.0006450443
41.000   3006.2725    44.5136   0.0692835503   2.5032585711   6.7473328799   2  4.4D-15  0.0D+00   2.361046    0.0010607717
42.000   3049.8281    42.5869   0.0673996069   2.4978930710   6.8546046553   2  2.7D-15  0.0D+00   2.361046    0.0016205073
43.000   3091.4244    40.5943   0.0654428122   2.4928316198   6.9683069434   2  4.9D-15  0.0D+00   2.361046    0.0023350797
44.000   3130.9935    38.5319   0.0633996671   2.4880723336   7.0894253362   2  2.6D-15  0.0D+00   2.361046    0.0032052051
45.000   3168.4635    36.3954   0.0612531062   2.4836142929   7.2191699242   2  2.2D-15  0.0D+00   2.361046    0.0042181676
46.000   3203.7583    34.1806   0.0589823104   2.4794575452   7.3590473064   2  6.7D-16  0.0D+00   2.361046    0.0053443930
47.000   3236.7971    31.8829   0.0565627497   2.4756031040   7.5109622721   2  1.1D-15  0.0D+00   2.361046    0.0065341108
48.000   3267.4950    29.4981   0.0539665741   2.4720529302   7.6773642878   2  1.3D-15  0.0D+00   2.361046    0.0077143693
49.000   3295.7631    27.0227   0.0511634986   2.4688098783   7.8614633171   2  2.2D-16  0.0D+00   2.361046    0.0087867447
50.000   3321.5095    24.4547   0.0481223659   2.4658775741   8.0675559435   2  2.2D-16  0.0D+00   2.361046    0.0096261178
51.000   3344.6420    21.7955   0.0448135876   2.4632601735   8.3015327128   2  1.3D-15  0.0D+00   2.361046    0.0100808197
52.000   3365.0721    19.0516   0.0412126675   2.4609619237   8.5716946490   2  5.7D-14  0.0D+00   2.361046    0.0099741237
53.000   3382.7221    16.2389   0.0373049516   2.4589864075   8.8901215624   2  2.8D-13  0.0D+00   2.361046    0.0091061972
54.000   3397.5369    13.3878   0.0330916168   2.4573353120   9.2750806294   2  1.7D-12  0.0D+00   2.361046    0.0072537304
55.000   3409.5017    10.5499   0.0285966481   2.4560065229   9.7555339398   2  1.1D-11  0.0D+00   2.361046    0.0041606480
56.000   3418.6677     7.8065   0.0238741458   2.4549913791  10.3802614752   2  7.8D-11  0.0D+00   2.361046   -0.0004939349
57.000   3425.1846     5.2741   0.0190147352   2.4542711018  11.2383370770   4  7.5D-14  0.0D+00   2.361046   -0.0071775687
58.000   3429.3359     3.1019   0.0141491994   2.4538129278  12.5121383430   4  1.5D-12  0.0D+00   2.361046   -0.0166871272
59.000   3431.5617     1.4483   0.0094468833   2.4535674646  14.6469906820   8  4.2D-13  0.0D+00   2.361046   -0.0305279994
60.000   3432.4448     0.4276   0.0051062558   2.4534701170  19.1308391191   8  1.7D-11  0.0D+00   2.361046   -0.0516763942
61.000   3432.6260     0.0272   0.0013357077   2.4534501414  37.4275200753  32  8.5D-11  0.0D+00   2.361046   -0.0861685674
*************************************************************************************************************************

For   v .GE. 35.00  inner wall extrapolated as:   V(R) =     -410.1832 + 0.12600573D+07*exp(-  2.36104606*R)
*************************************************************************************************************************
```

C.3: *Case (v): No Rotational Data: use a Morse Inner Wall*

This data set illustrates the type of situation discussed in § 2.5, a case for which one has vibrational data but little or no rotational data. As discussed in § 2.5, the program uses the vibrational data to determine Morse parameters $\mathfrak{D}_e$ and β, which are then combined with a read-in value of r_e and used to generate the inner-wall turning points. The regular RKR calculation of Eq. (2) is then used to define the outer wall of the potential. Although the molecular species in this example is a hydride (ArH^+), for which one might normally expect to use the Kaiser correction, the uncertainty associated with the inner wall makes such niceties pointless for this case.

```
 20 40  1 1  0  1 -1                   % IAN1 IMN1 IAN2 IMN2 CHARGE NDEGv NDEBv
'(v) NDE-based potential for Ar-H(+):  Morse Inner Wall Extrapolation'
 4 1  2 2  3 1  33.2D0  0.146D0        % NLR ITYPE IZP0 IZQ0 NP0 NQ0 VD XCN0
 -0.396754604292D-4  0.456933925968D-5  -0.392256864315D-7
  0.414470068478D-2
 1.28066d0                             % r_e  Morse minimum
  0  2  11.1d0                         % Kaiser NSV VEXT
  -0.4d0  0.2d0  1.6d0                 %(1) V1 DV V2
   2.0d0  1.0d0  32.d0                 %(2) V1 DV V2
```

Channel-6 output file for Case (v): No Rotational Data: use a Morse Inner Wall

```
(v) NDE-based potential for Ar-H(+):  Morse Inner Wall Extrapolation
**********************************************************************
RKR potential for Ca( 40)- H(  1)   with   Charge= 1
Reduced mass   ZMU=  0.98304686014   and constant   C_u/ZMU = 17.148347540284
    from atomic masses:  39.9625908640  &    1.0078250322(u)

Seek relative quadrature convergence 1.0D-10.   Bisect interval up to  5 times.
    performing 16-point Gaussian quadrature in each segment

NDE for  Gv  is an  (NP= 3/NQ= 1)  OUTER Pade  expansion in  (vD-v)  with
       X0(n=4)= 1.4600000D-01  and leading num. and denom. powers  2  &   2
       vD=   33.200000    D-G(v=-1/2)=  35609.923120
    Numerator coefficients are: -3.967546042920D-05  4.569339259680D-06
            -3.922568643150D-08
    Denominator coefficients :   4.144700684780D-03

NO rotational constants input, so inner wall of potential is Morse function.
  Input   Req= 1.280660(Angst)   plus   we= 2710.952  &  wexe= 61.66771 [cm-1]
  yields Morse with  De= 29793.805 [cm-1]   and   beta= 1.896347 [1/Angst.]

At  v00= -0.50000   Gv=  0.00000000   dG/dv=2710.9524   (1/2)d2G/dv2=-61.667709
                    Bv= 10.45573546   { ==>   Req= 1.280660000(A) }
                    alpha_e = 0.345654121

Calculate turning points at the  42 v-values
  -0.40  -0.20   0.00   0.20   0.40   0.60   0.80   1.00   1.20   1.40   1.60
   2.00   3.00   4.00   5.00   6.00   7.00   8.00   9.00  10.00  11.00  12.00
  13.00  14.00  15.00  16.00  17.00  18.00  19.00  20.00  21.00  22.00  23.00
  24.00  25.00  26.00  27.00  28.00  29.00  30.00  31.00  32.00

Resulting Turning Points:
    v        E(v)    dE(v)/dv       B(v)          Rmin(v)        Rmax(v)   NDIV  tst(f)   tst(g)    C(exp)       d(RMIN)
**************************************************************************************************************************
-0.400     270.4791  2698.6344  10.4557354585   1.2326674815   1.3334613636   2  2.1D-12  0.0D+00
-0.200     807.7496  2674.0913  10.4557354585   1.2002817408   1.3755273493   2  2.5D-13  0.0D+00
 0.000    1340.1238  2649.6715  10.4557354585   1.1792324431   1.4063390438   2  1.3D-13  0.0D+00
 0.200    1867.6263  2625.3741  10.4557354585   1.1628337797   1.4325816297   2  1.0D-13  0.0D+00
 0.400    2390.2815  2601.1982  10.4557354585   1.1491483678   1.4561922932   2  2.6D-13  0.0D+00
 0.600    2908.1136  2577.1429  10.4557354585   1.1372922990   1.4780549888   2  4.0D-14  0.0D+00
 0.800    3421.1467  2553.2073  10.4557354585   1.1267746500   1.4986608500   2  4.9D-14  0.0D+00
 1.000    3929.4045  2529.3905  10.4557354585   1.1172895727   1.5183160588   2  2.3D-14  0.0D+00
 1.200    4432.9107  2505.6914  10.4557354585   1.1086314197   1.5372266954   2  5.9D-14  0.0D+00
 1.400    4931.6888  2482.1091  10.4557354585   1.1006541543   1.5555393127   2  2.6D-14  0.0D+00
 1.600    5425.7621  2458.6426  10.4557354585   1.0932497144   1.5733625617   2  4.4D-16  0.0D+00
 2.000    6399.8859  2412.0524  10.4557354585   1.0798468264   1.6078561171   2  4.4D-14  0.0D+00
 3.000    8754.4466  2297.5257  10.4557354585   1.0522616825   1.6896812308   2  8.7D-15  0.0D+00
..........................................................................................................
................................ delete 25 intermediate lines of output ...................................
..........................................................................................................
29.000   35567.6034    38.9271  10.4557354585   0.8912739167   8.1741833465   2  2.4D-12  0.0D+00
30.000   35595.2410    17.9773  10.4557354585   0.8911669752  10.2995968034   2  1.1D-12  0.0D+00
31.000   35606.5707     6.0350  10.4557354585   0.8911231541  14.3470761119   4  4.4D-12  0.0D+00
32.000   35609.6222     1.0001  10.4557354585   0.8911113535  25.1220618327   8  1.4D-13  0.0D+00
**************************************************************************************************************************
```

C.4: *Cases (vi) & (vii):* MXR *Function for G_v With a Pure Dunham or* MXR *for B_v*

These two cases illustrate the data file setup associated with use of an MXR representation for G_v, combined with either a Dunham or an MXR representation for B_v. In the output for both cases we see that there are some convergence problems as $v \to v_{\mathfrak{D}}$ due to significant digit cancellations in the integrand argument $[G_v - G_{v'}]$. This cannot be avoided unless the entire calculation is performed in quadruple precision, but since no real additional physical accuracy would be attained, it would not be worth the trouble to do that. Note, too that both examples use $\mathrm{VEXT} > 0$, which indicates that a prior $\mathrm{VEXT} = 0$ calculation had been used to determine an appropriate value for VEXT for each case.

```
 3 7  3 7  +0  2  0                    % IAN1 IMN1 IAN2 IMN2 CHARGE NDEGv NDEBv
 '(vi) For Li2(A): MXR function for Gv  &  Dunham for Bv'
   9                                    % LMAXGv
   2.554976991440D+02 -1.591528931916D+00 4.320069610295D-03 -1.297800483407D-04
   5.126092802711D-06 -3.043543008425D-07 9.142950968846D-09 -1.496898654541D-10
   9.980517130870D-13
   55.d0  1.d0  9352.11494d0            % VS DVS DLIM
  3  1  2 2  7 0 113.2817653490D0 2.577D-08 % NLR ITYPE IZP0 IZQ0 NP0 NQ0 VD XCN0
   1.910501922487D-03 -3.893923351925D-04 2.334546248943D-05 -6.987656722521D-07
   1.155836220945D-08 -1.015514433411D-10 3.720613823813D-13
    17                                  % LMAXBv
   4.974826807719D-01 -5.451871858525D-03 -2.310449795574D-06 9.775126360220D-06
  -2.425290834207D-06 3.831066457326D-07 -4.243945514918D-08 3.342936415566D-09
  -1.887782854700D-10 7.703531741973D-12 -2.287056796063D-13 4.954101341163D-15
  -7.802622660609D-17 8.821305429325D-19 -6.966209130239D-21 3.645524469475D-23
  -1.135472319430D-25 1.593096618270D-28
  1  2   45.d0                          % Kaiser NSV VEXT
   -0.4d0  0.2d0  1.6d0                 %(1) V1 DV V2
    1.d0   1.0d0 113.d0                 %(2) V1 DV V2

  3 7  3 7  +0  2  2                    % IAN1 IMN1 IAN2 IMN2 CHARGE NDEGv NDEBv
 '(vii) For Li2(A): MXR function for both Gv  &  Bv'
   9                                    % LMAXGv
   2.554976991440D+02 -1.591528931916D+00 4.320069610295D-03 -1.297800483407D-04
   5.126092802711D-06 -3.043543008425D-07 9.142950968846D-09 -1.496898654541D-10
   9.980517130870D-13
   55.d0  1.d0  9352.11494d0            % VS DVS DLIM
  3  1  2 2  7 0 113.2817653490D0 2.577D-08 % NLR ITYPE IZP0 IZQ0 NP0 NQ0 VD XCN0
   1.910501922487D-03 -3.893923351925D-04 2.334546248943D-05 -6.987656722521D-07
   1.155836220945D-08 -1.015514433411D-10 3.720613823813D-13
    8                                   % LMAXBv
   4.974956434974D-01 -5.487758555749D-03 2.648227703650D-05 -1.139866232979D-06
   7.141138262611D-08 -4.445710119333D-09 1.443419023131D-10 -2.497993558364D-12
   1.725383416037D-14
  3   0 0  6 0  4.263D-08               % ITYPB IZP1 IZQ1 NP1 NQ1 XCN1
   2.114415071744D-01 -2.929745145298D-02 1.369881187153D-03 -3.136194459560D-05
   3.563240597730D-07 -1.610153741067D-09
  1  2   49.d0                          % Kaiser NSV VEXT
   -0.4d0  0.2d0  1.6d0                 %(1) V1 DV V2
    1.d0   1.0d0 114.d0                 %(2) V1 DV V2
```

Channel-6 output file for Case (vi): MXR Function for G_v Combined With a Pure Dunham Expansion for B_v

```
(vi) For Li2(A): MXR function for Gv  &  Dunham for Bv
*********************************************************************
RKR potential for Li( 7)-Li( 7)   with   Charge= 0
Reduced mass   ZMU=  3.50800171850   and constant   C_u/ZMU =  4.805479175537
```

```
    from atomic masses:   7.0160034370  &    7.0160034370(u)

Seek relative quadrature convergence 1.0D-10.   Bisect interval up to  5 times.
    performing 16-point Gaussian quadrature in each segment

Represent  Gv's  by Tellinghuisen-type MXR mixed representation:
================================
   9'th order Dunham for  v .le. VS   &   NDE for  v > VS,   with   VS= 55.0000
   with switching function   F_s = 1/[1 + exp{(v-VS)/DVS}]   with   DVS= 1.0000
    and a   sympotote energy (dissociation limit)   DLIM=  9352.1149 [cm-1]

The  9 Dunham  Gv  expansion coefficients are
       2.5549769914D+02 -1.5915289319D+00  4.3200696103D-03 -1.2978004834D-04
       5.1260928027D-06 -3.0435430084D-07  9.1429509688D-09 -1.4968986545D-10
       9.9805171309D-13

NDE for  Gv  is an  (NP= 7/NQ= 0)  OUTER Pade  expansion in  (vD-v)  with
       X0(n=3)= 2.5770000D-08  and leading num. and denom. powers  2  &   2
       vD=  113.281765     D-G(v=-1/2)=    9352.114940
    Numerator coefficients are:  1.910501922487D-03 -3.893923351925D-04
            2.334546248943D-05 -6.987656722521D-07  1.155836220945D-08
           -1.015514433411D-10  3.720613823813D-13

The 18 Dunham  Bv  expansion coefficients are
       4.9748268077D-01 -5.4518718585D-03 -2.3104497956D-06  9.7751263602D-06
      -2.4252908342D-06  3.8310664573D-07 -4.2439455149D-08  3.3429364156D-09
      -1.8877828547D-10  7.7035317420D-12 -2.2870567961D-13  4.9541013412D-15
      -7.8026226606D-17  8.8213054293D-19 -6.9662091302D-21  3.6455244695D-23
      -1.1354723194D-25  1.5930966183D-28

Calculate   Y00=  0.069258147    v(cor)= -0.0002710711    v(min)= -0.5002710711
    using    we= 255.4977    wexe= 1.591529    Be=  0.497483    ae= 0.00545187
    and corrected effective   De=  9352.184198 (after adding Y00)

At  v00= -0.50027   Gv=  0.00000000   dG/dv= 255.4986   (1/2)d2G/dv2= -1.591529
                    Bv=  0.49748416   { ==>   Req= 3.107983623(A) }
                    alpha_e = 0.005451872

Above   v =  45.000   extrapolate inner wall with exponential
       fitted to last 3 points ( & shift  RMAX  accordingly)

Calculate turning points at the 119 v-values
  -0.40  -0.20   0.00   0.20   0.40   0.60   1.00   2.00   3.00   4.00   5.00
   6.00   7.00   8.00   9.00  10.00  11.00  12.00  13.00  14.00  15.00  16.00
  17.00  18.00  19.00  20.00  21.00  22.00  23.00  24.00  25.00  26.00  27.00
  28.00  29.00  30.00  31.00  32.00  33.00  34.00  35.00  36.00  37.00  38.00
  39.00  40.00  41.00  42.00  43.00  44.00  45.00  46.00  47.00  48.00  49.00
  50.00  51.00  52.00  53.00  54.00  55.00  56.00  57.00  58.00  59.00  60.00
  61.00  62.00  63.00  64.00  65.00  66.00  67.00  68.00  69.00  70.00  71.00
  72.00  73.00  74.00  75.00  76.00  77.00  78.00  79.00  80.00  81.00  82.00
  83.00  84.00  85.00  86.00  87.00  88.00  89.00  90.00  91.00  92.00  93.00
  94.00  95.00  96.00  97.00  98.00  99.00 100.00 101.00 102.00 103.00 104.00
 105.00 106.00 107.00 108.00 109.00 110.00 111.00 112.00 113.00

Resulting Turning Points:
    v       E(v)    dE(v)/dv       B(v)            Rmin(v)         Rmax(v)   NDIV  tst(f)   tst(g)    C(exp)       d(RMIN)
*************************************************************************************************************************
-0.400     25.6031   255.1795   0.4969374800    3.0234372631    3.1972365663   2  1.6D-15  2.0D-15
-0.200     76.5754   254.5439   0.4958471565    2.9645029635    3.2655734419   2  6.7D-15  6.4D-15
 0.000    127.4208   253.9093   0.4947572489    2.9252417446    3.3142561635   2  5.9D-15  5.9D-15    8.335775
 0.200    178.1392   253.2757   0.4936680686    2.8941029057    3.3548345519   2  2.8D-15  2.3D-15    6.542694
 0.400    228.7311   252.6431   0.4925798647    2.8677259246    3.3906684110   2  2.1D-15  1.9D-15    5.697028
 0.600    279.1965   252.0114   0.4914928338    2.8445730747    3.4232948870   2  2.2D-15  2.0D-15    5.170596
 1.000    379.7488   250.7506   0.4893228659    2.8048360631    3.4820276524   2  1.0D-15  1.0D-15    4.714860
 2.000    628.9293   247.6138   0.4839253904    2.7279076041    3.6067170425   2  4.9D-15  4.8D-15    4.178673
..............................................................................................................
............................... delete 40 intermediate lines of output .......................................
..............................................................................................................
43.000   8062.0241   102.0111   0.2412555800    2.0485435822    7.1373528092   2  6.2D-15  1.7D-13    2.575810
44.000   8161.4881    96.9039   0.2324814935    2.0439678278    7.2771489537   2  3.1D-15  9.6D-14    2.616591
45.000   8255.8092    91.7289   0.2234973505    2.0396768355    7.4254977727   2  4.9D-15  2.6D-13    2.518026
46.000   8344.9314    86.5106   0.2143347759    2.0356645222    7.5833046780   2  5.1D-15  0.0D+00    2.518026    0.0000048059
47.000   8428.8260    81.2792   0.2050337064    2.0319242402    7.7515239817   2  3.6D-15  0.0D+00    2.518026    0.0000207800
48.000   8507.4973    76.0703   0.1956415038    2.0284485494    7.9311397917   2  1.4D-14  0.0D+00    2.518026    0.0000542433
49.000   8580.9874    70.9239   0.1862115850    2.0252290145    8.1231389712   2  9.4D-15  0.0D+00    2.518026    0.0001093876
50.000   8649.3802    65.8830   0.1768016272    2.0222560548    8.3284771833   2  2.3D-14  0.0D+00    2.518026    0.0001860396
..............................................................................................................
............................... delete 40 intermediate lines of output .......................................
..............................................................................................................
91.000   9349.9208     0.5433   0.0043654236    1.9930209958   52.7914090047  16  2.9D-12  0.0D+00    2.518026    0.0024228047
92.000   9350.4146     0.4468   0.0043678797    1.9930011274   57.0230330908  16  1.9D-13  0.0D+00    2.518026    0.0020614480
93.000   9350.8188     0.3637   0.0081788619    1.9929848672   61.8154981423  16  1.2D-11  0.0D+00    2.518026    0.0344422787
94.000   9351.1461     0.2927   0.0211356489    1.9929717016   67.2840618135  16  4.5D-12  0.0D+00    2.518026    0.1662930847
95.000   9351.4078     0.2325   0.0532459157    1.9929611712   73.5769464307  16  7.9D-12  0.0D+00    2.518026    0.4821753416
96.000   9351.6143     0.1819   0.1221249671    1.9929528655   80.8871496406  16  9.0D-12  0.0D+00    2.518026    0.9560124562
97.000   9351.7746     0.1399   0.2573510267    1.9929464185   89.4694692744  16  2.3D-12  0.0D+00    2.518026    1.4016999224
98.000   9351.8967     0.1055   0.5067819300    1.9929415054   99.6655747816  16  3.2D-11  0.0D+00    2.518026    1.6929584252
99.000   9351.9879     0.0778   0.9455438950    1.9929378394  111.9418090936  16  8.8D-11  0.0D+00    2.518026    1.8477777085
100.000  9352.0542     0.0558   1.6886134888    1.9929351698  126.9477011368  16  7.5D-12  0.0D+00    2.518026    1.9233261857
101.000  9352.1012     0.0389   2.9081747045    1.9929332799  145.6092531055   8  7.7D-11  0.0D+00    2.518026    1.9593707443
102.000  9352.1334     0.0261   4.8572547202    1.9929319852  169.2827714802  16  7.6D-11  0.0D+00    2.518026    1.9766194784
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 2.0D-10/1.3D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
103.000  9352.1546     0.0168   7.9015366849    1.9929311319  200.0186179979  16  2.0D-10  0.0D+00    2.518026    1.9849610307
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 5.1D-10/1.3D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
104.000  9352.1680     0.0103  12.5617284908    1.9929305947  241.0345672508  16  5.1D-10  0.0D+00    2.518026    1.9890365597
 *** STOP ITERATION:  At  NDIV= 32   tst(f)/(previous)= 7.4D-10/1.9D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
105.000  9352.1759     0.0059  19.5694488836    1.9929302748  297.6128692134  32  7.4D-10  0.0D+00    2.518026    1.9910408190
 *** STOP ITERATION:  At  NDIV= 32   tst(f)/(previous)= 1.3D-09/4.5D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
106.000  9352.1803     0.0032  29.9402950697    1.9929300969  378.9163489298  32  1.3D-09  0.0D+00    2.518026    1.9920274486
```

```
 *** CAUTION: 32 interval incomplete convergence:  tst(f) & tst(g)= 5.0D-10 0.0D+00  while  TOLER= 1.0D-10
107.000   9352.1826     0.0015  45.0685981563   1.9929300060 501.9793805852  32  5.0D-10  0.0D+00   2.518026   1.9925102054
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 4.4D-09/3.7D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
108.000   9352.1836     0.0006  66.8493803343   1.9929299645 701.4484689892  16  4.4D-09  0.0D+00   2.518026   1.9927428817
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 1.2D-08/3.6D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
109.000   9352.1840     0.0002  97.8342235426   1.99292994821056.9200299326  16  1.2D-08  0.0D+00   2.518026   1.9928519824
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 8.5D-08/6.7D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
110.000   9352.1842     0.0001 141.4291794992   1.99292994311786.3832793429  16  8.5D-08  0.0D+00   2.518026   1.9929008166
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 3.9D-07/1.9D-07   tst(g)/(previous)= 0.0D+00/0.0D+00
111.000   9352.1842     0.0000 202.1445232863   1.99292994193679.6496067163  16  3.9D-07  0.0D+00   2.518026   1.9929209996
 *** STOP ITERATION:  At  NDIV= 32   tst(f)/(previous)= 2.4D-05/3.0D-06   tst(g)/(previous)= 0.0D+00/0.0D+00
112.000   9352.1842     0.0000 285.9081211397   1.9929299418**************  32  2.4D-05  0.0D+00   2.518026   1.9929281646
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 4.8D-02/1.3D-02   tst(g)/(previous)= 0.0D+00/0.0D+00
113.000   9352.1842     0.0000 400.4564902950   1.9929299418**************  16  4.8D-02  0.0D+00   2.518026   1.9929298887
 *************************************************************************************************************************

 For   v .GE. 45.00  inner wall extrapolated as:   V(R) =    -520.9673 + 0.14922925D+07*exp(-  2.51802614*R)
 *************************************************************************************************************************
```

Channel-6 output file for Case (vii): MXR Functions for G_v and for B_v

```
 (vii) For Li2(A): MXR function for both Gv  &  Bv
 ************************************************************************
 RKR potential for Li(  7)-Li(  7)   with   Charge= 0
 Reduced mass   ZMU=  3.50800171850   and constant   C_u/ZMU =  4.805479175537
     from atomic masses:    7.0160034370  &     7.0160034370(u)

 Seek relative quadrature convergence 1.0D-10.   Bisect interval up to  5 times.
     performing 16-point Gaussian quadrature in each segment

 Represent  Gv's  by Tellinghuisen-type MXR mixed representation:
 ================================
    9'th order Dunham for  v .le. VS   &   NDE for  v > VS,   with   VS= 55.0000
    with switching function   F_s = 1/[1 + exp{(v-VS)/DVS}]   with   DVS= 1.0000
     and a   sympotote energy (dissociation limit)   DLIM=  9352.1149 [cm-1]

 The  9 Dunham  Gv  expansion coefficients are
         2.5549769914D+02 -1.5915289319D+00  4.3200696103D-03 -1.2978004834D-04
         5.1260928027D-06 -3.0435430084D-07  9.1429509688D-09 -1.4968986545D-10
         9.9805171309D-13

 NDE for  Gv  is an  (NP= 7/NQ= 0)  OUTER Pade  expansion in  (vD-v)  with
        X0(n=3)= 2.5770000D-08  and leading num. and denom. powers  2  &   2
        vD=  113.281765    D-G(v=-1/2)=   9352.114940
     Numerator coefficients are:  1.910501922487D-03 -3.893923351925D-04
              2.334546248943D-05 -6.987656722521D-07  1.155836220945D-08
             -1.015514433411D-10  3.720613823813D-13

 Represent  Bv's  by Tellinghuisen-type MXR mixed representation:
 ================================
    8'th order Dunham for  v .le. VS   &   NDE for  v > VS,   with   VS= 55.0000

 The  9 Dunham  Bv  expansion coefficients are
         4.9749564350D-01 -5.4877585557D-03  2.6482277036D-05 -1.1398662330D-06
         7.1411382626D-08 -4.4457101193D-09  1.4434190231D-10 -2.4979935584D-12
         1.7253834160D-14

 NDE for  Bv  is an  (NP= 6/NQ= 0) Exponential  expansion in  (vD-v)  with
        X1(n=3)= 4.2630000D-08  and leading num. and denom. powers  0  &   0
     Numerator coefficients are:  2.114415071744D-01 -2.929745145298D-02
              1.369881187153D-03 -3.136194459560D-05  3.563240597730D-07
             -1.610153741067D-09

 Calculate   Y00=  0.072227980    v(cor)= -0.0002826947    v(min)= -0.5002826947
     using    we= 255.4977    wexe= 1.591529     Be=  0.497496    ae= 0.00548776
     and corrected effective   De=  9352.187168 (after adding Y00)

 At  v00= -0.50028   Gv=  0.00000000   dG/dv= 255.4986   (1/2)d2G/dv2= -1.591529
                     Bv=  0.49749719   { ==>   Req= 3.107942903(A) }
                     alpha_e = 0.005487759

 Above   v =  49.000   extrapolate inner wall with exponential
        fitted to last 3 points ( & shift  RMAX  accordingly)

 Calculate turning points at the 119 v-values
   -0.40  -0.20   0.00   0.20   0.40   0.60   1.00   2.00   3.00   4.00   5.00
    6.00   7.00   8.00   9.00  10.00  11.00  12.00  13.00  14.00  15.00  16.00
   17.00  18.00  19.00  20.00  21.00  22.00  23.00  24.00  25.00  26.00  27.00
   28.00  29.00  30.00  31.00  32.00  33.00  34.00  35.00  36.00  37.00  38.00
   39.00  40.00  41.00  42.00  43.00  44.00  45.00  46.00  47.00  48.00  49.00
   50.00  51.00  52.00  53.00  54.00  55.00  56.00  57.00  58.00  59.00  60.00
   61.00  62.00  63.00  64.00  65.00  66.00  67.00  68.00  69.00  70.00  71.00
   72.00  73.00  74.00  75.00  76.00  77.00  78.00  79.00  80.00  81.00  82.00
   83.00  84.00  85.00  86.00  87.00  88.00  89.00  90.00  91.00  92.00  93.00
   83.00  84.00  85.00  86.00  87.00  88.00  89.00  90.00  91.00  92.00  93.00
   94.00  95.00  96.00  97.00  98.00  99.00 100.00 101.00 102.00 103.00 104.00
  105.00 106.00 107.00 108.00 109.00 110.00 111.00 112.00 113.00

 Resulting Turning Points:
     v        E(v)    dE(v)/dv       B(v)           Rmin(v)         Rmax(v)   NDIV  tst(f)   tst(g)    C(exp)       d(RMIN)
 *************************************************************************************************************************
 -0.400     25.6061   255.1795   0.4969471313   3.0233987865   3.1972081610   2  3.2D-15  3.4D-15
 -0.200     76.5784   254.5439   0.4958516691   2.9644780804   3.2655543825   2  2.7D-15  1.8D-15
  0.000    127.4237   253.9093   0.4947582466   2.9252261579   3.3142450914   2  8.9D-16  6.7D-16   8.337848
```

```
  0.200    178.1422   253.2757   0.4936668143    2.8940940095    3.3548294739   2  6.8D-15  6.1D-15    6.543548
  0.400    228.7341   252.6431   0.4925773248    2.8677217408    3.3906675968   2  2.4D-15  2.2D-15    5.696890
  0.600    279.1995   252.0114   0.4914897331    2.8445720595    3.4232969217   2  3.9D-15  3.1D-15    5.169723
  1.000    379.7518   250.7506   0.4893200731    2.8048380459    3.4820322503   2  2.9D-15  2.4D-15    4.713391
  2.000    628.9323   247.6138   0.4839263400    2.7279073455    3.6067188159   2  6.0D-15  6.0D-15    4.176945
 .....................................................................................................
 ................................ delete 40 intermediate lines of output ............................
 .....................................................................................................
 43.000   8062.0271   102.0111   0.2412589816    2.0486530117    7.1374628062   2  1.1D-14  8.2D-15    2.082971
 44.000   8161.4911    96.9039   0.2325109768    2.0440507973    7.2772324873   2  5.3D-15  4.0D-15    2.100804
 45.000   8255.8122    91.7289   0.2235482561    2.0397276757    7.4255491738   2  1.0D-14  7.3D-15    2.121922
 46.000   8344.9344    86.5106   0.2143966102    2.0356793188    7.5833200325   2  5.1D-15  2.7D-15    2.143082
 47.000   8428.8290    81.2792   0.2050918461    2.0319004009    7.7515006974   2  2.2D-14  1.9D-14    2.153211
 48.000   8507.5003    76.0703   0.1956805490    2.0283841176    7.9310759125   2  3.4D-15  4.4D-15    2.124768
 49.000   8580.9904    70.9239   0.1862199849    2.0251216503    8.1230321571   2  3.1D-15  5.2D-14    2.004384
 50.000   8649.3832    65.8830   0.1767764544    2.0221045150    8.3283261915   2  2.6D-14  0.0D+00    2.004384    0.0000026832
 51.000   8712.8062    60.9915   0.1674211497    2.0193228327    8.5478462775   2  2.4D-13  0.0D+00    2.004384    0.0000111121
 .....................................................................................................
 ................................ delete 40 intermediate lines of output ............................
 .....................................................................................................
 92.000   9350.4176     0.4468   0.0048343858    1.9921870677   57.0222195579  16  5.2D-12  0.0D+00    2.004384    0.0132731113
 93.000   9350.8218     0.3637   0.0042447604    1.9921703263   61.8146841289  16  5.8D-12  0.0D+00    2.004384    0.0161634256
 94.000   9351.1490     0.2927   0.0037078430    1.9921567709   67.2832474095  16  1.1D-12  0.0D+00    2.004384    0.0194191930
 95.000   9351.4108     0.2325   0.0032181566    1.9921459287   73.5761317144  16  9.6D-12  0.0D+00    2.004384    0.0230387210
 96.000   9351.6173     0.1819   0.0027709805    1.9921373769   80.8863346776  16  5.8D-12  0.0D+00    2.004384    0.0270095547
 97.000   9351.7776     0.1399   0.0023624202    1.9921307390   89.4686541216  16  2.3D-11  0.0D+00    2.004384    0.0313061514
 98.000   9351.8997     0.1055   0.0019894625    1.9921256803   99.6647594827  16  3.9D-11  0.0D+00    2.004384    0.0358874930
 99.000   9351.9908     0.0778   0.0016500049    1.9921219057  111.9409936979  16  1.5D-12  0.0D+00    2.004384    0.0406948615
100.000   9352.0572     0.0558   0.0013428443    1.9921191571  126.9468856490  32  4.9D-11  0.0D+00    2.004384    0.0456501274
101.000   9352.1042     0.0389   0.0010676020    1.9921172111  145.6084375683   8  9.3D-11  0.0D+00    2.004384    0.0506550656
 *** CAUTION: 32 interval incomplete convergence:  tst(f) & tst(g)= 1.1D-10 0.0D+00  while  TOLER= 1.0D-10
102.000   9352.1364     0.0261   0.0008245605    1.9921158781  169.2819558979  32  1.1D-10  0.0D+00    2.004384    0.0555923816
103.000   9352.1576     0.0168   0.0006143927    1.9921149995  200.0178024208   8  1.3D-11  0.0D+00    2.004384    0.0603292862
 *** STOP ITERATION:  At  NDIV=  8   tst(f)/(previous)= 3.8D-10/1.2D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
104.000   9352.1709     0.0103   0.0004377745    1.9921144464  241.0337516165   8  3.8D-10  0.0D+00    2.004384    0.0647244890
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 3.3D-10/1.3D-10   tst(g)/(previous)= 0.0D+00/0.0D+00
105.000   9352.1789     0.0059   0.0002949042    1.9921141171  297.6120536865  16  3.3D-10  0.0D+00    2.004384    0.0686393116
106.000   9352.1833     0.0032   0.0001849888    1.9921139338  378.9155337676  32  7.2D-11  0.0D+00    2.004384    0.0719530322
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 4.9D-09/2.8D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
107.000   9352.1856     0.0015   0.0001058115    1.9921138403  501.9785661328  16  4.9D-09  0.0D+00    2.004384    0.0745814353
 *** STOP ITERATION:  At  NDIV= 32   tst(f)/(previous)= 1.9D-08/2.5D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
108.000   9352.1866     0.0006   0.0000535269    1.9921137975  701.4476459811  32  1.9D-08  0.0D+00    2.004384    0.0764957264
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 8.4D-09/7.9D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
109.000   9352.1870     0.0002   0.0000228278    1.99211378071056.9192226031  16  8.4D-09  0.0D+00    2.004384    0.0777366891
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 5.8D-08/6.3D-09   tst(g)/(previous)= 0.0D+00/0.0D+00
110.000   9352.1871     0.0001   0.0000075505    1.99211377541786.3822265910  16  5.8D-08  0.0D+00    2.004384    0.0784169147
 *** CAUTION: 32 interval incomplete convergence:  tst(f) & tst(g)= 8.9D-08 0.0D+00  while  TOLER= 1.0D-10
111.000   9352.1872     0.0000   0.0000016323    1.99211377423679.6484935413  32  8.9D-08  0.0D+00    2.004384    0.0787037388
 *** STOP ITERATION:  At  NDIV= 32   tst(f)/(previous)= 2.5D-05/3.2D-06   tst(g)/(previous)= 0.0D+00/0.0D+00
112.000   9352.1872     0.0000   0.0000001442    1.9921137741***************  32  2.5D-05  0.0D+00    2.004384    0.0787795066
 *** STOP ITERATION:  At  NDIV= 16   tst(f)/(previous)= 6.1D-02/1.3D-02   tst(g)/(previous)= 0.0D+00/0.0D+00
113.000   9352.1872     0.0000   0.0000000003    1.9921137741***************  16  6.1D-02  0.0D+00    2.004384    0.0787927269
 ***********************************************************************************************************

 For   v .GE. 49.00  inner wall extrapolated as:   V(R) =   -2694.1259 + 0.65309251D+06*exp(-  2.00438358*R)
 ***********************************************************************************************************
```

Appendix F. Derivation of the RKR Equations

The first formal derivation of what is now known as the "RKR" method was due to O. Klein [3], and a version of his derivation is outlined here. Starting from the first-order JWKB or Bohr-Sommerfeld quantization condition

$$v + \frac{1}{2} \;=\; \frac{1}{\pi}\sqrt{\frac{2\mu}{\hbar^2}} \int_{r_1}^{r_2} [E - V(r)]^{1/2}\, dr \quad . \tag{23}$$

For the purpose of this derivation, it is notationally convenient to start by replacing v by v' and E by E'. We then take the derivative of this expression with respect to energy E', and next divide the range of integration into two parts to separate the repulsive and attractive regions:

$$\frac{dv'}{dE'} \;=\; \frac{1}{2\pi}\sqrt{\frac{2\mu}{\hbar^2}} \left\{ \int_{r_1}^{r_e} \frac{dr}{[E' - V(r)]^{1/2}} \;+\; \int_{r_e}^{r_2} \frac{dr}{[E' - V(r)]^{1/2}} \right\} \quad . \tag{24}$$

For a well-behaved single-minimum potential, there is a unique monotonic relationship between the distance variable r and the value of the potential energy function, $u = V(r)$ on each of the intervals $[r_1, r_e]$ and $[r_e, r_2]$. We may therefore re-write Eq. (24) with u replacing r as the independent variable in the two integrals:

$$\begin{aligned} \frac{dv'}{dE'} \;&=\; \frac{1}{2\pi}\sqrt{\frac{2\mu}{\hbar^2}} \left\{ \int_{E'}^{0} \frac{1}{[E' - u]^{1/2}} \frac{dr_1(u)}{du}\, du \;+\; \int_{0}^{E'} \frac{1}{[E' - u]^{1/2}} \frac{dr_2(u)}{du}\, du \right\} \\ &=\; \frac{1}{2\pi}\sqrt{\frac{2\mu}{\hbar^2}} \int_{0}^{E'} \left(\frac{dr_2(u)}{du} - \frac{dr_1(u)}{du} \right) \frac{du}{[E' - u]^{1/2}} \quad . \end{aligned} \tag{25}$$

We now introduce a mathematical gimmick (sometimes called an Abelian transformation[3]), which involves premultiplying both sides of Eq. (25) by the factor $dE'/[E - E']^{1/2}$ and integrating E' from 0 to E, to obtain

$$\begin{aligned} \int_0^E \frac{(dv'/dE')\, dE'}{[E - E']^{1/2}} \;&=\; \int_{v_{\rm min}}^{v(E)} \frac{dv'}{[E(v) - E(v')]^{1/2}} \\ &=\; \frac{1}{2\pi}\sqrt{\frac{2\mu}{\hbar^2}} \int_0^E dE' \left\{ \int_0^{E'} \left(\frac{dr_2(u)}{du} - \frac{dr_1(u)}{du} \right) \frac{du}{[(E - E')(E' - u)]^{1/2}} \right\} \quad , \end{aligned} \tag{26}$$

in which $v_{\rm min} = v(E{=}0)$ is the (non-integer) effective vibrational quantum number index associated with the potential minimum. If we then change the order of the double integration, and utilize the mathematical identity

$$\int_a^b \frac{dx}{[(b - x)(x - a)]^{1/2}} \;=\; \pi \quad , \tag{27}$$

we obtain

$$\int_{v_{\min}}^{v(E)} \frac{dv'}{[E(v)-E(v')]^{1/2}} = \frac{1}{2\pi}\sqrt{\frac{2\mu}{\hbar^2}} \int_0^E du \left\{ \left(\frac{dr_2(u)}{du} - \frac{dr_1(u)}{du} \right) \int_u^E \frac{dE'}{[(E-E')(E'-u)]^{1/2}} \right\}$$
$$= \frac{1}{2}\sqrt{\frac{2\mu}{\hbar^2}} \left\{ \int_0^E \frac{dr_2(u)}{du}\, du - \int_0^E \frac{dr_1(u)}{du}\, du \right\}$$
$$= \frac{1}{2}\sqrt{\frac{2\mu}{\hbar^2}} \left\{ \int_{r_e}^{r_2(E)} dr - \int_{r_e}^{r_1(E)} dr \right\}$$
$$= \frac{1}{2}\sqrt{\frac{2\mu}{\hbar^2}}\, [r_e(E(v)) - r_1(E(v))] \quad . \tag{28}$$

Rearrangement of this expression yields the first, or "vibrational", RKR equation

$$r_2(v) - r_1(v) = 2\sqrt{\frac{\hbar^2}{2\mu}} \int_{v_{\min}}^{v} \frac{dv'}{[E(v)-E(v')]^{1/2}} \equiv 2f \quad . \tag{29}$$

The derivation of the second, or "rotational", RKR equation proceeds in the same way, except that we first need to perform some manipulations to obtain the appropriate starting equation. The starting point is the recognition that for a rotating molecule (i.e., one with $J > 0$), the effective centrifugally-distorted potential appearing in the quantization condition of Eq. (23) is

$$V_J(r) = V(r) + \frac{\hbar^2}{2\mu}\frac{[J(J+1)]}{r^2} \quad , \tag{30}$$

so that the quantization condition may be re-written as

$$v(E,J) + \frac{1}{2} = \frac{1}{\pi}\sqrt{\frac{2\mu}{\hbar^2}} \int_{r_1}^{r_2} \left[E - V(r) - \frac{\hbar^2}{2\mu}\frac{[J(J+1)]}{r^2} \right]^{1/2} dr \quad . \tag{31}$$

For a given value of J, Eq. (31) tells us that there exists a unique mapping between v and E, and the chain rule of calculus tell us that in this case, for any function $\mathfrak{F}(E,J)$,

$$\left(\frac{\partial \mathfrak{F}(E,J)}{\partial [J(J+1)]} \right)_E = \left(\frac{\partial E}{\partial [J(J+1)]} \right)_v \left(\frac{\partial \mathfrak{F}}{\partial E} \right)_J \quad . \tag{32}$$

Application of this chain rule relationship to Eq. (31) then yields

$$\left(\frac{\partial v}{\partial [J(J+1)]} \right)_E = \left(\frac{\partial E}{\partial [J(J+1)]} \right)_v \left(\frac{\partial v}{\partial E} \right)_J \tag{33}$$
$$= -\frac{1}{2\pi}\sqrt{\frac{\hbar^2}{2\mu}} \int_{r_1}^{r_2} \frac{dr}{r^2 \left[E - V(r) - \frac{\hbar^2}{2\mu}\frac{[J(J+1)]}{r^2} \right]^{1/2}} \quad . \tag{34}$$

From the standard definition of the inertial rotational constant, we know that $\left.\frac{\partial E(v,J)}{\partial [J(J+1)]}\right|_{J=0} \equiv B_v$, so for $J=0$, Eq. (33) becomes

$$B_v \frac{dv}{dE} = -\frac{1}{2\pi}\sqrt{\frac{\hbar^2}{2\mu}} \int_{r_1}^{r_2} \frac{dr}{r^2\,[E - V(r)]^{1/2}} \quad , \tag{35}$$

in which the partial derivative has been replaced by a normal derivative, since when J is fixed (at $J=0$) there in only one independent variable.

Equation (35) provides a starting point that is the precise analog of Eq. (24) in the derivation of the RKR "f integral" result of Eq. (29). Proceeding precisely as before, to (i) replace variable names E and v with E' and v', respectively, (ii) split the range of integration into two parts at r_e, (iii) change the variable of integration from r to $u = V(r)$, (iv) multiply by $dE'/(E - E')^{1/2}$ and integrate E' from 0 to E, (v) change the order of integration and apply the identity of Eq. (27), and (vi) rearrange the result appropriately, then yields the second, or "rotational", RKR equation:

$$\frac{1}{r_1(v)} - \frac{1}{r_2(v)} = 2\sqrt{\frac{2\mu}{\hbar^2}} \int_{v_{\min}}^{v} \frac{B_{v'}\, dv'}{[E(v) - E(v')]^{1/2}} \equiv 2g \quad . \tag{36}$$

Combining Eqs. (29) and (36) then yields the final turning point expressions of Eqs. (5) and (6). Thus, for any case in which we have smooth functions that accurately describe the v-dependence of the vibrational energies G_v and inertial rotational constants B_v, Eqs. (29) and (29)-(5) may be used to generate the potential energy function in a pointwise manner.