Supplementary Material

This document contains Supplementary Material associated with the paper "**betaFIT**: A Computer Program to Fit Pointwise Potentials to Selected Analytic Functions", submitted to the *Journal of Quantitative Spectroscopy and Radiative Transfer* in February 2016. It consists of the three Appendices enumerated below. Note that Equation and Reference numbering appearing herein refer to those in the Journal Article.

Appendix A. Structure of the Input Data File

The logical structure and READ statements for inputting the parameters describing the system to be treated and specifying the type of fit to be carried out, is shown below. Appendix B then provides a detailed description of the nature and/or options associated with each of the input variables.

```
 #1    READ(5,*) PSEL, NTP, UNC, IROUND, LPPOT, prFIT, prDIFF
 #2    READ(5,*) Re, De, VMIN
 #3    READ(5,*) IFXRe, IFXDe, IFXVMIN
       IF(PSEL.EQ.2).OR.PSEL.EQ.3)) THEN
 #4        READ(5,*) NCMM, rhoAB, sVSR2, IDSTT, APSE, yMIN
           DO m=1, NCMM
 #5            READ(5,*) MMLR(m), CmVAL(m)
               ENDDO
           ENDIF
 #6    IF(PSEL.EQ.4) READ(5,*) as, bs
 #7    IF(UNC.GT.0.d0) READ(5,*) (RTP(i), VTP(i), i= 1,NTP)
 #8    IF(UNC.LE.0.d0) READ(5,*) (RTP(i), VTP(i), uVTP(i), i= 1,NTP)
   20  CONTINUE
 #9    READ(5,*, END= STOP) q, p, NS, NL, Rref
#10    IF(LPPOT.GT.0) READ(5,*) NPR, RPR1, dRPR
   {perform fit, and then repeatedly return here for another case}
       GO TO 20
```

Appendix B. Definitions and Descriptions of the Input Data File Parameters

Read integers specifying the type of potential being fitted to, the number of input potential function values and how they are to be weighted, and parameters controlling the fit procedure and printout.

#1. `READ(5,*) PSEL, NTP, UNC, IROUND, LPPOT, prFIT, prDIFF`

`PSEL` is an integer that specifies the type of analytic form to be used for the potential energy function.

If `PSEL` $=1$, use the Expanded Morse Oscillator (EMO) form of § 2.2. For $N_\beta = 0$ this yields the conventional 3-parameter Morse function.

If `PSEL` $=2$, use the Morse/Long-Range (MLR) potential form of § 2.3 which has one or more specified long-range inverse-power terms.

If `PSEL` $=3$, use the Double-Exponential/Long-Range (DELR) form of § 2.4 which has one or more specified long-range inverse-power terms.

If `PSEL` $=4$, use Seto's modification [74] of the Šurkus Generalized Potential Energy Function (GPEF) [27] of § 2.5. The parameters a_S, b_S, and q are input through READS #6 and 9.

- Dunham expansions are generated by setting $q = 1$, $a_S = 0$, and $b_S = 1$.
- SPF expansions are generated by setting $q = 1$, $a_S = 1$, and $b_S = 0$.
- Ogilvie–Tipping expansions are generated by setting $q = 1$ and $a_S = b_S = 0.5$.
- 'Hannover'-type polynomials [72, 75] are generated by setting $q = 1$ and $a_S = 1$

`NTP` is the number of potential function points to be read in.

If `UNC` > 0.0 it is the common (real number) uncertainty assigned to all of the potential function values. Input those points *via* READ #7.
If the input value of `UNC` ≤ 0.0, read in an independent uncertainty for each datum, as those points are input *via* READ #8.

`IROUND`: Setting (integer) `IROUND` $\neq 0$ causes the "sequential rounding and refitting" procedure of Ref. [77] to be implemented, with each parameter being rounded at the |`IROUND`|'th significant digit of its uncertainty. If `IROUND` > 0 the rounding is applied sequentially to the remaining free parameter with the largest relative uncertainty; if `IROUND` < 0 the rounding proceeds systematically from the last free parameter of the chosen model to the first (recommended). If `IROUND` $= 0$ the fit simply stops after full convergence and performs no parameter rounding.

`LPPOT` controls whether (`LPPOT` > 0) or not (`LPPOT` ≤ 0) **betaFIT** will print to Channel 8 a listing of potential energy and exponent coefficient values, on the range and mesh specified in READ #10.

`prFIT` is an integer flag that controls the level of printout from **betaFIT**. For `prFIT` ≤ 0 it prints only the final results for each case (normal setting). If `prFIT` $= 1$ it also prints the results of the initial linearized fit and of subsequent intermediate non-linear fits; the latter option creates more output, which may prove illuminating in cases for which the final fit fails to converge. If `prFIT` $= 2 - 5$ it also prints parameter changes and convergence tests in every non-linear fitting cycle. Normally, set `prFIT` $= 0$.

`prDIFF` is an integer specifying whether (for `prDIFF` > 0) or not (for `prDIFF` ≤ 0) the main output will include a listing of the residual discrepancies $\{y_{\rm calc}(i) - y_{\rm obs}(i)\}$ for each case. Normally, set `prDIFF` $= 0$.

#2. `READ(5,*) Re, De, VMIN`

`Re, De` and `VMIN` are the (real number) initial trial values for the equilibrium distance, well depth, and absolute energy at the potential minimum. respectively. Realistic (but not necessarily accurate) values of these parameters are required by the approximate linearized fit to Eq. (24), (25), or (26), which precedes non-linear fitting to Eq. (3), (6), or (19).

#3. `READ(5,*) IFXRe, IFXDe, IFXVMIN`

`IFXRe, IFXDe` and `IFXVMIN` are integers that control whether the values of `Re`, `De`, and/or `VMIN`, respectively, are to be varied in the fit (`IFXxx` ≤ 0), or to be held fixed at the input trial values (`IFXxx` > 0). While one would normally wish to set all three values ≤ 0, experience has shown that high-order fits with $\mathfrak{D}_e$ free may sometimes be unstable.

For the case of an MLR or DELR potential (`PSEL` $= 2$ or 3), read parameters specifying properties of the long-range tail function $u_{\rm LR}(r)$; for other cases, skip READ statements #4 and 5.

#4. `IF((PSEL.EQ.2).OR.(PSEL.EQ.3)) READ(5,*) NCMM, rhoAB, sVSR2, IDSTT, APSE, yMIN`

`NCMM` is the number of inverse-power long-range terms to be incorporated into $u_{\rm LR}(r)$ via Eq. (7) or (12), or to be included in the terms defining the 2×2 $u_{\rm LR}(r)$ function of Eq. (16) or the 3×3 diagonalization of Eq. (7) of Ref. [65].

For the 2×2 alkali-dimer cases, set `NCMM` $= 7$ with `MMLR`$(1) = 0$ or -1 and `MMLR`$(i > 1) = 3,\ 3,\ 6,\ 6,\ 8,$ and 8, while the input values of `CmVAL`(i) are $A_{\rm so}$, C_3^{Σ}, C_3^{Π}, C_6^{Σ}, C_6^{Π}, C_8^{Σ} and C_8^{Π} for $i = 1 - 7$, respectively, and

- For the $A\,^1\Sigma_u^+$ state of X_2, set `MMLR(1)= 0` to select the lower root of Eq. (16).
- For the $b\,^3\Pi_u$ state of X_2, set `MMLR(1)= -1` to select the upper root of Eq. (16).

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

- For the $1\,^3\Sigma_g^+$ state of X_2, set `MMLR(2)= -2` to select the lowest root of the 3×3 coupling matrix of Eq. (7) of Ref.[65].
- For the $B\,^1\Pi_u$ state of X_2, set `MMLR(2)= -3` to select the middle root of the 3×3 coupling matrix of Eq. (7) of Ref.[65].
- set `MMLR(2)= -4` to select the highest root of the 3×3 coupling matrix of Eq. (7) of Ref.[65].

`rhoAB` is the dimensionless system-dependent parameter `rhoAB` $= \rho = \rho^{\rm AB}$ appearing in the damping functions of Eqs. (13) and (14). If the read-in value of `rhoAB` ≤ 0.0 , omit damping functions, and define the long-range tail of the MLR or DELR potential using Eq. (7).

If integer `IDSTT` > 0 , the damping functions are represented by the generalized Douketis-Scoles type function of Eq. (13).

If integer `IDSTT` ≤ 0 , the damping functions are represented by the generalized Tang-Toennies function of Eq. (14).

If damping functions are used, integer `sVSR2` is twice the value of the very-short-range power parameter 's' of Eqs. (13)-(15), (`sVSR2` $\equiv 2\,s$). For generalized Tang-Toennies type functions, its allowed values are -4, -2, 0, 2, or 4, while for generalized Douketis-type functions, its allowed values are -4, -3, -2, -1, 0, 2, or 4.

If integer `APSE` ≤ 0, fit to a PE-MLR potential with $\beta(r)$ defined by Eq. (10). In this case, `yMIN` is a dummy parameter.

If integer `APSE` > 0, fit to an SE-MLR potential form with $\beta(r)$ defined by Eq. (17). In this case, the natural cubic spline function $\beta(r)$ is defined by its values at N_S equally spaced points on the interval $y_q^{\rm ref}(r) \in$ [`yMIN`, $y_q^{\rm ref}(r_e))$, with one point *at* `yMIN` and one near (but not too near) $y_q^{\rm ref}(r_e)$ and N_L equally spaced points on the interval $y_q^{\rm ref}(r) \in (y_q^{\rm ref}(r_e),\, +1]$, with the last point lying at $y_q^{\rm ref} = 1.0$. Note that $-1.0 \leq$ `yMIN` < 0.0, and that the total number of spline points is $N_S + N_L + 1$. Values of N_S and N_L are input via `READ` #9.

For an MLR or DELR potential (`PSEL` = 2 or 3), loop over the `NCMM` inverse-power terms, reading in the power `MMLR(m)`, and a value for that coefficient `CmVAL(m)`.

```
IF((PSEL.EQ.2).OR.(PSEL.EQ.3)) THEN
   DO m= 1,NCMM
#5.   READ(5,*) (MMLR(m), CmVAL(m)
      END DO
   END IF
```

If `PSEL`$=4$, read in the parameters defining the expansion variable in the GPEF potential of Eq. (22). For other cases, skip READ #6.

#6. `IF(PSEL.EQ.4) READ(5,*) as, bs`

In the GPEF radial expansion variable of Eq. (23): $a_S =$ `as` and $b_S =$ `bs`, while `q` is input below via READ #9.

Read the `NTP` distances `RTP`(i) and energies `VTP`(i) defining the potential function to be fitted. If `UNC` < 0.0, also read in an uncertainty `uVTP`(i) for each point.

#7. `IF(UNC.GT.0.d0) READ(5,*) (RTP(i), VTP(i), i = 1,NTP)`

#8. `IF(UNC.LE.0.d0) READ(5,*) (RTP(i), VTP(i), uVTP(i), i= 1,NTP)`

Finally, read in parameters specifying the type of fit to be performed. This READ statement is in a loop that allows *any* number of different fits to be performed in the same run. The code stops when the end of the data file is reached or the input value of the first parameter, `q`, is ≤ 0.

#9. `READ(5,*) q, p, NS, NL, RREF`

`q` and `p` are the integer powers q and p defining the radial variables $y_{\{q/p\}}^{\rm ref}(r)$ of Eqs. (2), (4) and (10), $z_q(r)$ of Eq. (23), or $y_p^{r_e}(r)$ of Eq. (1) and (6). Except for the case of an MLR potential, p is a dummy parameter that is internally set equal to q. Note that setting $q \leq 0$ causes the program to STOP.

For `PSEL` $= 1$ or 3, or `PSEL` $= 2$ with `APSE` ≤ 0, `NL` $\equiv N_\beta$ is the polynomial order of the potential function exponent coefficient expansion of Eq. (4) or (10), and `NS` is a dummy variable.

For `PSEL` $= 2$ and `APSE` > 0, N_S and N_L are the numbers of exponent-coefficient spline points on the intervals $y_q^{\rm ref}(r) \in$ [`yMIN`$, y_q^{\rm ref}(r_e))$ and $y_q^{\rm ref}(r) \in (y_q^{\rm ref}(r_e), +1.0]$, respectively (see READ #4).

For `PSEL` $= 4$, perform a series of fits with the order of the GPEF polynomial expansion ranging from `NS` to `NL`. For this case, p and `RREF` $\equiv r_{\rm ref}$ are dummy parameters.

`RREF` defines the reference distance in the potential function exponent expansion variable $y_{\{q/p\}}^{\rm ref}(r) = y_{\{q/p\}}(r; r_{\rm ref})$ of Eqs. (2) or (10) to be:

- the potential function equilibrium distance r_e (in general a variable), if `RREF` ≤ 0.
- the fixed read-in value of `RREF`, if `RREF` > 0.

For a GPEF potential, `RREF` is a dummy variable.

#10. `IF(LPPOT.GT.0) READ(5,*) NPR, RPR1, dRPR`

`NPR` specifies the number of distances at which the fitted potential function is to be calculated and written to Channel 8.

- If `NPR` ≤ 0, omit generation of potential function printout for this case.
- If `NPR` > 0, calculate and print potential function at `NPR` distances starting from $r =$ `RPR1` with a step size of $\Delta r =$ `dRPR`.

Appendix C. Illustrative Sample Input Data Files

Appendix C.1: Illustrative Input/Output for fits to an EMO potential form

This data file is a set of RKR turning points for ground-state NaH that was used to generate initial trial values of the EMO potential function parameters used in the direct-potential-fit data analysis of Ref. [45].

```
1  101  1.0  0  0 0 1                  % PSEL NTP UNC IROUND LPPOT prFIT prDIFF
1.88653358d0 15795.1d0 0.d0             % Re De VMIN
0 0 0                                   % IFXRe IFXDe IFXVMIN
   1.27263185744278  15779.01494490216
   1.27327384018599  15733.75964567196   1.27435125787419  15658.02169863633
   1.27583333934101  15554.27115742115   1.27769354944942  15424.75760065909
   1.27990913199516  15271.52292783471   1.28246073055685  15096.41408441944
   1.28533207261631  14901.09564985342   1.28850970563499  14687.06222657656
   1.29198277636327  14455.65057295593   1.29574284668412  14208.05142760175
   ..........................................................................
   ...................... OMIT 40 LINES ....................................
   ..........................................................................
   4.09966068317251  14455.65057295593   4.20012335281574  14687.06222657656
   4.31202810411714  14901.09564985342   4.43887297528275  15096.41408441944
   4.58582336531524  15271.52292783471   4.76096746621319  15424.75760065909
   4.97804002053615  15554.27115742115   5.26332726810017  15658.02169863633
   5.67804681677814  15733.75964567196   6.43542911797951  15779.01494490216

     5  0   0  11  -1.0
     5  0   0  11   2.0
     5  0   0  11   2.2
     5  0   0  11   2.3
     5  0   0  11   2.4
     5  0   0  12   2.3
     5  0   0  13   2.3
```

The following (truncated) listing of the Channel–6 Output from a fit of an EMO form to turning points for ground-state NaH illustrates a number of features of the code.

1. Since input parmeter `prDIFF` was set at `prDIFF` = 1, on completion of the fit for each case, the code provides a detailed listing of the residual discrepancies between the fitted function and the input data.

2. The changes in the quality of fit parameter $\overline{dd}$ for the first five cases show its dependence on the chosen value of the expansion center `RREF`.

3. The last two cases show how $\overline{dd}$ and the physically significant fit parameters $\mathfrak{D}_e =$ `De` and $r_e =$ `Re`, and their uncertainties, change on increasing the number of expansion parameters at the optimum `RREF` value.

4. At the very end of the treatment of for each case, the code examines the repulsive wall of the resulting function on the range from the innermost input point in to $r = 0$, and prints out a warning message if it encounters an inflection point, or if the function in that extrapolation region goes through a maximum and turns over. The output here shows that the fitted potential for Case (i), `RREF` $= r_e \approx 1.89$ Å, both has an inflection point and turns over, while all of those for larger `RREF` are well-behaved in the short-range extrapolation region.

Standard Channel-6 output for fits to an EMO potential form

```
Fit an  EMO potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000

Fit to  101 input turning points assuming common uncertainty  u(VTP)= 1.00D+00
------------------------------------------------------------------------------
   RTP       VTP     RTP       VTP     RTP       VTP     RTP       VTP
------------------------------------------------------------------------------
 1.27263  15779.015  1.27327  15733.760  1.27435  15658.022  1.27583  15554.271
 1.27769  15424.758  1.27991  15271.523  1.28246  15096.414  1.28533  14901.096
 1.28851  14687.062  1.29198  14455.651  1.29574  14208.051  1.29978  13945.321
 1.30410  13668.392  1.30869  13378.084  1.31356  13075.115  1.31870  12760.108
 1.32413  12433.604  1.32984  12096.067  1.33584  11747.896  1.34215  11389.427
 1.34877  11020.946  1.35572  10642.691  1.36303  10254.859  1.37072   9857.610
 1.37881   9451.076  1.38734   9035.358  1.39634   8610.537  1.40587   8176.670
 1.41597   7733.798  1.42671   7281.947  1.43816   6821.126  1.45041   6351.334
 1.46358   5872.557  1.47781   5384.772  1.49325   4887.943  1.51014   4382.030
 1.52877   3866.979  1.54955   3342.731  1.57307   2809.219  1.59445   2375.691
 1.60622   2156.674  1.61888   1936.148  1.63260   1714.107  1.64759   1490.547
 1.66418   1265.462  1.68283   1038.847  1.70431    810.697  1.72997    581.005
 1.76280    349.767  1.81307    116.978  1.88705      0.000  1.96770    116.978
 2.03136    349.767  2.07765    581.005  2.11684    810.697  2.15191   1038.847
 2.18422   1265.462  2.21453   1490.547  2.24332   1714.107  2.27089   1936.148
 2.29748   2156.674  2.32325   2375.691  2.37283   2809.219  2.43199   3342.731
 2.48888   3866.979  2.54410   4382.030  2.59809   4887.943  2.65117   5384.772
 2.70357   5872.557  2.75552   6351.334  2.80716   6821.126  2.85864   7281.947
 2.91009   7733.798  2.96163   8176.670  3.01337   8610.537  3.06543   9035.358
 3.11792   9451.076  3.17096   9857.610  3.22469  10254.859  3.27924  10642.691
 3.33477  11020.946  3.39147  11389.427  3.44956  11747.896  3.50927  12096.067
 3.57092  12433.604  3.63486  12760.108  3.70152  13075.115  3.77144  13378.084
 3.84526  13668.392  3.92382  13945.321  4.00816  14208.051  4.09966  14455.651
 4.20012  14687.062  4.31203  14901.096  4.43887  15096.414  4.58582  15271.523
 4.76097  15424.758  4.97804  15554.271  5.26333  15658.022  5.67805  15733.760
 6.43543  15779.015
------------------------------------------------------------------------------

Fit an  EMO(q= 5) potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
Use exponent expansion variable:   y_5(r)= [r^5 - Re^5]/[r^5 + Re^5]

Direct fit to  EMO{q= 5; Rref= Re   ; NL=11} potential:        dd= 4.41186D+00
 beta_{ 0}=  1.105264925267D+00 (+/- 1.3D-02)   PS= 1.8D-06   DSE= 4.78D+00
 beta_{ 1}= -1.517419880208D-01 (+/- 5.8D-02)   PS= 2.6D-06
 beta_{ 2}=  1.352971152980D-01 (+/- 1.9D-01)   PS= 3.5D-06
 beta_{ 3}=  1.702850451778D+00 (+/- 5.1D-01)   PS= 4.8D-06
 beta_{ 4}= -3.102380777674D-01 (+/- 1.1D+00)   PS= 6.4D-06
 beta_{ 5}= -8.130285163876D+00 (+/- 2.1D+00)   PS= 8.6D-06
 beta_{ 6}=  1.130859302642D-01 (+/- 3.1D+00)   PS= 1.1D-05
 beta_{ 7}=  1.925662619134D+01 (+/- 4.6D+00)   PS= 1.4D-05
 beta_{ 8}=  9.481179068060D-01 (+/- 4.3D+00)   PS= 1.8D-05
 beta_{ 9}= -2.205273423791D+01 (+/- 5.1D+00)   PS= 2.3D-05
```

```
 beta_{10}= -9.602705391040D-01 (+/- 2.3D+00)   PS= 2.7D-05
 beta_{11}=  9.997999047756D+00 (+/- 2.4D+00)   PS= 3.2D-05
       Re =  1.884459285 (+/- 0.001628849)      PS= 9.2D-07
       De = 15811.539216 (+/-    9.001965)      PS= 5.0D-02
     VMIN =      3.83112 (+/-    6.195505)      PS= 3.2D-02
============================================================================
     RTP       VTP     [c-o]  [c-o]/unc   RTP       VTP     [c-o]  [c-o]/unc
----------------------------------------------------------------------------
   1.27263  15779.01 -3.1366 -3.14D+00   1.27327  15733.76 -2.7082 -2.71D+00
   1.27435  15658.02 -2.0326 -2.03D+00   1.27583  15554.27 -1.1886 -1.19D+00
   1.27769  15424.76 -0.2615 -2.61D-01   1.27991  15271.52  0.6637  6.64D-01
   1.28246  15096.41  1.5084  1.51D+00   1.28533  14901.10  2.2046  2.20D+00
   1.28851  14687.06  2.6985  2.70D+00   1.29198  14455.65  2.9525  2.95D+00
   1.29574  14208.05  2.9465  2.95D+00   1.29978  13945.32  2.6785  2.68D+00
............................................................................
......................... omit 39 lines ....................................
............................................................................
   4.00816  14208.05  3.1661  3.17D+00   4.09966  14455.65  0.1536  1.54D-01
   4.20012  14687.06 -3.0760 -3.08D+00   4.31203  14901.10 -6.1114 -6.11D+00
   4.43887  15096.41 -8.4921 -8.49D+00   4.58582  15271.52 -9.7276 -9.73D+00
   4.76097  15424.76 -9.3160 -9.32D+00   4.97804  15554.27 -6.7695 -6.77D+00
   5.26333  15658.02 -1.6628 -1.66D+00   5.67805  15733.76  6.2310  6.23D+00
   6.43543  15779.01 16.4536  1.65D+01
------------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 1.196   V=  2.1519D+04
                           and turns over at   R= 1.018   V=  3.0635D+04
------------------------------------------------------------------------------

Fit an  EMO(q= 5) potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.0000^5]/[r^5 + 2.0000^5]

Direct fit to  EMO{q= 5; Rref= 2.000; NL=11} potential:        dd= 2.36087D+00
 beta_{ 0}=  1.119548739144D+00 (+/- 6.8D-03)   PS= 9.8D-07   DSE= 2.55849D+00
 beta_{ 1}= -6.631639048649D-02 (+/- 2.3D-02)   PS= 1.3D-06
 beta_{ 2}=  8.848302443800D-02 (+/- 8.9D-02)   PS= 1.6D-06
 beta_{ 3}=  8.030307399313D-01 (+/- 2.2D-01)   PS= 2.0D-06
 beta_{ 4}= -5.470309237480D-01 (+/- 4.7D-01)   PS= 2.6D-06
 beta_{ 5}= -3.559802128900D+00 (+/- 9.5D-01)   PS= 3.2D-06
 beta_{ 6}=  1.888862979595D+00 (+/- 1.2D+00)   PS= 4.1D-06
 beta_{ 7}=  8.219128631669D+00 (+/- 2.0D+00)   PS= 5.1D-06
 beta_{ 8}= -2.464699501918D+00 (+/- 1.4D+00)   PS= 6.3D-06
 beta_{ 9}= -9.253538400837D+00 (+/- 2.2D+00)   PS= 7.8D-06
 beta_{10}=  1.234002824781D+00 (+/- 6.6D-01)   PS= 9.6D-06
 beta_{11}=  4.225821000226D+00 (+/- 9.0D-01)   PS= 1.2D-05
       Re =  1.885894856 (+/- 0.000740151)      PS= 4.9D-07
       De = 15807.621833 (+/-    4.744166)      PS= 2.7D-02
     VMIN =     -2.62478 (+/-    3.369732)      PS= 1.7D-02
============================================================================
     RTP       VTP     [c-o]  [c-o]/unc   RTP       VTP     [c-o]  [c-o]/unc
----------------------------------------------------------------------------
   1.27263  15779.01 -2.6990 -2.70D+00   1.27327  15733.76 -2.3673 -2.37D+00
   1.27435  15658.02 -1.8400 -1.84D+00   1.27583  15554.27 -1.1729 -1.17D+00
```

```
   1.27769  15424.76 -0.4271 -4.27D-01   1.27991  15271.52  0.3356  3.36D-01
   1.28246  15096.41  1.0561  1.06D+00   1.28533  14901.10  1.6810  1.68D+00
   1.28851  14687.06  2.1651  2.17D+00   1.29198  14455.65  2.4730  2.47D+00
   1.29574  14208.05  2.5806  2.58D+00   1.29978  13945.32  2.4763  2.48D+00
............................................................................
......................... omit 39 lines ...................................
............................................................................
   4.00816  14208.05  2.7838  2.78D+00   4.09966  14455.65  1.5651  1.57D+00
   4.20012  14687.06  0.0231  2.31D-02   4.31203  14901.10 -1.6515 -1.65D+00
   4.43887  15096.41 -3.2207 -3.22D+00   4.58582  15271.52 -4.4010 -4.40D+00
   4.76097  15424.76 -4.8606 -4.86D+00   4.97804  15554.27 -4.2131 -4.21D+00
   5.26333  15658.02 -2.0199 -2.02D+00   5.67805  15733.76  2.1519  2.15D+00
   6.43543  15779.01  8.4090  8.41D+00
------------------------------------------------------------------------------

Fit an  EMO(q= 5) potential function to the input points
===========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.2000^5]/[r^5 + 2.2000^5]

Direct fit to  EMO{q= 5; Rref= 2.200; NL=11} potential:        dd= 9.17040D-01
 beta_{ 0}=  1.120317554435D+00 (+/- 1.3D-03)   PS= 3.8D-07   DSE= 9.93802D-01
 beta_{ 1}=  2.579419308219D-02 (+/- 5.3D-03)   PS= 4.5D-07
 beta_{ 2}=  4.493418815000D-02 (+/- 2.2D-02)   PS= 5.2D-07
 beta_{ 3}=  9.551163711660D-02 (+/- 6.0D-02)   PS= 6.1D-07
 beta_{ 4}=  9.400504108479D-02 (+/- 1.3D-01)   PS= 7.1D-07
 beta_{ 5}= -4.536180225524D-01 (+/- 3.0D-01)   PS= 8.2D-07
 beta_{ 6}= -1.076293378865D-01 (+/- 3.1D-01)   PS= 9.5D-07
 beta_{ 7}=  1.661252133761D+00 (+/- 6.6D-01)   PS= 1.1D-06
 beta_{ 8}=  1.488070765235D-01 (+/- 3.4D-01)   PS= 1.3D-06
 beta_{ 9}= -2.403610299837D+00 (+/- 6.9D-01)   PS= 1.5D-06
 beta_{10}=  8.928659265387D-02 (+/- 1.4D-01)   PS= 1.7D-06
 beta_{11}=  1.410694760231D+00 (+/- 2.7D-01)   PS= 1.9D-06
       Re =  1.887043501 (+/- 0.000262179)      PS= 1.9D-07
       De = 15796.715433 (+/-    2.056685)      PS= 1.0D-02
     VMIN =     -0.20435 (+/-    1.252471)      PS= 6.6D-03
============================================================================
     RTP       VTP     [c-o]  [c-o]/unc   RTP       VTP     [c-o]  [c-o]/unc
----------------------------------------------------------------------------
   1.27263  15779.01 -2.2945 -2.29D+00   1.27327  15733.76 -2.0244 -2.02D+00
   1.27435  15658.02 -1.5939 -1.59D+00   1.27583  15554.27 -1.0468 -1.05D+00
   1.27769  15424.76 -0.4313 -4.31D-01   1.27991  15271.52  0.2033  2.03D-01
   1.28246  15096.41  0.8095  8.09D-01   1.28533  14901.10  1.3435  1.34D+00
   1.28851  14687.06  1.7675  1.77D+00   1.29198  14455.65  2.0508  2.05D+00
   1.29574  14208.05  2.1714  2.17D+00   1.29978  13945.32  2.1166  2.12D+00
............................................................................
......................... omit 39 lines ...................................
............................................................................
   4.00816  14208.05  0.4839  4.84D-01   4.09966  14455.65  0.5803  5.80D-01
   4.20012  14687.06  0.5874  5.87D-01   4.31203  14901.10  0.4733  4.73D-01
   4.43887  15096.41  0.2105  2.10D-01   4.58582  15271.52 -0.2057 -2.06D-01
   4.76097  15424.76 -0.7238 -7.24D-01   4.97804  15554.27 -1.1837 -1.18D+00
   5.26333  15658.02 -1.2506 -1.25D+00   5.67805  15733.76 -0.3645 -3.65D-01
   6.43543  15779.01  2.1477  2.15D+00
```

```
--------------------------------------------------------------------------------

Fit an  EMO(q= 5) potential function to the input points
==========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.3000^5]/[r^5 + 2.3000^5]

Direct fit to  EMO{q= 5; Rref= 2.300; NL=11} potential:        dd= 8.62163D-01
 beta_{ 0}=  1.122813752765D+00 (+/- 8.1D-04)   PS= 3.6D-07   DSE= 9.34332D-01
 beta_{ 1}=  4.485234765113D-02 (+/- 3.4D-03)   PS= 4.1D-07
 beta_{ 2}=  3.712703462401D-02 (+/- 1.6D-02)   PS= 4.6D-07
 beta_{ 3}=  3.030828684494D-02 (+/- 4.4D-02)   PS= 5.2D-07
 beta_{ 4}=  3.837224844970D-01 (+/- 1.0D-01)   PS= 5.9D-07
 beta_{ 5}= -3.091507274247D-01 (+/- 2.4D-01)   PS= 6.7D-07
 beta_{ 6}= -1.073913606790D+00 (+/- 2.5D-01)   PS= 7.5D-07
 beta_{ 7}=  1.654753750375D+00 (+/- 5.7D-01)   PS= 8.4D-07
 beta_{ 8}=  1.451182241749D+00 (+/- 2.7D-01)   PS= 9.5D-07
 beta_{ 9}= -2.455171346716D+00 (+/- 6.0D-01)   PS= 1.1D-06
 beta_{10}= -5.163713061678D-01 (+/- 1.1D-01)   PS= 1.2D-06
 beta_{11}=  1.369044696219D+00 (+/- 2.3D-01)   PS= 1.3D-06
       Re =  1.886525078 (+/- 0.000230581)      PS= 1.8D-07
       De = 15794.995118 (+/-    2.055276)      PS= 9.8D-03
     VMIN =     -0.49645 (+/-    1.147599)      PS= 6.2D-03
==============================================================================
     RTP       VTP     [c-o]  [c-o]/unc   RTP       VTP     [c-o]  [c-o]/unc
------------------------------------------------------------------------------
   1.27263  15779.01 -1.7500 -1.75D+00   1.27327  15733.76 -1.5279 -1.53D+00
   1.27435  15658.02 -1.1745 -1.17D+00   1.27583  15554.27 -0.7272 -7.27D-01
   1.27769  15424.76 -0.2269 -2.27D-01   1.27991  15271.52  0.2845  2.85D-01
   1.28246  15096.41  0.7667  7.67D-01   1.28533  14901.10  1.1826  1.18D+00
   1.28851  14687.06  1.5002  1.50D+00   1.29198  14455.65  1.6938  1.69D+00
   1.29574  14208.05  1.7454  1.75D+00   1.29978  13945.32  1.6456  1.65D+00
..............................................................................
....................... omit 39 lines ........................................
..............................................................................
   4.00816  14208.05 -0.3308 -3.31D-01   4.09966  14455.65 -0.1585 -1.59D-01
   4.20012  14687.06  0.0865  8.65D-02   4.31203  14901.10  0.3397  3.40D-01
   4.43887  15096.41  0.5083  5.08D-01   4.58582  15271.52  0.4915  4.91D-01
   4.76097  15424.76  0.2223  2.22D-01   4.97804  15554.27 -0.2633 -2.63D-01
   5.26333  15658.02 -0.7301 -7.30D-01   5.67805  15733.76 -0.6440 -6.44D-01
   6.43543  15779.01  0.8079  8.08D-01
--------------------------------------------------------------------------------

Fit an  EMO(q= 5) potential function to the input points
==========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.4000^5]/[r^5 + 2.4000^5]

Direct fit to  EMO{q= 5; Rref= 2.400; NL=11} potential:        dd= 1.17879D+00
 beta_{ 0}=  1.128818331330D+00 (+/- 7.8D-04)   PS= 4.9D-07   DSE= 1.27746D+00
 beta_{ 1}=  5.638622149785D-02 (+/- 2.9D-03)   PS= 5.5D-07
 beta_{ 2}=  3.813323473370D-02 (+/- 1.5D-02)   PS= 6.1D-07
 beta_{ 3}=  5.350437182259D-02 (+/- 5.1D-02)   PS= 6.7D-07
 beta_{ 4}=  5.550413449163D-01 (+/- 1.1D-01)   PS= 7.4D-07
```

```
 beta_{ 5}= -5.435075308609D-01 (+/- 3.0D-01)   PS= 8.1D-07
 beta_{ 6}= -1.628251162324D+00 (+/- 2.9D-01)   PS= 9.0D-07
 beta_{ 7}=  2.493899072294D+00 (+/- 7.3D-01)   PS= 9.9D-07
 beta_{ 8}=  2.175527901947D+00 (+/- 3.3D-01)   PS= 1.1D-06
 beta_{ 9}= -3.415190696302D+00 (+/- 7.7D-01)   PS= 1.2D-06
 beta_{10}= -8.509462681555D-01 (+/- 1.4D-01)   PS= 1.3D-06
 beta_{11}=  1.690637922196D+00 (+/- 3.1D-01)   PS= 1.4D-06
       Re =  1.886542903 (+/- 0.000322148)      PS= 2.5D-07
       De = 15795.526650 (+/-    2.868420)      PS= 1.3D-02
     VMIN =      -2.59951 (+/-    1.461595)      PS= 8.5D-03
============================================================================
     RTP       VTP     [c-o]  [c-o]/unc   RTP       VTP     [c-o]  [c-o]/unc
----------------------------------------------------------------------------
   1.27263  15779.01 -0.8776 -8.78D-01   1.27327  15733.76 -0.7212 -7.21D-01
   1.27435  15658.02 -0.4744 -4.74D-01   1.27583  15554.27 -0.1661 -1.66D-01
   1.27769  15424.76  0.1715  1.72D-01   1.27991  15271.52  0.5059  5.06D-01
   1.28246  15096.41  0.8055  8.06D-01   1.28533  14901.10  1.0419  1.04D+00
   1.28851  14687.06  1.1908  1.19D+00   1.29198  14455.65  1.2336  1.23D+00
   1.29574  14208.05  1.1579  1.16D+00   1.29978  13945.32  0.9594  9.59D-01
............................................................................
....................... omit 39 lines ......................................
............................................................................
   4.00816  14208.05 -0.7553 -7.55D-01   4.09966  14455.65 -0.7572 -7.57D-01
   4.20012  14687.06 -0.5383 -5.38D-01   4.31203  14901.10 -0.1418 -1.42D-01
   4.43887  15096.41  0.3217  3.22D-01   4.58582  15271.52  0.6864  6.86D-01
   4.76097  15424.76  0.7732  7.73D-01   4.97804  15554.27  0.4696  4.70D-01
   5.26333  15658.02 -0.1441 -1.44D-01   5.67805  15733.76 -0.6338 -6.34D-01
   6.43543  15779.01 -0.1146 -1.15D-01
------------------------------------------------------------------------------

Fit an  EMO(q= 5) potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.3000^5]/[r^5 + 2.3000^5]

Direct fit to  EMO{q= 5; Rref= 2.300; NL=12} potential:        dd= 8.36916D-01
 beta_{ 0}=  1.123028735758D+00 (+/- 8.1D-04)   PS= 3.3D-07   DSE= 9.12291D-01
 beta_{ 1}=  4.266584120061D-02 (+/- 3.9D-03)   PS= 3.7D-07
 beta_{ 2}=  4.256860939165D-02 (+/- 1.6D-02)   PS= 4.2D-07
 beta_{ 3}=  8.122239040034D-02 (+/- 6.2D-02)   PS= 4.8D-07
 beta_{ 4}=  2.289939831197D-01 (+/- 1.7D-01)   PS= 5.4D-07
 beta_{ 5}= -5.226953490516D-01 (+/- 3.0D-01)   PS= 6.1D-07
 beta_{ 6}= -2.968694534486D-01 (+/- 7.2D-01)   PS= 6.9D-07
 beta_{ 7}=  2.020428247416D+00 (+/- 6.4D-01)   PS= 7.7D-07
 beta_{ 8}= -1.691107028350D-01 (+/- 1.4D+00)   PS= 8.7D-07
 beta_{ 9}= -2.735923904088D+00 (+/- 6.3D-01)   PS= 9.8D-07
 beta_{10}=  1.028730172954D+00 (+/- 1.4D+00)   PS= 1.1D-06
 beta_{11}=  1.448454463030D+00 (+/- 2.4D-01)   PS= 1.2D-06
 beta_{12}= -5.576205474969D-01 (+/- 4.9D-01)   PS= 1.4D-06
       Re =  1.886661449 (+/- 0.000255229)      PS= 1.6D-07
       De = 15795.309803 (+/-    2.031940)      PS= 9.0D-03
     VMIN =      -0.11136 (+/-    1.169897)      PS= 5.7D-03
============================================================================
     RTP       VTP     [c-o]  [c-o]/unc   RTP       VTP     [c-o]  [c-o]/unc
```

```
----------------------------------------------------------------------------
   1.27263  15779.01 -1.9513 -1.95D+00   1.27327  15733.76 -1.7125 -1.71D+00
   1.27435  15658.02 -1.3324 -1.33D+00   1.27583  15554.27 -0.8503 -8.50D-01
   1.27769  15424.76 -0.3096 -3.10D-01   1.27991  15271.52  0.2454  2.45D-01
   1.28246  15096.41  0.7720  7.72D-01   1.28533  14901.10  1.2307  1.23D+00
   1.28851  14687.06  1.5877  1.59D+00   1.29198  14455.65  1.8155  1.82D+00
   1.29574  14208.05  1.8946  1.89D+00   1.29978  13945.32  1.8144  1.81D+00
............................................................................
......................... omit 39 lines ....................................
............................................................................
   4.00816  14208.05 -0.0651 -6.51D-02   4.09966  14455.65  0.1190  1.19D-01
   4.20012  14687.06  0.3124  3.12D-01   4.31203  14901.10  0.4556  4.56D-01
   4.43887  15096.41  0.4748  4.75D-01   4.58582  15271.52  0.3027  3.03D-01
   4.76097  15424.76 -0.0821 -8.21D-02   4.97804  15554.27 -0.5915 -5.92D-01
   5.26333  15658.02 -0.9442 -9.44D-01   5.67805  15733.76 -0.5854 -5.85D-01
   6.43543  15779.01  1.2534  1.25D+00
------------------------------------------------------------------------------

Fit an  EMO(q= 5) potential function to the input points
==========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.3000^5]/[r^5 + 2.3000^5]

Direct fit to  EMO{q= 5; Rref= 2.300; NL=13} potential:        dd= 8.30343D-01
 beta_{ 0}=  1.123310907154D+00 (+/- 9.5D-04)   PS= 3.1D-07   DSE= 9.10497D-01
 beta_{ 1}=  4.205826554991D-02 (+/- 4.0D-03)   PS= 3.5D-07
 beta_{ 2}=  5.112211008707D-02 (+/- 2.2D-02)   PS= 4.0D-07
 beta_{ 3}=  5.974355983799D-02 (+/- 7.2D-02)   PS= 4.5D-07
 beta_{ 4}=  1.347152915931D-01 (+/- 2.3D-01)   PS= 5.1D-07
 beta_{ 5}= -2.428202240647D-01 (+/- 5.7D-01)   PS= 5.7D-07
 beta_{ 6}=  2.646211381774D-02 (+/- 9.1D-01)   PS= 6.5D-07
 beta_{ 7}=  9.058325473033D-01 (+/- 2.0D+00)   PS= 7.3D-07
 beta_{ 8}= -6.756566168943D-01 (+/- 1.7D+00)   PS= 8.2D-07
 beta_{ 9}= -7.058587535832D-01 (+/- 3.6D+00)   PS= 9.2D-07
 beta_{10}=  1.405502737721D+00 (+/- 1.5D+00)   PS= 1.0D-06
 beta_{11}= -3.112015127741D-01 (+/- 3.0D+00)   PS= 1.2D-06
 beta_{12}= -6.657217600534D-01 (+/- 5.2D-01)   PS= 1.3D-06
 beta_{13}=  5.898397494957D-01 (+/- 1.0D+00)   PS= 1.5D-06
       Re =  1.886771142 (+/- 0.000317119)      PS= 1.5D-07
       De = 15794.993714 (+/-    2.097280)      PS= 8.4D-03
     VMIN =     -0.17238 (+/-    1.172586)      PS= 5.4D-03
============================================================================
     RTP       VTP     [c-o]  [c-o]/unc   RTP       VTP     [c-o]  [c-o]/unc
----------------------------------------------------------------------------
   1.27263  15779.01 -2.0538 -2.05D+00   1.27327  15733.76 -1.8058 -1.81D+00
   1.27435  15658.02 -1.4107 -1.41D+00   1.27583  15554.27 -0.9092 -9.09D-01
   1.27769  15424.76 -0.3462 -3.46D-01   1.27991  15271.52  0.2325  2.32D-01
   1.28246  15096.41  0.7827  7.83D-01   1.28533  14901.10  1.2639  1.26D+00
   1.28851  14687.06  1.6410  1.64D+00   1.29198  14455.65  1.8854  1.89D+00
   1.29574  14208.05  1.9769  1.98D+00   1.29978  13945.32  1.9045  1.90D+00
............................................................................
......................... omit 39 lines ....................................
............................................................................
   4.00816  14208.05 -0.1658 -1.66D-01   4.09966  14455.65 -0.0180 -1.80D-02
```

```
   4.20012  14687.06  0.1728  1.73D-01   4.31203  14901.10  0.3514  3.51D-01
   4.43887  15096.41  0.4395  4.40D-01   4.58582  15271.52  0.3549  3.55D-01
   4.76097  15424.76  0.0504  5.04D-02   4.97804  15554.27 -0.4195 -4.20D-01
   5.26333  15658.02 -0.8089 -8.09D-01   5.67805  15733.76 -0.5863 -5.86D-01
   6.43543  15779.01  1.0321  1.03D+00
 ------------------------------------------------------------------------------
```

Appendix C.2: Illustrative Input/Output for fits to a PE-MLR potential form

To fit the same set of NaH turning points to an PE-MLR potential with the damped, three-term long-range tail,

$$u_{\rm LR}(r) = D_6(r)\,\frac{C_6}{r^6} + D_8(r)\,\frac{C_8}{r^8} + D_{10}(r)\,\frac{C_{10}}{r^{10}} \quad ,$$

the input data file is largely the same as that for the EMO case of Appendix C,1 except that its first three lines are replaced by the following:

```
2  101  1.0  0  0 0 0                 % PSEL NTP UNC IROUND LPPOT prFIT prDIFF
1.88753358d0 15799.2281   -1.04964   % Re De VMIN    1.88653358d0
0 0 0                                % IFXRe IFXDe IFXVMIN
3  0.687d0 -2 1    -1  -0.8          % NCMM rhoAB sVSR2 IDSTT APSE yMIN
6  357502.d0                         % MMLR(1) CmVAL(1)
8  5.41796d6                         % MMLR(2) CmVAL(2)
10 1.1292d8                          % MMLR(3) CmVAL(3)
```

Also, for this case, be sure to set the exponent expansion variable parameter q to a non-zero value:

```
      3  5   0  11  -1.0            %  q p NS NL RREF
      3  5   0  11   2.0            %  q p NS NL RREF
      3  5   0  11   2.2            %  q p NS NL RREF
      3  5   0  11   2.4            %  q p NS NL RREF
      3  5   0  11   2.6            %  q p NS NL RREF
      3  5   0  12   2.4            %  q p NS NL RREF
```

As was the case for the EMO potential in the previous subsection, the results summarized below show that there is a marked dependence on the expansion centre RREF, although in this case the apparent optimum value is slightly larger, RREF $= 2.4$. In this case, inner-wall inflections were not encountered for any of these examples.

Standard Channel-6 output for fits to a PE-MLR potential form

```
Fit an  MLR potential function to the input points
===========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281

Fit to  101 input turning points assuming common uncertainty  u(VTP)= 1.00D+00
--------------------------------------------------------------------------------
   RTP       VTP      RTP       VTP      RTP       VTP      RTP       VTP
--------------------------------------------------------------------------------
 1.27263  15779.015  1.27327  15733.760  1.27435  15658.022  1.27583  15554.271
 1.27769  15424.758  1.27991  15271.523  1.28246  15096.414  1.28533  14901.096
 1.28851  14687.062  1.29198  14455.651  1.29574  14208.051  1.29978  13945.321
 ...............................................................................
 ...................... omit 20 lines ..........................................
 ...............................................................................
 4.20012  14687.062  4.31203  14901.096  4.43887  15096.414  4.58582  15271.523
 4.76097  15424.758  4.97804  15554.271  5.26333  15658.022  5.67805  15733.760
 6.43543  15779.015
--------------------------------------------------------------------------------
```

```
Fit an  MLR(q= 3 p= 5)  potential function to the input points
==========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
Use exponent expansion variable:   y_3(r)= [r^3 - Re^3]/[r^3 + Re^3]
MLR polynomial exponent function is:
                            beta(R)= betaINF*y_5 + (1-y_5)*Sum{beta_i*[y_3q]^i}
     in which   y_{p/q}(r)= [r^{p/q} - Re^{p/q}]/[r^{p/q} + Re^{p/q}]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767

Direct fit to  MLR{q= 3, p= 5; Rref= Re  ; NL=11} potential:   dd= 4.14881D+00
 beta_{ 0}=  5.210088470815D-02 (+/- 6.7D-03)   PS= 8.1D-07   DSE= 4.50D+00
 beta_{ 1}= -4.879372718807D+00 (+/- 4.4D-02)   PS= 1.6D-06
 beta_{ 2}= -8.606172148099D+00 (+/- 1.9D-01)   PS= 3.3D-06
 beta_{ 3}= -1.382865040240D+01 (+/- 8.1D-01)   PS= 6.4D-06
 beta_{ 4}= -1.044718123736D+01 (+/- 2.2D+00)   PS= 1.3D-05
 beta_{ 5}=  1.702488392838D+01 (+/- 6.7D+00)   PS= 2.4D-05
 beta_{ 6}= -2.331478528767D+01 (+/- 1.3D+01)   PS= 4.7D-05
 beta_{ 7}= -1.797582329953D+02 (+/- 2.8D+01)   PS= 9.2D-05
 beta_{ 8}= -2.006694410039D+01 (+/- 3.5D+01)   PS= 1.8D-04
 beta_{ 9}=  3.716231851855D+02 (+/- 5.7D+01)   PS= 3.4D-04
 beta_{10}= -1.560911646360D+01 (+/- 3.6D+01)   PS= 6.5D-04
 beta_{11}= -3.992266560589D+02 (+/- 5.0D+01)   PS= 1.2D-03
       Re =  1.888286861 (+/- 0.001186455)      PS= 1.7D-06
       De = 15785.766189 (+/-    7.525562)      PS= 4.0D-02
     VMIN =     -5.86263 (+/-    5.458515)      PS= 3.0D-02
-------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
==========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.0000^3]/[r^3 + 2.0000^3]
MLR polynomial exponent function is:
                            beta(R)= betaINF*y_5 + (1-y_5)*Sum{beta_i*[y_3q]^i}
     in which   y_{p/q}(r)= [r^{p/q} - 2.0000^{p/q}]/[r^{p /q} + 2.0000^{p/q}]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767

Direct fit to  MLR{q= 3, p= 5; Rref= 2.00; NL=11} potential:   dd= 2.44653D+00
 beta_{ 0}=  4.093516943273D-02 (+/- 3.7D-03)   PS= 4.6D-07   DSE= 2.65132D+00
 beta_{ 1}= -4.935069403448D+00 (+/- 2.4D-02)   PS= 8.3D-07
 beta_{ 2}= -8.514666846007D+00 (+/- 9.3D-02)   PS= 1.5D-06
 beta_{ 3}= -1.213597618057D+01 (+/- 4.6D-01)   PS= 2.6D-06
 beta_{ 4}= -9.468006567354D+00 (+/- 9.6D-01)   PS= 4.6D-06
 beta_{ 5}= -2.568598352127D-01 (+/- 3.9D+00)   PS= 8.0D-06
 beta_{ 6}= -3.648974865239D+01 (+/- 4.6D+00)   PS= 1.4D-05
```

```
 beta_{ 7}= -9.101826340894D+01 (+/- 1.5D+01)   PS= 2.4D-05
 beta_{ 8}=  3.677217498557D+01 (+/- 1.0D+01)   PS= 4.2D-05
 beta_{ 9}=  1.583277280902D+02 (+/- 2.9D+01)   PS= 7.2D-05
 beta_{10}= -8.212652173533D+01 (+/- 8.7D+00)   PS= 1.3D-04
 beta_{11}= -1.840820046665D+02 (+/- 2.2D+01)   PS= 2.2D-04
       Re =  1.888413048 (+/- 0.000702775)      PS= 1.1D-06
       De = 15787.926244 (+/-    4.439478)      PS= 2.2D-02
     VMIN =     -0.63715 (+/-    3.224455)      PS= 1.8D-02
------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
=========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.2000^3]/[r^3 + 2.2000^3]
MLR polynomial exponent function is:
                            beta(R)= betaINF*y_5 + (1-y_5)*Sum{beta_i*[y_3q]^i}
     in which   y_{p/q}(r)= [r^{p/q} - 2.2000^{p/q}]/[r^{p /q} + 2.2000^{p/q}]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767

Direct fit to  MLR{q= 3, p= 5; Rref= 2.20; NL=11} potential:   dd= 9.27589D-01
 beta_{ 0}=  3.204338918334D-02 (+/- 1.0D-03)   PS= 1.7D-07   DSE= 1.00523D+00
 beta_{ 1}= -4.964463783558D+00 (+/- 5.8D-03)   PS= 2.6D-07
 beta_{ 2}= -8.303452855978D+00 (+/- 2.5D-02)   PS= 4.0D-07
 beta_{ 3}= -1.090568997298D+01 (+/- 1.2D-01)   PS= 6.1D-07
 beta_{ 4}= -1.054696879501D+01 (+/- 3.3D-01)   PS= 9.3D-07
 beta_{ 5}= -1.078163489171D+01 (+/- 9.7D-01)   PS= 1.4D-06
 beta_{ 6}= -2.861775086289D+01 (+/- 1.8D+00)   PS= 2.1D-06
 beta_{ 7}= -3.212474097215D+01 (+/- 3.8D+00)   PS= 3.2D-06
 beta_{ 8}=  2.782725424717D+01 (+/- 4.0D+00)   PS= 4.9D-06
 beta_{ 9}=  3.437917774194D+01 (+/- 7.2D+00)   PS= 7.4D-06
 beta_{10}= -6.091004316522D+01 (+/- 3.3D+00)   PS= 1.1D-05
 beta_{11}= -6.174097209273D+01 (+/- 5.3D+00)   PS= 1.7D-05
       Re =  1.886896673 (+/- 0.000241382)      PS= 4.6D-07
       De = 15793.596991 (+/-    1.701155)      PS= 7.6D-03
     VMIN =      1.66845 (+/-    1.216849)      PS= 6.7D-03
------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
=========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.4000^3]/[r^3 + 2.4000^3]
MLR polynomial exponent function is:
                            beta(R)= betaINF*y_5 + (1-y_5)*Sum{beta_i*[y_3q]^i}
     in which   y_{p/q}(r)= [r^{p/q} - 2.4000^{p/q}]/[r^{p /q} + 2.4000^{p/q}]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
```

```
Linearized fit uses    beta(INF)=  3.01699767

Direct fit to  MLR{q= 3, p= 5; Rref= 2.40; NL=11} potential:   dd= 7.42387D-01
 beta_{ 0}=  3.313575213993D-02 (+/- 4.8D-04)   PS= 1.3D-07   DSE= 8.04529D-01
 beta_{ 1}= -4.944989249107D+00 (+/- 2.2D-03)   PS= 1.8D-07
 beta_{ 2}= -8.111093878132D+00 (+/- 1.6D-02)   PS= 2.6D-07
 beta_{ 3}= -1.024508938500D+01 (+/- 5.7D-02)   PS= 3.5D-07
 beta_{ 4}= -1.073354816102D+01 (+/- 2.6D-01)   PS= 4.9D-07
 beta_{ 5}= -1.231210515970D+01 (+/- 4.7D-01)   PS= 6.8D-07
 beta_{ 6}= -1.945737005742D+01 (+/- 1.6D+00)   PS= 9.3D-07
 beta_{ 7}= -1.178929272879D+01 (+/- 1.7D+00)   PS= 1.3D-06
 beta_{ 8}=  1.635150487244D+01 (+/- 4.0D+00)   PS= 1.8D-06
 beta_{ 9}=  3.259898843233D+00 (+/- 3.6D+00)   PS= 2.4D-06
 beta_{10}= -3.847795647841D+01 (+/- 3.8D+00)   PS= 3.3D-06
 beta_{11}= -2.642501965810D+01 (+/- 3.4D+00)   PS= 4.6D-06
       Re =  1.886597347 (+/- 0.000197294)      PS= 4.0D-07
       De = 15799.930613 (+/-    1.479211)      PS= 5.8D-03
     VMIN =     -0.54682 (+/-    0.913083)      PS= 5.4D-03
-------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
==========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.6000^3]/[r^3 + 2.6000^3]
MLR polynomial exponent function is:
                            beta(R)= betaINF*y_5 + (1-y_5)*Sum{beta_i*[y_3q]^i}
     in which   y_{p/q}(r)= [r^{p/q} - 2.6000^{p/q}]/[r^{p /q} + 2.6000^{p/q}]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767

Direct fit to  MLR{q= 3, p= 5; Rref= 2.60; NL=11} potential:   dd= 9.55160D-01
 beta_{ 0}=  3.980898651584D-02 (+/- 4.2D-04)   PS= 1.7D-07   DSE= 1.03511D+00
 beta_{ 1}= -4.881969506407D+00 (+/- 2.1D-03)   PS= 2.2D-07
 beta_{ 2}= -7.833359056552D+00 (+/- 1.5D-02)   PS= 2.8D-07
 beta_{ 3}= -9.525398825469D+00 (+/- 6.4D-02)   PS= 3.6D-07
 beta_{ 4}= -9.954013610836D+00 (+/- 2.7D-01)   PS= 4.7D-07
 beta_{ 5}= -1.022034579066D+01 (+/- 6.0D-01)   PS= 6.0D-07
 beta_{ 6}= -1.038374353275D+01 (+/- 1.9D+00)   PS= 7.8D-07
 beta_{ 7}= -3.193792804081D+00 (+/- 2.0D+00)   PS= 1.0D-06
 beta_{ 8}=  4.245677766366D+00 (+/- 5.5D+00)   PS= 1.3D-06
 beta_{ 9}= -8.535748150242D+00 (+/- 3.0D+00)   PS= 1.7D-06
 beta_{10}= -2.052808170929D+01 (+/- 6.1D+00)   PS= 2.1D-06
 beta_{11}= -9.504534584677D+00 (+/- 3.9D+00)   PS= 2.7D-06
       Re =  1.887027361 (+/- 0.000213213)      PS= 5.5D-07
       De = 15802.039320 (+/-    2.263062)      PS= 7.2D-03
     VMIN =     -1.21139 (+/-    1.186543)      PS= 6.9D-03
-------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
==========================================================
```

```
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.4000^3]/[r^3 + 2.4000^3]
MLR polynomial exponent function is:
                            beta(R)= betaINF*y_5 + (1-y_5)*Sum{beta_i*[y_3q]^i}
     in which   y_{p/q}(r)= [r^{p/q} - 2.4000^{p/q}]/[r^{p /q} + 2.4000^{p/q}]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767

Direct fit to  MLR{q= 3, p= 5; Rref= 2.40; NL=12} potential:   dd= 7.15443D-01
 beta_{ 0}=  3.300413932349D-02 (+/- 4.7D-04)   PS= 1.2D-07   DSE= 7.79877D-01
 beta_{ 1}= -4.945583500792D+00 (+/- 2.2D-03)   PS= 1.7D-07
 beta_{ 2}= -8.119265356272D+00 (+/- 1.7D-02)   PS= 2.3D-07
 beta_{ 3}= -1.015542438849D+01 (+/- 8.9D-02)   PS= 3.2D-07
 beta_{ 4}= -1.060517345501D+01 (+/- 2.7D-01)   PS= 4.5D-07
 beta_{ 5}= -1.350191289319D+01 (+/- 1.0D+00)   PS= 6.2D-07
 beta_{ 6}= -2.052194568318D+01 (+/- 1.7D+00)   PS= 8.5D-07
 beta_{ 7}= -5.718827624214D+00 (+/- 5.0D+00)   PS= 1.2D-06
 beta_{ 8}=  2.165279842465D+01 (+/- 5.7D+00)   PS= 1.6D-06
 beta_{ 9}= -9.978675422381D+00 (+/- 1.1D+01)   PS= 2.2D-06
 beta_{10}= -5.085795570827D+01 (+/- 1.0D+01)   PS= 3.0D-06
 beta_{11}= -1.595420962611D+01 (+/- 8.8D+00)   PS= 4.2D-06
 beta_{12}=  1.053095524828D+01 (+/- 8.2D+00)   PS= 5.7D-06
       Re =  1.886538596 (+/- 0.000197045)      PS= 3.7D-07
       De = 15798.678698 (+/-    1.731526)      PS= 5.3D-03
     VMIN =     -0.10324 (+/-    0.950094)      PS= 4.9D-03
------------------------------------------------------------------------------
```

Appendix C.3: Illustrative Input/Output for fits to an SE-MLR potential form

To fit the same set of NaH turning points to an MLR potential with the same damped, three-term long-range tail described at the beginning of Appendix C.2 to a `SE-MLR` functions, the first seven lines of the data file are the same as those for the `PE-MLR` case described above, except that in input line #4 one must set `APSE` > 0, rather than ≤ 0, and the definitions of the parameters `NS` and `NL` input via `READ` #9 has changed (see Appendix B).

```
2  101  1.0  0  0  0 1                  % PSEL NTP UNC IROUND LPPOT prFIT prDIFF
1.88753358d0 15799.2281   -1.04964    % Re De VMIN    1.88653358d0
0 1 0                                 % IFXRe IFXDe IFXVMIN
3  0.687d0 -2 1     1  -1.0           % NCMM rhoAB sVSR2 IDSTT APSE yMIN
6  357502.d0                          % MMLR(1) CmVAL(1)
8  5.41796d6                          % MMLR(2) CmVAL(2)
10 1.1292d8                           % MMLR(3) CmVAL(3)
```

Also, for this case, remember that `NS` has physical significance, and should be greater than zero.

```
  3  5   2  11   2.8
  3  5   3  11   2.8
  3  5   4  11   2.8
  3  5   4  11   3.0
  3  5   4  11   3.3
  3  5   4  11   3.6
```

The results shown below indicate that an SE-MLR model for these data requires `NS` ≥ 4 and that the best expansion centre is close to `Rref` $= 3.3$ Å.

These results also illustrate a fit-stabilization feature of the code. If the value of $\overline{\texttt{dd}}$ in a particular step of the non-linear fit is *larger* than the value from the previous step, the parameter changes are scaled back by a factor of (1/4), sometimes more than once, until the fit becomes stable and a progressive decrease of $\overline{\texttt{dd}}$ from one iteration step to the next is regained. This fit-stabilization seems to have been required in the early stages of all of the SE-MLR cases considered here, but the procedure succeeds, and all of those fits all eventually converged fully. Note that none of these cases yield potentials with inflection or turnover in the repulsive inner wall extrapolation region.

Standard Channel-6 output for fits to an SE-MLR potential form

```
Fit an  MLR potential function to the input points
=========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281

Fit to  101 input turning points assuming common uncertainty  u(VTP)= 1.00D+00
------------------------------------------------------------------------------
   RTP       VTP     RTP       VTP     RTP       VTP     RTP       VTP
------------------------------------------------------------------------------
 1.27263  15779.015  1.27327  15733.760  1.27435  15658.022  1.27583  15554.271
 1.27769  15424.758  1.27991  15271.523  1.28246  15096.414  1.28533  14901.096
 1.28851  14687.062  1.29198  14455.651  1.29574  14208.051  1.29978  13945.321
 .............................................................................
 .................... omit 20 lines ..........................................
 .............................................................................
```

```
 4.20012  14687.062  4.31203  14901.096  4.43887  15096.414  4.58582  15271.523
 4.76097  15424.758  4.97804  15554.271  5.26333  15658.022  5.67805  15733.760
 6.43543  15779.015
------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
===============================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.8000^3]/[r^3 + 2.8000^3]
Use Pashov natural spline exponent based on   2 yq^{ref} values for  r < r_e
                                        and  11 yq^{ref} values for  r > r_e
     in which   y_{p/q}(r)= [r^{p/q} - 2.8000^{p/q}]/[r^{p /q} + 2.8000^{p/q}]
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  14  yq^{ref} values:
  -1.0000000 -0.7654949 -0.5809898 -0.4418089 -0.3026280 -0.1634471 -0.0242662
   0.1149146  0.2540955  0.3932764  0.5324573  0.6716382  0.8108191  1.0000000
 & define beta(y_q^{ref}(r)) as a natural cubic spline
                                   through points at the  14  yq^{ref} values:
  -1.0000000 -0.7600000 -0.5800000 -0.4400000 -0.3000000 -0.1600000 -0.0200000
   0.1100000  0.2500000  0.3900000  0.5300000  0.6700000  0.8100000  1.0000000
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767
 SE-MLR Linearization:  NS= 2,  NL= 11,  R_{ref}=  2.800  yields   dd=  0.01795

At Iteration  2  RMSD= 7.5D+01  RMSD/RMSDB= 1.3D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 1.8D+01  RMSD/RMSDB= 3.0D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 7.0D+01  RMSD/RMSDB= 9.8D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 2.0D+01  RMSD/RMSDB= 2.8D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 6.5D+01  RMSD/RMSDB= 7.2D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 2.2D+01  RMSD/RMSDB= 2.4D+00  Scale PC by  (1/4)**2
At Iteration  5  RMSD= 6.1D+01  RMSD/RMSDB= 5.2D+00  Scale PC by  (1/4)**1

Direct fit to  MLR{q= 3; Rref= 2.80 ; NS= 2, NL=11}  potential:    dd= 5.25D+00
yqPSE{ 1}= -1.0000000   beta_{ 1}=  4.5680742378D-02(+/- 2.3D-03)   PS= 1.2D-05
yqPSE{ 2}= -0.7600000   beta_{ 2}=  4.7234545615D-02(+/- 1.2D-03)   PS= 1.6D-06
yqPSE{ 3}= -0.5800000   beta_{ 3}=  2.5114254801D-02(+/- 3.6D-03)   PS= 7.4D-06
yqPSE{ 4}= -0.4400000   beta_{ 4}=  4.5595126007D-02(+/- 1.0D-02)   PS= 2.1D-05
yqPSE{ 5}= -0.3000000   beta_{ 5}=  4.1112049197D-02(+/- 5.6D-03)   PS= 4.1D-05
yqPSE{ 6}= -0.1600000   beta_{ 6}=  4.2568249431D-02(+/- 3.8D-03)   PS= 3.8D-05
yqPSE{ 7}= -0.0200000   beta_{ 7}=  5.4939864005D-02(+/- 2.9D-03)   PS= 3.3D-05
yqPSE{ 8}=  0.1100000   beta_{ 8}=  8.5009383229D-02(+/- 2.8D-03)   PS= 3.4D-05
yqPSE{ 9}=  0.2500000   beta_{ 9}=  1.5555290037D-01(+/- 3.3D-03)   PS= 4.1D-05
yqPSE{10}=  0.3900000   beta_{10}=  3.0241496494D-01(+/- 5.2D-03)   PS= 6.2D-05
yqPSE{11}=  0.5300000   beta_{11}=  5.7788392412D-01(+/- 1.1D-02)   PS= 1.3D-04
yqPSE{12}=  0.6700000   beta_{12}=  1.0489222890D+00(+/- 4.7D-02)   PS= 4.1D-04
yqPSE{13}=  0.8100000   beta_{13}=  1.7832112424D+00(+/- 1.6D-01)   PS= 2.0D-03
yqPSE{14}=  1.0000000   beta_{14}=  3.0169976694D+00(+/- 0.0D+00)   PS= 0.0D+00
       Re =  1.890665802 (+/- 0.001413291)      PS= 3.0D-06
       De = 15797.626330 (+/-   14.239695)      PS= 3.7D-02
     VMIN =      2.78239 (+/-    6.432840)      PS= 3.6D-02
------------------------------------------------------------------------------
```

```
Fit an  MLR(q= 3 p= 5)  potential function to the input points
==========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.8000^3]/[r^3 + 2.8000^3]
Use Pashov natural spline exponent based on   3 yq^{ref} values for  r < r_e
                                        and  11 yq^{ref} values for  r > r_e
     in which   y_{p/q}(r)= [r^{p/q} - 2.8000^{p/q}]/[r^{p /q} + 2.8000^{p/q}]
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  15  yq^{ref} values:
  -1.0000000 -0.8436633 -0.6873265 -0.5809898 -0.4418089 -0.3026280 -0.1634471
  -0.0242662  0.1149146  0.2540955  0.3932764  0.5324573  0.6716382  0.8108191
   1.0000000
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  15  yq^{ref} values:
  -1.0000000 -0.8400000 -0.6800000 -0.5800000 -0.4400000 -0.3000000 -0.1600000
  -0.0200000  0.1100000  0.2500000  0.3900000  0.5300000  0.6700000  0.8100000
   1.0000000
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                               C 6= 3.57502000D+05
                                               C 8= 5.41796000D+06
                                               C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767
 SE-MLR Linearization:  NS= 3,  NL= 11,  R_{ref}=  2.800  yields   dd=  0.01676

At Iteration  2  RMSD= 3.9D+01  RMSD/RMSDB= 1.8D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 9.9D+00  RMSD/RMSDB= 4.6D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 3.6D+01  RMSD/RMSDB= 1.1D+01  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 1.1D+01  RMSD/RMSDB= 3.4D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 3.4D+01  RMSD/RMSDB= 6.7D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 1.2D+01  RMSD/RMSDB= 2.4D+00  Scale PC by  (1/4)**2
At Iteration  5  RMSD= 3.2D+01  RMSD/RMSDB= 4.7D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 7.0D+00  RMSD/RMSDB= 3.5D+00  Scale PC by  (1/4)**1

Direct fit to  MLR{q= 3; Rref= 2.80 ; NS= 3, NL=11}  potential:    dd= 1.93D+00
yqPSE{ 1}= -1.0000000   beta_{ 1}=  1.5586787285D-02(+/- 2.6D-03)   PS= 1.1D-05
yqPSE{ 2}= -0.8400000   beta_{ 2}=  5.8731989588D-02(+/- 3.5D-04)   PS= 6.6D-07
yqPSE{ 3}= -0.6800000   beta_{ 3}=  5.0180480041D-02(+/- 1.7D-03)   PS= 1.9D-06
yqPSE{ 4}= -0.5800000   beta_{ 4}=  5.3212804373D-02(+/- 3.4D-03)   PS= 5.8D-06
yqPSE{ 5}= -0.4400000   beta_{ 5}=  3.4998962935D-02(+/- 4.0D-03)   PS= 2.6D-05
yqPSE{ 6}= -0.3000000   beta_{ 6}=  3.0920084725D-02(+/- 2.6D-03)   PS= 1.6D-05
yqPSE{ 7}= -0.1600000   beta_{ 7}=  3.4834452510D-02(+/- 1.8D-03)   PS= 1.3D-05
yqPSE{ 8}= -0.0200000   beta_{ 8}=  4.8725589622D-02(+/- 1.4D-03)   PS= 1.1D-05
yqPSE{ 9}=  0.1100000   beta_{ 9}=  7.9127111739D-02(+/- 1.2D-03)   PS= 1.2D-05
yqPSE{10}=  0.2500000   beta_{10}=  1.5016189972D-01(+/- 1.3D-03)   PS= 1.4D-05
yqPSE{11}=  0.3900000   beta_{11}=  2.9707725862D-01(+/- 2.0D-03)   PS= 2.2D-05
yqPSE{12}=  0.5300000   beta_{12}=  5.7279127231D-01(+/- 4.2D-03)   PS= 4.5D-05
yqPSE{13}=  0.6700000   beta_{13}=  1.0437327895D+00(+/- 1.7D-02)   PS= 1.4D-04
yqPSE{14}=  0.8100000   beta_{14}=  1.7791126428D+00(+/- 5.9D-02)   PS= 7.0D-04
yqPSE{15}=  1.0000000   beta_{15}=  3.0169976694D+00(+/- 0.0D+00)   PS= 0.0D+00
       Re =  1.885872644 (+/- 0.000801836)      PS= 1.0D-06
       De = 15804.398946 (+/-    5.293832)      PS= 1.3D-02
     VMIN =     -3.96925 (+/-    2.458376)      PS= 1.2D-02
----------------------------------------------------------------------------
```

```
Fit an  MLR(q= 3 p= 5)  potential function to the input points
=============================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.8000^3]/[r^3 + 2.8000^3]
Use Pashov natural spline exponent based on   4 yq^{ref} values for  r < r_e
                                        and  11 yq^{ref} values for  r > r_e
     in which   y_{p/q}(r)= [r^{p/q} - 2.8000^{p/q}]/[r^{p /q} + 2.8000^{p/q}]
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.8827475 -0.7654949 -0.6482424 -0.5809898 -0.4418089 -0.3026280
  -0.1634471 -0.0242662  0.1149146  0.2540955  0.3932764  0.5324573  0.6716382
   0.8108191  1.0000000
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.8800000 -0.7600000 -0.6400000 -0.5800000 -0.4400000 -0.3000000
  -0.1600000 -0.0200000  0.1100000  0.2500000  0.3900000  0.5300000  0.6700000
   0.8100000  1.0000000
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767
 SE-MLR Linearization:  NS= 4,  NL= 11,  R_{ref}=  2.800  yields   dd=  0.01639

At Iteration  2  RMSD= 1.2D+01  RMSD/RMSDB= 1.5D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 3.2D+00  RMSD/RMSDB= 4.2D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 1.1D+01  RMSD/RMSDB= 9.0D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 3.5D+00  RMSD/RMSDB= 2.9D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 1.0D+01  RMSD/RMSDB= 5.9D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 3.8D+00  RMSD/RMSDB= 2.2D+00  Scale PC by  (1/4)**2
At Iteration  5  RMSD= 9.6D+00  RMSD/RMSDB= 4.3D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 2.2D+00  RMSD/RMSDB= 3.0D+00  Scale PC by  (1/4)**1

Direct fit to  MLR{q= 3; Rref= 2.80 ; NS= 4, NL=11}  potential:    dd= 7.06D-01
yqPSE{ 1}= -1.0000000   beta_{ 1}= -3.5869928514D-02(+/- 2.9D-03)   PS= 3.1D-06
yqPSE{ 2}= -0.8800000   beta_{ 2}=  4.7795674362D-02(+/- 3.5D-04)   PS= 4.0D-07
yqPSE{ 3}= -0.7600000   beta_{ 3}=  5.3665497092D-02(+/- 3.2D-04)   PS= 2.9D-07
yqPSE{ 4}= -0.6400000   beta_{ 4}=  4.3945334619D-02(+/- 1.3D-03)   PS= 1.1D-06
yqPSE{ 5}= -0.5800000   beta_{ 5}=  4.1252721503D-02(+/- 2.3D-03)   PS= 2.8D-06
yqPSE{ 6}= -0.4400000   beta_{ 6}=  3.4937264386D-02(+/- 1.4D-03)   PS= 1.4D-05
yqPSE{ 7}= -0.3000000   beta_{ 7}=  3.2752105669D-02(+/- 9.9D-04)   PS= 5.6D-06
yqPSE{ 8}= -0.1600000   beta_{ 8}=  3.6330684137D-02(+/- 7.0D-04)   PS= 4.7D-06
yqPSE{ 9}= -0.0200000   beta_{ 9}=  4.9960960599D-02(+/- 5.3D-04)   PS= 4.0D-06
yqPSE{10}=  0.1100000   beta_{10}=  8.0320075656D-02(+/- 4.7D-04)   PS= 4.1D-06
yqPSE{11}=  0.2500000   beta_{11}=  1.5126503998D-01(+/- 5.0D-04)   PS= 4.9D-06
yqPSE{12}=  0.3900000   beta_{12}=  2.9817637358D-01(+/- 7.4D-04)   PS= 7.5D-06
yqPSE{13}=  0.5300000   beta_{13}=  5.7383197465D-01(+/- 1.5D-03)   PS= 1.6D-05
yqPSE{14}=  0.6700000   beta_{14}=  1.0447268081D+00(+/- 6.4D-03)   PS= 4.9D-05
yqPSE{15}=  0.8100000   beta_{15}=  1.7796771323D+00(+/- 2.2D-02)   PS= 2.4D-04
yqPSE{16}=  1.0000000   beta_{16}=  3.0169976694D+00(+/- 0.0D+00)   PS= 0.0D+00
       Re =  1.886997694 (+/- 0.000330635)      PS= 3.6D-07
       De = 15800.839271 (+/-    2.026075)      PS= 4.5D-03
     VMIN =     -0.38756 (+/-    1.054322)      PS= 4.4D-03
------------------------------------------------------------------------------
```

```
Fit an  MLR(q= 3 p= 5)  potential function to the input points
==========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 2.8000^3]/[r^3 + 2.8000^3]
Use Pashov natural spline exponent based on   5 yq^{ref} values for  r < r_e
                                        and  11 yq^{ref} values for  r > r_e
     in which   y_{p/q}(r)= [r^{p/q} - 2.8000^{p/q}]/[r^{p /q} + 2.8000^{p/q}]
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  17  yq^{ref} values:
  -1.0000000 -0.9061980 -0.8123959 -0.7185939 -0.6247919 -0.5809898 -0.4418089
  -0.3026280 -0.1634471 -0.0242662  0.1149146  0.2540955  0.3932764  0.5324573
   0.6716382  0.8108191  1.0000000
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  17  yq^{ref} values:
  -1.0000000 -0.9000000 -0.8100000 -0.7100000 -0.6200000 -0.5800000 -0.4400000
  -0.3000000 -0.1600000 -0.0200000  0.1100000  0.2500000  0.3900000  0.5300000
   0.6700000  0.8100000  1.0000000
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767
 SE-MLR Linearization:  NS= 5,  NL= 11,  R_{ref}=  2.800  yields   dd=  0.01780

At Iteration  2  RMSD= 1.6D+01  RMSD/RMSDB= 1.2D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 4.5D+00  RMSD/RMSDB= 3.4D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 1.5D+01  RMSD/RMSDB= 7.9D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 5.0D+00  RMSD/RMSDB= 2.6D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 1.4D+01  RMSD/RMSDB= 5.5D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 5.3D+00  RMSD/RMSDB= 2.1D+00  Scale PC by  (1/4)**2
At Iteration  5  RMSD= 1.3D+01  RMSD/RMSDB= 4.1D+00  Scale PC by  (1/4)**1

Direct fit to  MLR{q= 3; Rref= 2.80 ; NS= 5, NL=11}  potential:    dd= 1.27D+00
yqPSE{ 1}= -1.0000000   beta_{ 1}= -8.3138717664D-02(+/- 6.2D-02)   PS= 1.9D-05
yqPSE{ 2}= -0.9000000   beta_{ 2}=  3.4666560489D-02(+/- 8.8D-03)   PS= 2.7D-06
yqPSE{ 3}= -0.8100000   beta_{ 3}=  5.7906310320D-02(+/- 3.8D-04)   PS= 3.7D-07
yqPSE{ 4}= -0.7100000   beta_{ 4}=  4.8853085594D-02(+/- 9.7D-04)   PS= 1.6D-06
yqPSE{ 5}= -0.6200000   beta_{ 5}=  4.1968870726D-02(+/- 3.2D-03)   PS= 4.3D-06
yqPSE{ 6}= -0.5800000   beta_{ 6}=  3.5249189113D-02(+/- 5.7D-03)   PS= 1.1D-05
yqPSE{ 7}= -0.4400000   beta_{ 7}=  3.1585170187D-02(+/- 2.9D-03)   PS= 2.6D-05
yqPSE{ 8}= -0.3000000   beta_{ 8}=  3.1935906617D-02(+/- 1.7D-03)   PS= 9.6D-06
yqPSE{ 9}= -0.1600000   beta_{ 9}=  3.5827671542D-02(+/- 1.2D-03)   PS= 8.0D-06
yqPSE{10}= -0.0200000   beta_{10}=  4.9550733019D-02(+/- 9.3D-04)   PS= 6.8D-06
yqPSE{11}=  0.1100000   beta_{11}=  7.9976936969D-02(+/- 8.4D-04)   PS= 7.0D-06
yqPSE{12}=  0.2500000   beta_{12}=  1.5094401015D-01(+/- 8.9D-04)   PS= 8.4D-06
yqPSE{13}=  0.3900000   beta_{13}=  2.9788227722D-01(+/- 1.3D-03)   PS= 1.3D-05
yqPSE{14}=  0.5300000   beta_{14}=  5.7354196059D-01(+/- 2.8D-03)   PS= 2.7D-05
yqPSE{15}=  0.6700000   beta_{15}=  1.0444557029D+00(+/- 1.2D-02)   PS= 8.4D-05
yqPSE{16}=  0.8100000   beta_{16}=  1.7794002647D+00(+/- 3.9D-02)   PS= 4.1D-04
yqPSE{17}=  1.0000000   beta_{17}=  3.0169976694D+00(+/- 0.0D+00)   PS= 0.0D+00
       Re =  1.886841728 (+/- 0.000586908)      PS= 6.1D-07
       De = 15799.280735 (+/-    3.812146)      PS= 7.7D-03
     VMIN =      1.17017 (+/-    2.187489)      PS= 7.4D-03
------------------------------------------------------------------------------
```

```
Fit an  MLR(q= 3 p= 5)  potential function to the input points
==========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 3.0000^3]/[r^3 + 3.0000^3]
Use Pashov natural spline exponent based on   4 yq^{ref} values for  r < r_e
                                        and  11 yq^{ref} values for  r > r_e
     in which   y_{p/q}(r)= [r^{p/q} - 3.0000^{p/q}]/[r^{p /q} + 3.0000^{p/q}]
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.9002980 -0.8005961 -0.7008941 -0.6511921 -0.5056292 -0.3600663
  -0.2145034 -0.0689404  0.0766225  0.2221854  0.3677483  0.5133112  0.6588742
   0.8044371  1.0000000
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.9000000 -0.8000000 -0.7000000 -0.6500000 -0.5000000 -0.3600000
  -0.2100000 -0.0600000  0.0700000  0.2200000  0.3600000  0.5100000  0.6500000
   0.8000000  1.0000000
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767
 SE-MLR Linearization:  NS= 4,  NL= 11,  R_{ref}=  3.000  yields   dd=  0.02000

At Iteration  2  RMSD= 1.2D+01  RMSD/RMSDB= 1.6D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 3.3D+00  RMSD/RMSDB= 4.5D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 1.1D+01  RMSD/RMSDB= 8.4D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 3.6D+00  RMSD/RMSDB= 2.8D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 1.0D+01  RMSD/RMSDB= 5.6D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 3.9D+00  RMSD/RMSDB= 2.1D+00  Scale PC by  (1/4)**2
At Iteration  5  RMSD= 9.7D+00  RMSD/RMSDB= 4.2D+00  Scale PC by  (1/4)**1

Direct fit to  MLR{q= 3; Rref= 3.00 ; NS= 4, NL=11}  potential:    dd= 6.63D-01
yqPSE{ 1}= -1.0000000   beta_{ 1}= -3.0682876802D-02(+/- 2.5D-03)   PS= 2.9D-06
yqPSE{ 2}= -0.9000000   beta_{ 2}=  4.8564990052D-02(+/- 3.0D-04)   PS= 3.6D-07
yqPSE{ 3}= -0.8000000   beta_{ 3}=  5.3570995482D-02(+/- 2.5D-04)   PS= 2.8D-07
yqPSE{ 4}= -0.7000000   beta_{ 4}=  4.3963693787D-02(+/- 9.3D-04)   PS= 1.0D-06
yqPSE{ 5}= -0.6500000   beta_{ 5}=  4.1100230092D-02(+/- 1.8D-03)   PS= 2.8D-06
yqPSE{ 6}= -0.5000000   beta_{ 6}=  3.4397049223D-02(+/- 1.0D-03)   PS= 1.0D-05
yqPSE{ 7}= -0.3600000   beta_{ 7}=  3.3124366030D-02(+/- 6.7D-04)   PS= 4.8D-06
yqPSE{ 8}= -0.2100000   beta_{ 8}=  3.9892441679D-02(+/- 5.1D-04)   PS= 3.8D-06
yqPSE{ 9}= -0.0600000   beta_{ 9}=  6.2024345473D-02(+/- 4.1D-04)   PS= 3.6D-06
yqPSE{10}=  0.0700000   beta_{10}=  1.0536028741D-01(+/- 4.4D-04)   PS= 4.1D-06
yqPSE{11}=  0.2200000   beta_{11}=  2.0842146591D-01(+/- 6.1D-04)   PS= 5.5D-06
yqPSE{12}=  0.3600000   beta_{12}=  3.9153801828D-01(+/- 1.1D-03)   PS= 9.4D-06
yqPSE{13}=  0.5100000   beta_{13}=  7.2454347811D-01(+/- 2.6D-03)   PS= 2.2D-05
yqPSE{14}=  0.6500000   beta_{14}=  1.2155112559D+00(+/- 1.2D-02)   PS= 7.4D-05
yqPSE{15}=  0.8000000   beta_{15}=  1.9746372564D+00(+/- 4.1D-02)   PS= 3.9D-04
yqPSE{16}=  1.0000000   beta_{16}=  3.0169976694D+00(+/- 0.0D+00)   PS= 0.0D+00
       Re =  1.887036478 (+/- 0.000241412)      PS= 3.4D-07
       De = 15799.201871 (+/-    2.265718)      PS= 4.2D-03
     VMIN =     -0.30192 (+/-    0.991473)      PS= 4.1D-03
-------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
```

```
==========================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 3.3000^3]/[r^3 + 3.3000^3]
Use Pashov natural spline exponent based on   4 yq^{ref} values for  r < r_e
                                        and  11 yq^{ref} values for  r > r_e
     in which   y_{p/q}(r)= [r^{p/q} - 3.3000^{p/q}]/[r^{p /q} + 3.3000^{p/q}]
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.9211840 -0.8423681 -0.7635521 -0.7347362 -0.5815783 -0.4284205
  -0.2752627 -0.1221048  0.0310530  0.1842108  0.3373687  0.4905265  0.6436843
   0.7968422  1.0000000
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.9200000 -0.8400000 -0.7600000 -0.7300000 -0.5800000 -0.4200000
  -0.2700000 -0.1200000  0.0300000  0.1800000  0.3300000  0.4900000  0.6400000
   0.7900000  1.0000000
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767
 SE-MLR Linearization:  NS= 4,  NL= 11,  R_{ref}=  3.300  yields   dd=  0.02446

At Iteration  2  RMSD= 1.4D+01  RMSD/RMSDB= 1.7D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 3.8D+00  RMSD/RMSDB= 4.8D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 1.3D+01  RMSD/RMSDB= 8.8D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 4.2D+00  RMSD/RMSDB= 2.8D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 1.2D+01  RMSD/RMSDB= 5.8D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 4.5D+00  RMSD/RMSDB= 2.2D+00  Scale PC by  (1/4)**2
At Iteration  5  RMSD= 1.1D+01  RMSD/RMSDB= 4.2D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 4.2D+00  RMSD/RMSDB= 7.0D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 2.3D+00  RMSD/RMSDB= 3.9D+00  Scale PC by  (1/4)**2
At Iteration  2  RMSD= 2.0D+00  RMSD/RMSDB= 3.3D+00  Scale PC by  (1/4)**3
At Iteration  2  RMSD= 1.9D+00  RMSD/RMSDB= 3.2D+00  Scale PC by  (1/4)**4

Direct fit to  MLR{q= 3; Rref= 3.30 ; NS= 4, NL=11}  potential:    dd= 5.84D-01
yqPSE{ 1}= -1.0000000   beta_{ 1}= -1.7194328115D-02(+/- 1.7D-03)   PS= 2.4D-06
yqPSE{ 2}= -0.9200000   beta_{ 2}=  5.1264448776D-02(+/- 2.2D-04)   PS= 2.8D-07
yqPSE{ 3}= -0.8400000   beta_{ 3}=  5.2785077077D-02(+/- 2.1D-04)   PS= 2.7D-07
yqPSE{ 4}= -0.7600000   beta_{ 4}=  4.3442209629D-02(+/- 6.8D-04)   PS= 8.5D-07
yqPSE{ 5}= -0.7300000   beta_{ 5}=  4.0417221051D-02(+/- 1.2D-03)   PS= 1.9D-06
yqPSE{ 6}= -0.5800000   beta_{ 6}=  3.3189860905D-02(+/- 7.6D-04)   PS= 5.9D-06
yqPSE{ 7}= -0.4200000   beta_{ 7}=  3.4647034796D-02(+/- 4.1D-04)   PS= 3.6D-06
yqPSE{ 8}= -0.2700000   beta_{ 8}=  4.8620673772D-02(+/- 3.6D-04)   PS= 3.0D-06
yqPSE{ 9}= -0.1200000   beta_{ 9}=  8.6005568773D-02(+/- 4.1D-04)   PS= 3.2D-06
yqPSE{10}=  0.0300000   beta_{10}=  1.6685132947D-01(+/- 6.5D-04)   PS= 4.2D-06
yqPSE{11}=  0.1800000   beta_{11}=  3.2037473123D-01(+/- 1.2D-03)   PS= 6.8D-06
yqPSE{12}=  0.3300000   beta_{12}=  5.7548209562D-01(+/- 2.6D-03)   PS= 1.4D-05
yqPSE{13}=  0.4900000   beta_{13}=  9.8720496373D-01(+/- 7.6D-03)   PS= 4.0D-05
yqPSE{14}=  0.6400000   beta_{14}=  1.5630728772D+00(+/- 4.1D-02)   PS= 1.5D-04
yqPSE{15}=  0.7900000   beta_{15}=  2.3111526683D+00(+/- 1.3D-01)   PS= 7.1D-04
yqPSE{16}=  1.0000000   beta_{16}=  3.0169976694D+00(+/- 0.0D+00)   PS= 0.0D+00
       Re =  1.886974676 (+/- 0.000146706)      PS= 3.0D-07
       De = 15796.164772 (+/-    3.211541)      PS= 3.7D-03
     VMIN =      0.25811 (+/-    0.885330)      PS= 3.6D-03
```

```
-------------------------------------------------------------------------------

Fit an  MLR(q= 3 p= 5)  potential function to the input points
=============================================================
    with initial   VMIN=      -1.0496   Re= 1.88753358   De= 15799.2281
 Use exponent expansion variable:   y_3(r)= [r^3 - 3.6000^3]/[r^3 + 3.6000^3]
Use Pashov natural spline exponent based on   4 yq^{ref} values for  r < r_e
                                        and  11 yq^{ref} values for  r > r_e
     in which   y_{p/q}(r)= [r^{p/q} - 3.6000^{p/q}]/[r^{p /q} + 3.6000^{p/q}]
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.9370105 -0.8740209 -0.8110314 -0.7980419 -0.6391290 -0.4802161
  -0.3213032 -0.1623903 -0.0034774  0.1554355  0.3143484  0.4732613  0.6321742
   0.7910871  1.0000000
 & define beta(y_q^{ref}(r)) as a natural spline through points at the  16  yq^{ref} values:
  -1.0000000 -0.9300000 -0.8700000 -0.8100000 -0.7900000 -0.6300000 -0.4800000
  -0.3200000 -0.1600000  0.0000000  0.1500000  0.3100000  0.4700000  0.6300000
   0.7900000  1.0000000
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
Linearized fit uses    beta(INF)=  3.01699767
 SE-MLR Linearization:  NS= 4,  NL= 11,  R_{ref}=  3.600  yields   dd=  0.02846

At Iteration  2  RMSD= 1.8D+01  RMSD/RMSDB= 1.7D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 4.3D+00  RMSD/RMSDB= 4.2D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 1.7D+01  RMSD/RMSDB= 1.2D+01  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 4.9D+00  RMSD/RMSDB= 3.6D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 1.6D+01  RMSD/RMSDB= 7.5D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 5.3D+00  RMSD/RMSDB= 2.6D+00  Scale PC by  (1/4)**2
At Iteration  5  RMSD= 1.5D+01  RMSD/RMSDB= 5.1D+00  Scale PC by  (1/4)**1
At Iteration  5  RMSD= 5.7D+00  RMSD/RMSDB= 2.0D+00  Scale PC by  (1/4)**2
At Iteration  6  RMSD= 1.4D+01  RMSD/RMSDB= 3.8D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 1.1D+01  RMSD/RMSDB= 1.5D+01  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 6.1D+00  RMSD/RMSDB= 8.8D+00  Scale PC by  (1/4)**2
At Iteration  2  RMSD= 5.4D+00  RMSD/RMSDB= 7.7D+00  Scale PC by  (1/4)**3
At Iteration  2  RMSD= 5.2D+00  RMSD/RMSDB= 7.4D+00  Scale PC by  (1/4)**4
At Iteration  4  RMSD= 3.1D+00  RMSD/RMSDB= 4.3D+00  Scale PC by  (1/4)**1
At Iteration  4  RMSD= 1.8D+00  RMSD/RMSDB= 2.6D+00  Scale PC by  (1/4)**2
At Iteration  4  RMSD= 1.6D+00  RMSD/RMSDB= 2.3D+00  Scale PC by  (1/4)**3
At Iteration  4  RMSD= 1.6D+00  RMSD/RMSDB= 2.2D+00  Scale PC by  (1/4)**4

Direct fit to  MLR{q= 3; Rref= 3.60 ; NS= 4, NL=11}  potential:    dd= 6.93D-01
yqPSE{ 1}= -1.0000000   beta_{ 1}= -1.4436314143D-03(+/- 1.5D-03)   PS= 3.6D-06
yqPSE{ 2}= -0.9300000   beta_{ 2}=  5.5253176536D-02(+/- 4.6D-04)   PS= 2.9D-07
yqPSE{ 3}= -0.8700000   beta_{ 3}=  5.2283860031D-02(+/- 4.7D-04)   PS= 3.9D-07
yqPSE{ 4}= -0.8100000   beta_{ 4}=  4.4152721372D-02(+/- 7.0D-04)   PS= 1.1D-06
yqPSE{ 5}= -0.7900000   beta_{ 5}=  4.1302297252D-02(+/- 1.0D-03)   PS= 2.3D-06
yqPSE{ 6}= -0.6300000   beta_{ 6}=  3.2224967772D-02(+/- 8.2D-04)   PS= 5.5D-06
yqPSE{ 7}= -0.4800000   beta_{ 7}=  3.7117729608D-02(+/- 4.6D-04)   PS= 3.7D-06
yqPSE{ 8}= -0.3200000   beta_{ 8}=  6.2549013811D-02(+/- 7.2D-04)   PS= 3.4D-06
yqPSE{ 9}= -0.1600000   beta_{ 9}=  1.2724804674D-01(+/- 1.5D-03)   PS= 4.2D-06
yqPSE{10}=  0.0000000   beta_{10}=  2.5944401604D-01(+/- 3.1D-03)   PS= 6.5D-06
```

```
yqPSE{11}=  0.1500000   beta_{11}=  4.6902225039D-01(+/- 6.5D-03)   PS= 1.3D-05
yqPSE{12}=  0.3100000   beta_{12}=  7.9765582128D-01(+/- 1.7D-02)   PS= 3.1D-05
yqPSE{13}=  0.4700000   beta_{13}=  1.2594053426D+00(+/- 5.2D-02)   PS= 9.9D-05
yqPSE{14}=  0.6300000   beta_{14}=  1.9422405192D+00(+/- 3.2D-01)   PS= 3.9D-04
yqPSE{15}=  0.7900000   beta_{15}=  2.7670029549D+00(+/- 1.0D+00)   PS= 1.8D-03
yqPSE{16}=  1.0000000   beta_{16}=  3.0169976694D+00(+/- 0.0D+00)   PS= 0.0D+00
       Re =  1.886810484 (+/- 0.000149086)      PS= 3.6D-07
       De = 15793.435584 (+/-   10.855866)      PS= 4.3D-03
     VMIN =      0.39415 (+/-    1.002140)      PS= 4.3D-03
------------------------------------------------------------------------------
```

Appendix C.4: Illustrative Input/Output for fits to a DELR potential form

To fit the same set of NaH turning points to a DELR potential that has the same damped three-term long-range tail used for the MLR potentials, the first five lines in the above MLR data file remain unchanged except that the value of PSEL in the first line is set equal to 3 rather than 2:

```
3  101  1.0  0  0  0 0                  % PSEL NTP UNC IROUND LPPOT prFIT prDIFF
1.88653358d0 15795.1d0 0.d0             % Re De VMIN
0 0 0                                   % IFXRe IFXDe IFXVMIN
3  0.687d0 -2 1    0 -0.8               % NCMM rhoAB sVSR2 IDSTT APSE yMIN
6  357502.d0                            % MMLR(1) CmVAL(1)
8  5.41796d6                            % MMLR(2) CmVAL(2)
10 1.1292d8                             % MMLR(3) CmVAL(3)
```

For this case, as for the EMO, parameter q and NS are dummy variables.

```
5  0   0  11  -1.0                      % q p NS NL RREF
5  0   0  11   2.0                      % q p NS NL RREF
5  0   0  11   2.2                      % q p NS NL RREF
5  0   0  11   2.5                      % q p NS NL RREF
5  0   0  12   2.2                      % q p NS NL RREF
5  0   0  13   2.2                      % q p NS NL RREF
```

While the fits to the DELR model are of reasonable quality, the results presented below show that all of the predicted potentials have potential energy inflection or inflection and turnover behaviour in the short-range extrapolation region. This printout also shows the steps of the iterative convergence to determine an internally consistent initial value of $\beta(r_e)$ (printed there as beta_0) as part of the 'linearization' step discussed in § 3.1, as well as the fact that the 'stabilization' procedure of damping preliminary estimates of parameter changes is again applied to good effect.

Standard Channel-6 output for fits to a DELR potential form

```
Fit an DELR potential function to the input points
==========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000

Fit to  101 input turning points assuming common uncertainty  u(VTP)= 1.00D+00
------------------------------------------------------------------------------
   RTP       VTP     RTP       VTP     RTP       VTP     RTP       VTP
------------------------------------------------------------------------------
 1.27263  15779.015  1.27327  15733.760  1.27435  15658.022  1.27583  15554.271
 1.27769  15424.758  1.27991  15271.523  1.28246  15096.414  1.28533  14901.096
 1.28851  14687.062  1.29198  14455.651  1.29574  14208.051  1.29978  13945.321
 .............................................................................
 .................... omit 20 lines .........................................
 .............................................................................
 4.20012  14687.062  4.31203  14901.096  4.43887  15096.414  4.58582  15271.523
 4.76097  15424.758  4.97804  15554.271  5.26333  15658.022  5.67805  15733.760
 6.43543  15779.015
------------------------------------------------------------------------------

Fit an DELR(q= 5) potential function to the input points
```

```
==========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
Use exponent expansion variable:   y_5(r)= [r^5 - Re^5]/[r^5 + Re^5]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
  Start with this long-range tail and   beta(0)=  1.000000
     which yields initial values of   AA= 1.5795100D+04   BB= 3.1590200D+04
Update  beta_0  from   1.000000   to   3.072425   by  2.1D+00 :   DSE= 1.9D+02
     which yields initial values of   AA= 1.5795100D+04   BB= 3.1590200D+04
 Converge on   beta_0=   3.072425   Next change=  0.0D+00
At Iteration  2  RMSD= 2.8D+01  RMSD/RMSDB= 5.2D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 2.1D+01  RMSD/RMSDB= 2.4D+00  Scale PC by  (1/4)**1

Direct fit to DELR{q= 5; Rref= Re   ; NL=11} potential:        dd= 4.78262D+00
 beta_{ 0}=  1.096028033539D+00 (+/- 1.5D-02)   PS= 2.1D-06   DSE= 5.18D+00
 beta_{ 1}= -1.594669654759D-01 (+/- 6.2D-02)   PS= 2.9D-06
 beta_{ 2}=  2.211374559204D-01 (+/- 2.1D-01)   PS= 3.9D-06
 beta_{ 3}=  1.832748391143D+00 (+/- 5.4D-01)   PS= 5.4D-06
 beta_{ 4}= -6.691196964007D-01 (+/- 1.2D+00)   PS= 7.2D-06
 beta_{ 5}= -8.804150247692D+00 (+/- 2.2D+00)   PS= 9.6D-06
 beta_{ 6}=  8.293716298867D-01 (+/- 3.4D+00)   PS= 1.3D-05
 beta_{ 7}=  2.084388004213D+01 (+/- 4.8D+00)   PS= 1.6D-05
 beta_{ 8}=  2.917329297754D-01 (+/- 4.7D+00)   PS= 2.1D-05
 beta_{ 9}= -2.381095397877D+01 (+/- 5.4D+00)   PS= 2.5D-05
 beta_{10}= -7.367887820992D-01 (+/- 2.5D+00)   PS= 3.0D-05
 beta_{11}=  1.074842106181D+01 (+/- 2.6D+00)   PS= 3.6D-05
       AA=  1.577524366966D+04     BB=  3.004165737795D+04
       Re =  1.884053335 (+/- 0.001731281)      PS= 9.9D-07
       De = 15818.839066 (+/-    9.629776)      PS= 5.4D-02
     VMIN =      3.80623 (+/-    6.704738)      PS= 3.5D-02
------------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 1.077   V=  2.8404D+04
                           and turns over at   R= 1.028   V=  2.9941D+04
------------------------------------------------------------------------------

Fit an DELR(q= 5) potential function to the input points
==========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.0000^5]/[r^5 + 2.0000^5]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
  Start with this long-range tail and   beta(0)=  1.000000
     which yields initial values of   AA= 1.6107459D+04   BB= 3.0052801D+04
Update  beta_0  from   1.000000   to   0.697576   by -3.0D-01 :   DSE= 2.0D+01
     which yields initial values of   AA= 1.7044815D+04   BB= 3.0990158D+04
Update  beta_0  from   0.697576   to   0.802965   by  1.1D-01 :   DSE= 3.1D+01
     which yields initial values of   AA= 1.6638008D+04   BB= 3.0583351D+04
Update  beta_0  from   0.802965   to   0.751895   by -5.1D-02 :   DSE= 2.6D+01
```

```
     which yields initial values of   AA= 1.6820897D+04   BB= 3.0766240D+04
Update  beta_0  from   0.751895   to   0.773980   by  2.2D-02 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6738848D+04   BB= 3.0684190D+04
Update  beta_0  from   0.773980   to   0.763884   by -1.0D-02 :   DSE= 2.7D+01
     which yields initial values of   AA= 1.6775768D+04   BB= 3.0721110D+04
Update  beta_0  from   0.763884   to   0.768390   by  4.5D-03 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6759170D+04   BB= 3.0704512D+04
Update  beta_0  from   0.768390   to   0.766357   by -2.0D-03 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6766635D+04   BB= 3.0711977D+04
Update  beta_0  from   0.766357   to   0.767270   by  9.1D-04 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6763278D+04   BB= 3.0708620D+04
Update  beta_0  from   0.767270   to   0.766859   by -4.1D-04 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6764788D+04   BB= 3.0710130D+04
Update  beta_0  from   0.766859   to   0.767044   by  1.8D-04 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6764109D+04   BB= 3.0709451D+04
Update  beta_0  from   0.767044   to   0.766960   by -8.3D-05 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6764414D+04   BB= 3.0709756D+04
Update  beta_0  from   0.766960   to   0.766998   by  3.7D-05 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6764277D+04   BB= 3.0709619D+04
Update  beta_0  from   0.766998   to   0.766981   by -1.7D-05 :   DSE= 2.8D+01
     which yields initial values of   AA= 1.6764339D+04   BB= 3.0709681D+04
 Converge on   beta_0=   0.766989   Next change=  7.6D-06
At Iteration  2  RMSD= 9.9D+02  RMSD/RMSDB= 3.5D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 5.6D+02  RMSD/RMSDB= 2.0D+00  Scale PC by  (1/4)**2
At Iteration  3  RMSD= 8.7D+02  RMSD/RMSDB= 2.4D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 1.7D+01  RMSD/RMSDB= 5.1D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 1.3D+01  RMSD/RMSDB= 2.4D+00  Scale PC by  (1/4)**1

Direct fit to DELR{q= 5; Rref= 2.000; NL=11} potential:        dd= 2.69052D+00
 beta_{ 0}=  1.115238978199D+00 (+/- 8.0D-03)   PS= 1.1D-06   DSE= 2.91573D+00
 beta_{ 1}= -7.531906244057D-02 (+/- 2.8D-02)   PS= 1.5D-06
 beta_{ 2}=  1.335971644609D-01 (+/- 1.1D-01)   PS= 1.9D-06
 beta_{ 3}=  8.808096498560D-01 (+/- 2.6D-01)   PS= 2.4D-06
 beta_{ 4}= -7.613235210522D-01 (+/- 5.6D-01)   PS= 3.0D-06
 beta_{ 5}= -3.915835295026D+00 (+/- 1.1D+00)   PS= 3.8D-06
 beta_{ 6}=  2.388786493452D+00 (+/- 1.4D+00)   PS= 4.7D-06
 beta_{ 7}=  9.071198057864D+00 (+/- 2.4D+00)   PS= 5.9D-06
 beta_{ 8}= -3.013477237059D+00 (+/- 1.7D+00)   PS= 7.4D-06
 beta_{ 9}= -1.023038220333D+01 (+/- 2.5D+00)   PS= 9.1D-06
 beta_{10}=  1.470678360645D+00 (+/- 7.7D-01)   PS= 1.1D-05
 beta_{11}=  4.656746246037D+00 (+/- 1.1D+00)   PS= 1.4D-05
       AA=  1.573131200787D+04     BB=  2.999689794039D+04
       Re =  1.885857883 (+/- 0.000839587)      PS= 5.6D-07
       De = 15815.029715 (+/-    5.333498)      PS= 3.1D-02
     VMIN =     -2.91840 (+/-    3.840617)      PS= 1.9D-02
----------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 1.109   V=  2.9913D+04
                           and turns over at   R= 1.106   V=  3.0935D+04
----------------------------------------------------------------------------

Fit an DELR(q= 5) potential function to the input points
==========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.2000^5]/[r^5 + 2.2000^5]
```

```
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
  Start with this long-range tail and   beta(0)=  1.000000
     which yields initial values of   AA= 1.6106589D+04   BB= 3.0057083D+04
Update  beta_0  from   1.000000   to   1.022514   by  2.3D-02 :   DSE= 2.1D+01
     which yields initial values of   AA= 1.6059115D+04   BB= 3.0009608D+04
Update  beta_0  from   1.022514   to   1.016341   by -6.2D-03 :   DSE= 2.0D+01
     which yields initial values of   AA= 1.6071923D+04   BB= 3.0022417D+04
Update  beta_0  from   1.016341   to   1.018004   by  1.7D-03 :   DSE= 2.0D+01
     which yields initial values of   AA= 1.6068458D+04   BB= 3.0018951D+04
Update  beta_0  from   1.018004   to   1.017554   by -4.5D-04 :   DSE= 2.0D+01
     which yields initial values of   AA= 1.6069395D+04   BB= 3.0019888D+04
Update  beta_0  from   1.017554   to   1.017675   by  1.2D-04 :   DSE= 2.0D+01
     which yields initial values of   AA= 1.6069141D+04   BB= 3.0019635D+04
Update  beta_0  from   1.017675   to   1.017642   by -3.3D-05 :   DSE= 2.0D+01
     which yields initial values of   AA= 1.6069210D+04   BB= 3.0019703D+04
 Converge on   beta_0=   1.017651   Next change=  8.9D-06
At Iteration  2  RMSD= 8.9D+02  RMSD/RMSDB= 3.2D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 5.4D+02  RMSD/RMSDB= 2.8D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 6.4D+00  RMSD/RMSDB= 4.8D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 4.8D+00  RMSD/RMSDB= 2.4D+00  Scale PC by  (1/4)**1

Direct fit to DELR{q= 5; Rref= 2.200; NL=11} potential:        dd= 1.07508D+00
 beta_{ 0}=  1.120054915325D+00 (+/- 1.5D-03)   PS= 4.6D-07   DSE= 1.16507D+00
 beta_{ 1}=  2.367014196637D-02 (+/- 6.5D-03)   PS= 5.4D-07
 beta_{ 2}=  4.288720491111D-02 (+/- 2.7D-02)   PS= 6.3D-07
 beta_{ 3}=  1.551527342711D-01 (+/- 7.3D-02)   PS= 7.3D-07
 beta_{ 4}=  7.460219393705D-02 (+/- 1.6D-01)   PS= 8.5D-07
 beta_{ 5}= -7.557980059175D-01 (+/- 3.6D-01)   PS= 9.9D-07
 beta_{ 6}=  3.977498493378D-02 (+/- 3.8D-01)   PS= 1.1D-06
 beta_{ 7}=  2.369802042151D+00 (+/- 8.1D-01)   PS= 1.3D-06
 beta_{ 8}= -1.138686364056D-01 (+/- 4.1D-01)   PS= 1.5D-06
 beta_{ 9}= -3.180687841061D+00 (+/- 8.4D-01)   PS= 1.8D-06
 beta_{10}=  2.480246442829D-01 (+/- 1.7D-01)   PS= 2.0D-06
 beta_{11}=  1.745284303283D+00 (+/- 3.3D-01)   PS= 2.3D-06
       AA=  1.573528800283D+04     BB=  2.999082702308D+04
       Re =  1.887142276 (+/- 0.000308311)      PS= 2.2D-07
       De = 15802.863880 (+/-    2.359170)      PS= 1.2D-02
     VMIN =     -0.13237 (+/-    1.468316)      PS= 7.8D-03
------------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 1.115   V=  3.0397D+04
------------------------------------------------------------------------------

Fit an DELR(q= 5) potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.5000^5]/[r^5 + 2.5000^5]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
```

```
                                                C10= 1.12920000D+08
  Start with this long-range tail and   beta(0)=  1.000000
     which yields initial values of   AA= 1.6106668D+04   BB= 3.0056695D+04
Update  beta_0  from   1.000000   to   1.122595   by  1.2D-01 :   DSE= 2.8D+01
!!! CAUTION !!! Iteration to optimize  beta(0)  not converged after 21 tries
At Iteration  2  RMSD= 5.8D+02  RMSD/RMSDB= 3.0D+00  Scale PC by  (1/4)**1

Direct fit to DELR{q= 5; Rref= 2.500; NL=11} potential:        dd= 1.73281D+00
 beta_{ 0}=  1.136035235987D+00 (+/- 8.2D-04)   PS= 7.4D-07   DSE= 1.87785D+00
 beta_{ 1}=  7.065877030306D-02 (+/- 3.1D-03)   PS= 8.1D-07
 beta_{ 2}=  4.521847619940D-02 (+/- 1.6D-02)   PS= 8.8D-07
 beta_{ 3}=  1.390910506407D-01 (+/- 6.7D-02)   PS= 9.5D-07
 beta_{ 4}=  6.396183428634D-01 (+/- 1.3D-01)   PS= 1.0D-06
 beta_{ 5}= -1.119556659625D+00 (+/- 4.2D-01)   PS= 1.1D-06
 beta_{ 6}= -1.723194156717D+00 (+/- 3.9D-01)   PS= 1.2D-06
 beta_{ 7}=  4.177231794800D+00 (+/- 1.0D+00)   PS= 1.3D-06
 beta_{ 8}=  2.115753467498D+00 (+/- 5.0D-01)   PS= 1.4D-06
 beta_{ 9}= -5.349248254522D+00 (+/- 1.1D+00)   PS= 1.5D-06
 beta_{10}= -7.471162356997D-01 (+/- 2.3D-01)   PS= 1.7D-06
 beta_{11}=  2.453472662871D+00 (+/- 4.6D-01)   PS= 1.8D-06
       AA=  1.570858272946D+04     BB=  2.996260328312D+04
       Re =  1.887508614 (+/- 0.000407822)      PS= 3.6D-07
       De = 15800.741543 (+/-    4.132711)      PS= 2.0D-02
     VMIN =     -4.39415 (+/-    2.128574)      PS= 1.3D-02
------------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 1.121   V=  3.0386D+04
------------------------------------------------------------------------------

Fit an DELR(q= 5) potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.2000^5]/[r^5 + 2.2000^5]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
  Start with this long-range tail and   beta(0)=  1.000000
     which yields initial values of   AA= 1.6106139D+04   BB= 3.0059298D+04
Update  beta_0  from   1.000000   to   1.022495   by  2.2D-02 :   DSE= 2.1D+01
!!! CAUTION !!! Iteration to optimize  beta(0)  not converged after 22 tries
At Iteration  2  RMSD= 9.2D+02  RMSD/RMSDB= 3.4D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 5.5D+02  RMSD/RMSDB= 2.7D+00  Scale PC by  (1/4)**1
At Iteration  2  RMSD= 5.0D+00  RMSD/RMSDB= 4.7D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 3.8D+00  RMSD/RMSDB= 2.4D+00  Scale PC by  (1/4)**1

Direct fit to DELR{q= 5; Rref= 2.200; NL=12} potential:        dd= 9.20842D-01
 beta_{ 0}=  1.117451257005D+00 (+/- 1.6D-03)   PS= 3.7D-07   DSE= 1.00378D+00
 beta_{ 1}=  4.009260991753D-02 (+/- 7.4D-03)   PS= 4.4D-07
 beta_{ 2}=  1.147058960475D-02 (+/- 2.5D-02)   PS= 5.1D-07
 beta_{ 3}= -4.059409622099D-02 (+/- 9.5D-02)   PS= 5.9D-07
 beta_{ 4}=  6.325120276734D-01 (+/- 2.2D-01)   PS= 6.9D-07
 beta_{ 5}= -6.055857090936D-03 (+/- 4.3D-01)   PS= 8.0D-07
 beta_{ 6}= -2.457041501434D+00 (+/- 9.1D-01)   PS= 9.2D-07
```

```
 beta_{ 7}=  1.024126476239D+00 (+/- 8.9D-01)   PS= 1.1D-06
 beta_{ 8}=  4.860152413486D+00 (+/- 1.8D+00)   PS= 1.2D-06
 beta_{ 9}= -2.005426995757D+00 (+/- 8.7D-01)   PS= 1.4D-06
 beta_{10}= -4.412006859282D+00 (+/- 1.7D+00)   PS= 1.6D-06
 beta_{11}=  1.340156242175D+00 (+/- 3.3D-01)   PS= 1.9D-06
 beta_{12}=  1.675119094981D+00 (+/- 6.0D-01)   PS= 2.2D-06
       AA=  1.573544546428D+04     BB=  2.998806310486D+04
       Re =  1.886565358 (+/- 0.000336176)      PS= 1.8D-07
       De = 15800.893936 (+/-    2.142385)      PS= 9.8D-03
     VMIN =      0.25044 (+/-    1.272230)      PS= 6.3D-03
------------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 1.118   V=  3.0340D+04
                           and turns over at   R= 1.117   V=  3.0709D+04
------------------------------------------------------------------------------

Fit an DELR(q= 5) potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358   De= 15795.1000
 Use exponent expansion variable:   y_5(r)= [r^5 - 2.2000^5]/[r^5 + 2.2000^5]
uLR(r) inverse-power terms incorporate DS damping with  rhoAB= 0.6870000
       defined to give very short-range damped uLR-term behaviour  r^{-2/2}
                                                C 6= 3.57502000D+05
                                                C 8= 5.41796000D+06
                                                C10= 1.12920000D+08
  Start with this long-range tail and   beta(0)=  1.000000
     which yields initial values of   AA= 1.6106671D+04   BB= 3.0056680D+04
Update  beta_0  from   1.000000   to   1.027003   by  2.7D-02 :   DSE= 1.7D+01
!!! CAUTION !!! Iteration to optimize  beta(0)  not converged after 23 tries
At Iteration  2  RMSD= 4.6D+00  RMSD/RMSDB= 4.3D+00  Scale PC by  (1/4)**1
At Iteration  3  RMSD= 3.5D+00  RMSD/RMSDB= 2.3D+00  Scale PC by  (1/4)**1

Direct fit to DELR{q= 5; Rref= 2.200; NL=13} potential:        dd= 9.19631D-01
 beta_{ 0}=  1.117448400383D+00 (+/- 1.6D-03)   PS= 3.5D-07   DSE= 1.00840D+00
 beta_{ 1}=  3.973357385637D-02 (+/- 7.9D-03)   PS= 4.1D-07
 beta_{ 2}=  1.789346858692D-02 (+/- 3.8D-02)   PS= 4.8D-07
 beta_{ 3}= -5.526890121379D-02 (+/- 1.1D-01)   PS= 5.6D-07
 beta_{ 4}=  5.809783360345D-01 (+/- 3.4D-01)   PS= 6.5D-07
 beta_{ 5}=  1.403203325449D-01 (+/- 7.8D-01)   PS= 7.5D-07
 beta_{ 6}= -2.289228853671D+00 (+/- 1.3D+00)   PS= 8.7D-07
 beta_{ 7}=  4.937200044856D-01 (+/- 2.6D+00)   PS= 1.0D-06
 beta_{ 8}=  4.585149542944D+00 (+/- 2.3D+00)   PS= 1.2D-06
 beta_{ 9}= -1.078074120069D+00 (+/- 4.5D+00)   PS= 1.3D-06
 beta_{10}= -4.185569035483D+00 (+/- 2.1D+00)   PS= 1.6D-06
 beta_{11}=  5.494146056872D-01 (+/- 3.9D+00)   PS= 1.8D-06
 beta_{12}=  1.600272867548D+00 (+/- 7.4D-01)   PS= 2.1D-06
 beta_{13}=  2.642139873974D-01 (+/- 1.3D+00)   PS= 2.4D-06
       AA=  1.573473763341D+04     BB=  2.998735713564D+04
       Re =  1.886576309 (+/- 0.000341277)      PS= 1.7D-07
       De = 15800.877733 (+/-    2.153027)      PS= 9.3D-03
     VMIN =      0.14316 (+/-    1.384214)      PS= 5.9D-03
------------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 1.118   V=  3.0334D+04
------------------------------------------------------------------------------
```

Appendix C.5: Illustrative Input/Output for fits to a GPEF potential form

To fit the same set of NaH turning points to a GPEF potential using the Šurkus q = 1 expansion variable, the first three lines in the EMO data file of Appendix C.1 are replaced by the following:

```
 4  101  1.0  -2  0  0 0                        % PSEL NTP UNC IROUND LPPOT prFIT prDIFF
 1.88653358d0 0.d0 0.d0                          % Re De VMIN
 0 1 0                                           % IFXRe IFXDe IFXVMIN
  1.d0  1.d0                                     % a_S b_S
```

For this case, both p and $r_{\rm ref}$ are dummy variables, but q may be important.

```
     4  0   13  16  0.0
     2  0   10  13  0.0
```

The first set of GPEF case considered here performs fits to GPEF potentials represented by polynomial expansions with orders ranging from 13 to 16 in the Šurkus variable $z_4(r) = (r^4 - {r_e}^4)/(r^4 + {r_e}^4)$, while the second set consists of expansions with orders ranging from 10 to 13 the radial variable $z_2(r) = (r^2 - {r_e}^2)/(r^2 + {r_e}^2)$.

As an illustration of the results of application of the 'Sequential Rounding and Refitting' (SRR) procedure, this set of fits was performed with parameter IROUND in line #1 of the data file set at -3. As can be seen, all of the parameters are rounded compactly, and comparisons with results obtained without performing any rounding show that with one exception, a case in which the rounding algorithm forced VMIN $= 0.66(\pm 1.84)$ to be precisely zero, to the three significant digits shown, that parameter rounding had *no effect* on the final $\overline{dd}$ values.

Standard Channel-6 output for fits to GPEF potential forms

```
 Fit an GPEF potential function to the input points
 ===========================================================
     with initial   VMIN=       0.0000   Re= 1.88653358
 GPEF expansion variable is:   y= (R^q - Re^q)//(  1.00000*R^q  +1.00000*Re^q)

 Fit to  101 input turning points assuming common uncertainty  u(VTP)= 1.00D+00
 -----------------------------------------------------------------------------
    RTP       VTP      RTP       VTP      RTP       VTP      RTP       VTP
 -----------------------------------------------------------------------------
  1.27263  15779.015  1.27327  15733.760  1.27435  15658.022  1.27583  15554.271
  1.27769  15424.758  1.27991  15271.523  1.28246  15096.414  1.28533  14901.096
  1.28851  14687.062  1.29198  14455.651  1.29574  14208.051  1.29978  13945.321
  1.30410  13668.392  1.30869  13378.084  1.31356  13075.115  1.31870  12760.108
  1.32413  12433.604  1.32984  12096.067  1.33584  11747.896  1.34215  11389.427
  1.34877  11020.946  1.35572  10642.691  1.36303  10254.859  1.37072   9857.610
  1.37881   9451.076  1.38734   9035.358  1.39634   8610.537  1.40587   8176.670
  1.41597   7733.798  1.42671   7281.947  1.43816   6821.126  1.45041   6351.334
  1.46358   5872.557  1.47781   5384.772  1.49325   4887.943  1.51014   4382.030
  1.52877   3866.979  1.54955   3342.731  1.57307   2809.219  1.59445   2375.691
  1.60622   2156.674  1.61888   1936.148  1.63260   1714.107  1.64759   1490.547
  1.66418   1265.462  1.68283   1038.847  1.70431    810.697  1.72997    581.005
  1.76280    349.767  1.81307    116.978  1.88705      0.000  1.96770    116.978
  2.03136    349.767  2.07765    581.005  2.11684    810.697  2.15191   1038.847
  2.18422   1265.462  2.21453   1490.547  2.24332   1714.107  2.27089   1936.148
  2.29748   2156.674  2.32325   2375.691  2.37283   2809.219  2.43199   3342.731
```

```
 2.48888   3866.979  2.54410   4382.030  2.59809   4887.943  2.65117   5384.772
 2.70357   5872.557  2.75552   6351.334  2.80716   6821.126  2.85864   7281.947
 2.91009   7733.798  2.96163   8176.670  3.01337   8610.537  3.06543   9035.358
 3.11792   9451.076  3.17096   9857.610  3.22469  10254.859  3.27924  10642.691
 3.33477  11020.946  3.39147  11389.427  3.44956  11747.896  3.50927  12096.067
 3.57092  12433.604  3.63486  12760.108  3.70152  13075.115  3.77144  13378.084
 3.84526  13668.392  3.92382  13945.321  4.00816  14208.051  4.09966  14455.651
 4.20012  14687.062  4.31203  14901.096  4.43887  15096.414  4.58582  15271.523
 4.76097  15424.758  4.97804  15554.271  5.26333  15658.022  5.67805  15733.760
 6.43543  15779.015
-------------------------------------------------------------------------------

Fit an GPEF potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358
GPEF expansion variable is:   y= (R^4 - Re^4)/(  1.00000*R^4  +1.00000*Re^4)

Fit to a GPEF{q=4;  N=13} potential yields:                       DSE= 3.11D+00
    c_{ 0} =  1.6954770000D+04 (+/- 2.4D+02)    PS= 4.1D-02
    c_{ 1} = -6.5805600000D-01 (+/- 9.2D-02)    PS= 2.9D-06
    c_{ 2} =  1.6717780000D+00 (+/- 2.7D-01)    PS= 3.4D-06
    c_{ 3} =  7.1294000000D-01 (+/- 1.3D+00)    PS= 3.7D-06
    c_{ 4} = -9.0453700000D+00 (+/- 2.3D+00)    PS= 4.1D-06
    c_{ 5} = -7.6276000000D+00 (+/- 8.1D+00)    PS= 4.4D-06
    c_{ 6} =  5.1817000000D+01 (+/- 1.1D+01)    PS= 4.7D-06
    c_{ 7} =  1.3315900000D+01 (+/- 2.6D+01)    PS= 5.1D-06
    c_{ 8} = -1.4196400000D+02 (+/- 3.5D+01)    PS= 5.4D-06
    c_{ 9} =  1.0900000000D+01 (+/- 3.8D+01)    PS= 5.7D-06
    c_{10} =  1.9970300000D+02 (+/- 6.1D+01)    PS= 6.0D-06
    c_{11} = -6.8210000000D+01 (+/- 1.7D+01)    PS= 6.3D-06
    c_{12} = -1.1279000000D+02 (+/- 4.4D+01)    PS= 6.6D-06
    c_{13} =  6.2100000000D+01 (+/- 1.8D+01)    PS= 6.9D-06
     VMIN =       4.37000 (+/-    3.984955)     PS= 1.9D-02
       Re =  1.886360000 (+/- 0.001070016)      PS= 7.7D-07

Fit to a GPEF{q=4;  N=14} potential yields:                       DSE= 1.68D+00
    c_{ 0} =  1.7862814000D+04 (+/- 1.8D+02)    PS= 2.1D-02
    c_{ 1} = -6.4413600000D-01 (+/- 4.5D-02)    PS= 1.4D-06
    c_{ 2} =  1.2133000000D-01 (+/- 2.5D-01)    PS= 1.6D-06
    c_{ 3} =  1.4417100000D+00 (+/- 6.3D-01)    PS= 1.8D-06
    c_{ 4} =  8.2963300000D+00 (+/- 2.6D+00)    PS= 2.0D-06
    c_{ 5} = -1.9475230000D+01 (+/- 4.3D+00)    PS= 2.1D-06
    c_{ 6} = -4.5151000000D+01 (+/- 1.4D+01)    PS= 2.3D-06
    c_{ 7} =  1.0256930000D+02 (+/- 1.8D+01)    PS= 2.4D-06
    c_{ 8} =  1.3209090000D+02 (+/- 4.1D+01)    PS= 2.6D-06
    c_{ 9} = -3.1738300000D+02 (+/- 4.9D+01)    PS= 2.7D-06
    c_{10} = -1.4942500000D+02 (+/- 5.5D+01)    PS= 2.9D-06
    c_{11} =  5.1321000000D+02 (+/- 8.1D+01)    PS= 3.0D-06
    c_{12} = -4.2750000000D+01 (+/- 2.3D+01)    PS= 3.2D-06
    c_{13} = -3.3502000000D+02 (+/- 5.5D+01)    PS= 3.3D-06
    c_{14} =  1.5200000000D+02 (+/- 2.1D+01)    PS= 3.5D-06
     VMIN =      -1.95000 (+/-    2.326215)     PS= 9.9D-03
       Re =  1.886241000 (+/- 0.000561144)      PS= 3.9D-07
```

```
Fit to a GPEF{q=4;  N=15} potential yields:                        DSE= 9.68D-01
    c_{ 0} =  1.7712147000D+04 (+/- 1.1D+02)    PS= 1.1D-02
    c_{ 1} = -4.4966310000D-01 (+/- 4.0D-02)    PS= 7.7D-07
    c_{ 2} =  2.6352100000D-01 (+/- 1.4D-01)    PS= 8.9D-07
    c_{ 3} = -2.5529770000D+00 (+/- 7.0D-01)    PS= 9.9D-07
    c_{ 4} =  7.8680630000D+00 (+/- 1.5D+00)    PS= 1.1D-06
    c_{ 5} =  1.7603780000D+01 (+/- 6.1D+00)    PS= 1.2D-06
    c_{ 6} = -5.6636290000D+01 (+/- 8.4D+00)    PS= 1.3D-06
    c_{ 7} = -7.7490600000D+01 (+/- 2.9D+01)    PS= 1.3D-06
    c_{ 8} =  2.4945730000D+02 (+/- 3.0D+01)    PS= 1.4D-06
    c_{ 9} =  1.4642700000D+02 (+/- 7.5D+01)    PS= 1.5D-06
    c_{10} = -6.0238800000D+02 (+/- 7.5D+01)    PS= 1.6D-06
    c_{11} = -4.7332000000D+01 (+/- 9.6D+01)    PS= 1.7D-06
    c_{12} =  7.5276000000D+02 (+/- 1.2D+02)    PS= 1.7D-06
    c_{13} = -2.0114000000D+02 (+/- 3.7D+01)    PS= 1.8D-06
    c_{14} = -3.7860000000D+02 (+/- 8.0D+01)    PS= 1.9D-06
    c_{15} =  1.9210000000D+02 (+/- 2.9D+01)    PS= 2.0D-06
     VMIN =     -1.33000 (+/-    1.341352)      PS= 5.4D-03
       Re =  1.887734000 (+/- 0.000393329)      PS= 2.1D-07

Fit to a GPEF{q=4;  N=16} potential yields:                        DSE= 4.28D-01
    c_{ 0} =  1.7365240000D+04 (+/- 6.0D+01)    PS= 4.8D-03
    c_{ 1} = -5.1617830000D-01 (+/- 1.9D-02)    PS= 3.3D-07
    c_{ 2} =  1.0487507000D+00 (+/- 1.1D-01)    PS= 3.8D-07
    c_{ 3} = -1.5688180000D+00 (+/- 3.4D-01)    PS= 4.2D-07
    c_{ 4} = -4.0029810000D+00 (+/- 1.5D+00)    PS= 4.6D-07
    c_{ 5} =  1.1575200000D+01 (+/- 2.9D+00)    PS= 5.0D-07
    c_{ 6} =  3.6704220000D+01 (+/- 1.1D+01)    PS= 5.4D-07
    c_{ 7} = -8.0632400000D+01 (+/- 1.3D+01)    PS= 5.7D-07
    c_{ 8} = -1.5490380000D+02 (+/- 4.6D+01)    PS= 6.1D-07
    c_{ 9} =  3.2721090000D+02 (+/- 3.9D+01)    PS= 6.4D-07
    c_{10} =  3.5954600000D+02 (+/- 1.1D+02)    PS= 6.8D-07
    c_{11} = -8.2242700000D+02 (+/- 9.4D+01)    PS= 7.1D-07
    c_{12} = -3.5440500000D+02 (+/- 1.3D+02)    PS= 7.5D-07
    c_{13} =  1.1628200000D+03 (+/- 1.5D+02)    PS= 7.8D-07
    c_{14} = -8.7740000000D+01 (+/- 5.0D+01)    PS= 8.1D-07
    c_{15} = -6.9850000000D+02 (+/- 9.8D+01)    PS= 8.5D-07
    c_{16} =  3.0570000000D+02 (+/- 3.3D+01)    PS= 8.8D-07
     VMIN =      0.58900 (+/-    0.628318)      PS= 2.3D-03
       Re =  1.887326000 (+/- 0.000181818)      PS= 8.9D-08
------------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 0.687   V=  1.6750D+06
------------------------------------------------------------------------------

Fit an GPEF potential function to the input points
=========================================================
    with initial   VMIN=       0.0000   Re= 1.88653358
GPEF expansion variable is:   y= (R^2 - Re^2)/(  1.00000*R^2  +1.00000*Re^2)

Fit to a GPEF{q=2;  N=10} potential yields:                        DSE= 1.99D+00
    c_{ 0} =  6.9611180000D+04 (+/- 1.5D+02)    PS= 6.8D-02
    c_{ 1} = -1.0901849000D+00 (+/- 1.6D-02)    PS= 1.5D-06
    c_{ 2} =  1.1668120000D+00 (+/- 5.6D-02)    PS= 2.1D-06
    c_{ 3} = -1.4994000000D+00 (+/- 3.0D-01)    PS= 2.8D-06
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    c_{ 4} = -9.7302000000D-01 (+/- 7.2D-01)    PS= 3.6D-06
    c_{ 5} =  4.0608000000D+00 (+/- 2.1D+00)    PS= 4.7D-06
    c_{ 6} =  8.7485000000D+00 (+/- 5.7D+00)    PS= 5.9D-06
    c_{ 7} = -1.6034000000D+01 (+/- 4.1D+00)    PS= 7.4D-06
    c_{ 8} = -4.0712000000D+01 (+/- 1.7D+01)    PS= 9.2D-06
    c_{ 9} =  8.7610000000D+01 (+/- 2.0D+01)    PS= 1.1D-05
    c_{10} = -4.2330000000D+01 (+/- 7.3D+00)    PS= 1.4D-05
     VMIN =      2.08000 (+/-    1.765044)      PS= 1.5D-02
       Re =  1.887366000 (+/- 0.000262137)      PS= 6.1D-07

 Fit to a GPEF{q=2;  N=11} potential yields:                       DSE= 2.00D+00
    c_{ 0} =  6.9875540000D+04 (+/- 2.2D+02)    PS= 6.4D-02
    c_{ 1} = -1.0830568000D+00 (+/- 1.7D-02)    PS= 1.4D-06
    c_{ 2} =  9.9781900000D-01 (+/- 1.1D-01)    PS= 1.9D-06
    c_{ 3} = -1.4133400000D+00 (+/- 3.0D-01)    PS= 2.6D-06
    c_{ 4} =  1.5898200000D+00 (+/- 1.7D+00)    PS= 3.4D-06
    c_{ 5} =  3.8140000000D-01 (+/- 3.0D+00)    PS= 4.4D-06
    c_{ 6} = -6.4770000000D+00 (+/- 1.1D+01)    PS= 5.5D-06
    c_{ 7} =  2.1397000000D+01 (+/- 2.3D+01)    PS= 6.9D-06
    c_{ 8} = -2.8817000000D+01 (+/- 1.8D+01)    PS= 8.6D-06
    c_{ 9} = -2.3060000000D+01 (+/- 6.9D+01)    PS= 1.1D-05
    c_{10} =  7.6030000000D+01 (+/- 7.1D+01)    PS= 1.3D-05
    c_{11} = -4.0700000000D+01 (+/- 2.4D+01)    PS= 1.6D-05
     VMIN =      0.00000 (+/-    1.969521)      PS= 1.4D-02
       Re =  1.887425000 (+/- 0.000265521)      PS= 5.7D-07

 Fit to a GPEF{q=2;  N=12} potential yields:                       DSE= 8.20D-01
    c_{ 0} =  7.0369124000D+04 (+/- 1.0D+02)    PS= 2.4D-02
    c_{ 1} = -1.1531881000D+00 (+/- 1.1D-02)    PS= 5.2D-07
    c_{ 2} =  7.7764940000D-01 (+/- 5.1D-02)    PS= 7.3D-07
    c_{ 3} =  1.0271270000D+00 (+/- 2.8D-01)    PS= 9.8D-07
    c_{ 4} =  3.1022300000D+00 (+/- 7.1D-01)    PS= 1.3D-06
    c_{ 5} = -3.2600610000D+01 (+/- 3.7D+00)    PS= 1.7D-06
    c_{ 6} =  1.7269500000D+01 (+/- 5.0D+00)    PS= 2.1D-06
    c_{ 7} =  2.0850960000D+02 (+/- 2.2D+01)    PS= 2.6D-06
    c_{ 8} = -3.6587800000D+02 (+/- 3.6D+01)    PS= 3.3D-06
    c_{ 9} = -2.3601300000D+02 (+/- 3.6D+01)    PS= 4.0D-06
    c_{10} =  1.1298200000D+03 (+/- 1.1D+02)    PS= 4.9D-06
    c_{11} = -1.0472000000D+03 (+/- 1.1D+02)    PS= 6.0D-06
    c_{12} =  3.2170000000D+02 (+/- 3.4D+01)    PS= 7.3D-06
     VMIN =     -1.17100 (+/-    0.830402)      PS= 5.5D-03
       Re =  1.886691000 (+/- 0.000132571)      PS= 2.2D-07

 Fit to a GPEF{q=2;  N=13} potential yields:                       DSE= 8.02D-01
    c_{ 0} =  7.0419395000D+04 (+/- 1.1D+02)    PS= 2.2D-02
    c_{ 1} = -1.1430833000D+00 (+/- 1.3D-02)    PS= 4.8D-07
    c_{ 2} =  7.2124050000D-01 (+/- 7.1D-02)    PS= 6.7D-07
    c_{ 3} =  7.6974100000D-01 (+/- 3.6D-01)    PS= 9.0D-07
    c_{ 4} =  4.5866400000D+00 (+/- 1.5D+00)    PS= 1.2D-06
    c_{ 5} = -3.0309220000D+01 (+/- 4.1D+00)    PS= 1.5D-06
    c_{ 6} = -1.3167000000D+00 (+/- 1.7D+01)    PS= 1.9D-06
    c_{ 7} =  2.1231090000D+02 (+/- 2.2D+01)    PS= 2.4D-06
    c_{ 8} = -2.6365200000D+02 (+/- 9.9D+01)    PS= 3.0D-06
    c_{ 9} = -3.7730700000D+02 (+/- 1.3D+02)    PS= 3.7D-06
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    c_{10} =  9.9406000000D+02 (+/- 1.6D+02)    PS= 4.5D-06
    c_{11} = -5.7203000000D+02 (+/- 4.4D+02)    PS= 5.5D-06
    c_{12} = -9.0700000000D+01 (+/- 3.7D+02)    PS= 6.7D-06
    c_{13} =  1.2350000000D+02 (+/- 1.1D+02)    PS= 8.1D-06
     VMIN =     -1.40500 (+/-    0.839689)      PS= 5.0D-03
       Re =  1.886775000 (+/- 0.000150644)      PS= 2.0D-07
-----------------------------------------------------------------------------
*** CAUTION *** inner wall has inflection at   R= 0.267   V=  5.4870D+07
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