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FORTTRAN Subroutines for Generating
XC(fit) Potential Energy Functions
for H₂-Kr and H₂-Ar

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Chemical Physics Research Report

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This manual describes subroutines `XCfitH2Kr` and `XCfitH2Ar`, which uses the XC(fit) potential function models of Refs.(1,2) to generate values of the three-dimensional potential energy functions for all possible diatom-isotopologue forms of H₂-Kr and H₂-Ar.

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I. General Considerations

Dynamical calculations for an atom-diatom system are generally either classical, simply requiring values of the potential energy function itself for a particular system configuration, or quantum-mechanical coupled-channel calculations which require diagonal and off-diagonal radial channel potential functions associated with various combinations of exit-channel diatom vibration-rotational levels. Alternately, in some classical calculations one might wish to assume an average over the very fast diatom stretching motion. Because of the complexity of the XC(fit) potential function form, some comments regarding how our potential function subroutines³ may be used to accomplish these varying aims are presented here. Note that while the subroutine names and some remarks in the following refer to the H₂-Kr system, the discussion applies equally to the reported XC(fit) potentials for H₂-Ar.¹

The calling sequence for our potential function subroutines has the form

```
SUBROUTINE XCfitH2Kr(Vpot, Rcm, CSttheta, rd, XI, MN1, MN2)
```

in which $R_{cm} = |\vec{R}| = R$ is the length of vector \vec{R} which runs from the centre of mass of the hydrogen diatom to the rare gas atom, $rd = |\vec{r}| = r$ is the diatom bond length, $CSttheta \equiv \cos \theta = \vec{R} \cdot \vec{r} / |\vec{R}| |\vec{r}|$, and $Vpot$ is the value of the potential energy function for the specified system configuration. In order to provide a systematic description of interactions involving heteronuclear hydrogen isotopologues such as HD, we adopt the convention that \vec{r} is defined to point from the heavier to the lighter component of the diatom. Thus, $\theta = 0$ would correspond to the collinear alignment D-H—Kr while $\theta = \pi$ corresponds to H-D—Kr. Finally, MN1 and MN2 are the integer mass numbers identifying the particular isotopic form of diatomic hydrogen, and XI is an array which is defined below.

II. Interactions Involving Homonuclear Hydrogen: H₂, D₂ or T₂

Since the XC(fit) potentials of Refs. 1,2 were determined from data for complexes formed from the homonuclear hydrogen species H₂ and D₂, the Jacobi coordinates (R, θ, r) in terms of which they are defined assume that the diatom centre of mass lies precisely in the middle of the diatom bond. In this coordinate frame, the XC(fit) potentials may be written as finite power series in the diatom stretching coordinate $\xi \equiv (r - r_0)/r_0$,

$$V(R, \theta, \xi) = \sum_{k=0}^{k_{max}} \xi^k V_k(R, \theta) \quad (1)$$

in which the fixed reference distance $r_0 = 1.448739 a_0$ was chosen to be the expectation value of r for H₂ in its ground ro-vibrational level,^{4,5} and $k_{max} = 5$ and 4, respectively, for the H₂-Kr and H₂-Ar systems. The central part of the potential function calculation then involves generating values of the expansion coefficients $V_k(R, \theta)$ for any specified values of the bond-midpoint Jacobi coordinates $R = R_{mid}$ and $\theta = \theta_{mid}$. This is done by the internal subroutine

```
SUBROUTINE Vkh2Kr(R, CSttheta, VK)
```

which returns values of $VK(k) = V_k(R_{mid}, \theta_{mid})$ for $k = 0 - k_{max}$. To calculate a value of the potential energy for a given instantaneous 3-D system configuration of a system involving homonuclear hydrogen (H₂, D₂ or T₂), the main potential subroutine XCfitH2Kr calls internal subroutine Vkh2Kr which returns values of those expansion coefficients, after which the potential function value is generated from the power series sum of Eq. (1). In this case the H-isotope mass numbers MN1 = MN2 and the array XI are dummy variables.

Many dynamical calculations make the approximation that the rapid hydrogen diatom stretching motion may be frozen out or averaged over. This approximation may be invoked simply by specifying a particular value for the bond length r and generating the potential in the manner described above. However, the more correct approach would be to average over that stretching motion for the particular diatom (v, j) state involved in the interaction under consideration. Because of the simple power series form of Eq. (1), values of this vibrationally averaged potential are readily generated as

$$\bar{V}_{v,j}(R, \theta) \equiv \langle v, j | V(R, \theta, \xi) | v, j \rangle = \sum_{k=0}^{k_{\max}} \langle v, j | \xi^k | v, j \rangle V_k(R, \theta) = \sum_{k=0}^{k_{\max}} \langle \xi^k \rangle_{v,j} V_k(R, \theta) \quad (2)$$

The diatom-stretching expectation values $\langle v, j | \xi^k | v, j \rangle = \langle \xi^k \rangle_{v,j}$ appearing in Eq. (2) have been tabulated for all possible vibration-rotation levels of all isotopologues of diatomic hydrogen,³⁻⁵ or may readily be generated from the accurately known potential function for ground-state molecular hydrogen^{3,4} using standard methods.⁶

Potential function subroutine `XCfith2Kr` treats the input value of $r = \text{rd}$ both as a flag and as a bond length. For $\text{rd} \geq 0.0$ the subroutine returns the value of the normal 3-D potential function for the configuration (R, θ, r) , using Eqs. (1) to generate it in the manner described above. However, if the input value of $r = \text{rd}$ is set < 0 , the subroutine assumes that the appropriate expectation values $\langle \xi^k \rangle_{v,j}$ have been provided in the $(k_{\max}+1)$ -element array `XI(k)` for $k=0 - k_{\max}$. The subroutine then uses these quantities to generate the desired vibrationally averaged potential function value from Eq. (2).

Full three-dimensional coupled-channel calculations which take account of all three internal degrees of freedom require the radial channel potential functions

$$V_{v',j'}^{v',j'}(R, \theta) \equiv \langle v', j' | V(R, \theta, \xi) | v', j' \rangle = \sum_{k=0}^{k_{\max}} \langle v', j' | \xi^k | v', j' \rangle V_k(R, \theta) = \sum_{k=0}^{k_{\max}} \langle \xi^k \rangle_{v',j'}^{v',j'} V_k(R, \theta) \quad (3)$$

The requisite diagonal and off-diagonal matrix elements of powers of the diatom stretching coordinate $\langle \xi^k \rangle_{v',j'}^{v',j'} \equiv \langle v', j' | \xi^k | v', j' \rangle$ may be readily generated from the accurately known potential function for ground-state molecular hydrogen^{3,4} using standard methods.⁶ For this type of application, a user may wish to modify subroutine `XCfith2Kr` to import all required sets of $\langle v', j' | \xi^k | v', j' \rangle$ matrix elements and perform the appropriate sums at the same time, so as to avoid repetitious redundant evaluations of the $V_k(R, \theta)$ values.

For the user's convenience, matrix elements of this type for a range of vibration-rotation levels of the six isotopologues of diatomic hydrogen are tabulated in the Appendix below.

III. Kr with Heteronuclear Hydrogen: HD, HT or DT

For the heteronuclear species HD, HT or DT, dynamical calculations require the use of Jacobi coordinates based on the centre of mass of the diatom, which in this case is *not* located at the bond-midpoint (see Fig. 1). As discussed in Ref. 7, the relationship between the bond-midpoint coordinates $(R_{\text{mid}}, \theta_{\text{mid}}, r)$ in terms of which the potential is defined, and the centre-of-mass coordinates $(R_{\text{cm}}, \theta_{\text{cm}}, r)$ used for dynamical calculations, is given by the expressions

$$R_{\text{mid}} = R_{\text{cm}} [1 + 2(\delta/R_{\text{cm}}) \cos \theta_{\text{cm}} + (\delta/R_{\text{cm}})^2]^{1/2} \quad (4)$$

$$\begin{aligned} \cos \theta_{\text{mid}} &= (\cos \theta_{\text{cm}} + \delta/R_{\text{cm}}) / [1 + 2(\delta/R_{\text{cm}}) \cos \theta_{\text{cm}} + (\delta/R_{\text{cm}})^2]^{1/2} \\ &= (R_{\text{cm}} \cos \theta_{\text{cm}} + \delta) / R_{\text{mid}} \end{aligned} \quad (5)$$

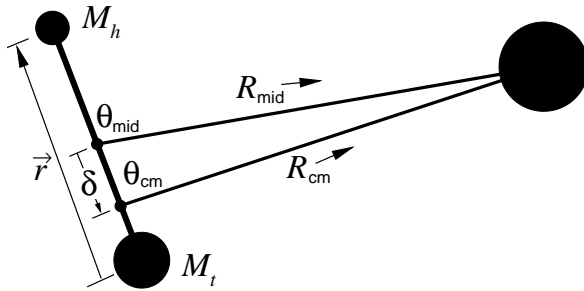


Fig. 1. Relation between centre-of-mass ($R_{\text{cm}}, \theta_{\text{cm}}$) and bond-midpoint ($R_{\text{mid}}, \theta_{\text{mid}}$) Jacobi coordinates for an atom-diatom system.

in which the displacement of the diatom centre-of-mass from the bond-midpoint is (see Fig. 1)

$$\delta = \frac{M_h - M_t}{2(M_h + M_t)} r = -\frac{|M_h - M_t|}{2(M_h + M_t)} r_0 (\xi + 1) \quad (6)$$

where M_h and M_t are, respectively, the masses of the atoms at the head and tail of the diatomic bond vector \vec{r} . The sign of δ is determined by the convention chosen for the direction of \vec{r} (typically, $M_h \leq M_t$), and the angle θ is determined by combining the definition of \vec{r} with the convention that \vec{R} points from the centre of mass of the diatom to the atom: $\cos \theta = \vec{R} \cdot \vec{r} / |\vec{R}| |\vec{r}|$. For $M_h \neq M_t$, if one only requires values of the potential function at a particular 3-D system configuration, the input parameter $\text{rd} = r$ is > 0 and subroutine `XCfitH2Kr` simply uses Eqs. (4)–(6) to determine the values of R_{mid} and $\cos \theta_{\text{mid}}$ defined by the input (centre-of-mass) values of R_{cm} and $\cos \theta_{\text{cm}}$. For those R_{mid} and $\cos \theta_{\text{mid}}$ values, `VkH2Kr` returns values of $V_k(R_{\text{mid}}, \theta_{\text{mid}})$ which on substitution into Eq. (1) yield the desired potential function value. On the other hand, if one requires vibrationally averaged functions of the form of Eq. (2) or (3), the problem is more complicated.

It is important to realize that for heteronuclear hydrogen ($M_h \neq M_t$), the transformation of Eqs. (4)–(6) must be performed *before* any diatom vibrational averaging is performed. However, the power series expansion of Eq. (1) is defined in terms of the coordinates $(R, \theta) = (R_{\text{mid}}, \theta_{\text{mid}})$, and the potential function obtained on converting to the centre-of-mass coordinates $(R_{\text{cm}}, \theta_{\text{cm}})$ is no longer a simple finite power series in ξ . This means that Eqs. (2) or (3) cannot be used to define the radial functions required for coupled-channel calculations. Rather, the functions $\bar{V}_{v,j}(R_{\text{cm}}, \theta_{\text{cm}}) \equiv \langle v, j | V(R_{\text{cm}}, \theta_{\text{cm}}, \xi) | v, j \rangle$ or $V_{v,j}^{v',j'}(R_{\text{cm}}, \theta_{\text{cm}}) \equiv \langle v', j' | V(R_{\text{cm}}, \theta_{\text{cm}}, \xi) | v, j \rangle$ would in principle have to be evaluated numerically for each required combination of $(R_{\text{cm}}, \theta_{\text{cm}})$ values, using the radial wavefunction(s) $\varphi_{v,j}(r) = |v, j\rangle$ for the diatom vibration-rotation level(s) in question. This “correct” procedure for taking account of the effect of an isotopic centre-of-mass displacement on the diatom vibrational averaging for an atom–diatom (or diatom–diatom) potential energy surface is straightforward in principle, since it involves the evaluation of one-dimensional radial overlap integrals generated from known potentials⁴ using standard methods.⁶ However, the fact that this averaging must be performed for every required combination of $(R_{\text{cm}}, \theta_{\text{cm}})$ values would make it somewhat tedious to implement.

Fortunately, Ref. 7 showed that the introduction of an orthogonal polynomial representation for the ξ -dependence of the potential energy function can greatly simplify the problem of generating the vibrationally averaged functions required for coupled-channel calculations. However, to our knowledge, that approach has not been tested previously.

For any particular system geometry, the value of the potential energy function is clearly the same, no matter which coordinate system is used. As a result, with the centre-of-mass and bond-midpoint

coordinates related by Eqs. (4) – (6), we can write

$$U(R_{\text{cm}}, \theta_{\text{cm}}, \xi) = V(R_{\text{mid}}, \theta_{\text{mid}}, \xi) = \sum_{k=0}^{k_{\text{max}}} \xi^k V_k(R_{\text{mid}}, \theta_{\text{mid}}) \quad (7)$$

$$= \sum_j T_j(\xi) S_j(R_{\text{cm}}, \theta_{\text{cm}}) \quad (8)$$

in which $\{T_j(\xi)\}$ is a set of orthonormal polynomial functions of ξ defined on the interval $[a, b]$ with weight function $w(\xi)$. This in turn implies that

$$S_j(R_{\text{cm}}, \theta_{\text{cm}}) = \int_a^b w(\xi) T_j(\xi) U(R_{\text{cm}}, \theta_{\text{cm}}, \xi) d\xi = \sum_{i=0}^{k'_{\text{max}}} w_i T_j(\xi_i) U(R_{\text{cm}}, \theta_{\text{cm}}, \xi_i) \quad (9)$$

in which ξ_i and w_i are the $(k'_{\text{max}} + 1)$ points and weights associated with a quadrature scheme based on the orthogonal polynomials $\{T_j(\xi)\}$. If a finite expansion in terms of the $S_j(R_{\text{cm}}, \theta_{\text{cm}})$ functions yields an accurate description of the potential, re-writing the polynomials $T_j(\xi)$ as simple power series in ξ and collecting coefficients of the same order would allow us to write

$$U(R_{\text{cm}}, \theta_{\text{cm}}, \xi) = \sum_{k=0}^{k'_{\text{max}}} \xi^k U_k(R_{\text{cm}}, \theta_{\text{cm}}) \quad (10)$$

in which $U_k(R_{\text{cm}}, \theta_{\text{cm}})$ are simple linear combinations of the $S_j(R_{\text{cm}}, \theta_{\text{cm}})$ values determined from the quadrature procedure of Eq. (9). With the potential now re-expanded in the centre-of-mass coordinates as a simple power series in ξ , tabulated sets of values of $\langle \xi^k \rangle_{v,j}^{v',j'}$ values may be used to generate the vibrational averaged potential in the usual manner

$$U_{v,j}^{v',j'}(R_{\text{cm}}, \theta_{\text{cm}}) \equiv \langle v', j' | U(R_{\text{cm}}, \theta_{\text{cm}}, \xi) | v, j \rangle = \sum_{k=0}^{k'_{\text{max}}} \langle \xi^k \rangle_{v,j}^{v',j'} U_k(R_{\text{cm}}, \theta_{\text{cm}}) \quad (11)$$

For the above approach to be practically useful, it is essential that only a modest number of orthogonal polynomials $T_j(\xi)$ be required in the expansion of Eq. (8). We have examined the convergence of this approach for the $\text{H}_2\text{-Kr}$ system using normalized Legendre polynomials, for which $[a, b] = [-1, +1]$ and $w(\xi) = 1$. For the cases of HD-Kr (for which $\delta/r = 0.166496$) and HT-Kr (for which $\delta/r = 0.249539$), the potential function for a range of system configurations $(R_{\text{cm}}, \theta_{\text{cm}}, \xi)$ was calculated in two ways: (i) using the exact transformation of Eqs. (4) – (6) in Eq. (1), and (ii) using the finite expansion of Eq. (10) with various choices of expansion order k'_{max} . While Method (i) is exact, it does not provide the transformed potential in a form which allows the vibrational averaging to be performed in the simple manner of Eq. (11), so we wish to test the efficacy of Method (ii).

For various choices of the expansion order k'_{max} and a range of values of R , the root mean square of the discrepancies associated with using Method (ii), $\overline{\text{err}}_{\text{rms}}$, were calculated by averaging over ξ (on the interval $[-0.9, +0.9]$) and over $\cos \theta_{\text{cm}} \in [-1, +1]$. The results are plotted in the upper segment of Fig. 2; results for HD-Kr are shown as solid curves and those for HT-Kr as dotted curves. It is clear that when the order k'_{max} of the orthogonal polynomial expansion is the same as that ($k_{\text{max}} = 5$) of the $V_k(R_{\text{mid}}, \theta_{\text{mid}})$ expansion in terms of which the potential is defined, the approximate Method (ii) yields significant discrepancies. However, as $k'_{\text{max}} - k_{\text{max}}$ increases those discrepancies rapidly become negligibly small, especially in the Van der Waals potential well and low-energy repulsive wall region.

In view of the above, the procedure of Method (ii) is implemented by subroutine `XCfitH2Kr` whenever the input parameters `MN1` \neq `MN2` indicate that the species considered involves heteronuclear hydrogen, and the input value of `rd` $<$ 0 signals that vibrationally averaged potential function values are desired. In view of the convergence studies illustrated by Fig. 2, the resulting expansion in $U_k(R_{\text{cm}}, \theta_{\text{cm}})$ is of order $k'_{\text{max}} = 8$, so for the H₂-Kr system the input array `XI(k)` should be dimensioned externally for $k = 0 - 8$.

It is important to remember that the full physical domain of the diatom stretching expansion variable, $[-1, \infty)$, is somewhat wider than the domain $[-1, +1]$ on which the Legendre polynomials we use for $\{T_j(\xi)\}$ are defined. However, the spectroscopic data used to determine the XC(fit) potential only corresponds to diatomic hydrogen bond lengths spanning the interval $(-0.26, +0.33)$, defined as the distance between the inner and outer classical turning points for H₂($v = 1, j = 2$),⁸ while the *ab initio* points defining the XC-type model potential span the interval $\xi \in [-0.24, +0.31]$. Since the present XC(fit) model potential function does not attempt to incorporate a reliable means of extrapolating beyond this region, it is clear that the present potential function may not behave realistically outside this ξ interval, and hence should only be used with great care there. In practice, therefore, the limitations associated with the $[-1, +1]$ domain of Legendre polynomials or the $\xi \in [-0.9, +0.9]$ of the tests associated with Fig. 2 introduce no significant errors.

IV. Subroutine Calling Sequence & Parameter Definitions

SUBROUTINE `XCfitH2Kr(Vpot, Rcm, CStheta, rd, XI, MN1, MN2)`

- `Vpot` is the (REAL*8) value returned for the potential energy at the specified system configuration, in atomic units (hartees).
- `Rcm` is the (REAL*8) distance from the diatom centre of mass to the Kr atom *textttRcm* = $R \equiv R_{\text{cm}}$, in atomic units (bohr).
- `rd` is the (REAL*8) diatomic hydrogen bond length $r \equiv \text{rd}$, in atomic units (bohr).
- `CStheta` is the (REAL*8) cosine of the angle between $\vec{R} = \vec{R}_{\text{cm}}$ and \vec{r} , where \vec{R} points from the diatom centre of mass to the Kr atom and \vec{r} points from the heavier to the lighter hydrogen atom isotope (for `MN1`=`MN2` the direction of \vec{r} is, of course, irrelevant).
- `XI` For `rd` $<$ 0, this is the array of (REAL*8) values of $\overline{\xi_{v,j}^k}$ or $(\xi^k)_{v,j}^{v',j'}$ (for $k = 0 - k_{\text{max}}$ or k'_{max}) required by Eqs. (2), (3) or (11). For `rd` $>$ 0 it is a dummy array ignored by the subroutine.
- `MN1` & `MN2` are the (INTEGER*4) atomic mass numbers of the atomic isotopes of hydrogen forming the diatom.

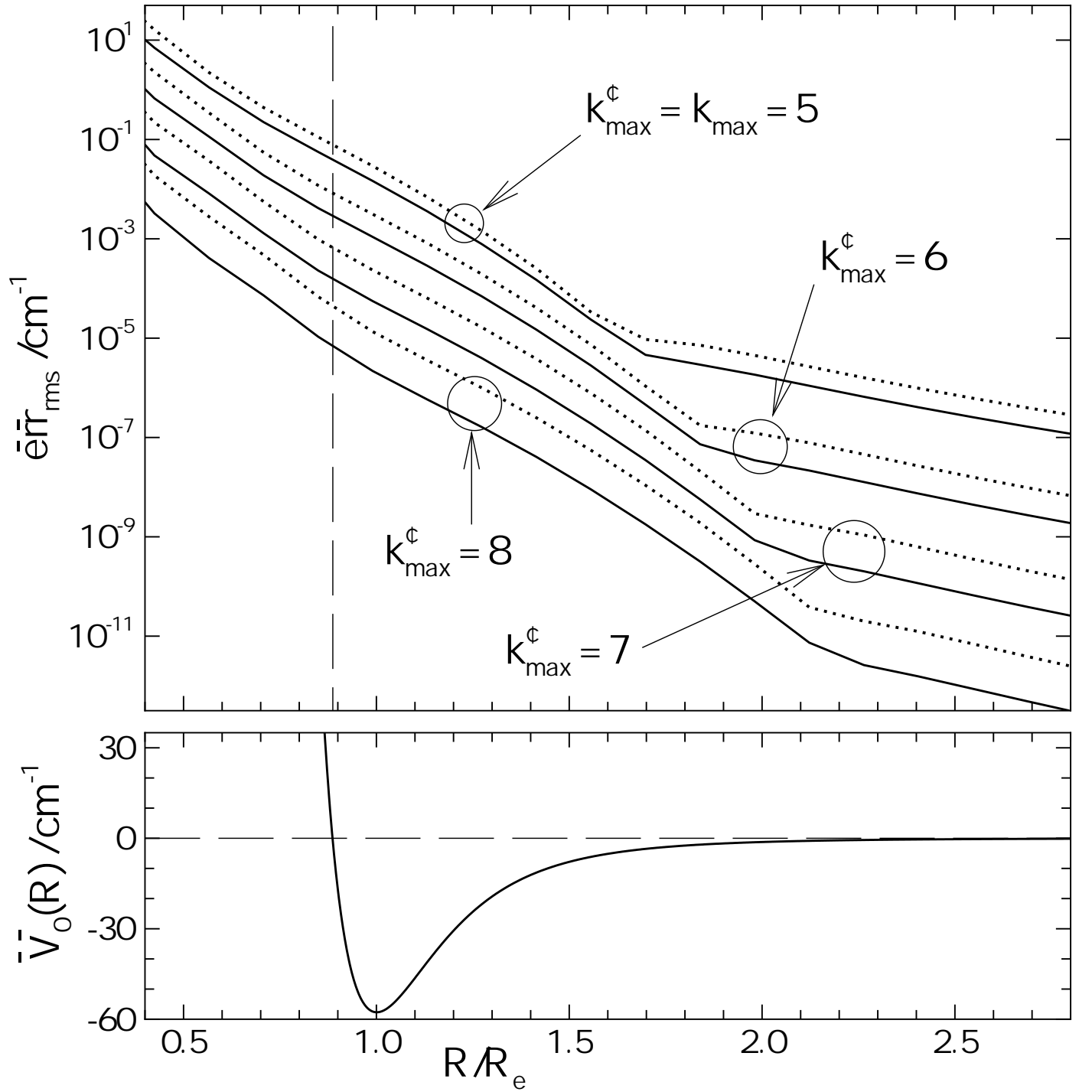


Fig. 2. *Upper:* Root mean square discrepancies $\bar{\epsilon}_{\text{rms}}$ associated with use of the truncated transformation of Eq.(10) for HD-Kr (solid curves) and HT-Kr (dotted curves), for various choices of the final expansion order k_{max}^{ζ} . *Lower:* isotropic $\xi = 0$ potential for HD-Kr on the same radial scale.

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- ³ See the “Potential Functions” link at <http://leroy.uwaterloo.ca>.
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- ⁷ W.-K. Liu, J. E. Grabenstetter, R. J. Le Roy, and F. McCourt, *J. Chem. Phys.* **68**, 5028 (1978).
- ⁸ A more meaningful estimate of the range of ξ values to which the data are most sensitive would probably be the much narrower interval $[-0.0098, +0.0714]$ defined by the average values $\bar{\xi}_{v,j} = \langle v, j | \xi | v, j \rangle$ associated with the H₂ and D₂ levels forming the observed bimer complexes.

Appendix: Subroutine Listing

Expectation values and matrix elements of powers of $XI = \xi = (r - r_0)/r_0$ for $r_0 = 1.448739$ bohr.

Kolos/Le Roy-Schwartz potential for ground state H2: Get expectation values

v'	J'	v''	J''	FREQ	$\langle v', J' XI^{**k} v'', J'' \rangle$	for k=0	to	MORDR= 5	
0	0	0	0	1.00000000	-0.00000023	0.01344075	0.00029486	0.00055228	0.00004018
0	1	0	1	1.00000000	0.00150453	0.01346204	0.00035631	0.00055582	0.00004450
0	2	0	0	0.99981095	0.00225187	0.01347177	0.00038685	0.00055761	0.00004666
0	2	0	2	1.00000000	0.00450607	0.01351816	0.00047950	0.00056401	0.00005325
0	3	0	1	0.99948010	0.00524217	0.01352774	0.00050969	0.00056596	0.00005541
0	3	0	3	1.00000000	0.00898877	0.01363589	0.00066527	0.00057910	0.00006668
0	4	0	2	0.99899597	0.00970482	0.01364507	0.00069489	0.00058128	0.00006883
0	4	0	4	1.00000000	0.01493014	0.01385453	0.00091569	0.00060447	0.00008525
1	0	0	0	0.00000000	0.11488352	0.00507707	0.00493553	0.00056822	0.00037517
1	0	0	2	0.01914028	0.11557406	0.00589122	0.00501788	0.00062913	0.00038656
1	0	1	0	1.00000000	0.06670045	0.04538130	0.00704041	0.00370591	0.00093026
1	1	0	1	0.00000000	0.11496427	0.00543137	0.00496991	0.00059982	0.00038094
1	1	0	3	0.03178904	0.11618515	0.00679133	0.00511638	0.00070266	0.00040111
1	1	1	1	1.00000000	0.06826830	0.04565174	0.00726303	0.00376014	0.00096202
1	2	0	0	-0.01904002	0.11439401	0.00532336	0.00495562	0.00060197	0.00038112
1	2	0	2	0.00000000	0.11512578	0.00613961	0.00504350	0.00066371	0.00039323
1	2	0	4	0.04423693	0.11699597	0.00805183	0.00527002	0.00081107	0.00042430
1	2	1	0	0.99944467	0.06902406	0.04577392	0.00737230	0.00378666	0.00097776
1	2	1	2	1.00000000	0.07139607	0.04620638	0.00771190	0.00387278	0.00102694
1	3	0	1	-0.03151358	0.11403449	0.00583469	0.00500408	0.00065606	0.00039133
1	3	0	3	0.00000000	0.11536810	0.00720115	0.00516588	0.00076141	0.00041354
1	3	0	5	0.05639743	0.11805661	0.00967746	0.00549569	0.00095767	0.00045873
1	3	1	1	0.99847284	0.07209690	0.04630671	0.00781762	0.00389866	0.00104255
1	3	1	3	1.00000000	0.07606825	0.04707247	0.00839455	0.00405232	0.00112795
1	4	0	2	-0.04370571	0.11360532	0.00668832	0.00509474	0.00074277	0.00040906
1	4	0	4	0.00000000	0.11569128	0.00861518	0.00535126	0.00089557	0.00044423
1	4	0	6	0.06819561	0.11941218	0.01167526	0.00581496	0.00114757	0.00050801
1	4	1	2	0.99705088	0.07667757	0.04713943	0.00849425	0.00407708	0.00114330
1	4	1	4	1.00000000	0.08226259	0.04829010	0.00932307	0.00431168	0.00126986

Kolos/Le Roy-Schwartz potential for ground state D2: Get expectation values

v'	J'	v''	J''	FREQ	$\langle v', J' XI^{**k} v'', J'' \rangle$	for k=0	to	MORDR= 5	
0	0	0	0	1.00000000	-0.00978972	0.00949220	-0.00013214	0.00026816	0.00000064
0	1	0	1	1.00000000	-0.00904092	0.00948470	-0.00011084	0.00026817	0.00000166
0	2	0	0	0.99993291	-0.00866709	0.00948075	-0.00010022	0.00026818	0.00000216
0	2	0	2	1.00000000	-0.00754533	0.00947311	-0.00006831	0.00026839	0.00000368
0	3	0	1	0.99981456	-0.00717300	0.00946918	-0.00005775	0.00026843	0.00000418
0	3	0	3	1.00000000	-0.00530692	0.00946418	-0.00000461	0.00026920	0.00000673
0	4	0	2	0.99963926	-0.00493747	0.00946027	0.00000586	0.00026929	0.00000723
0	4	0	4	1.00000000	-0.00233154	0.00946795	0.00008024	0.00027117	0.00001082

Kolos/Le Roy-Schwartz potential for ground state T2: Get expectation values

v'	J'	v''	J''	FREQ	$\langle v', J' XI^{**k} v'', J'' \rangle$	for k=0	to	MORDR= 5	
0	0	0	0	1.00000000	-0.01407250	0.00783729	-0.00022942	0.00018070	-0.00000510
0	1	0	1	1.00000000	-0.01357367	0.00782707	-0.00021777	0.00018042	-0.00000465
0	2	0	0	0.99996336	-0.01332428	0.00782188	-0.00021196	0.00018028	-0.00000442
0	2	0	2	1.00000000	-0.01257690	0.00780816	-0.00019453	0.00017993	-0.00000375
0	3	0	1	0.99989855	-0.01232775	0.00780297	-0.00018874	0.00017981	-0.00000353
0	3	0	3	1.00000000	-0.01108398	0.00778357	-0.00015978	0.00017937	-0.00000241
0	4	0	2	0.99980216	-0.01083543	0.00777840	-0.00015402	0.00017926	-0.00000219
0	4	0	4	1.00000000	-0.00909754	0.00775780	-0.00011361	0.00017895	-0.00000063

Kolos/Le Roy-Schwartz potential for ground state HD: Get expectation values

v'	J'	v''	J''	FREQ	$\langle v', J' XI^{**k} v'', J'' \rangle$	for $k=0$	to	MORDR= 8	
0	0	0	0	1.00000000	-0.00449500	0.01159911	0.00006306	0.00040629	0.00001654
				0.00002436	0.00000244	0.00000214			
0	1	0	1	1.00000000	-0.00336895	0.01160251	0.00010248	0.00040752	0.00001888
				0.00002456	0.00000264	0.00000217			
0	2	0	0	0.99987699	-0.00280818	0.01160373	0.00012211	0.00040816	0.00002005
				0.00002466	0.00000274	0.00000219			
0	2	0	2	1.00000000	-0.00112136	0.01161694	0.00018135	0.00041054	0.00002360
				0.00002501	0.00000305	0.00000224			
0	3	0	1	0.99966086	-0.00056579	0.01161813	0.00020082	0.00041125	0.00002477
				0.00002512	0.00000316	0.00000226			
0	3	0	3	1.00000000	0.00223890	0.01165753	0.00029986	0.00041640	0.00003077
				0.00002580	0.00000369	0.00000236			
0	4	0	2	0.99934267	0.00278504	0.01165864	0.00031905	0.00041723	0.00003194
				0.00002593	0.00000379	0.00000238			
0	4	0	4	1.00000000	0.00669895	0.01174660	0.00045859	0.00042671	0.00004054
				0.00002709	0.00000458	0.00000255			
1	0	0	0	0.00000000	0.10676343	0.00310889	0.00386946	0.00032015	0.00024454
				0.00003814	0.00002291	0.00000549			
1	0	0	2	0.01546806	0.10717239	0.00366746	0.00391081	0.00035506	0.00024952
				0.00004136	0.00002364	0.00000589			
1	0	1	0	1.00000000	0.05297054	0.03799071	0.00466102	0.00255433	0.00052268
				0.00025605	0.00007366	0.00003499			
1	1	0	1	0.00000000	0.10681960	0.00335391	0.00388663	0.00033842	0.00024706
				0.00003994	0.00002331	0.00000572			
1	1	0	3	0.02571298	0.10754402	0.00428602	0.00396028	0.00039710	0.00025588
				0.00004540	0.00002458	0.00000642			
1	1	1	1	1.00000000	0.05413672	0.03815333	0.00479839	0.00258137	0.00053871
				0.00026051	0.00007600	0.00003582			
1	2	0	0	-0.01540720	0.10649760	0.00328433	0.00387926	0.00033998	0.00024713
				0.00004031	0.00002338	0.00000578			
1	2	0	2	0.00000000	0.10693196	0.00384374	0.00392345	0.00037521	0.00025243
				0.00004359	0.00002415	0.00000620			
1	2	0	4	0.03583592	0.10804500	0.00515198	0.00403762	0.00045865	0.00026597
				0.00005149	0.00002610	0.00000722			
1	2	1	0	0.99963772	0.05470575	0.03822763	0.00486621	0.00259465	0.00054667
				0.00026273	0.00007717	0.00003624			
1	2	1	2	1.00000000	0.05646457	0.03848628	0.00507476	0.00263738	0.00057128
				0.00026978	0.00008081	0.00003756			
1	3	0	1	-0.02554531	0.10630638	0.00364325	0.00390337	0.00037145	0.00025160
				0.00004359	0.00002413	0.00000622			
1	3	0	3	0.00000000	0.10710051	0.00457804	0.00398492	0.00043110	0.00026128
				0.00004924	0.00002552	0.00000696			
1	3	0	5	0.04578259	0.10870684	0.00626728	0.00415153	0.00054096	0.00028089
				0.00005988	0.00002833	0.00000837			
1	3	1	1	0.99900124	0.05700609	0.03854891	0.00514107	0.00265041	0.00057920
				0.00027204	0.00008199	0.00003799			
1	3	1	3	1.00000000	0.05994528	0.03900488	0.00549347	0.00272622	0.00062147
				0.00028459	0.00008834	0.00004036			
1	4	0	2	-0.03551129	0.10607801	0.00424192	0.00394883	0.00042157	0.00025935
				0.00004881	0.00002540	0.00000694			
1	4	0	4	0.00000000	0.10732528	0.00555630	0.00407842	0.00050709	0.00027461
				0.00005710	0.00002758	0.00000803			
1	4	0	6	0.05550408	0.10955866	0.00763491	0.00431316	0.00064597	0.00030212
				0.00007098	0.00003153	0.00000993			
1	4	1	2	0.99806425	0.06044083	0.03904982	0.00555724	0.00273883	0.00062931
				0.00028688	0.00008954	0.00004081			
1	4	1	4	1.00000000	0.06456601	0.03973176	0.00605988	0.00285378	0.00069107
				0.00030607	0.00009903	0.00004446			

Kolos/Le Roy-Schwartz potential for ground state HT: Get expectation values

v'	J'	v''	J''	FREQ	<v',J' XI**k v'',J''>	for k=0	to	MORDR= 8
0	0	0	0	1.00000000	-0.00614569	0.01093501	-0.00000677	0.00035946 0.00001035
				0.00002012	0.00000164	0.00000164		
0	1	0	1	1.00000000	-0.00514529	0.01093396	0.00002617	0.00036018 0.00001218
				0.00002024	0.00000179	0.00000166		
0	2	0	0	0.99989680	-0.00464666	0.01093306	0.00004258	0.00036055 0.00001310
				0.00002031	0.00000186	0.00000167		
0	2	0	2	1.00000000	-0.00314805	0.01093789	0.00009204	0.00036201 0.00001587
				0.00002053	0.00000209	0.00000170		
0	3	0	1	0.99971525	-0.00265315	0.01093699	0.00010833	0.00036244 0.00001678
				0.00002060	0.00000216	0.00000171		
0	3	0	3	1.00000000	-0.00016101	0.01095878	0.00019088	0.00036575 0.00002144
				0.00002104	0.00000254	0.00000178		
0	4	0	2	0.99944742	0.00032708	0.01095786	0.00020698	0.00036628 0.00002235
				0.00002112	0.00000262	0.00000179		
0	4	0	4	1.00000000	0.00380558	0.01101435	0.00032302	0.00037260 0.00002900
				0.00002188	0.00000318	0.00000190		

Kolos/Le Roy-Schwartz potential for ground state DT: Get expectation values

v'	J'	v''	J''	FREQ	<v',J' XI**k v'',J''>	for k=0	to	MORDR= 8
0	0	0	0	1.00000000	-0.01182686	0.00869953	-0.00018511	0.00022400 -0.00000275
				0.00000963	0.00000015	0.00000059		
0	1	0	1	1.00000000	-0.01120315	0.00869018	-0.00016890	0.00022382 -0.00000205
				0.00000964	0.00000019	0.00000059		
0	2	0	0	0.99994889	-0.01089154	0.00868536	-0.00016081	0.00022373 -0.00000170
				0.00000964	0.00000021	0.00000059		
0	2	0	2	1.00000000	-0.00995713	0.00867384	-0.00013653	0.00022358 -0.00000065
				0.00000966	0.00000028	0.00000060		
0	3	0	1	0.99985861	-0.00964628	0.00866904	-0.00012848	0.00022351 -0.00000030
				0.00000967	0.00000030	0.00000060		
0	3	0	3	1.00000000	-0.00809157	0.00865521	-0.00008811	0.00022352 0.00000145
				0.00000972	0.00000041	0.00000061		
0	4	0	2	0.99972461	-0.00778227	0.00865044	-0.00008011	0.00022348 0.00000179
				0.00000973	0.00000043	0.00000061		
0	4	0	4	1.00000000	-0.00561057	0.00864130	-0.00002370	0.00022401 0.00000425
				0.00000983	0.00000058	0.00000062		