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Parametrization of the hybrid potential for pairs of neutral atoms

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Abstract. The hybrid form is a combination of the Rydberg potential and the London inverse-sixth-power energy. It is accurate at all relevant distance scales and simple enough for use in all-atom simulations of biomolecules. One may compute the parameters of the hybrid potential for the ground state of a pair of neutral atoms from their internuclear separation, the depth and curvature of their potential at its minimum, and from their van der Waals coefficient of dispersion C_6.

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1 The hybrid form

Commercial molecular-modeling codes use pair potentials chosen more for speed than for accuracy. They use the harmonic potential

$$V_h(r) = -E_0 + \frac{k}{2}\,(r - r_0)^2 \qquad (1)$$

for covalently bonded pairs of neutral atoms and the Lennard-Jones potential [1]

$$V_{LJ}(r) = E_0 \left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6} \right] \qquad (2)$$

for unbonded pairs. The recently introduced hybrid potential [2]

$$V(r) = a e^{-b\,r}\,(1 - c\,r) - \frac{C_6}{r^6 + d\,r^{-6}} \qquad (3)$$

is nearly as fast and much more accurate. It is fast enough for use in all-atom simulations of biomolecules and accurate at all biologically relevant distance scales when its parameters are suitably chosen. How to choose them is the focus of this paper. Formulas are derived for a, b, c, and d in terms of the internuclear separation r_0, the depth E_0 and curvature k of the potential at its minimum, and the van der Waals coefficient C_6 of the pair. The hybrid potential therefore is applicable to pairs of neutral atoms for which no empirical potential is available. Its eventual incorporation into TINKER [3], Amber [4], and other such codes is a goal of this work.

The hybrid potential is a combination of the Rydberg formula used in spectroscopy and the London formula for pairs of atoms. The terms involving a, b, and c were proposed by Rydberg to incorporate spectroscopic data, but were largely ignored until recently. The constant C_6 is the coefficient of the London tail. The new term $d\,r^{-6}$ cures the London singularity. As $r \to 0$, $V(r) \to a$, finite; as $r \to \infty$, $V(r)$ approaches the London term, $V(r) \to -C_6/r^6$. In a perturbative analysis [5], the a, b, c terms arise in first order, and the C_6 term in second order.

When fitted to spectroscopically determined potentials for the ground states of H_2, N_2, O_2, Ar–Ar, and Kr–Kr, the hybrid form is four orders of magnitude more accurate than the harmonic and Lennard-Jones potentials and five times more accurate than the Morse [6], Varnshi [7], and Hulburt-Hirschfelder [8] potentials [2]. It also yields accurate second virial coefficients and heats of vaporization [2]. Its simplicity recommends it as a teaching tool and as a practical form for computation.

How does one find the parameters a, b, c, and d when an empirical potential is not available? For many pairs of neutral atoms, spectroscopists have measured the internuclear separation r_0, the well depth $E_0 = |V(r_0)|$ and curvature $k = V''(r_0)$ at the minimum of the potential, and the London coefficient C_6. These input parameters are discussed in Section 2 with an emphasis on the curvature k and its relation to the vibrational frequency of the ground state and to the energy D_0 needed to dissociate the ground state. Section 3 develops a rule of thumb for the parameter d to which the hybrid form is relatively insensitive. Section 4 derives formulas for the hybrid parameters a, b, and c in terms of r_0, E_0, k, C_6, and d and plots the resulting hybrid potentials for the 11 pairs H_2, N_2, O_2, NO, OH, I_2, Li_2, Na_2, K_2, Ar–Ar, and Kr–Kr.

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2 Input parameters

In addition to the well depth $E_0 = |V(r_0)|$, the internuclear separation r_0 at the minimum, and the London or van der Waals coefficient C_6, the curvature $k = V''(r_0)$ of the potential at r_0 often is available either directly or in the guise of the energy of dissociation D_0.

Near r_0, the motion of the internuclear separation r is described by the Lagrangian

$$L = \frac{1}{2}\,\mu\,\dot{r}^2 - \frac{1}{2}\,k\,(r - r_0)^2 \tag{4}$$

in which $\mu = m_1 m_2/(m_1 + m_2)$ is the reduced mass of the two atoms of mass m_1 and m_2. To lowest order in $r - r_0$, the ground state then has energy

$$E_g = \frac{1}{2}\hbar\omega - E_0 \tag{5}$$

in which ω is the (angular) vibrational frequency of the ground state. The curvature k is related to ω by

$$k = \mu\omega^2. \tag{6}$$

In the chemical-physics literature, the depth E_0 and separation r_0 are labeled D_e and r_e, and the angular frequency $\omega = 2\pi\nu$ is expressed as a frequency ω_e in inverse centimeters: $\omega_e = \omega/(2\pi c)$ where c is the speed of light. In these terms and in cgs units, $k = 4\pi^2 c^2 \mu \omega_e^2$. The energy of dissociation is $D_0 = -E_g = E_0 - \hbar\omega/2$, and so the curvature $k = V''(r_0)$ is related to the difference between it and the well depth $E_0 = D_e$ by

$$k = 4\mu(E_0 - D_0)^2/\hbar^2 = 4\mu(D_e - D_0)^2/\hbar^2. \tag{7}$$

The values of the input parameters are listed in Table 1. The internuclear separation r_0 at the minimum of the potential well $V(r)$ and its depth $E_0 = V(r_0)$ are from [9] for H_2, NO, OH, and I_2, and from [10] for O_2. The curvature $k = V''(r_0)$ of the potential at its minimum is from [9] for H_2, O_2, NO, OH, and I_2. The van der Waals coefficient C_6 is from [11] for H_2; from [12] for NO; from [13] for OH; and from [14] for O_2, I_2, Ar–Ar, and Kr–Kr. The values of r_0, E_0, and k for Ar–Ar and Kr–Kr respectively are from [15, 16]. The values of r_0, E_0, k, and C_6 for N_2, Li_2, Na_2, and K_2 respectively are from [14,17–22].

3 A rule of thumb

The d-term of the hybrid form is a trick to avoid the $1/r^6$ singularity of the London term. It has no other justification. Luckily, the quality of the fit is not sensitive to the precise value of the parameter d, and so we need only a good rule of thumb for that parameter. To develop an approximate formula that estimates this parameter, we first find values of a, b, c, and d that provide good fits of the hybrid form $V(r)$ to empirical potentials for the 11 pairs H_2, N_2, O_2, NO, OH, I_2, Li_2, Na_2, K_2, Ar–Ar, and Kr–Kr of neutral atoms.

Table 1. The depth $E_0 = V(r_0)$ of the potential well $V(r)$, the internuclear separation r_0 and the curvature $k = V''(r_0)$ at the minimum $r = r_0$, and the van der Waals coefficient C_6 for 11 pairs of neutral atoms.

	E_0 (eV)	r_0 (Å)	k (eV Å^{-2})	C_6 (eV Å^6)
H_2	4.7467	0.7417	35.8861	3.88338
$^{14}N_2$	9.8995	1.09768^a	143.2245	14.382
O_2	5.2136	1.2075	73.4726	9.3215
NO	6.609	1.1590	99.5676	11.245
OH	4.624	0.9707	48.6196	6.854
I_2	1.5571	2.668	10.7378	230.05
$^7Li_2$	1.0559	2.6730	1.5752	829.33
Na_2	0.74664	3.0786	1.0706	929.76
K_2	0.55183	3.9243	0.61375	2328.6
Ar_2	0.01234	3.757	0.0691	38.4213
Kr_2	0.01735	4.017	0.0896	77.6791

[a] Extra digits are included to avoid round-off errors.

Table 2. The values of the coefficients a, b, c, and d that fit the hybrid potential $V(r)$ (Eq. (3)) to RKR data for H_2, N_2, O_2, NO, OH, I_2, Li_2, Na_2, and K_2 and to empirical potentials for Ar–Ar and Kr–Kr while respecting equations (15, 17, 19, 20). The rms errors $\Delta V(r)$ for $r \geq f\,r_0$ are also listed.

	a (eV)	b (Å^{-1})	c (Å^{-1})	d (Å^{12})	f, ΔV (eV)
H_2	47.796	2.9632	2.5406	12.2	0.68, 0.086
N_2	3752.644	4.3533	1.1777	34.8	0.81, 0.088
O_2	2901.580	4.2173	1.0510	59.8	0.84, 0.039
NO	3809.497	4.4196	1.0943	47.0	0.81, 0.077
OH	377.804	3.6909	1.4668	32.5	0.80, 0.023
I_2	14361.15	2.8013	0.4351	2.08e5^b	0.88, 0.039
Li_2	199.481	1.6200	0.5101	2.85e6	0.86, 0.016
Na_2	231.900	1.5311	0.4292	9.40e6	0.81, 0.009
K_2	325.051	1.3409	0.3269	9.94e7	0.85, 0.008
Ar_2	1987.943	2.6517	0.2978	8.10e7	0.70, 0.00009
Kr_2	1875.462	2.3661	0.2789	5.72e8	0.90, 0.00018

[b] 2.083e5 = 2.083×10^5.

Empirical potentials obtained from spectroscopic data [10,23,24] by the RKR (Rydberg [25], Klein [26], Rees [27]) method are available from [9] for H_2, NO, and I_2; from [28] for OH; from [17] for N_2; from [10] for O_2; from [18] for Li_2; from [19] for Na_2; from [29] for K_2; from [15] for Ar–Ar; and from [16] for Kr–Kr.

Section 4 contains formulas (15, 17, 19, 20) for a, b, and c in terms of E_0, r_0, k, C_6, and d that ensure that the hybrid form $V(r)$ goes through the minimum $(r_0, -E_0)$ with curvature k. For each pair of atoms, I found the value of d that best fits the hybrid form $V(r)$ to the empirical potential of the pair for $r \geq f\,r_0$ in which $0 \leq f \leq 1$. The resulting values of a, b, c, and d are listed in Table 2 along with the fractions f and the root-mean-square (rms) errors $\Delta V(r)$ for $r \geq f\,r_0$. Figures 1–11 show that the fitted hybrid forms V_f (dashes, dark blue) nicely follow the points (diamonds, cyan) of the empirical potentials for the 11 pairs of neutral atoms H_2, N_2, O_2, NO, OH, I_2, Li_2, Na_2, K_2, Ar–Ar, and Kr–Kr. The fitted $V_f(r)$'s go through the empirical minima with the right curvatures and closely trace the empirical potentials, at least for $r \geq f r_0$. Figure 1 for molecular hydrogen adds the harmonic potential

V_h (dot-dash, magenta), which fits only near the minimum at $r = r_0$. Figure 2 for molecular nitrogen and Figure 10 for a pair of argon atoms include the Lennard-Jones potential V_{LJ} (dot-dash, magenta), which is accurate only near r_0.

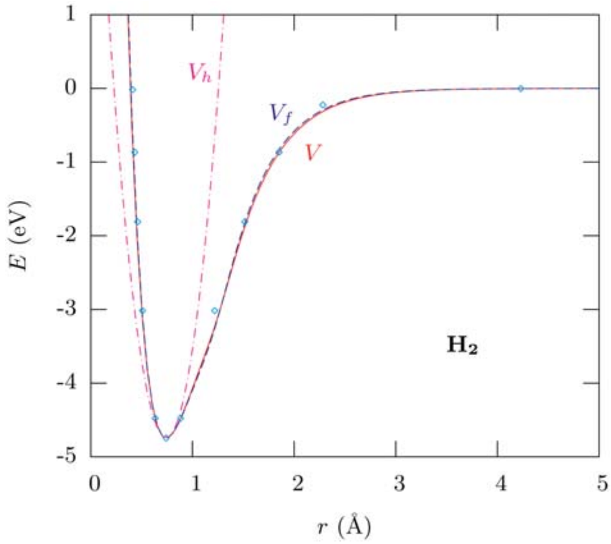

Fig. 1. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of molecular hydrogen (diamonds, cyan) and gives the correct London tail for $r > 3$ Å nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue). In all the figures, the values of C_6 used in V and V_f are from Table 1. The harmonic form V_h (dot-dash, magenta) fits only near the minimum.

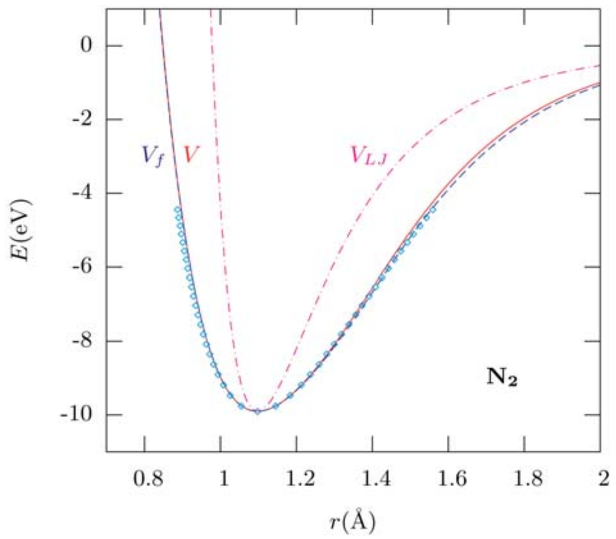

Fig. 2. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of molecular nitrogen (diamonds, cyan) nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue). The Lennard-Jones form V_{LJ} (dot-dash, magenta) fits only near the minimum.

Table 3. Values of the coefficients a, b, c, and d obtained by equations (8, 15, 17, 19, 20) from the values of E_0, r_0, k, and C_6 of Table 3.

	a (eV)	b (Å^{-1})	c (Å^{-1})	d (Å^{12})	f, ΔV
H_2	45.01	2.907	2.5663	16.7	0.68, 0.087
N_2	4059.02	4.435	1.1762	27.7	0.81, 0.111
O_2	2868.48	4.246	1.0539	40.7	0.84, 0.068
NO	4040.42	4.496	1.0946	34.0	0.81, 0.156
OH	491.96	3.942	1.4478	19.8	0.81, 0.053
I_2	16125.67	2.832	0.4350	2.79e5	0.88, 0.041
Li_2	148.93	1.516	0.5161	4.01e6	0.86, 0.028
Na_2	278.20	1.595	0.4275	7.33e6	0.81, 0.012
K_2	359.65	1.381	0.3273	7.30e7	0.85, 0.012
Ar_2	4994.79	2.921	0.2959	3.12e7	0.70, 0.012
Kr_2	9610.07	2.805	0.2759	6.23e7	0.90, 0.0004

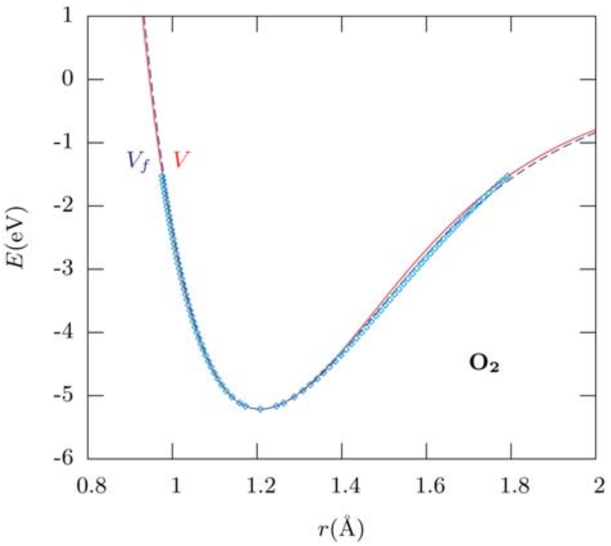

Fig. 3. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of molecular oxygen (diamonds, cyan) nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

The fitted values of the parameter d in Table 2 are less well defined than those of a, b, and c. The empirical rule of thumb

$$d = 7.1\,\text{Å}^{12} + 2.89\,\frac{C_6^3}{E_0^3\,r_0^6} + 0.468\,\frac{E_0}{\text{eV}}\,\frac{r_0^{13}}{\text{Å}} \qquad (8)$$

gives the 11 values of d listed in Table 3 and roughly approximates those of Table 2.

4 Three formulas

Suppose we use the rule (8) for the fudge-factor d and take the London coefficient C_6 from Table 1. How do we find the parameters a, b, and c that make the hybrid potential $V(r)$ have its minimum at $r = r_0$ with $V(r_0) = -E_0$ and with curvature $V''(r_0) = k$?

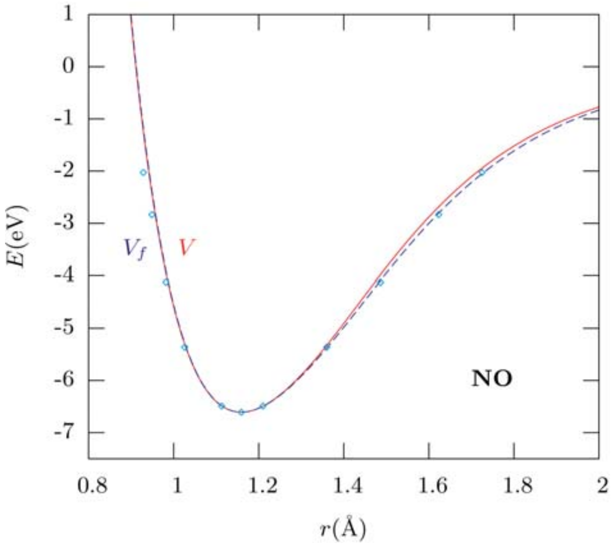

Fig. 4. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of nitric oxide (diamonds, cyan) nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

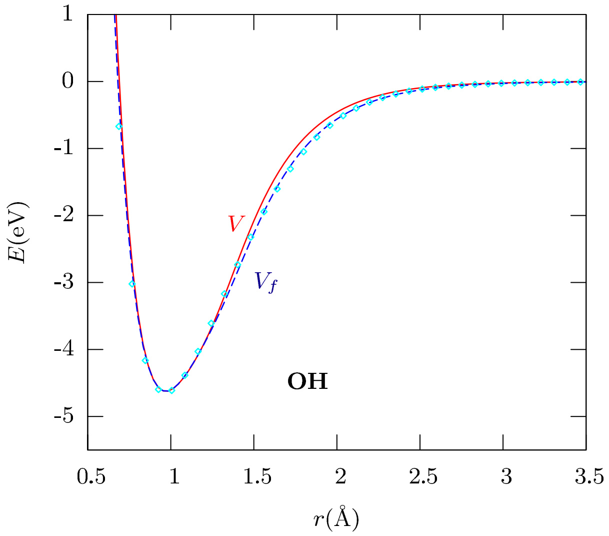

Fig. 5. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of the hydroxyl radical (diamonds, cyan) slightly less well than the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

Let us write the hybrid form as the sum

$$V(r) = v(r) + w(r) \tag{9}$$

of the a, b, c terms $v(r)$

$$v(r) = a\,e^{-br}(1 - c\,r) \tag{10}$$

and the C_6, d terms $w(r)$

$$w(r) = -\frac{C_6}{r^6 + d\,r^{-6}}. \tag{11}$$

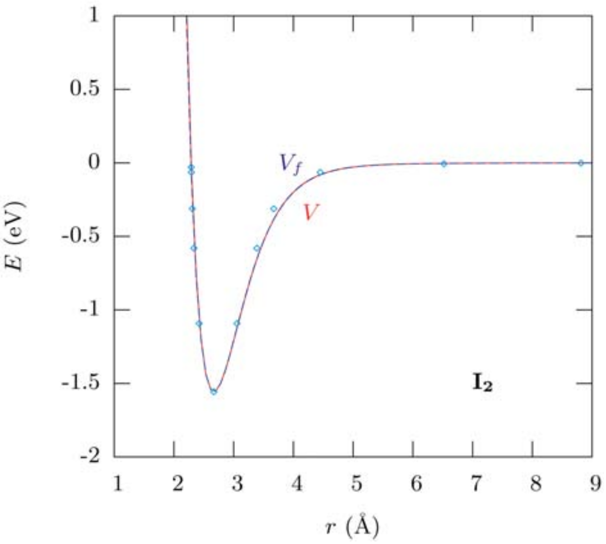

Fig. 6. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of molecular iodine (diamonds, cyan) nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

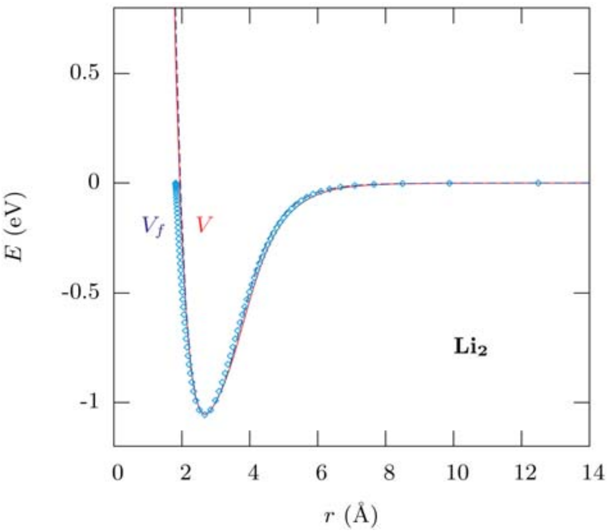

Fig. 7. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of the lithium dimer (diamonds, cyan) nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

Since C_6 and d are given, the function $w(r)$ and its derivatives

$$w'(r) = 6\,C_6\,r^5\,\frac{r^{12} - d}{(r^{12} + d)^2} \tag{12}$$

and

$$w''(r) = -6\,C_6\,r^4\,\frac{(7r^{12} - d)(r^{12} - 5d)}{(r^{12} + d)^3} \tag{13}$$

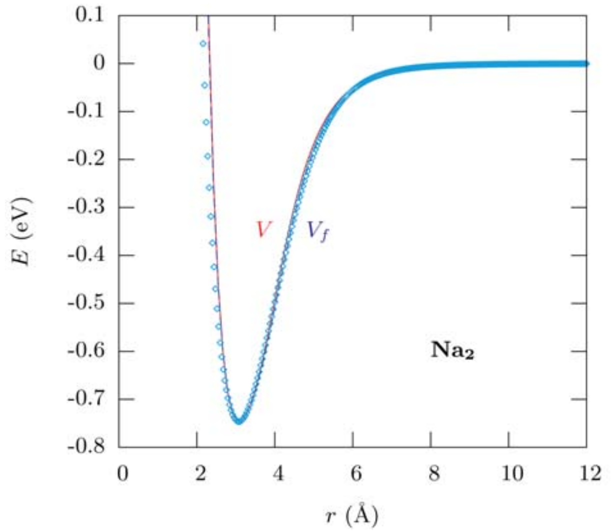

Fig. 8. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of the sodium dimer (diamonds, cyan) well, but not quite as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

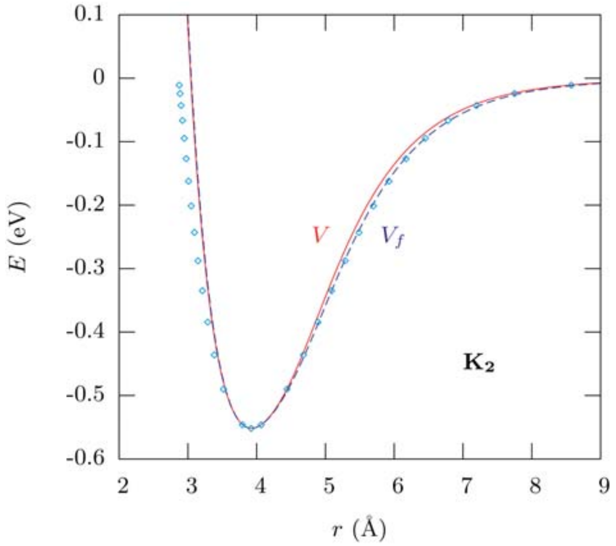

Fig. 9. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of the potassium dimer (diamonds, cyan) well, but not quite as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

are determined. The condition that $V(r_0) = -E_0$ then is

$$a\, e^{-b r_0}(1 - c\, r_0) = -w(r_0) - E_0 \tag{14}$$

which implies that a is

$$a = -(w(r_0) + E_0)\, e^{b r_0}/(1 - c\, r_0). \tag{15}$$

The condition that $V'(r_0) = 0$ is

$$a\, e^{-b r_0}(b + c - b\, c\, r_0) = w'(r_0) \tag{16}$$

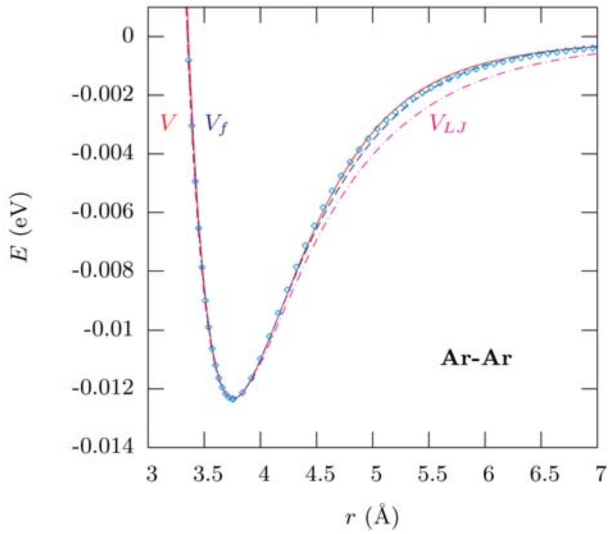

Fig. 10. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of the argon dimer (diamonds, cyan) nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue). The Lennard-Jones form V_{LJ} fitted to the minimum (dot-dash, magenta) is too low for $r > 4$ Å.

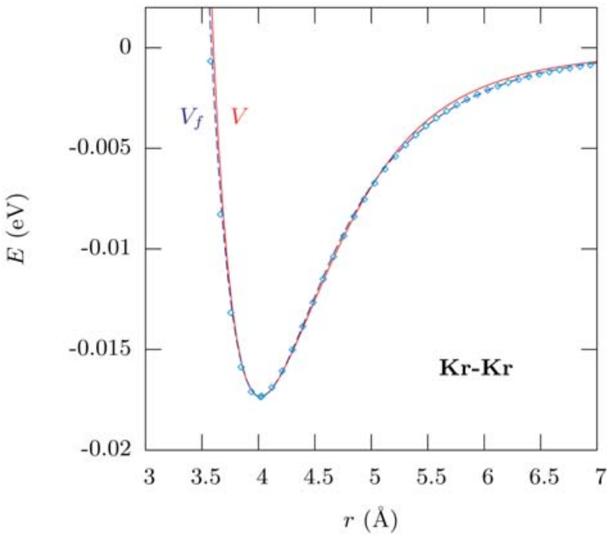

Fig. 11. (Color online) The hybrid form V with the calculated coefficients (a, b, c, and d, Tab. 3) (solid, red) fits the RKR spectral points for the ground state of the krypton dimer (diamonds, cyan) nearly as well as does the hybrid form V_f with the fitted coefficients (a, b, c, and d, Tab. 2) (dashes, dark blue).

which together with (15) gives b as

$$b = -c/(1 - c\, r_0) - w'(r_0)/(w(r_0) + E_0). \tag{17}$$

Finally, the condition $V''(r_0) = k$ is

$$a\, b e^{-b r_0}(b - b\, c\, r_0 + 2\, c) = k - w''(r_0) \tag{18}$$

which with (15) for a and (17) for b is a quadratic equation for c with roots

$$c = \left[r_0 \pm \sqrt{\frac{(w(r_0) + E_0)^2}{w'(r_0)^2 + (k - w''(r_0))(w(r_0) + E_0)}} \right]^{-1}. \tag{19}$$

The minus sign implies

$$c > 1/r_0 \Longleftrightarrow 1 - c\, r_0 < 0 \tag{20}$$

while the plus sign implies

$$c < 1/r_0 \Longleftrightarrow 1 - c\, r_0 > 0. \tag{21}$$

A covalently bonded pair will have $v(r_0) < 0$, which implies $1 - cr_0 < 0$ and so $c > 1/r_0$, which entails the minus sign. One may choose the minus sign for the 11 pairs of neutral atoms considered in this paper. A further discussion of the choice of sign appears in the Appendix.

If one uses the rule of thumb (8) for d and the values of r_0, E_0, k, and C_6 from Table 1, then one may find c from condition (19) with a choice of sign, and then b from (17), and then a from (15). The resulting values of a, b, c, and d for the 11 pairs of neutral atoms H_2, N_2, O_2, NO, OH, I_2, Li_2, Na_2, K_2, Ar–Ar, and Kr–Kr are listed in Table 3 for the case of a minus sign in equation (19); also shown are the rms errors $\Delta V(r)$ for $r \geq f r_0$ for the f's of Table 2. Figures 1–11 show the hybrid form V with these values of a, b, c, and d and with the C_6's of Table 1 as solid red curves. They closely trace the empirical potentials (diamonds, cyan) and the fitted hybrid forms V_f (dashes, dark blue).

5 Conclusions

By using equations (8, 15, 17, 19, 20), one may build an accurate hybrid potential (3) for the ground state of a pair of neutral atoms from their internuclear separation, the depth and curvature of their potential at its minimum, and from their van der Waals coefficient C_6. The hybrid potential therefore is applicable to pairs of neutral atoms for which no empirical potential is available. Given the differences between it and the Lennard-Jones, harmonic, Morse, Varnshi, and Hulburt-Hirschfelder potentials, it would be worthwhile to examine the consequences of these differences in Monte Carlo searches for low-energy states of biomolecules and in numerical simulations of phase transitions and reactions far from equilibrium.

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Table 4. The values of the coefficients a, b, c, and d that best fit the hybrid potential $V(r)$ (Eq. (3)) to RKR data for Li_2, Na_2, and K_2 and to empirical potentials for Ar–Ar and Kr–Kr while respecting equations (15, 17, 19) with a plus sign in (19). $\Delta V(r)$ is the rms error in V for $r \geq f\, r_0$.

	a (eV)	b (Å^{-1})	c (Å^{-1})	d (Å^{12})	f, ΔV (eV)
Li_2	1136.21	1.8218	0.3225	869.0	0.77, 0.037
Na_2	648.22	1.5692	0.3034	2692.0	0.90, 0.004
K_2	500.31	1.2673	0.2486	33770.0	0.70, 0.012
Ar_2	1754.01	2.7054	0.2620	1.57e5	0.70, 0.001
Kr_2	2725.43	2.5622	0.2485	1.0e6	0.90, 0.0003

Appendix: The choice of sign

The choice of the minus sign in equation (19) implies that the fudge factor d must exceed a certain lower limit. The parameter a is the value of the potential $V(r)$ at $r = 0$ and so must be positive. The minus-sign inequalities (20) imply that $1 - cr_0 < 0$. Thus equation (15) will give a positive value for a only if

$$w(r_0) + E_0 > 0 \tag{A.1}$$

which by (11) implies the lower limit

$$d > \frac{C_6\, r_0^6}{E_0} - r_0^{12} \tag{A.2}$$

on the fudge factor d. The values of d listed in Tables 2 and 3 satisfy this constraint.

The choice of the plus sign in equation (19) implies two upper limits on the fudge factor d. The plus-sign inequalities (21) imply that $1 - cr_0 > 0$. Thus equation (15) will give a positive value for a only if

$$w(r_0) + E_0 < 0 \tag{A.3}$$

which by (11) implies the upper limit

$$d < \frac{C_6\, r_0^6}{E_0} - r_0^{12} \tag{A.4}$$

on the fudge factor d. The right-hand-side of this inequality is negative for the pairs N_2, O_2, NO, and I_2 and less than unity for the pairs H_2 and OH, as may be seen from the values of C_6, r_0, and E_0 listed in Table 1. Thus the minus sign is required for the pairs N_2, O_2, NO, and I_2 and strongly indicated for the pairs H_2 and OH.

The second upper limit on d arises because both b and c must be positive ($b > 0$ because $v(r)$ must vanish as $r \to \infty$, and $c > 0$ because $c < 0$ implies $v(r) > 0$). Thus if the positive sign is chosen in the formula (19) for c, then $1 - cr_0 > 0$, and also $w(r_0) + E_0 < 0$ by (A.3), and so equation (17) will give a positive value for b only if $w'(r_0) > 0$, which by (12) implies the upper limit

$$d < r_0^{12}. \tag{A.5}$$

The curves displayed in Figures 1–11 all correspond to the choice of a minus sign in equation (19). But for the five pairs Li_2, Na_2, K_2, Ar–Ar, and Kr–Kr, one also may get good fits to the empirical data by using the plus sign (21). The resulting values of a, b, c, and d appear in Table 4. The d's obey (A.4 and A.5).

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