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Born-Mayer-Type Interatomic Potential for Neutral Ground-State Atoms with $Z = 2$ to $Z = 105$[*]

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Born-Mayer parameters are given which permit, with good accuracy (to within 6%), a greatly simplified computation of a previously derived interatomic potential, $U(R)$, based on the Thomas-Fermi-Dirac (TFD) approximation. The numerical values of A and b appearing in $U(R) = A\exp(-bR)$ are tabulated in two sets of commonly used units for 104 homonuclear pairs of neutral ground-state atoms having $Z = 2$ to $Z = 105$. Approximate lower and upper limits of applicability, R_l and R_u, are also listed, as is the magnitude of the maximum percent error (ϵ) for each fit. R_l is generally $\sim 1.5a_0$ ($a_0 = 0.52917$ Å), while $R_u \sim 3.5a_0$. The effective upper limit probably lies at ~ 6–$8a_0$. Also, with the aid of the given table and the combining rule $U_{12} \simeq (U_{11}U_{22})^{1/2}$, the interaction energies of a total of 5356 heteronuclear diatoms can readily be obtained.

I. INTRODUCTION

An interatomic potential U, based on the Thomas-Fermi-Dirac (TFD) approximation,[1–4] has been derived elsewhere[5] and found to be reasonably reliable for some 36 like[6] and unlike[7] rare-gas atom pairs, respectively, at internuclear separations R ranging from $\sim 0.01a_0$ to $\sim 6a_0$. In each of the latter cases as well as in similar calculations, by the author, for a large number of other pairs of atoms,[8] one interesting and invariably recurring feature is the following: Upon plotting the potential U on a logarithmic scale versus internuclear separation R on a linear scale, there always exists a considerable interval of R over which the curve $U(R)$ is almost exactly linear.[6,7] In this interval of "linearity," therefore, the potential can be expressed in the so-called Born-Mayer form,[9,10] i.e.,

$$U(R) = Ae^{-bR}, \quad R_l \leqslant R \leqslant R_u, \tag{I.1}$$

where R_l and R_u, respectively, denote the lower and upper limits of the interval, and the parameters A and b are constants for a given pair of atoms. The numerical values of R_l and R_u are typically $\sim 1.5a_0$ ($a_0 = 0.52917$ Å) and $\sim 3.5a_0$, respectively. It should be emphasized, however, that because of certain peculiar properties[6,7] of the finite TFD atoms, the actual maximal values of R_u are not readily obtainable within the framework of this approximation, and hence the numerical values of R_u given in Table II should be considered merely as lower bounds. Indeed, extrapolations of this linear portion of $U(R)$ to $R \sim 6a_0$ and beyond were generally found[6,7] to agree to within order of magnitude, and often much better, with the empirical values of $U(R)$ at these distances.

Now, the original analytic form of $U(R)$, as derived in Ref. 5, is of considerably greater complexity than relation (I.1), requires detailed knowledge of TFD electron-density distributions, screening functions, and the evaluation of a fairly complicated two-center integral.[5] By contrast, the functional form (I.1) is not only known to be approximately correct[9–11] for U_r, the repulsive part of the total potential, but also possesses the additional advantage of being exceedingly convenient to handle in practice, i.e., in the very large class of calculations[12–19] involving U itself as well as its derivatives and/or integrals.

It is the purpose of this paper, therefore, to facilitate such calculations by making the analytically complicated TFD potential available, for the first time, in the simplified form (I.1) for all homonuclear and heteronuclear pairs of neutral ground-state atoms having $Z = 2$ to $Z = 105$.

II. THE BORN-MAYER PARAMETERS

Obtained by a least-squares fit to the appropriate TFD data,[5–8] the numerical values of A and b are given (in two commonly used sets of units[20]: $e^2/a_0 = 27.210$ eV, and eV; $a_0 = 0.52917$ Å, and Å) in Table I, as is the magnitude of the maximal percent error (ϵ) for each fit. Table II lists the corresponding values of R_l and R_u, respectively.

In using these tables, the nature of the entries for R_u, discussed in Sec. I, should be borne in mind, i.e., the entry for a given atom gives but an "apparent" R_u, or a lower bound on how far out relation (I.1) is applicable. The actual upper limit of applicability can be expected[6,7] to be considerably higher ($\sim 6 - 8a_0$).

Table I can also be used to calculate interatomic potentials for pairs of unlike atoms if the well-known empirical "combining rule"[21–24]

$$U_{12} \simeq (U_{11}U_{22})^{1/2} \tag{II.1}$$

is used, in which the subscripts refer, in brief, to Z_1 and Z_2, i.e., to the respective atomic numbers of the interacting atoms. In a recent detailed numerical study,[7] this widely used rule was found to be remarkably accurate, mostly to within ~ 0.01

TABLE I. Numerical values of Born-Mayer parameters A and b for neutral ground-state TFD atoms with $Z=2$ to $Z=105$. (ϵ is the magnitude of the maximum % error for each fit.)

Atomic number Z	Chemical symbol	A		b		ϵ
		(e^2/a_0)	(eV)	(a_0^{-1})	(Å^{-1})	(%)
2	He	8.6047	234.13	2.207 79	4.172 17	4.1
3	Li	16.109	438.33	2.120 81	4.007 80	4.2
4	Be	24.599	699.34	2.059 04	3.891 07	4.7
5	B	35.606	968.84	2.027 71	3.831 87	4.1
6	C	48.367	1316.1	2.015 92	3.809 59	4.5
7	N	62.840	1709.9	2.009 00	3.796 51	5.1
8	O	78.771	2143.4	2.004 74	3.788 46	5.0
9	F	96.267	2619.4	2.002 29	3.783 83	5.1
10	Ne	114.72	3121.5	1.999 54	3.778 63	5.6
11	Na	134.56	3661.4	1.998 99	3.777 59	5.8
12	Mg	140.72	3829.0	1.956 94	3.698 13	4.9
13	Al	157.85	4295.1	1.946 81	3.678 99	4.2
14	Si	186.39	5071.7	1.958 88	3.701 80	4.3
15	P	205.67	5596.3	1.951 37	3.687 60	3.9
16	S	222.99	6067.6	1.940 26	3.666 61	3.7
17	Cl	235.64	6411.8	1.924 49	3.636 81	3.6
18	Ar	255.82	6960.9	1.919 01	3.626 45	3.6
19	K	277.95	7563.0	1.916 34	3.621 41	3.6
20	Ca	298.57	8124.1	1.910 44	3.610 26	3.4
21	Sc	319.62	8696.9	1.905 44	3.600 81	3.2
22	Ti	343.72	9352.6	1.904 02	3.598 12	3.2
23	V	366.70	9977.9	1.900 77	3.591 98	3.2
24	Cr	389.77	10 606	1.897 94	3.586 63	3.1
25	Mn	414.53	11 279	1.896 07	3.583 10	2.9
26	Fe	438.46	11 931	1.893 00	3.577 30	3.0
27	Co	463.35	12 608	1.891 16	3.573 82	3.0
28	Ni	487.72	13 271	1.888 18	3.568 19	2.7
29	Cu	511.53	13 919	1.884 57	3.561 37	2.7
30	Zn	539.78	14 687	1.884 24	3.560 74	2.8
31	Ga	564.68	15 365	1.880 99	3.554 60	2.8
32	Ge	590.33	16 063	1.879 03	3.550 90	2.8
33	As	618.26	16 823	1.878 33	3.549 58	2.7
34	Se	645.35	17 560	1.876 88	3.546 84	2.8
35	Br	672.43	18 297	1.874 95	3.543 19	2.9
36	Kr	703.70	19 148	1.875 20	3.543 66	2.8
37	Rb	731.90	19 915	1.873 73	3.540 88	2.9
38	Sr	763.87	20 785	1.873 95	3.541 30	2.8
39	Y	792.10	21 553	1.872 49	3.538 54	2.8
40	Zr	819.91	22 310	1.870 42	3.534 63	2.9
41	Nb	850.89	23 153	1.869 90	3.533 65	2.9
42	Mo	881.65	23 990	1.869 26	3.532 44	3.0
43	Tc	911.85	24 811	1.864 89	3.524 18	3.1
44	Ru	941.72	25 624	1.867 23	3.528 60	3.1
45	Rh	972.66	26 466	1.866 43	3.527 09	3.1
46	Pd	1005.2	27 352	1.865 99	3.526 26	3.0
47	Ag	1040.7	28 318	1.866 57	3.527 35	3.1
48	Cd	1071.1	29 145	1.865 21	3.524 78	3.2
49	In	1102.6	30 002	1.864 16	3.522 80	3.3
50	Sn	1140.2	31 025	1.865 10	3.524 58	3.4
51	Sb	1171.4	31 874	1.863 82	3.522 16	3.5
52	Te	1199.4	32 636	1.861 36	3.517 51	3.5
53	I	1231.2	33 501	1.860 20	3.515 32	3.6
54	Xe	1265.2	34 426	1.859 80	3.514 56	3.5

TABLE I (*continued*)

Atomic number Z	Chemical symbol	A		b		ϵ
		(e^2/a_0)	(eV)	(a_0^{-1})	(Å^{-1})	(%)
55	Cs	1298.9	35 343	1.859 01	3.513 07	3.4
56	Ba	1336.4	36 363	1.859 56	3.514 11	3.5
57	La	1370.2	37 283	1.858 91	3.512 88	3.5
58	Ce	1403.3	38 184	1.857 96	3.511 08	3.5
59	Pr	1436.0	39 074	1.856 79	3.508 87	3.6
60	Nd	1471.5	40 040	1.856 64	3.508 59	3.6
61	Pm	1508.4	41 044	1.856 51	3.508 34	3.7
62	Sm	1544.3	42 020	1.856 21	3.507 78	3.7
63	Eu	1580.5	43 005	1.856 06	3.507 49	3.8
64	Gd	1615.9	43 969	1.855 71	3.506 83	3.7
65	Tb	1651.4	44 935	1.855 12	3.505 72	3.8
66	Dy	1688.7	45 950	1.855 13	3.505 73	3.8
67	Ho	1724.9	46 935	1.854 65	3.504 83	3.8
68	Er	1765.1	48 028	1.854 93	3.505 36	3.6
69	Tm	1801.4	49 016	1.854 49	3.504 52	3.7
70	Yb	1842.3	50 129	1.854 89	3.505 28	3.8
71	Lu	1879.8	51 149	1.854 59	3.504 71	3.8
72	Hf	1914.1	52 083	1.853 44	3.502 54	3.8
73	Ta	1952.7	53 133	1.853 46	3.502 58	3.9
74	W	1991.2	54 181	1.853 00	3.501 71	4.0
75	Re	2028.1	55 185	1.852 31	3.500 41	4.0
76	Os	2067.9	56 268	1.852 40	3.500 58	4.0
77	Ir	2104.6	57 266	1.851 90	3.499 63	4.0
78	Pt	2144.2	58 344	1.851 91	3.499 65	4.0
79	Au	2185.7	59 473	1.852 04	3.499 89	4.1
80	Hg	2230.0	60 678	1.852 54	3.500 84	4.1
81	Tl	2270.7	61 786	1.852 46	3.500 69	4.1
82	Pb	2311.8	62 904	1.852 58	3.500 92	4.2
83	Bi	2349.2	63 922	1.851 64	3.499 14	4.2
84	Po	2395.9	65 192	1.852 24	3.500 27	4.1
85	At	2434.6	66 246	1.851 73	3.499 31	4.1
86	Rn	2476.5	67 386	1.851 63	3.499 12	4.2
87	Fr	2517.4	68 499	1.851 37	3.498 63	4.2
88	Ra	2623.0	71 372	1.863 68	3.521 89	5.7
89	Ac	2665.6	72 531	1.863 60	3.521 74	5.6
90	Th	2716.9	73 927	1.864 70	3.523 82	5.3
91	Pa	2761.1	75 130	1.864 80	3.524 01	5.2
92	U	2806.6	76 368	1.865 19	3.524 75	5.0
93	Np	2850.8	77 570	1.865 18	3.524 73	4.7
94	Pu	2895.1	78 776	1.865 32	3.524 99	4.5
95	Am	2940.2	80 003	1.865 44	3.525 22	4.3
96	Cm	2981.6	81 129	1.864 87	3.524 14	4.2
97	Bk	3027.6	82 381	1.865 11	3.524 59	4.2
98	Cf	3072.8	83 611	1.865 06	3.524 50	4.1
99	Es	3115.2	84 765	1.864 56	3.523 55	4.2
100	Fm	3160.0	85 984	1.864 61	3.523 65	4.2
101	Md	3207.8	87 284	1.864 85	3.524 10	4.2
102	No	3253.6	88 531	1.864 95	3.524 29	4.2
103	Lw	3300.2	89 798	1.865 11	3.524 59	4.2
104	-	3346.4	91 056	1.864 99	3.524 37	4.3
105	-	3393.9	92 348	1.865 25	3.524 86	4.3

TABLE II. Numerical values of R_l and R_u, in atomic units ($a_0 = 0.52917$ Å) for neutral ground-state TFD atoms having $Z = 2$ to $Z = 105$. *Actual* upper limits are probably ~6–8a_0 (see text).

Z	R_l	Z	R_u
2–11	1.0	2, 3, 5–9	3.0
>11	1.5	4, 13–87	3.5
		10–12; 88–105	4.0

to ~1%, rising but rarely to a few percent. In terms of Eq. (I. 1), one therefore has

$$U_{12}(R) \simeq \left(A_1 A_2 e^{-(b_1+b_2)R}\right)^{1/2}$$

or

$$U_{12}(R) \simeq A_{12} e^{-b_{12}R}, \qquad \text{(II. 2)}$$

where $A_{12} = (A_1 A_2)^{1/2}$ is but the geometric mean of A_1, A_2; and b_{12} is simply the arithmetic mean of b_1, b_2. Thus any or all of the interaction potentials for a total of $(104)(103)/2! = 5356$ unlike pairs of atoms can also be calculated quite simply with the aid of Table I.[25]

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[25] From a strictly quantum-mechanical point of view it might be held that, for a given pair of atoms, the parameter A ought to assume different values depending upon the various angular-momentum states of the interacting atoms. This, however, is completely outside the capabilities of the TFD approximation. For the latter, in order to render the model soluble, customarily assumes spherically symmetric electron distributions and vanishing angular momenta for *all* atoms (and ions). See, e.g., Ref. 4(b), pp. 140 and 162. Similarly, states of chemical binding do not occur in the TFD approximation, as has been shown by J. W. Sheldon, Phys. Rev. 99, 1291 (1955), and by E. Teller, Rev. Mod. Phys. 34, 627 (1962).