

Interaction universality and scaling laws for interaction potentials between closed-shell atoms and ions

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A universal scaling scheme is developed for closed-shell interactions. The exchange energies (total energies minus the Coulombic energies) are found to scale with two parameters to universal interaction curves for noble gas–noble gas, alkali ion–noble gas, and halogen ion–noble gas interactions. The interaction potentials constructed from the universal interaction curves agree well with experimentally determined potentials, and also successfully reproduce measured ion mobilities and diffusion coefficients. The universal interactions can be viewed not just as a correlation scheme, but also as operating to extend the range of the potentials for a number of ion–atom systems to both larger and smaller distances than are presently probed by direct measurements. They also provide the basis for predictions of potentials for systems lacking experimental measurements. In the case of the noble gases, they reduce by two the number of parameters required for the formulation of an accurate extended principle of corresponding states.

I. INTRODUCTION

The interaction potentials between noble gas atoms have been accurately determined from inversion of equilibrium, scattering, and transport data.^{1,2} A similar situation has been developed over the past few years for the interactions of alkali and halide ions with noble gas atoms.³ Most of the information has come from the inversion of ion mobility data,^{4–7} with a substantial supplement on the short-range repulsion from scattering measurements with fast ion beams.^{8–11}

Since all these atoms and ions have similar closed-shell electronic structures, it is not surprising that a number of attempts have been made to find similarities and correlations among the potentials. One early result was a correlation of the repulsive potentials on the basis of parameters suggested by a delta-function model for the electron–nucleus attractions.¹² In the region of the potential well, a correlation of potentials is responsible for the fact that the noble gases and their mixtures follow a principle of corresponding states with great accuracy.¹³ However, such a correlation does *not* hold for the corresponding ion–atom potentials,^{3,14,15} for reasons that are discussed later. More recent efforts have concentrated on models in which a short-range repulsion is combined with a series of long-range attraction terms.^{16–22} The essential problem is the repulsion, since the attraction terms are known; some approaches have used one or more terms of the Born–Mayer type whose parameters are determined from a few selected experimental measurements or theoretical calculations, and others have relied on self-consistent-field or other *ab initio* calculations. The considerable

success of these semiempirical approaches strongly suggests that an underlying simple correlation may exist.

The purpose of this paper is to find such a correlation; it is both more general and less ambitious than most of the above-cited approaches, in that only a general correlation is sought, not independent predictions. The results nevertheless have predictive power, in that the potentials for unknown systems can be accurately estimated from the potentials for known systems.

The procedure is to start with the experimentally determined potentials, subtract the attraction terms, and see whether the remaining “exchange” potentials can be correlated into a single universal function with a minimum of adjustable parameters.

The attraction terms consist of the asymptotic expressions for the long-range induction and dispersion energies, multiplied by a suitable damping function to account for electron overlap and exchange. We find that the exchange potentials can be correlated with only two parameters per system, one for energy and one for distance. Three different “universal” functions seem, however, to be required, one each for atom–atom, alkali ion–atom, and halogen ion–atom interactions. Nevertheless, the results do not unambiguously rule out the existence of a single universal function, since the deviations from complete universality occur in the region where the results are sensitive to experimental errors in the starting potentials, uncertainty in the damping functions, and truncation of the induction and dispersion energy series.

One immediate benefit of this procedure occurs for the atom–atom potentials of the noble gases. The simple principle of corresponding states does not hold perfectly for the noble gases: if the potentials are scaled together in the vicinity of the potential well, then systematic deviations are found

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in both the long-range attractive tails and the short-range repulsive walls. The result is that an improved principle of corresponding states requires two additional parameters for the repulsion and at least one additional (known) parameter for the attraction, for a total of five.¹³ The present procedure, in contrast, requires only two parameters to correlate the exchange potentials over the entire range of interest.

The motivation for the present procedure comes from the fact that a principle of corresponding states does *not* hold, even approximately, for ion-atom systems. Consideration of the nature of the potentials readily reveals the reason. The interaction between the noble gas atoms depends symmetrically on the properties of both atoms, and so might conceivably have a universal shape, but the interaction of an alkali or halogen ion with a noble gas atom does not have this symmetric character. In particular, the induction potential (i.e., the charge-induced dipole, quadrupole, etc., energies) depends only on the properties of the atom and not on the particular ion involved, since all the ions have the same charge, but the other components of the potential depend on both the ion and atom. Thus, for example, the potentials for $\text{Li}^+ + \text{Xe}$ and $\text{Cs}^+ + \text{Xe}$ have identical long-range induction tails, but the rest of the potentials differ markedly because Cs^+ is a much larger and more polarizable ion than Li^+ . The potentials therefore have inherently different shapes, and if the potential minima, say, are scaled together, the rest of the potentials will not coincide. An obvious way out of this difficulty is first to subtract off the induction energy and then examine the remainder of the potential for a scaling relation (i.e., whether the potentials all have the same shape). A great improvement is thereby achieved, which can be further improved by also subtracting off the dispersion energy before seeking a correlation. As already mentioned, this procedure substantially improves the accuracy with which the noble gases follow a principle of corresponding states. It also brings the ion-atom potentials into conformity with a principle of corresponding states (i.e., a scaling relation).

It should be mentioned that the crucial feature that makes the foregoing procedure possible is the existence of damping functions to determine the induction and dispersion energies at *all* internuclear separations from their known long-range asymptotic behavior. Such damping functions by now have a fairly elaborate history, which has been reviewed by Tang and Toennies.¹⁶

The "universal" interactions that we have obtained have been checked in two ways; first, by comparing them with the best known experimentally determined potentials, where in most of the cases the agreement is within the uncertainties of the reference potentials, and second, by using them to calculate ion mobilities and diffusion coefficients for direct comparison with experiments. Again, in most of the cases the present interactions reproduce the ion-transport properties within the experimental uncertainties.

The determined scaling parameters of the exchange energies vary smoothly along the periodic table and in similar fashion with the parameters of the delta-function model.¹² The linear correlation of these two sets of parameters was further used to predict new halogen ion-noble gas poten-

tials. Their accuracy is expected to vary within 10–30 % over the entire range of interest.

II. UNIVERSAL INTERACTIONS

The model to be used for obtaining the exchange interactions consists of two parts; the exchange energy part V_{ex} and the Coulombic energy part V_c , multiplied by a suitable damping function $h(R)$,

$$V(R) = V_{\text{ex}}(R) + V_c(R)h(R), \quad (1)$$

where R is the separation. In the case of atom-atom interactions, the Coulombic energy is just the dispersion energy,

$$V_c(R) = V_{\text{dis}}(R), \quad (2)$$

whereas in the case of ion-atom interactions it includes the induction energy,

$$V_c(R) = V_{\text{dis}}(R) + V_{\text{ind}}(R). \quad (3)$$

These energies are approximated here by their long-range asymptotic expressions, truncated after the R^{-8} terms,

$$-V_{\text{dis}}(R) = C_6/R^6 + C_8/R^8, \quad (4)$$

$$-V_{\text{ind}}(R) = e^2\alpha_d/2R^4 + e^2\alpha_q/2R^6 + e^2\alpha_o/2R^8, \quad (5)$$

where C_l are dispersion coefficients and the α_l are l -pole polarizabilities of the atoms (d = dipole, q = quadrupole, o = octopole). As a damping function we use the one recommended by Ahlrichs, Penco, and Scoles,²³

$$h(R) = \begin{cases} \exp[-(1.28R_m/R - 1)^2] & \text{for } R < 1.28R_m \\ 1 & \text{for } R \geq 1.28R_m \end{cases}, \quad (6)$$

where R_m is the position of the potential minimum. Although more elaborate damping functions have by now been developed,¹⁶ the data available at the present time do not justify their use.

The reason for terminating the series after the R^{-8} terms is that almost nothing is known about the hexadecapole polarizabilities needed to calculate the R^{-10} term of the induction energy. For consistency, we have therefore also terminated the dispersion energy at the same place, even though reasonable estimates of the C_{10} coefficients are sometimes available.

We can now use this model to test whether the exchange energies follow a simple scaling law,

$$V_{\text{ex}}(R) = v_o V_{\text{ex}}^*(R^*), \quad (7)$$

where $V_{\text{ex}}^*(R^*)$, with $R^* = R/\rho$, is a universal function, and v_o and ρ are energy and distance scaling parameters, respectively. We calculate these exchange energies using the formula of Eq. (1) and empirical potentials determined from experiments.

For small R we used empirical potentials obtained from beam-scattering experiments: those of Rol and co-workers²⁴ for atom-atom interactions, and those of Refs. 8–11 for ion-atom interactions, hereafter called beam potentials. For atom-atom interactions at larger R we used multiproperty potentials,²⁵ which accurately reproduce various equilibrium, transport, and scattering data. For ion-atom interactions at larger R we used potentials determined from the

direct inversion of ion mobility data by Viehland and Kirkpatrick,⁵⁻⁷ hereafter called mobility potentials.

To calculate the induction energies we used polarizabilities from a variety of experimental and theoretical sources, as listed in Table I. To calculate the C_6 dispersion coefficients we used the method of Koutselos and Mason,²⁶ in which the numbers of equivalent electrons is the same in an isoelectronic series of closed-shell atoms and ions. These numbers of equivalent electrons were calculated for the five homonuclear pairs of noble-gas atoms, using their accurately known C_6 coefficients; from these values the C_6 coefficients for all the unlike atom-atom and ion-atom interactions were obtained.²⁶ The C_8 coefficients could then be calculated from the corresponding C_6 coefficients plus dipole and quadrupole polarizabilities.^{26,27} The essential input data and the calculated numbers of equivalent electrons are given in Table I.

Once V_{ex} is obtained by subtracting the damped induction and dispersion energies from the empirical total potential, the existence of the two-parameter scaling law of Eq. (7) can be inferred by seeing whether plots of $\ln V_{ex}$ vs $\ln R$ for the various systems can be brought into coincidence on a single universal curve by parallel translation. In this way we found that to a good approximation the noble gas-noble gas, alkali ion-noble gas, and halogen ion-noble gas V_{ex} interactions each lie on a different "universal" curve. We have fitted these three curves by double-exponential functions,

$$V_{ex}^*(R^*) = Ae^{-aR^*} - Be^{-bR^*}, \quad (8)$$

where A , a , B , and b are dimensionless parameters, summarized in Table II. Since the parallel-translation procedure is only relative (the whole group of curves can be translated *en masse*), the magnitudes of these parameters depend on the choice of some system as a reference, that is a system for which we make the (arbitrary) choice of $v_o = 1$ and $\rho = 1$. We have chosen Ar-Ar as the reference system. The quantities $v_o A$, $v_o B$, a/ρ , and b/ρ are invariant, and have the same values whatever choice is made for the reference system.

The three $V_{ex}^*(R^*)$ curves are shown in Fig. 1, with the positions of the minima marked for the typical systems Ar-Ar, $K^+ - Ar$, and $Cl^- - Ar$. It can be seen that the differences among these three V_{ex}^* curves occur mostly at large internuclear separations, where the attraction energy dominates. It is thus possible that these differences are not real, but are only caused by the magnification of relatively small errors in the empirical potentials and in the calculated Coulombic energies, caused by taking the difference between two quantities of comparable magnitude. Errors in the empirical potentials are largely caused by experimental errors, and errors in the calculated Coulombic energies would result from use of an approximate damping function and from termination of the asymptotic series. Improvements in accuracy might then lead to a single truly universal $V_{ex}^*(R^*)$ curve, but the data available at the present time are not adequate to test this possibility properly.

We turn next to summarizing and testing the accuracy of the results of the foregoing scheme of universal exchange interactions.

TABLE I. Parameters used to determine induction and dispersion energies.

Atom	$\alpha_d (a_0^3)$	$\alpha_q (a_0^5)$	$\alpha_o (a_0^3)$	$C_6 (e^2 a_0^3)$	N
He	1.3831 ^a	2.4434 ^a	10.614 ^a	1.461 ^a	1.434
Ne	2.663 ^b	7.48 ^s	34.27 ⁱ	6.87 ^l	4.443
Ar	11.08 ^b	54.14 ^h	531.2 ⁱ	67.2 ^l	5.902
Kr	16.74 ^b	97.08 ^h	1411 ^k	133 ^l	6.704
Xe	27.29 ^b	191.9 ^h	3683 ^k	301 ^m	7.925
Li ⁺	0.1925 ^c	0.118 ^h			1.434
Na ⁺	1.00 ^d	1.68 ^h			4.443
K ⁺	5.47 ^d	16.4 ^h			5.902
Rb ⁺	9.11 ^d	35.8 ^h			6.704
Cs ⁺	15.8 ^e	85.5 ^h			7.925
F ⁻	10.5 ^{e,f}	61.1 ^h			4.443
Cl ⁻	28.1 ^e	262 ^h			5.902
Br ⁻	36.4 ^e	348 ^h			6.704
I ⁻	54.7 ^e	537 ^h			7.925

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III. SUMMARY AND TESTS OF THE UNIVERSAL INTERACTIONS

In determining the numerical values of the scaling parameters v_o and ρ , we have given consideration to the fact that we expect the values to vary smoothly both within an isoelectronic sequence (e.g., Ar-Ar, $K^+ - Ar$, $Cl^- - Ar$) and within a family of the periodic table (e.g., $K^+ - He$, $K^+ - Ne$, $K^+ - Ar$, $K^+ - Kr$, $K^+ - Xe$). It turns out that this can be done without any appreciable sacrifice in the accuracy of fitting. The advantage is that it enhances the ability of the model to predict new closed-shell interactions, both by virtue of the smoothness and by bringing the parameters into conformity with those of the delta-function model.¹²

The final potentials as calculated from the assigned values of v_o and ρ can be tested by comparison either directly with empirical potentials based on experimental data, or in-

TABLE II. Dimensionless parameters for the universal exchange interactions of Eq. (8).

System	A	a	B	b
Noble gas-noble gas	170.80	1.6203	68.510	1.5143
Alkali ion-noble gas	146.98	1.5024	70.198	1.4041
Halogen ion-noble gas	104.55	1.7361	-.0072267	.44857

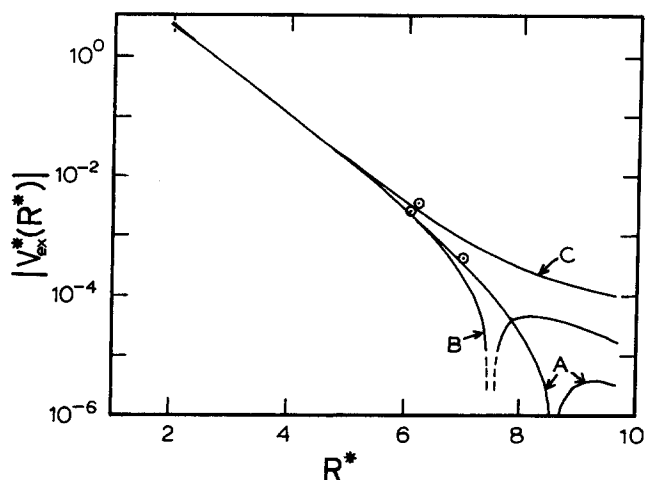


FIG. 1. Universal exchange interactions of Eq. (8): (A) noble gas-noble gas systems; (B) alkali ion-noble gas systems; (C) halogen ion-noble gas systems. The circles indicate the positions of the potential minima for the typical systems Ar-Ar, $K^+ - Ar$, and $Cl^- - Ar$. Note the logarithmic scale.

directly with the experimental data. In the case of the noble gas-noble gas interactions, the empirical potentials are so accurately known that the testing can be satisfactorily carried out on the potentials themselves. However, the ion-atom empirical potentials are less accurately known, in part because they are based largely only on ion mobility data, and we have therefore also examined the agreement between cal-

culated and experimental ion mobilities and diffusion coefficients.

A. Noble gas-noble gas interactions

The results for the noble gases are summarized in Table III, which includes the dispersion coefficients, the scaling parameters ν_0 and ρ , and the calculated values of the positions (R_m) and depths (ϵ) of the potential wells. The calculated R_m and ϵ are compared with the experimental multiproperty values in the last columns of the table. The agreement is within about 1%, indicating that the scaled potentials agree very well with the experimental ones in the vicinity of the potential minimum. The potentials at larger R will automatically agree well because accurate values of C_6 and C_8 have been used in both. The sort of agreement obtained is shown in Fig. 2 for the typical system Ar-Ar. The other noble-gas systems are very similar.

The agreement between the calculated and experimental potentials in the short-range repulsive region is illustrated in Fig. 3 for the typical system Ar-Ar. The agreement is within the accuracy of the experimental potentials. The other noble-gas systems are very similar.

In summary, the present scaled potentials agree within experimental uncertainty with multiproperty potentials at intermediate and large R , and with the beam potentials at small R . The former experimental potentials are known within a few percent and the latter ones within 10-15 %.

TABLE III. Potential parameters for noble gas systems.

System	$C_6(e^2a_0^2)$	$C_8(e^2a_0^2)$	$\nu_0(e^2/a_0)$	$\rho(a_0)$	$R_m(a_0)$	$\epsilon \times 10^3$ (e^2/a_0)	$\frac{(R_m)_{calc}}{(R_m)_{exp}}$	$\frac{\epsilon_{calc}}{\epsilon_{exp}}$	Experimental potential
HeHe	1.4609	14.546	0.08167	0.7935	5.66	0.0344	1.01	1.01	a
Ne	3.1458	36.785	0.1585	0.8098	5.76	0.0683	1.01	0.99	b
Ar	9.7725	159.74	0.2101	0.9321	6.61	0.0940	1.01	1.00	c
Kr	13.544	247.82	0.2768	0.9648	6.98	0.0967	1.00	0.99	d
Xe	19.952	416.31	0.2914	1.031	7.52	0.0919	1.01	1.02	e
NeNe	6.8700	91.902	0.4103	0.8133	5.91	0.134	1.01	1.00	f
Ar	20.640	378.20	0.8822	0.8934	6.65	0.210	1.00	1.00	g
Kr	28.401	577.40	0.9574	0.9334	6.97	0.220	1.00	1.00	g
Xe	41.541	952.67	1.021	0.9893	7.41	0.223	1.01	1.00	g
ArAr	67.200	1570.9	1.000	1.000	7.06	0.459	0.99	1.01	h
Kr	94.300	2399.3	1.316	1.025	7.32	0.529	1.00	1.00	i
Xe	140.60	3961.4	1.470	1.075	7.66	0.597	1.00	1.00	j
KrKr	133.00	3662.4	1.512	1.058	7.52	0.630	0.99	1.00	k
Xe	199.44	6043.3	1.784	1.101	7.82	0.752	0.99	1.02	j
XeXe	301.00	9965.6	2.911	1.123	8.19	0.897	0.99	1.00	l

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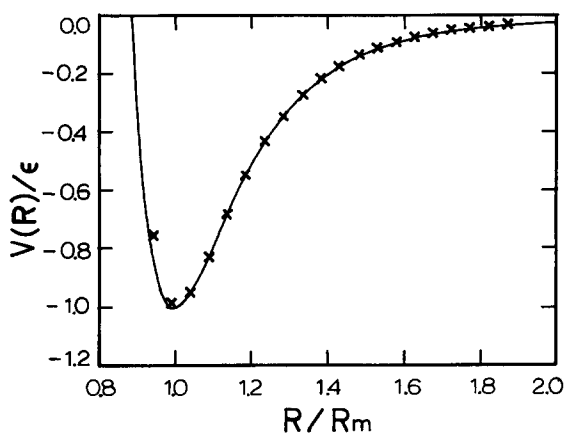


FIG. 2. Comparison of calculated (solid curve) and experimental multiproperty (crosses) potentials for the typical system Ar-Ar in the region of the minimum.

B. Alkali ion-noble gas interactions

The results for the alkali ion-noble gas systems are summarized in Table IV, including the comparison of the calculated R_m and ϵ values with the experimental mobility ones. Here the agreement is only within several percent, a somewhat poorer result than for the noble-gas systems. The main cause of this is the fact that the mobility potentials are not as accurately established as are the noble-gas multiproperty potentials.

No comparisons of R_m and ϵ are given in Table IV for the systems $\text{Rb}^+ - \text{He}$, $\text{Cs}^+ - \text{He}$, and $\text{Cs}^+ - \text{Ne}$. These systems have shallow potential wells that are not accurately probed by the mobility data, and in addition for the latter two systems conflicting results have been obtained from different types of experimental information. These systems are discussed in more detail below, as is the system $\text{K}^+ - \text{Ar}$, which shows somewhat larger deviations in R_m and ϵ than do the other systems, and for which there are also some con-

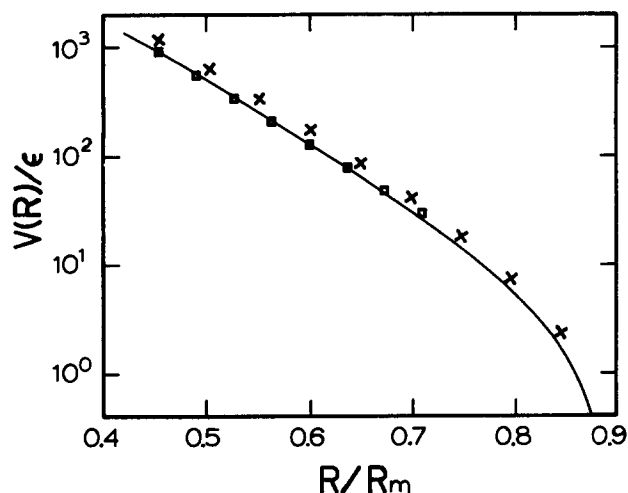


FIG. 3. Comparison of short-range repulsive potentials for Ar-Ar. Solid curve, present calculations; crosses, multiproperty potential (Table III); squares, beam potential (Ref. 24).

flicting experimental results. Furthermore, for three other systems there are no beam-scattering measurements to probe the short-range interactions ($\text{Li}^+ - \text{Xe}$, $\text{Na}^+ - \text{Xe}$, $\text{K}^+ - \text{Xe}$).

In all of the above cases the scaling procedure for $V_{\text{ex}}^*(R^*)$ can be viewed as filling gaps in experimental information and helping to resolve conflicts in experimental results. Because of the uncertainties involved, however, we have considered it necessary to see how well all the scaled potentials reproduce the original ion mobility and diffusion measurements, as described next.

The complicated kinetic-theory computational procedures for calculating mobilities and diffusion coefficients from given ion-atom potentials have been described elsewhere in detail²⁸ and need not be repeated here. Suffice it to say that the successive approximations involved were carried to high enough order that the results had converged to about the usual experimental accuracy. Both the experiments and the calculations correspond to a fixed temperature (usually 300 K) and varying electric field strength. The latter is expressed as the single combined variable E/N , the ratio of the electric field strength to the gas number density, whose customary unit is the Townsend (Td), with $1 \text{ Td} = 10^{-17} \text{ V cm}^2$. The mobility itself varies inversely with N , and is therefore customarily reported as a standard value (K_o), referred to a standard gas density N_o corresponding to an ideal gas at standard conditions of 0°C and 1 atm ($N_o = 2.687 \times 10^{19} \text{ molecules/cm}^3$). The diffusion coefficients parallel and perpendicular to the field, however, are customarily reported as ND_{\parallel} and ND_{\perp} . Although these products are independent of N , they vary strongly with E/N , roughly as $(E/N)^2$, which makes comparisons unwieldy. A simple way to remove this dominant quadratic dependence on E/N is to define dimensionless diffusion coefficients, $\tilde{D}_{\parallel,\perp}$, as follows:

$$\tilde{D}_{\parallel,\perp} \equiv eND_{\parallel,\perp}/N_o K_{\text{pol}} kT_{\text{pol}}, \quad (9)$$

$$kT_{\text{pol}} \equiv kT + \frac{1}{2}M(v_d)_{\text{pol}}^2, \quad (10)$$

$$(v_d)_{\text{pol}} = (N_o K_{\text{pol}})(E/N), \quad (11)$$

where e is the ionic charge, k is Boltzmann's constant, K_{pol} is the limiting standard mobility at $T = 0$ and $E/N = 0$, T_{pol} is an effective ion temperature that would result if the mobility always had the constant value $K_o = K_{\text{pol}}$, $(v_d)_{\text{pol}}$ is the drift velocity corresponding to this constant mobility, and M is the mass of the neutral atom. In the limit of $T = 0$ and $E/N = 0$, the mobility and diffusion are dominated by the long-range R^{-4} polarization component of the potential, as given in Eq. (5), and K_{pol} can therefore be calculated from knowledge of the dipole polarizability of the atom and the ion-atom reduced mass.²⁹ It is the effective ion temperature that is responsible for the strong dependence of $D_{\parallel,\perp}$ on E/N .

We have made detailed comparisons between calculated and measured ion mobilities and diffusion coefficients for all the alkali ion-noble gas systems.³⁰ Since the agreement is satisfactory for most of the systems, we give only a statistical summary, and discuss the three somewhat anomalous systems separately ($\text{K}^+ - \text{Ar}$, $\text{Cs}^+ - \text{He}$, $\text{Cs}^+ - \text{Ne}$). Because of the length of the results we restrict the statistical summary to a comparison only with the measurements reported by the

TABLE IV. Potential parameters for alkali ion–noble gas systems.^a

Systems	$C_6(e^2 a_0^6)$	$C_8(e^2 a_0^8)$	$v_0(e^2/a_0)$	$\rho(a_0)$	$R_m(a_0)$	$\epsilon \times 10^3$ (e^2/a_0)	$\frac{(R_m)_{\text{calc}}}{(R_m)_{\text{exp}}}$	$\frac{\epsilon_{\text{calc}}}{\epsilon_{\text{exp}}}$
Li ⁺ He	0.2962	2.044	0.1135	0.7185	3.64	2.70	1.00	1.00
Ne	0.6742	5.502	0.3211	0.7174	3.89	2.41	0.99	0.98
Ar	1.842	23.79	0.5730	0.8701	4.53	9.90	1.00	0.99
Kr	2.483	36.85	0.7201	0.9088	4.58	14.5	1.00	0.99
Xe	3.546	61.71	0.8753	0.9740	4.75	20.2	1.00	1.00
Na ⁺ He	1.424	13.17	0.2063	0.7640	4.55	1.30	0.99	1.03
Ne	3.199	34.16	0.5646	0.7607	4.70	2.37	1.02	0.98
Ar	9.010	140.1	0.9767	0.8745	5.10	6.85	1.00	0.98
Kr	12.22	214.1	1.064	0.9394	5.42	8.08	0.99	1.00
Xe	17.57	353.5	1.208	1.023	5.88	9.48	1.04	1.00
K ⁺ He	5.835	72.05	0.2690	0.8589	5.49	0.749	1.01	0.89
Ne	12.58	177.8	0.7254	0.8534	5.61	1.43	1.01	0.98
Ar	38.97	741.8	1.202	0.9478	5.87	4.51	1.06	0.96
Kr	54.01	1137	1.282	1.014	6.24	5.17	1.02	0.98
Xe	79.45	1883	1.596	1.053	6.34	7.84	1.00	1.02
Rb ⁺ He	8.800	126.2	0.3474	0.8868	5.85	0.646
Ne	18.76	304.5	0.9348	0.8855	6.02	1.20	1.01	0.98
Ar	59.71	1266	1.207	1.023	6.60	2.97	1.02	0.94
Kr	83.31	1936	1.612	1.044	6.69	4.22	1.00	0.99
Xe	123.4	3201	1.852	1.083	6.73	6.56	1.00	0.97
Cs ⁺ He	13.69	236.4	0.5092	0.9241	6.38	0.535
Ne	28.87	556.0	1.132	0.9217	6.38	1.10
Ar	94.39	2301	1.605	1.031	6.76	3.05	1.03	0.97
Kr	132.6	3510	1.908	1.060	6.85	4.26	1.04	0.98
Xe	197.9	5785	1.922	1.170	7.61	4.26	0.98	1.02

^a Experimental values of R_m and ϵ are from Refs. 5 and 6.

Georgia Tech group,^{31–46} which are very extensive and which adequately depict the performance of the present scheme.

Since both the experiments and the computations contain uncertainties which vary with E/N , we use statistical measures that make allowance for this fact. These measures are defined as⁶

$$\delta \equiv n^{-1} \sum_{i=1}^n [(Q_i/q_i - 1)/(|\Delta Q_i| + |\Delta q_i|)], \quad (12)$$

$$\chi^2 \equiv n^{-1} \sum_{i=1}^n [(Q_i/q_i - 1)^2/(|\Delta Q_i| + |\Delta q_i|)^2], \quad (13)$$

where n is the number of data points, $|\Delta Q_i|$ is the absolute value of the estimated fractional uncertainty in the measured value Q_i of a particular property, and $|\Delta q_i|$ is the corresponding fractional uncertainty in the calculated value q_i . These definitions are designed to prevent a few large discrepancies from overwhelming the measures when the discrepancies are mainly only of the order of the uncertainties in the measurements and calculations. A positive value of δ indicates that the measurements lie above the calculations, and vice versa. A value of $|\delta|$ that is appreciably less than unity indicates that the overall agreement is comparable to the uncertainties, on the average. A value of χ that is less than unity indicates that there is little scatter in the experimental data and that the agreement with the calculations is fairly uniform over the whole range of E/N .

The statistical summary is presented in Table V, and includes values of δ and χ as obtained from the mobility potentials. Since these potentials were obtained largely by

fitting the mobility data indicated, their values of δ and χ represent about the best fit possible. The most important general conclusion to be drawn from Table V is that our values of δ and χ are usually small and comparable in magnitude to the ones obtained for the mobility potentials.

We now turn to the three systems for which some anomalies appear. Various potentials for $K^+ - Ar$ as obtained from different measurements do not agree as well as expected, as discussed in detail by Viehland.⁶ In the foregoing work this manifests itself by somewhat poorer agreement for R_m and ϵ (Table IV), although the values of δ and χ are reasonable (Table V). Direct comparison shows that our present scaled potential does reproduce the transport data fairly well, as shown in Figs. 4 and 5 for K_o and $\tilde{D}_{||}$. The agreement is satisfactory, although perhaps not optimal. We conclude that the scaled potential is adequate, in view of the inconsistencies that exist in the various types of experimental data.

The mobility potentials for $Cs^+ - He$ and $Cs^+ - Ne$ determined in Ref. 6 from the variation of K_o with E/N at 300 K do not agree with earlier mobility potentials deduced from the variation of K_o with T at $E/N \approx 0$,⁴⁷ and they are also not consistent with the beam potentials.¹¹ In addition, they do not fit smoothly into the present scheme with reasonable scaling parameters. We have therefore used the earlier mobility and beam potentials to obtain first approximations for the scaling parameters, and then made small adjustments in the parameters to obtain smoothness with respect to the other systems (Table IV). The resulting scaled potentials reproduce adequately the transport coefficients as a function of E/N , as shown by the values of δ and χ in Table V and by

TABLE V. Deviations between measured and calculated transport coefficients of alkali ions in noble gases.

System	Data type	Data reference	Range of E/N (Td)	Data points	Data accuracy(%)	Deviations ^a			
						Mobility ^b		Present model	
						δ	χ	δ	χ
Li ⁺ He	K_o	34	2-200	31	3	-0.35	0.24	-0.70	0.33
	K_o	38	2-226	102	2	-0.03	0.41	0.39	0.48
	$D_{ }$	35	2-150	26	5	0.87	0.65	0.90	0.40
	$D_{ }$	38	2-150	25	7	0.40	0.37	0.76	0.47
Li ⁺ Ne	K_o	34	3-90	24	2	0.14	0.37	-0.05	0.42
	$D_{ }$	35	3-90	15	5	0.98	0.39	0.75	0.46
Li ⁺ Ar	K_o	34	6-200	27	2	0.55	0.67	-0.48	0.53
	$D_{ }$	35	6-200	17	5			2.42	0.40
Li ⁺ Kr	K_o	45	7-195	36	2	0.14	0.54	0.27	0.51
	$D_{ }$	46	7-195	11	15	0.64	0.31	1.12	0.42
Li ⁺ Xe	K_o	45	10-200	32	3	-0.46	0.54	-0.60	0.44
	$D_{ }$	46	10-200	15	15	-0.08	0.30	0.23	0.64
Na ⁺ He	K_o	34	4-175	23	2	0.05	0.22	-0.16	0.34
	$D_{ }$	35	4-175	23	5	1.40	0.48	1.47	0.72
Na ⁺ Ne	K_o	34	4-200	25	2	0.03	0.19	0.07	0.23
	$D_{ }$	35	4-200	14	5	0.80	0.46	0.69	0.50
Na ⁺ Ar	K_o	34	6-500	35	2	0.10	0.27	0.24	0.34
	$D_{ }$	35	6-500	24	5	0.70	0.45	1.26	0.82
Na ⁺ Kr	K_o	43	7-515	46	4	0.12	0.20	0.09	0.41
	$D_{ }$	43	7-515	26	10	0.09	0.44	0.54	0.45
Na ⁺ Xe	K_o	43	7-500	49	5	-0.06	0.19	0.22	0.43
	$D_{ }$	43	7-500	33	10	0.26	0.73	1.03	0.85
K ⁺ He	K_o	32	1-152	57	2	0.36	0.37	-0.28	0.20
	$D_{ }$	33	1-152	57	7	0.61	0.42	0.32	0.40
K ⁺ Ne	K_o	32	1-203	44	2	-0.06	0.11	0.29	0.28
	$D_{ }$	33	1-203	44	7	-0.04	0.14	-0.43	0.13
K ⁺ Ar	K_o	31	1-610	43	3	0.14	0.25	0.49	0.48
	$D_{ }$	31	1-610	32	7	0.46	0.63	0.50	0.41
K ⁺ Kr	K_o	44	8-700	53	2	0.07	0.27	0.08	0.28
	$D_{ }$	44	8-700	39	9	0.56	0.40	0.55	0.43
K ⁺ Xe	K_o	44	7-805	45	2	0.31	0.44	0.28	0.34
	$D_{ }$	44	7-700	32	9	0.41	0.45	0.73	0.54
Rb ⁺ He	K_o	36	4-120	32	2	-0.02	0.22	0.08	0.20
	$D_{ }$	37	4-120	32	8	-0.69	0.41	-0.62	0.38
Rb ⁺ Ne	K_o	36	3-500	41	2	-0.02	0.22	0.51	0.21
	$D_{ }$	37	3-500	41	9	-0.22	0.26	0.10	0.24
Rb ⁺ Ar	K_o	36	2-500	38	2	0.09	0.39	-0.72	0.41
	$D_{ }$	37	2-500	38	8	0.12	0.45	0.07	0.51
Rb ⁺ Kr	K_o	42	9-865	59	2	-0.16	0.37	0.11	0.19
	$D_{ }$	40	9-500	31	7	0.40	0.58	0.97	0.56
Rb ⁺ Xe	K_o	42	10-710	56	2	-0.08	0.27	0.17	0.37
	$D_{ }$	40	10-710	39	6	-0.22	0.47	0.33	0.43
Cs ⁺ He	K_o	41	5-130	34	3	0.01	0.26	0.49	0.22
	$D_{ }$	41	5-130	32	10-50	0.50	0.35	0.67	0.43
Cs ⁺ Ne	K_o	41	3-300	40	2	-0.09	0.24	0.64	0.23
	$D_{ }$	41	3-300	40	10	3.25	0.59	0.79	0.28
Cs ⁺ Ar	K_o	39	6-500	51	2	0.08	0.30	0.31	0.30
	$D_{ }$	40	6-500	51	8	0.86	0.70	0.85	0.66
Cs ⁺ Kr	K_o	39	7-505	51	2	-0.00	0.30	-0.01	0.42
	$D_{ }$	40	7-505	38	8	0.10	0.59	0.70	0.56
Cs ⁺ Xe	K_o	39	10-660	47	2	0.04	0.27	-0.24	0.33
	$D_{ }$	40	10-660	35	10	0.43	0.42	0.59	0.39

^a The definitions of δ and χ are given in Eqs. (12) and (13).

^b Results from Ref. 6 and from additional calculations.

direct comparisons. The latter are illustrated in Fig. 6 for the mobility of Cs⁺ in He; the results for Cs⁺-Ne are similar, and the diffusion coefficients are also satisfactorily reproduced. In addition, the transport and scattering data themselves have previously been shown to be mutually consistent.⁴⁸ We conclude that the scaled potentials for Cs⁺-He

and Cs⁺-Ne are probably more reliable than the original mobility potentials.

Finally, it should be mentioned that, after the present analysis was finished,³⁰ a new determination of the Li⁺-He and Li⁺-Ar potentials appeared,⁴⁹ including new transport measurements. For both systems the new determina-

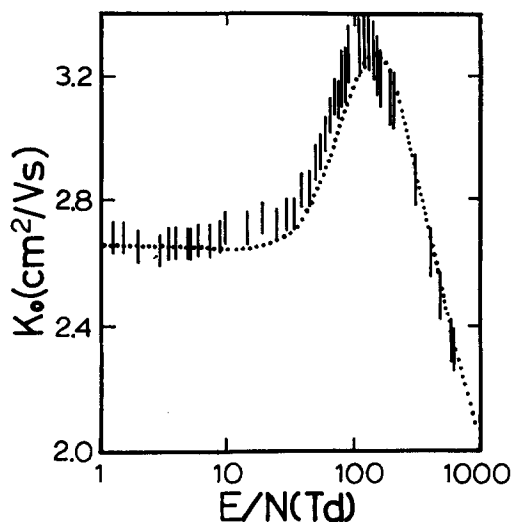


FIG. 4. Comparison of calculated and measured mobilities for K^+ in Ar. The dotted curve is calculated from the present potential, and the error bars represent measurements from Ref. 31.

tion decreased the R_m values by about 3% and increased the ϵ values by about 10%. Since these changes tend to compensate each other when properties are calculated, we did not feel it worthwhile to make a complete reanalysis of these systems to produce only small changes in the values of v_o and ρ given in Table IV.

In summary, the present scaled potentials agree with the available transport and scattering data within experimental uncertainties. We estimate that the scaled potentials for the alkali ion–noble gas interactions are accurate to about 10–20% over their entire range of R .

C. Halogen ion–noble gas interactions

The results for the halogen ion–noble gas systems are summarized in Table VI, including the comparison of the calculated R_m and ϵ values with the experimental mobility

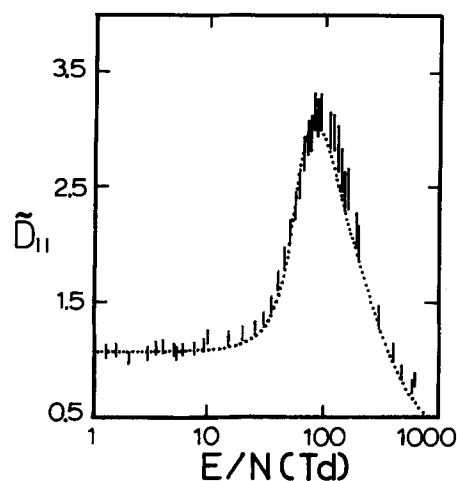


FIG. 5. Same as Fig. 4, for the diffusion coefficient parallel to the field.

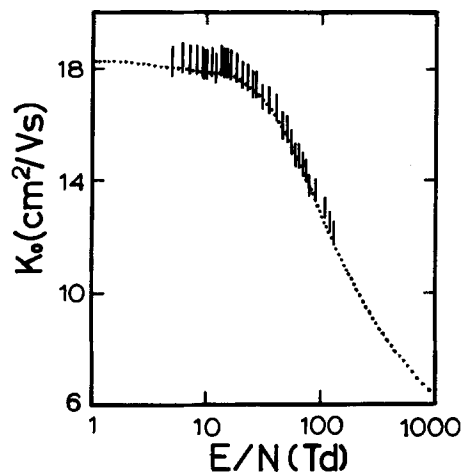


FIG. 6. Comparison of calculated and measured mobilities for Cs^+ in He. The dotted curve is calculated from the present potential, and the error bars represent measurements from Ref. 41.

ones. The data available for the halogen ions are less extensive than for the alkali ions, a fact that is made evident by the absence of four systems from Table VI (F^- –Ne, I^- –Ne, Kr, Xe), by the absence of potential wells from the mobility potentials for all six systems in Table VI that involve He or Ne, and by poorer agreement between calculated and experimental R_m and ϵ values. We consider each of these three points in turn.

The absence of four systems from Table VI suggests that it would be worthwhile to try to develop a scheme to predict the scaling parameters v_o and ρ , for instance from the parameters of the delta-function model. Such a prediction scheme is discussed in Sec. IV.

The absence of potential wells from the mobility potentials of six systems in Table VI means that the scaling procedure can be viewed as operating in a predictive mode for these systems, extending the knowledge of $V(R)$ to larger R than covered by direct measurement. This also applies to $V(R)$ at small R , since there are beam data for only the six systems Cl^- –He, Ne, Ar, and Br^- –He, Ne, Ar.

The poorer agreement for R_m and ϵ values turns out to be within experimental uncertainties of the mobility potentials over their ranges of R , which are about 10–15% in the best cases and about 20–25% in the worst.⁷ To establish this fact we have made detailed comparisons, both of the scaled and mobility potentials themselves, and of the calculated and experimental transport properties.³⁰ For the present discussion it is sufficient to report just a statistical summary of the comparison with the transport measurements of the NOAA^{50–52} and Georgia Tech^{53–59} groups. The statistical comparisons are given in Table VII. The general conclusion to be drawn is that our values of δ and χ are acceptably small and comparable in magnitude to the ones obtained from the mobility potentials, which were fitted to the data, except for a few cases discussed below.

The first case that we note is F^- –Xe, for which the agreement for R_m and ϵ is not so good (Table VI). This is reflected by the poor agreement for K_o at high-field strengths shown by large values of δ and χ in Table VII.

TABLE VI. Potential parameters for halogen ion–noble gas systems.^a

System	$C_6(e^2 a_0^6)$	$C_8(e^2 a_0^8)$	$v_0(e^2/a_0)$	$\rho(a_0)$	$R_m(a_0)$	$\epsilon \times 10^3$ (e^2/a_0)	$\frac{(R_m)_{\text{calc}}}{(R_m)_{\text{exp}}}$	$\frac{\epsilon_{\text{calc}}}{\epsilon_{\text{exp}}}$
F ⁻ -He	8.658	157.5	0.09414	0.9797	5.63	0.563
Ar	60.11	1524	0.5180	1.028	5.46	5.20	1.04	1.03
Kr	84.69	2325	0.4200	1.105	5.01	9.98	1.07	0.99
Xe	126.9	3834	0.4143	1.206	5.10	13.3	1.10	0.84
Cl ⁻ -He	18.44	462.0	0.2026	1.008	6.53	0.360
Ne	38.00	1034	0.9543	0.9269	6.50	0.695
Ar	131.6	4292	1.330	1.020	6.25	3.68	1.05	0.97
Kr	187.7	6535	1.436	1.085	6.70	3.94	1.03	1.05
Xe	285.2	10753	1.568	1.122	6.45	7.62	1.07	1.05
Br ⁻ -He	22.82	589.2	0.2342	1.068	7.52	0.184
Ne	46.87	1313	1.018	0.9463	6.71	0.634
Ar	163.6	5462	1.662	1.033	6.63	2.95	1.04	0.98
Kr	233.9	8322	1.722	1.097	7.00	3.40	1.03	1.04
Xe	356.3	13705	1.789	1.144	6.85	6.14	1.07	0.99
I ⁻ -He	31.43	852.2	0.2858	1.118	8.36	0.112
Ar	227.3	7876	2.049	1.053	6.94	2.64	1.02	0.94

^a Experimental values of R_m and ϵ are from Ref. 7.

However, the disagreement for the mobilities is really just slightly beyond the range of experimental uncertainty, as shown in Fig. 7, so that the situation is not serious. The disagreement for the longitudinal diffusion coefficients appears more serious, but here there is doubt about the analysis of the swarm measurements.⁶⁰ Similar remarks apply to F⁻-Kr.

The second case is Br⁻-Ne, which has unusually large values of δ and χ in Table VII. The reason is that we have put greater emphasis on the beam data¹⁰ at small R in order to obtain more consistent values of the scaling parameters v_0 and ρ . The actual discrepancy between the transport and beam data is not too large, corresponding to about 7% in K_0 , as shown by an earlier direct comparison of the measurements.⁴⁸

In summary, the present scaled potentials for the halogen ion–noble gas interactions give reasonable agreement with the available transport and scattering data. However, the data available for the halogen ions are more limited than for the alkali ions, so our estimate of the uncertainty of the scaled potentials has to be increased to about 15–25% over their entire range of R .

IV. PREDICTION OF NEW POTENTIALS

The repulsive branches of the potentials for the interactions of closed-shell atoms and ions have been rather well correlated by parameters suggested by a delta-function model for the electron–nucleus attractions.¹² A connection between these parameters and the present scaling parameters v_0 and ρ would allow the prediction of the currently unmeasured potentials for the systems F⁻-Ne and I⁻-Ne, Kr, Xe. Such a connection is established in this section.

The delta-function model leads to a repulsive potential of simple exponential form,

$$V(R) = V_0 e^{-BR/\sigma}, \quad (14)$$

where σ is a distance-scaling parameter that is obtained from

Hartree–Fock–Slater calculations of atomic charge densities,⁶¹ and β is a universal constant whose numerical value depends on the choice of a reference system for σ . When the Ar–Ar potential is chosen as a reference system so that $\sigma_{\text{Ar}} = 1$, then $\beta = 3.66 \text{ \AA}^{-1}$ (for R in \AA); only the ratio β/σ is invariant to the choice of reference system. The parameter V_0 is related by the model to β/σ and to the number of electrons n in the atom or ion,

$$V_0 = \gamma n (\beta/\sigma), \quad (15)$$

where γ is a constant for a given family of the periodic table.

Values of n , σ , and γ are given in Table VIII for interactions between like closed-shell species. The unlike interactions are obtained from the combination rules,^{62,63}

$$\sigma_{12} = \frac{1}{2}(\sigma_1 + \sigma_2), \quad (16)$$

$$[(V_0)_{12}/\sigma_{12}]^{2\sigma_{12}} = [(V_0)_1/\sigma_1]^{\sigma_1} [(V_0)_2/\sigma_2]^{\sigma_2}. \quad (17)$$

We have found that a simple linear correlation between these parameters and the present scaling parameters v_0 and ρ holds fairly accurately among members of an isoelectronic series. For example, we find

$$\frac{(v_0)_{\text{F}^- \text{He}} - (v_0)_{\text{NeHe}}}{(V_0)_{\text{F}^- \text{He}} - (V_0)_{\text{NeHe}}} \approx \frac{(v_0)_{\text{NeHe}} - (v_0)_{\text{Na}^+ \text{He}}}{(V_0)_{\text{NeHe}} - (V_0)_{\text{Na}^+ \text{He}}}, \quad (18)$$

$$\frac{\rho_{\text{F}^- \text{He}} - \rho_{\text{NeHe}}}{\sigma_{\text{F}^- \text{He}} - \sigma_{\text{NeHe}}} \approx \frac{\rho_{\text{NeHe}} - \rho_{\text{Na}^+ \text{He}}}{\sigma_{\text{NeHe}} - \sigma_{\text{Na}^+ \text{He}}}. \quad (19)$$

From such relations it is straightforward to calculate the parameters of those halogen ion–noble gas interactions for which no direct measurements exist. These parameters are summarized in Table IX. We estimate that the overall accuracy of the resulting $V(R)$ is about 10–20% for large R and about 20–30% for small R , except for I⁻-Xe, which is probably somewhat less accurate. Testing of these predictions awaits further transport or scattering measurements.

TABLE VII. Deviations between measured and calculated transport coefficients of halogen ions in noble gases.

	Data type	Data reference	$T(K)$	Range of $E/N(Td)$	Data points	Data accuracy (%)	Deviations ^a			
							Mobility ^b		Present model	
							δ	χ	δ	χ
F ⁻ He	K_o	51	297	0-50	32	5	0.28	0.38	1.07	1.23
				50-100	12	4	0.09	0.27	0.59	0.65
				100-250	8	4	0.00	0.22	0.30	0.46
F ⁻ Ar	K_o	50	297	0-37	13	5	-0.16	0.24	0.26	0.72
				146-350	17	4	0.08	0.26	0.04	0.20
F ⁻ Kr	K_o	54	300	0-38	20	2	0.02	0.75	0.78	1.53
				158-300	13	2	-0.83	1.43	-3.34	3.53
F ⁻ Xe	K_o	54	300	0-40	22	3	0.12	0.70	-0.33	1.11
				190-310	4	5	0.24	0.51	-1.03	1.14
	$D_{ }$	54	300	0-40	22	15			0.39	3.29
				190-310	4	20			-5.02	5.28
Cl ⁻ He	K_o	49	297	0-50	26	5	-0.08	0.17	-0.85	0.86
				50-100	15	4	-0.04	0.10	-1.09	1.10
				100-250	18	4	-0.10	0.23	-0.84	0.86
Cl ⁻ Ne	K_o	52	300	0-60	25	2	-0.14	0.50	-0.87	0.95
				60-200	9	2	0.14	0.55	-0.59	0.81
				200-405	6	2	0.69	0.84	0.13	0.44
	$D_{ }$	53	300	0-60	25	10	0.04	0.52	-0.20	0.52
				60-200	9	10	0.66	0.73	0.40	0.56
				200-405	6	10	1.71	1.89	0.96	1.01
Cl ⁻ Ar	K_o	52	300	0-45	22	3	-0.06	0.79	0.61	0.87
				165-450	19	3	-0.19	0.40	-0.79	0.83
Cl ⁻ Kr	K_o	52	300	0-40	23	2	-0.11	0.33	-1.63	1.67
				145-450	12	2	0.02	0.39	0.50	0.60
	$D_{ }$	53	300	0-40	23	10	0.09	0.37	-0.15	0.45
				145-450	12	10	0.66	0.72	0.91	0.98
Cl ⁻ Xe	K_o	55	300	0-40	18	2	0.27	0.35	-1.19	1.29
				160-250	7	2	-0.53	0.60	0.79	0.88
				250-500	8	2	-0.47	0.59	0.17	0.23
	$D_{ }$	53	300	0-40	18	10	0.63	1.04	0.52	0.96
				160-250	7	10	0.47	0.51	0.83	0.87
				250-500	8	10	0.09	0.45	0.13	0.62
Br ⁻ He	K_o	49	297	0-50	32	5	-0.04	0.12	0.13	0.22
				50-100	15	4	0.10	0.13	0.03	0.08
	K_o	58	300	100-250	15	4	0.36	0.39	0.13	0.17
				0-60	21	2	0.11	0.39	-1.77	1.78
Br ⁻ Ne	K_o	56	300	60-200	15	2	-0.08	0.22	-1.54	1.55
				200-500	5	2	0.44	0.79	-1.46	1.60
	$D_{ }$	56	300	0-60	21	10	-0.92	0.99	-1.35	1.39
				60-200	15	10	-0.38	0.56	-1.26	1.33
				200-500	5	10	1.44	1.51	-0.12	0.31
Br ⁻ Ar	K_o	49	297	0-70	18	5	0.11	0.25	-0.27	0.44
				115-250	18	5	0.03	0.24	-0.43	0.47
	K_o	57	300	250-450	11	5	-0.02	0.16	-0.36	0.38
				0-50	7	2	-0.10	0.77	-1.76	1.89
Br ⁻ Kr	K_o	56	300	195-500	27	2	-0.01	0.36	-0.55	0.61
				0-50	7	10	-0.36	0.67	0.44	0.80
	$D_{ }$	56	300	195-500	27	10	0.05	0.27	0.42	0.52
				0-65	19	2	-0.27	0.84	-1.77	1.91
Br ⁻ Xe	K_o	57	300	280-400	4	2	-0.10	0.31	-0.45	0.63
				400-1000	8	2	-0.10	0.28	-0.50	0.59
				0-65	19	10	-0.07	0.40	-0.19	0.54
	$D_{ }$	56	300	280-400	4	10	0.38	0.49	-0.00	0.19
				400-1000	8	10	-0.47	0.78	-0.74	0.90
				0-50	34	5	0.03	0.13	-0.01	0.14
I ⁻ He	K_o	49	297	50-100	15	4	0.11	0.20	-0.01	0.16
				100-250	15	4	0.14	0.19	-0.15	0.20
I ⁻ Ar	K_o	50	297	0-55	20	5	0.03	0.10	-0.00	0.11
				55-160	23	5	-0.02	0.14	-0.32	0.46
				160-500	22	4	-0.09	0.27	-0.94	0.96

^a The definitions of δ and χ are given in Eqs. (12) and (13).^b Results from Ref. 7 and from additional calculations.

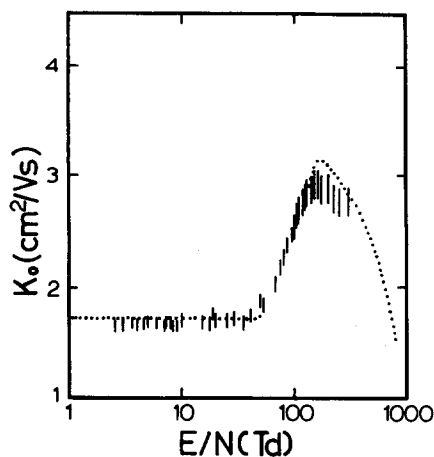


FIG. 7. Comparison of calculated and measured mobilities for F^- in Xe. The dotted curve is calculated from the present potential, and the error bars represent measurements from Ref. 53.

V. DISCUSSION

The main result of this work is that the exchange energies of noble gas–noble gas, alkali ion–noble gas, and halogen ion–noble gas interactions scale with only two parameters, each to a different universal interaction curve. Total potentials are then obtained by adding on the damped longer range Coulombic energies. We estimate that the resulting $V(R)$ are accurate within a few percent for the noble gas systems, within about 10–20% for the alkali ion systems, and within about 15–20% for the halogen ion systems. These uncertainties are generally no worse than the uncertainties of the corresponding potentials as obtained directly from experiments. The correlation, however, extends many experimental $V(R)$ to larger and smaller R than covered by the experiments.

The connection of the scaling parameters with the parameters of the delta-function model enabled predictions to

TABLE VIII. Parameters of the delta-function model, Eqs. (14) and (15).^a

	n	σ	$\gamma(eV \cdot \text{\AA}^2)$
He	2	0.840	6.83
Ne	10	0.791	18.7
Ar	18	1.000	18.7
Kr	36	1.087	18.7
Xe	54	1.214	18.7
Li^+	2	0.511	17.4
Na^+	10	0.618	35.4
K^+	18	0.828	35.4
Rb^+	36	0.920	35.4
Cs^+	54	1.042	35.4
F^-	10	1.040	8.5
Cl^-	18	1.232	8.5
Br^-	36	1.317	8.5
I^-	54	1.446	8.5

^aThe results are normalized to $\sigma_{Ar} = 1$.

TABLE IX. Parameters for predicted halogen ion–noble gas potentials.

System	$C_6(e^2 a_0^6)$	$C_8(e^2 a_0^8)$	$v_0(e^2/a_0)$	$\rho(a_0)$	$R_m(a_0)$	$\epsilon \times 10^3$ (e^2/a_0)
F^- –Ne	18.17	367.4	0.2791	0.8890	4.61	2.79
I^- –Ne	64.21	1886	0.9363	1.081	8.66	0.148
I^- –Kr	326.3	12014	1.680	1.157	7.55	2.61
I^- –Xe	499.2	19817	3.758	1.061	6.45	9.59

be made for the $V(R)$ curves for four halogen ion–noble gas systems for which no experimental measurements were available.

In the case of the noble gas interactions the present universal correlation reduces the number of parameters required for the formulation of a corresponding-states principle by two. In the case of the ion–atom systems it quantifies the failure of ion transport data to follow a corresponding-states principle, since only the exchange energies follow a universal scaling rule.

The fundamental reasons for the scaling universality are not obvious. On the one hand, the universality may reflect some deep order in the quantum mechanics of interacting closed-shell systems. On the other hand, the universality may merely reflect the fact that $V_{ex}(R)$ is a rather featureless curve, so that it is not surprising that only two parameters are required to characterize it.

Finally, we expect similar scaling principles to hold for other closed-shell systems, such as those involving doubly charged alkaline-earth ions, but lack of data at present prevent such applications.

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