Determination of the Interatomic Potential of Krypton

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(Received 10 May 1973)

New measurements of the differential collision cross section for Kr + Kr are presented and, together with previously published data, are analyzed in terms of a Morse–Spline–van der Waals interatomic potential function. By means of a least-squares fitting procedure a potential is obtained which best describes the measurements. This potential also predicts second virial coefficients and vibrational-level spacings that agree well with experiment. Some of the difficulties that arise in attempting the inversion of scattering data in this and similar systems are discussed. Finally, we present a comparison with some low-temperature solid-state data.

I. INTRODUCTION

Recently, under the crossfire of molecular beams,[1,2] spectroscopy,[3] and the reanalysis of bulk properties in terms of flexible multiparameter potential functions,[4-6] the long-standing problem of the realistic description of the ground-state interaction of two argon atoms has been essentially solved. Small discrepancies obviously remain, but we now appear to be almost at the point where even the nature of many-body forces in condensed phases can be discussed quantitatively.

It is then logical and useful to apply the same techniques to the next-heavier noble gas, krypton. There are at least four reasons for carrying out such a study. First, the availability of a radioactive Kr isotope has generated a series of data referring to experiments which are particular to this gas.[7,8] Second, the precise knowledge of the interatomic forces in krypton will allow a check on the validity of combination rules for interactions between unlike molecules.[9] Third, it may also allow for the determination of how strictly the principle of corresponding states holds,[10,11] and finally, the important problem of the three-body-forces contribution to condensed-phase properties needs to be examined in more than the one system in which it has been studied so far—argon.[5,6]

In 1971, working along the same lines as for Ar_2, Bobetic[12] produced a potential for the Kr_2

dimer.[13] As with the Bobetic-Barker potential for Ar_2, the Bobetic Kr_2 potential was shown to describe inadequately the differential collision cross sections for the Kr + Kr system that were first measured by Cavallini *et al.*[14] Moreover, a recent calculation[15] of the lattice constant of solid Kr at high temperatures confirms the inadequacy of Bobetic's Kr_2 potential. Differential collision cross sections for the Kr + Kr system were also obtained at one energy by Schafer, Siska, and Lee[16] and the data fitted by a potential of the Morse–Spline–van der Waals (MSV) form. An improved analysis of the same data produced a new set of MSV parameters that are quoted by Docken and Schafer[17] in their recent study of the spectroscopic levels of the Kr_2 dimer. However, it appears that neither of these MSV potentials is entirely satisfactory when solid-state properties are considered. Accordingly, in an attempt to resolve this problem, we have extended the differential collision cross-section measurements for Kr + Kr to a lower energy than those in previously published results.[14] A potential for Kr_2 is obtained by fitting the experimental data to cross sections calculated with a MSV potential function along with the added constraint provided by the spacings of the first few vibrational levels of the Kr_2 dimer. Our potential is compared with other existing Kr_2 potentials. Finally, we compare experimental second virial coefficient and solid-state properties with values calculated starting from our potential.

II. EXPERIMENTAL

The experimental setup has been previously described.[18] It makes use of a crossed out-of-plane beam geometry with an angular resolution of about 0.5°. The relative energies of collision of the three series of data used to obtain the potential are reported in Table I, along with the Mach number of the supersonic primary beam and the temperature of the secondary multichannel beam source. The resulting velocity resolution full width at half-maximum (FWHM) is, in any case, about 15%. No measurements have been performed at lower energies because of suspected primary-beam condensation.

Beam velocities and Mach numbers have been determined by beam analysis with a slotted-disk velocity selector. A leveling off of a Mach-number-versus-beam-parameters curve (increasing pressure and decreasing stagnation temperature) has been taken as indication of beam condensation.

III. ANALYSIS

The experimental results are compared in the LAB system with the calculated cross sections as outlined below.

Following Munn and Smith,[19] and adopting their notation, we calculate numerically the approximate "low-resolution" scattering amplitudes

$$|f^+(\theta)|^2 + |f^-(\theta)|^2 + |f^+(\pi - \theta)|^2 + |f^-(\pi - \theta)|^2 ,$$

where the contribution from the $\pi - \theta$ angle accounts for the lack of mass selectivity of our detector. We then convert the cross section to the LAB system and perform the averaging over the relative velocity, which is constructed using 81 different points. Finally, at small angles, we take into account the loss in resolution due to the non-negligible detector height (detector dimensions 0.3×3.0 mm; detector-scattering center distance 55 mm). The present data were found to be inappropriate (see Sec. V) for a direct inversion procedure, mainly because the damping and shifting of the rainbow oscillations by the finite velocity resolution was too large.

TABLE I. E is the relative energy of collision; k is Boltzmann's constant; M is the primary-beam Mach number; and T is the secondary-beam source temperature.

E/k (K)	M	T (K)
916	13.5	91
760	18.7	91
613	20.1	85

We then decided to adopt a fitting procedure, but, in order to save some advantages of the inversion method, we deduced the starting potential for the fit using inversion techniques.

We started from the measured positions of the rainbow oscillations, applied a correction due to the finite resolution, and determined the deflection function as described in Ref. 20. Then the potential was obtained by direct integration over the deflection function.[20] Thus the range of the potential to which the data are sensitive and a well-behaved starting potential are obtained. In order to determine finer details of the potential and to account for an exact averaging process, the points obtained by inversion were fitted to an analytical potential as follows:

$$V(r) = \epsilon f_M(x, \beta), \quad 0 < r < r_1$$

$$V(r) = \sum_{k=0}^{3} a_k z^k, \quad r_1 < r < r_2 \text{ with } z = (r - r_1)/(r_2 - r_1)$$

$$V(r) = -C_6 r^{-6} - C_8 r^{-8}, \quad r_2 < r < \infty$$

$$f_M = e^{2\beta(1-x)} - 2e^{\beta(1-x)}, \quad x = r/r_m$$

ϵ is the potential minimum and r_m is the internuclear distance corresponding to the minimum. This form of the potential has been chosen in order to decouple the repulsive part and the minimum from the asymptotic part of the potential, which can be varied independently.[21]

The long-range attraction is described by a dispersion potential including dipole-dipole and dipole-quadrupole terms. The well and the short-range repulsion are represented by a Morse potential. The different parts are connected by a cubic spline function

$$V(r) = \sum_{k=0}^{3} a_k z^k \text{ with } z = (r - r_1)/(r_2 - r_1).$$

The coefficients a_k are completely determined by the two end points of the interval and the first derivatives at these points. The special requirements of this type of spline function provide a continuous connection with a continuous first and nonzero second derivative at the connection points.

The final adjustment of the free parameters was then performed using a nonlinear least-squares procedure[22] to find the minimum of

$$\chi_k^2 = \sum_{i=1}^{N_k} [(I_{ik}^{obs} - C_k I_{ik}^{cal})/\Delta I_{ik}^{obs}]^2 ,$$

k is the index of a single group of data (e.g., the differential cross sections belonging to one energy) with N_k data points. I_{ik}^{obs} is the measured and I_{ik}^{cal} the calculated data point in the LAB system for each measured value. ΔI_{ik}^{obs} is the error of the

reference point. C_k is an additional free parame-
ter employed in order to adjust the absolute value
of the cross section. The criterion that a poten-
tial fits the data is that

$$\chi_{tot}^2 = \sum_{k=1}^{n} \chi_k^2$$

is minimal, where n is the number of data sets.
$N_k = 23, 24,$ and 22 for $k = 1, 2,$ and 3, respectively.

It should be noted that the significance of χ^2 as
a statistical measure of the compatibility between
a model and a data set is only valid if the data
represent a complete statistical distribution or if
the model fully describes the physics. Unfortu-
nately, in almost all physical applications, both
of these conditions break down. Therefore the χ^2
values should be considered as a quantitative
measure to distinguish between models. In addi-
tion, they provide the possibility of extracting
error bounds for the best-fit parameters.

IV. RESULTS

The procedure described above was applied to
three different sets of data. $k = 1, 2,$ and 3 cor-
respond to relative energies of collision E/k
$= 916, 760,$ and 613 K, respectively. The parame-
ter C_6 was fixed at the value $C_6/k = 908\,000$ K Å^6,
in order to agree with the most recent theoretical
estimate.[23] After some preliminary experimenta-
tion, the connection points were fixed at $r_1 = 4.5$ Å
and $r_2 = 5.0$ Å. The parameters ϵ, r_m, $C = C_8/C_6$,
and the normalization constant C_k were left free
in the minimization procedure. Unfortunately, the
χ^2 were found to be energy dependent such that the
lowest energy produced the largest χ^2. However,
condensation of the primary beam, or other ener-
gy-dependent experimental errors, such as over-
estimation of energy resolution, could not be
excluded. We account for this by giving a greater
weight to the data at higher energies. The relative
importance of the measurements has been esti-
mated by comparing the amplitude of the calcu-
lated cross-section oscillations with the measured
ones at the three different energies.

The parameter β was fixed at the values 6.2
and 6.3, which were indicated as the most likely
values to give agreement with the slope of the
level spacings versus level number plot of the
spectroscopy data recently obtained by Tanaka.[24]
Potential Nos. 2 and 3 of Table II were so ob-
tained. Afterwards all parameters were kept con-
stant and β changed to 6.1 and 6.4, obtaining po-
tential Nos. 1 and 4. If a Morse potential is
assumed in the bowl (as we did), the slope is
simply related to β, but one has to keep in mind
that only for the first few levels can one approxi-

TABLE II. Results of the fitting of scattering and
virial data. $\chi_{1,2,3}^2$ are the χ^2 values corresponding to
the three experimental energies: $1 = 916$ K, $2 = 760$ K,
and $3 = 613$ K. $\chi_{1+2+3}^2 = \chi_1^2 + \chi_2^2 + \chi_3^2$. χ_4^2 is the χ^2 value ob-
tained by comparison with virial-coefficient data for Kr
obtained from Ref. 25. $\chi_{tot}^2 = \chi_{1+2+3}^2 + \chi_4^2$.

Potential	ϵ/k (K)	r_m (Å)	χ_1^2	χ_2^2	χ_3^2	χ_{1+2+3}^2	χ_4^2	χ_{tot}^2
Ref. 12	197.7	4.01	311	186	82	579	45	624
Ref. 17	198.8	4.11	71	49	38	158	28	186
Present 1 $\beta = 6.1$	200	4.03	46	53	49	148	30	178
Present 2 $\beta = 6.2$	200	4.03	47	49	48	144	13	157
Present 3 $\beta = 6.3$	200	4.03	49	47	48	144	18	162
Present 4 $\beta = 6.4$	200	4.03	53	46	48	147	43	190
Solid state	200	4.012	61	52	49	162	19	181

mate the potential with a Morse form.

The results are summarized in Table II along
with the results of a fit to the virial coefficient
data for Kr.[25] In the same table, corresponding
numbers are reported for the Kr potentials pro-
posed by Bobetic[12] and Schafer.[17] The χ^2 value for
an "adequate" model and a "good" set of data
should be the expectation value; that is, the num-
ber of degrees of freedom (equal to the number of
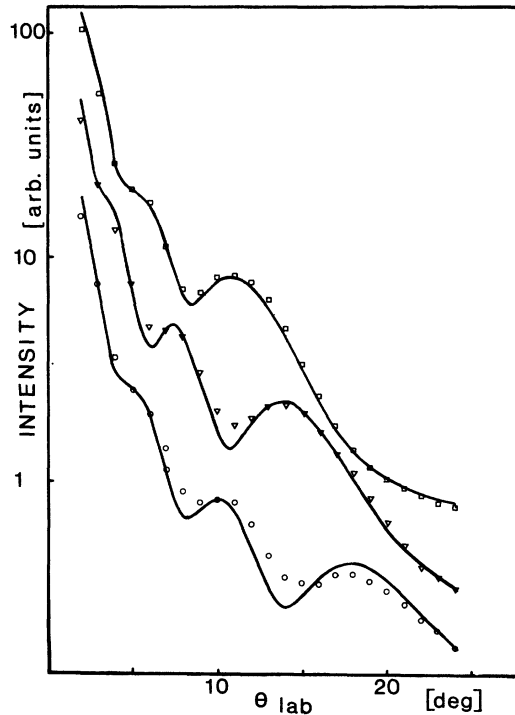data points minus the number of free parameters).

FIG. 1. Differential-collision cross-section data for
Kr compared with calculations (full line) using potential
No. 3 obtained with the best-fit procedure described in
the text (potential No. 2 gives indistinguishable results).
$E/k = \square$, 916 K; ∇, 760 K; $\bigcirc$, 613 K.

TABLE III. Potential parameters for potential No. 2 and 3.

Parameter	Potential No 2	Potential No 3
C_6/k (K Å^6)	908 000	908 000
C_8/C_6	10.9 ± 2	10.9 ± 2
ϵ/k (K)	200 ± 4	200 ± 4
r_m (Å)	4.03 ± 0.04	4.03 ± 0.04
r_1 (Å)	4.5	4.5
r_2 (Å)	5.0	5.0
β	6.2	6.3
a_0 (K)	-147.01	-145.84
a_1 (K Å^{-1})	76.856	78.034
a_2 (K Å^{-2})	-18.172	-24.022
a_3 (K Å^{-3})	4.8747	8.3822

The χ^2 values of Table II are still too high. This could be due to the inflexibility of the model or the incompleteness of the data set (for instance errors in the energy calibration and/or the averaging procedure). Nevertheless, it is possible to derive error bounds for the parameters by renormalizing the χ^2 to the expectation values. Figure 1 displays in graphical form some of the results. Potential parameters for the two best potentials (Nos. 2 and 3) are listed in Table III.

V. DISCUSSION

A. Possibility of an Inversion Procedure

Since an inversion procedure[20,26,27] is the most elegant tool for determining the potential from the measured cross section, we first investigated this possibility. At each of the three energies two or three (at the lowest energy) rainbow maxima were resolved. Due to the finite-velocity resolution (15% FWHM) the positions of these extrema were shifted and the amplitude of the oscil-
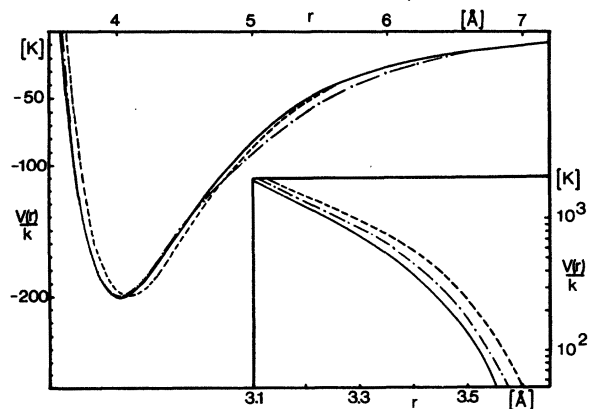

FIG. 2. Present potential No. 3 for Kr (full line) compared with potential of Ref. 17 (broken line) and Ref. 12 (dash-dotted line).

lations damped. This could be verified by trial calculations performed using the averaging procedure described above. The procedure of Ref. 20 needs as input information a well-resolved rainbow structure (at least five extrema, this condition being met by the present data), the rapid oscillations, and some additional requirements for the continuity of the deflection function. If the rapid oscillations are not resolved, some other information can be used, such as the amplitudes of the rainbow oscillations or the large-angle scattering.[28,29] As can be seen from Figs. 1 and 2, the present data can only be inverted if the amplitudes of the rainbow extrema, (i.e., the cross section itself) are used as input. Nearly the same criteria hold for other inversion procedures.[26,27] For example, in Ref. 26 adjusting the poles in the complex-momentum plane requires a comparison with the cross-section data themselves.[30] In all cases the cross sections should not be affected by any kind of an averaging process. Since the deconvolution of our data seems to be impossible, there remains the possibility of performing the averaging of the cross section directly, but such a procedure requires the generation of phase shifts at different energies from the data at one energy, and hence all the advantages of an inversion process are lost.

B. Scattering data

As can be seen in Table II both our best-fit potential and the potential of Ref. 17 describe the scattering data quite well. Not unexpectedly, the scattering results are rather insensitive to r_m. However, it is disappointing that both the present minimalization procedure and that of Schafer et al. should produce r_m values that differ by as much as 2%. The fact that, this difference notwithstanding, the two potentials, which are compared in Fig. 2, give very similar differential collision cross sections is, however, not surprising, and is in agreement with the findings of Boyle,[31] who recently analyzed the reliability of potentials extracted from rainbow data. A useful complement to the analysis of Boyle has been recently reported by Farrar et al.[32] in a paper in which they show the use of wide-angle scattering and/or virial-coefficient data for the resolution of such ambiguities. In the present work we have chosen to constrain our fit with the spectroscopic properties of the dimer. In Fig. 2 the potential of Ref. 12 is also reported. The value of r_m is the same as for our potential, but the outer attractive wall has quite a different slope. Therefore, scattering efficiently discriminates between the two (see Table II and Ref. 14).

C. Spectroscopy

Recently, Tanaka[24] has extended the uv spectroscopy measurements already performed on argon[3] to Kr dimers. As specified in Sec. IV., we have already used part of the information contained in the spectroscopy results as a constraint to our potential model. Nevertheless, since the slope of the level-spacing-versus-vibrational-quantum-number plot (which gives β for our model) is not the only information contained in the spectroscopic data, it is worthwhile to perform a direct comparison of the experimental-level spacings with the values calculated for $^{84}Kr\,^{84}Kr$ from our potential. Sixteen bound levels were found in this way, and their spacings are reported in Table IV.

Figure 3 compares the experimental vibrational spacings with those calculated by Docken and Schafer[14] and with the ones calculated with our potential No. 3. The agreement between the predictions of both potentials with experimental data is rather good. The agreement between the two sets of predictions notwithstanding, the differences between the two potentials are once again not surprising, since the level spacings are related only to the width of the potential well. As can be seen in Fig. 2, the well widths of the two potentials are very similar, particularly for the deeper levels. When spectroscopists succeed in resolving the rotational structure of the vibrational spectrum, they should be able to readily distinguish between different r_m values. The ϵ/k value obtained from the experimental-level spacings using Le Roy's

method[33] is 199.2 (± 0.7) K, which is in pleasingly good agreement with the present results.

D. Gaseous Bulk Properties

Comparisons between predictions of the present Kr potentials and experimental virial-coefficient data are reported in Fig. 4. Except for the lowest temperatures, the agreement is generally good. However, we do not attach too much importance to this agreement because the experimental data do not span a range of reduced temperatures wide enough to offer a narrow constraint to the potential. For this reason we did not calculate viscosity coefficients.

VI. SOLID-STATE PROPERTIES

Kr crystallizes into a face-centered cubic solid at 115.8 K. The lattice constant,[34] isothermal compressibility,[35,36] and heat capacity[37] are known as a function of temperature all the way down to liquid-He temperatures, and some information is also available on the elastic constants.[38] Procedures for evaluating the partition function, and hence the thermodynamic properties, exist.[39,40] In particular, if the temperature is quite low (less than $\frac{1}{3}$ of the melting temperature) the standard techniques of lattice dynamics apply, while at higher temperatures it is necessary to
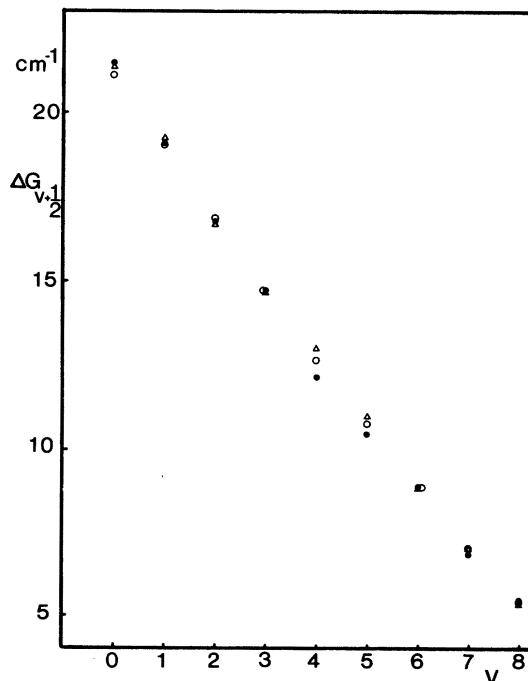
TABLE IV. $^{84}Kr_2$ ground-state vibrational spacings: a are the values calculated from present potential No. 2; b are the values calculated from present potential No. 3; c are the experimental values: Ref. 24.

v	$\Delta G_{v+1/2}$ (cm^{-1})		
	a	b	c
0	21.08	21.39	21.56
1	19.06	19.26	19.09
2	16.83	16.81	16.76
3	14.86	14.74	14.76
4	13.17	13.10	12.23
5	11.13	11.07	10.49
6	9.07	9.00	8.92
7	7.18	7.11	6.92
8	5.48	5.42	5.54
9	4.00	3.94	
10	2.74	2.69	
11	1.72	1.68	
12	0.94	0.90	
13	0.39	0.38	
14	0.09	0.08	

FIG. 3. $^{84}Kr_2$ ground-state vibrational spacings: ●, experiment (Ref. 24); △, present potential No. 3; ○, potential of Ref. 17.
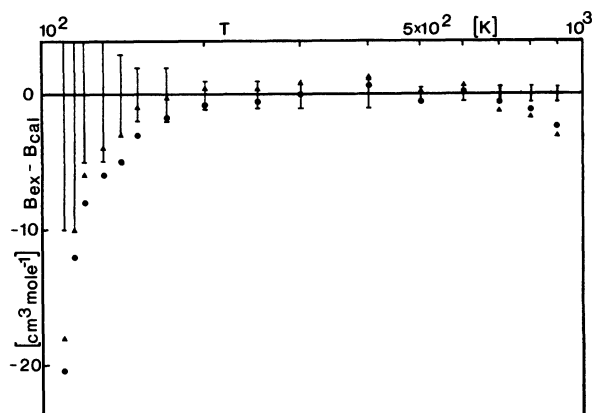
FIG. 4. Virial-coefficient data for Kr (Ref. 25) compared with values calculated from our potential Nos. 2 (▲) and 3 (●). The vertical bars represent the error in the experimental values.

use computer-simulation techniques such as Monte Carlo calculations.

In this preliminary study of solid Kr we will restrict ourselves to 0 K, where the complications due to vibrational anharmonicity are reduced. We shall adopt the working hypothesis that the potential energy of the solid can be expanded as

$$V = \sum_{i > j} \phi_{(i,j)}^{(12)} + \sum_{i > j > k} \phi_{(i,j,k)}^{(123)} ,$$

where i, j, k label atoms in the crystal, $\phi^{(12)}$ is the two-body potential just determined, and $\phi^{(123)}$ is the three-body potential. We shall further assume that $\phi^{(123)}$ is adequately approximated by the long-range–triple-dipole–Axilrod-Teller-Muto (ATM) form:

$$\phi_{(i,j,k)}^{(123)} = \nu(1 + 3 \cos\theta_1 \cos\theta_2 \cos\theta_3)(R_1 R_2 R_3)^{-3} ,$$

with $\nu = 220.4 \times 10^{-12}$ erg Å^9. This force can be regarded as the screening of the pairwise long-range induced dipole interactions between atoms by the other atoms of the solid. The third virial coefficient of argon, as well as both its solid and liquid properties, appears to be satis-

factorily explained by this approach.[4-6,15]

We have evaluated the free energy and pressure as a function of the volume at 0 K using a self-consistent phonon scheme,[41] and in this way we have obtained the ground-state energy, pressure, and the bulk modulus (inverse compressibility). The results are shown in Table V, both with and without the three-body ATM force. As can be seen, the scattering potential obtained in the present paper with the three-body ATM force produces data in fairly good agreement with experiment. The pressure-volume data, together with some theoretical predictions, are displayed in graphical form in Fig. 5.

Before concluding this section a few general remarks are in order about the information on the position of the potential minimum available through solid-state properties.

In the classical solid at 0 K, if we have only interactions between the 12 nearest neighbors in the fcc lattice, and if the forces are pairwise additive, the inversion symmetry of the crystal demands that the atoms all sit at the potential minimum r_m. In a real solid, the range of the potential extends beyond the nearest neighbors and is attractive [the six second-neighbors are at $\sqrt{2}\, r_m$, where the potential is assumed to be $-(C_6/r^6) - (C_8/r^8)$]. This causes the crystal to collapse, so that the nearest-neighbor distance r_{NN} is less than r_m. The exact magnitude of this effect can readily be evaluated, once C_6 and C_8 are known, and amounts to $r_m - r_{NN} = 0.08$ Å for Kr. The next effect to be considered is that of three-body forces. The long-range ATM forces arise as a screening of the two-body London (van der Waals) forces by the other atoms in the solid. This effect is also exactly known and causes $r_m - r_{NN} = -0.04$ Å in krypton. Little is known about short-range-exchange many-body forces, except that they are believed to be smaller than ATM forces. Finally, we must consider the thermal motion of the atoms, which at 0 K is due to the zero-point energy. This causes the crystal to dilate such that $r_m - r_{NN} = -0.02$ Å. These three effects are essentially model independent. The r_{NN} in Kr is

TABLE V. Values of energy E, pressure P, bulk modulus $1/\chi_T$, and debye Θ at 27.10 cm³ mole⁻¹ and 0 K. Pot. A =present 2; Pot. B=present 3; Pot. C=same form as present 3, shifting r_m to 4.012 Å.

	Pot. A+ATM	Pot. A	Pot. B+ATM	Pot. B	Pot. C+ATM	Pot. C	Expt.
E (K)	−1340	−1459	−1338	−1457	−1344	−1463	−1342 ± 5 [a]
P (bar)	+445	−650	+497	−597	1	−1094	∼0 [b]
$1/\chi_T$ (Kbar)	36.2	31.8	37.7	33.3	34.6	30.2	34.4 ± 0.4 [c]
Θ_D (K)	70.0	69.7	71.5	71.2	69.4	⋯	71.9 ± 0.2 [d]

[a] Reference 35.
[b] Reference 32.
[c] References 33 and 34.
[d] Reference 42.

NEAREST-NEIGHBOR SEPARATION (Å)
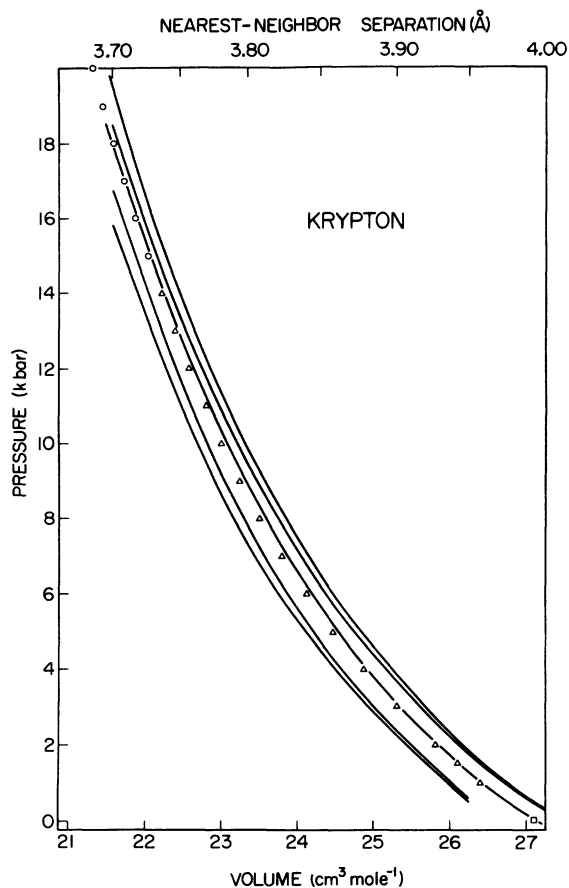
KRYPTON

VOLUME (cm³ mole⁻¹)

FIG. 5. Pressure-volume solid-state data for Kr. O and Δ experiment (Ref. 43). Full lines represent calculations with potential (from low to high): No. 2, No. 3, No. 3 (with r_m shifted to 4.012 + ATM force), No. 2 + ATM, No. 3 + ATM.

known experimentally to be $3.99\,225 \pm 0.00\,005$ Å at 4.25 K. We then have the following equations:

$$r_m = r_{NN} + 0.08 - 0.04 - 0.02 = 4.01 \text{ Å}$$

or

$$r_m = r_{NN} + 0.08 - 0.02 = 4.05 \text{ Å},$$

depending upon whether or not the three-body forces are present. Schafer's value of 4.11 Å for r_m will produce about a 4% error in the zero-pressure volume of the solid, even if there is no three-body effect on the pressure. This result is totally unacceptable.

From the foregoing we conclude that in contrast to the work of Schafer et al., our results are consistent with the hypothesis that the ATM force is the only one important for the energy, that at least 50% of it contributes to the pressure, and possibly slightly less to the bulk modulus. This conclusion, if taken at face value, appears to

complement the finding of Dymond and Alder[44] for argon. Nevertheless, on these grounds alone we cannot claim strictly that for the pressure and the bulk modulus the hypothesis is either demonstrated or refuted, since the errors in our r_m, although roughly equal to 1%, are still too large. More convincing evidence for this hypothesis can be obtained by examining Table V and Fig. 5 in detail. Here we see that a mere shift of r_m from 4.03 to 4.012 Å gives an almost perfect fit to the zero-temperature PV data of the solid if the ATM three-body force is included. Moreover, this "solid-state" potential is only marginally worse for gas properties than our best two potentials (see Table II). Unfortunately, this "solid-state" MSV potential gives the worst value for the low-temperature Debye Θ in the solid! (see Table V). Since this latter property is relatively insensitive to three-body forces, it appears to add weight to our "gas" potentials. It is therefore impossible at present to reconcile completely a single MSV potential plus the three-body ATM forces with all the gas and solid-state data. The difficulty may be due to inadequacies in the MSV functional form, the ATM three-body approximation, errors in the experiments, or any suitable combination of the three.

VII. CONCLUSIONS

Through the analysis of scattering measurements, a potential has been obtained for Kr that also describes spectroscopic and bulk gaseous properties quite well. Solid-state data are consistent with the hypothesis that three-body forces are present in the solid, and that for the energy they are quantitatively accounted for by the ATM triple-dipole term. For the pressure this happens to be at least good to 50%. In order for this latter hypothesis to be tested with 10% precision a non-condensed state property is needed that yields the r_m parameter of the potential with about a 1‰ precision. This must await a new generation of experiments.

Within the limits outlined in Sec. V, the present potential is believed to be accurate in the attractive and the low-energy repulsive region. Modifications of the higher-energy repulsive branch may be needed in order to describe high-temperature transport properties or other properties that are sensitive to changes in that part of the potential.

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