POTENTIALS OF REPULSIVE INTERACTION BETWEEN ATOMS OF NOBLE GASES

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Abstract

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POTENTIALS OF REPULSIVE INTERACTION BETWEEN ATOMS OF NOBLE GASES

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The study of the forces of interaction of atoms and molecules in the region of repulsion is of great practical and theoretical interest. In a fairly wide interval of interparticle distances the repulsive interaction of atoms can be described by a power law of the form $V(r) = K/r^s$, with constant values of K and s. For such a potential the classical theory of scattering gives a simple relation between the effective cross section for scattering through small angles and the parameters of the potential, the relative energy of the interacting particles, and the aperture. Using data on the scattering of fast beams of neutral atoms, in the present work, by a method analogous to that described in ([1]), the parameters of the potential functions K and s have been obtained for the heavy noble gases (Kr, Xe) and their combinations with light gases.

Table 1

Values of the parameter of the potential $V = K/r^s$ [eV] for the systems studied

System	Experimental K	Experimental s	Experimental Δr, Å	Combined K	Combined s
Kr–Kr	1382	7.7	2.4–3.02	–	–
Xe–Xe	463	6.35	2.48–3.09	–	–
He–Kr	45.3	5.52	1.67–2.04	61.5	5.8
Ne–Kr	437	7.65	2.15–2.52	330	7.67
Ar–Kr	855	6.92	2.4–3.1	486	6.88
He–Xe	35.2	5.2	1.73–2.2	36.1	5.12
Ne–Xe	210	6.76	2–2.56	190	7
Ar–Xe	292	5.9	2.48–3.27	282	6.25
Kr–Xe	875	7.1	2.44–3	802	7.02

Table 1 gives the parameters of the potential functions for the gases studied and the range of distances in which these parameters are valid, i.e., may be regarded as constant. The data obtained make it possible, for all combinations of pairs of noble-gas atoms, to test the empirical combining rule widely used for describing the properties of gas mixtures in the low-temperature region ([2]).

The values of the combined parameters for interaction potentials of the form $V_{ij} = K_{ij}/r^{s_{ij}}$ are determined from the relations

$$s_{ij} = \frac{1}{2}(s_{ii} + s_{jj}), \qquad K_{ij} = \sqrt{K_{ii}K_{jj}},$$

where the indices i and j denote the kind of atom. The values of the parameters found in this way are also given in Table 1.

The distances for which the parameter values are valid are found as the arithmetic mean of the corresponding distances for the combined homogeneous systems. The values of the potential parameters for atoms of the light noble gases were taken from work ([1]).

Comparison of the combined values with those found experimentally (comparison of the values of the potential energy themselves is more meaningful) reveals, for all systems, good fulfillment of the combining rule. In this case the values of the interaction energies agree to within 15-20% for all systems, except Ne–Kr and Ar–Kr, where the agreement is somewhat worse. This discrepancy is apparently explained by the fact that

that as the steepness of the potential s increases, the accuracy in determining the other parameter K decreases markedly, since the value of K is proportional to the experimentally found value of the effective scattering cross section to the power $s/2$. For identical errors in determining the effective cross sections, the error in determining K grows as s increases; apparently for this reason, at lower values of s, the agreement between the experimental and combined potentials is much better and, in individual cases, the discrepancy does not exceed 10%.

A comparison of the potential curves for Xe–Xe and Kr–Kr with the experimental data ([3]) reveals a noticeable discrepancy for Xe–Xe and good agreement for Kr–Kr. For the heavy gases, the systematic discrepancy of the values of s with the data of work ([3]), noted in ([1]), by an amount approximately equal to 2, is retained.

When the data obtained are compared with the results of theoretical calculations based on the statistical model ([4]), one may expect that for heavy gases, owing to the greater validity of the statistical model, the agreement will be better. Unfortunately, in this case practically all the experimental data turn out to refer to distances exceeding the limiting radii of the model ([4]). For these distances the data obtained can be compared only with extrapolated calculated values. Such a comparison showed that for the systems Kr–Kr and Xe–Xe, over the entire interval studied, the calculated values are approximately twice as large as the experimental ones. For mixed systems the agreement with the results of ([4]) is somewhat better. Such a discrepancy apparently makes the extrapolation of calculations performed for the Thomas–Fermi–Dirac model to distances exceeding the limiting radius insufficiently justified.

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REFERENCES

1. A. B. Kamnev, V. B. Leonas, DAN, **162**, No. 4 (1965).
2. J. Hirschfelder et al., *Molecular Theory of Gases and Liquids*, IL, 1961.
3. J. Amdur, E. A. Mason, *Phys. Fluids*, **1**, 370 (1958).
4. A. A. Abrahamson, *Phys. Rev.*, **130**, 693 (1963); **133A**, 990 (1964).

Note: Figure translations are in progress. See original paper for figures.