# INTERACTION POTENTIALS OF H, He ATOMS AND H$_{2}$ MOLECULES

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Fig. 1

Figure 1: Fig. 1

## Abstract

## Full Text

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# INTERACTION POTENTIALS OF H, He ATOMS AND $H_2$ MOLECULES

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The investigation of interatomic short-range forces for H and He atoms and $H_2$ molecules is of considerable practical and theoretical interest. In practical terms, information on the interaction forces (potential) is valuable, since it makes it possible to calculate the kinetic properties (coefficients of viscosity, diffusion, etc.) of gases containing these components. Data on the potential function for $H_2$—$H_2$ and H—$H_2$ in the interaction-energy range 0.25-2.5 eV make it possible, by methods of kinetic theory, to calculate the values of the transport coefficients of hydrogen in the temperature interval 2500-25 000° K. The study of these systems is also of interest in view of the fact that only for them are accurate quantum-mechanical calculations of the interaction energy possible. Comparison of experimental data and calculations makes it possible to check the correctness of the available theoretical results and the validity of the approximations used in the calculation.

A well-developed method for determining short-range interatomic forces is the study of the elastic scattering of fast beams of neutral particles on gas targets (1). In the present work, using an apparatus analogous to that described earlier (2), the dependences of the effective total cross sections for elastic scattering $Q(\theta_0)$ on the energy $E$ were investigated in the range 600-4000 eV for the systems H—He, H—$H_2$, He—He, He—$H_2$, and $H_2$—$H_2$.

**Fig. 1**

Figure 1 shows, on a double logarithmic scale, the dependences of $Q(\theta_0)$ on $E$ for these systems. To obtain the cross-section values for the systems He—He, $H_2$—$H_2$, and H—He, the values in Fig. 1 should be multiplied by scale factors equal, respectively, to 1.2, 0.95, and 0.54.

The absolute values of the cross sections were obtained by averaging over a large number ($\sim 10$) of separate measurements, as a rule with a threefold repetition of independent measurements of the entire curve. Under these conditions, a deviation from monotonic behavior of ±2.0% is considered to exceed the limits of the measurement error, and therefore the dependence of $Q(\theta_0)$ on $E$ for the H–$H_2$ system is "anomalous."

In the case of scattering through small angles with a spherically symmetric interaction potential of the form $V = K/r^n$, the effective total scattering cross section $Q(\theta_0, E)$ in the classical approximation can be described by the expression ($^3$)

$$Q(\theta_0, E) = \pi \left(KC(n)/\theta_0 E\right)^{2/n}, \tag{1}$$

where $E$ is the energy of the beam particles; $C(n)$ is a numerical factor depending on $n$; $\theta_0$ is the effective angular aperture of the detector, which determines the minimum deflection angle. A relation of the form (1) makes it possible, from the experimental dependence $Q(\theta_0)$ on $E$ (if it is linear), to immediately find the value of $n$. With the aid of $n$, the effective mean aperture $\theta_0$ is calculated comparatively simply, and then also the second parameter of the potential, $K$. The range of distances $\Delta r$ of closest approach realized in such an experiment is determined in the classical approximation by the relation, obvious for scattering through small angles, $Q(\theta_0, E) = \pi r^2$, i.e. $r_{\max} = (Q(\theta_0, E_{\min})/\pi)^{1/2}$ and $r_{\min} = (Q(\theta_0, E_{\max})/\pi)^{1/2}$.

**Table 1**

| System | $K$, eV • Å$^n$ | $n$ | $\Delta r$, Å |
|---|---|---|---|
| H–$H_2$ | 0.94 | 4.15 | 1.24–1.00 |
| H–He | 1.2 | 2.7 | 1.35–0.79 |
| He–He | 4.33 | 5.86 | 1.53–1.10 |
| He–$H_2$ | 5.0 | 3.8 | 1.89–1.15 |
| $H_2$–$H_2$ | 14.1 | 5.87 | 1.95–1.34 |

In the experiments described, the effective angular aperture of the detector $\theta_0$ was about $2 \cdot 10^{-3}$ rad; the scattering cross sections of the H–$H_2$ system were measured with detectors having different $\theta_0$ ($1.3 \cdot 10^{-3}, 2 \cdot 10^{-3}$, and $3.2 \cdot 10^{-3}$ rad), and therefore the energy scale in Fig. 1 for this system is normalized to $\theta_0 = 2 \cdot 10^{-3}$ rad. According to the well-known Massey criterion, quantum effects may appear under these conditions. However, a stricter estimate, carried out on the basis of Ref. ($^4$), shows that allowance for quantum effects is necessary only for the H–$H_2$ and H–He systems. In this case the total scattering cross section is expressed in the form ($^4$)

$$Q(0) = F(n)(K\pi/hv)^{2/(n-1)}, \tag{2}$$

where $F(n)$ is a numerical factor depending on $n$; $h$ is Planck' s constant; $v$ is the relative velocity.

Table 1 gives the parameters of the potentials $K$ and $n$ obtained by us for the systems studied, and the intervals of distances in which the quoted values are valid. The results for the H–$H_2$, He–$H_2$, and H–He systems can be compared with data from theoretical calculations. This comparison reveals very good agreement with the calculation of Ref. ($^5$) for the potential of the He–$H_2$ system and poorer agreement with the calculations for the H–He system ($^6$,$^7$ ). Numerous works have been devoted to the theoretical study of the potential surfaces of the $H_3$ system, for example ($^8$), and, in particular, the results of the latter showed a strong nonsphericity of the force field of the interaction between H and $H_2$. Therefore the "anomalous" behavior of the dependence $Q(\theta_0)$ on $E$ for H–$H_2$ (Fig. 1) can be explained by the influence of this effect. Owing to the strong nonsphericity, relation (2) can be applied only to the initial part of the dependence $Q(\theta_0, E)$, i.e. in the region of relatively large distances of closest approach. For smaller distances of closest approach, as follows from the data of Fig. 1, the potential energy of the H–$H_2$ interaction depends on distance much more strongly; however, quantitative treatment of the experimental data in this case is difficult. The second break in the $Q(\theta_0 E)$ curve for H–$H_2$, in the region of 3.6 keV, can apparently be explained by a transition to classical scattering; in particular, this is indicated indirectly by the close agreement of the values of the parameter $n$ determined from (2) for the energy region below 3.6 keV and from (1) for higher energies. Another possible explanation of this break is connected with allowance for a nonadiabatic transition as a result of the crossing of the electronic levels of the $H_3$ system ($^9$).

The effective spherically symmetric interaction potential for H—$H_2$, proposed in work ($^{10}$), agrees poorly with the experimental data corresponding to the initial part of the dependence of $Q(\theta_0)$ on $E$ (Table 1).

It is interesting to note that the interaction potential for $H_2$—$H_2$ obtained in work ($^{10}$) agrees well with the data of the experiment described. Experimental study of the systems H—$H_2$, H—He and He—He was carried out in works ($^{11-13}$), and their results agree well with those described only in the case of the He—He system; the discrepancy for the other systems can apparently be explained by the imperfection of the apparatus used in these measurements ($^{11,12}$).

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