

QUANTUM TRANSPORT PROPERTIES OF GASEOUS PARA AND ORTHO-HYDROGEN AT LOW TEMPERATURES

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Received 18 November 1986

Revised manuscript received 29 January 1987

UDC 539.19

Original scientific paper

The viscosity, heat conductivity and diffusion coefficients of para- and ortho-hydrogen and their mixtures are investigated quantum mechanically using the modified Buckingham potential function for a temperature range 1.85 K—22.2 K. The calculations were carried out for various para-ortho concentrations. Our results are compared with available theoretical and experimental data; the agreement with both is fairly good. Also, the calculations show that the viscosity and heat conductivity of ortho-hydrogen is smaller than those of para-hydrogen in accordance with the measurements of Becker and Stehl. The thermal diffusion factor of para- and ortho-hydrogen is calculated for different concentrations.

1. Introduction

Much effort and time has been devoted over the years to the quantum and classical transport theory of low and moderately dense gases of light diatomic molecules¹⁻¹⁴). The transport properties of light gases at low temperatures show interesting quantum effects. The deviations from the results of the classical theory are due

to the wave nature of the molecules (diffraction effects) and also those effects which owe their existence to the statistics of the particles (symmetry effects). The diffraction effects are of importance when the de Broglie wavelength associated with the molecules is of the order of magnitude of the molecular dimensions.

Therefore it is important to carry out calculations of these properties at low temperatures based on accurate quantum mechanical expressions and using a reliable potential field for the molecular interaction.

For the case of para- and ortho-hydrogen, there have been several studies on the transport properties of para-para-hydrogen, ortho-ortho-hydrogen and their mixtures⁹⁻¹²⁾ since the very earlier work of Halpern and Gwathmey¹⁵⁾ who drew attention to the fact that pure symmetry effects would lead to a difference in viscosity of para- and ortho-hydrogen. The difference in viscosity between ortho- and para-hydrogen has been measured experimentally^{16,17)}, and it was found that the viscosity of ortho-hydrogen is smaller than that of para-hydrogen, contrary to the earlier theoretical expectations. The discrepancy between theory and experiment has been discussed by Takayanagi and Ohno¹⁸⁾ who came to the conclusion that most probably the non spherical character of the intermolecular forces, possible combined with formations of $(H_2)_2$ complexes might be the source of the discrepancies. Cohen et al.¹⁾ used the Lennard-Jones potential in their quantum mechanical calculations. Their calculations on the concentration dependence of viscosity show that para-hydrogen has a greater viscosity than ortho-hydrogen.

In view of the obvious interest in studying this system, we thought it is to be important to start new quantum mechanical calculations of all the transport properties of para-hydrogen and ortho-hydrogen and their mixtures at low temperatures using the modified Buckingham potential field¹⁹⁾. Our calculations are valid only for temperatures where inelastic collisions resulting in rotational excitation are very rare.

The modified Buckingham potential is somewhat more flexible than the Lennard-Jones potential, since it permits the variation of the low velocity collision diameter as compared to the separation at the minimum molecular separation^{25,26)}.

A goal of this work is to obtain a detailed understanding of the scattering process of the considered system. Another goal is to develop techniques for computing also to modify the potential parameters of the interaction potential in order to obtain improved results than given those by Cohen et al.¹⁾.

The skeleton of this paper is divided as follows: In section 2 we give the phase shifts which are needed for the calculation of the transport properties. All the cross sections calculated from the phase shifts are stated in section 3. We deduce in section 4 all the transport coefficients for pure para-hydrogen, pure ortho-hydrogen and ortho-para hydrogen mixtures.

2. Phase shifts

Scattering cross sections are determined by the phase shifts $\delta_l(k)$. The phase shifts are functions of the angular momentum quantum number l and the wave number k . They are obtained from the asymptotic behaviour of wave function for large relative separation of two hydrogen molecules. Our calculations assume spherically symmetric potential of the molecule, so that the para-para, para-ortho and

ortho-ortho systems are represented by one interaction. In this way the transport properties are expressed in terms of one set of phase shifts. We used the modified Buckingham potential¹⁹⁾ to describe the interaction of two hydrogen molecules

$$U(r) = \frac{\epsilon}{1 - 6/\alpha} \left\{ \frac{6}{\alpha} \exp [\alpha (1 - r/r_m)] - (r_m/r)^6 \right\}, \quad (1)$$

where r is the separation distance between the molecules, ϵ is the minimum potential energy, r_m is the value of r for which $U(r)$ is a minimum and α is an additional parameter which may be considered a measure of the steepness of the repulsion energy. This potential is a three-constant potential with the parameters ϵ , r_m and α which includes in the induced — dipole — induced — dipole interaction. We took the values of these three constants to be $\epsilon/K = 37.3$ K, $r_m = 3.337 \cdot 10^{-8}$ cm, $\alpha = 14$ (see the method of determination of the potential parameters in Ref. 20), K is Boltzmann's constant.

We used Eq. (1) to evaluate the phase shifts for the relative motion of two hydrogen molecules. Phase shifts for large l were calculated from Born's method²¹⁾, which gives the phase shifts in the following form

$$\delta_l = -\frac{\pi}{2} \int_0^{\infty} U(r) [J_{l+1/2}(kr)]^2 r dr, \quad (2)$$

where $J_{l+1/2}(kr)$ is the Bessel function of the half integral order. When l is small, the WKD approximation²²⁾ was used. This approximation gives the following expression for δ_l

$$\delta_l = \frac{\pi}{4} + \frac{l\pi}{2} - kr_l + \int_{r_l}^{\infty} \left[\sqrt{k^2 - U(r) - \frac{l(l+1)}{r^2}} - k \right] dr, \quad (3)$$

where r_l is the largest zero of

$$F(r) = k^2 - U(r) - \frac{l(l+1)}{r^2}. \quad (4)$$

The phase shifts lying between those determined by Born's and WKD methods are calculated by interpolation. A detailed description of the methods we used to solve and evaluate Eqs. (2) and (3) for $U(r)$ given by Eq. (1) are found in a separate article²⁰⁾. In Fig. 1 we illustrate the phase shifts for the relative motion of two hydrogen molecules for different values of orbital angular momentum quantum number l as functions of kr_m . All the calculations were carried out on a Perkin Elmar 1625 system computer at El Minia University. These phase shifts can be used for pure para-hydrogen and pure ortho-hydrogen as well as for their mixtures. The behaviour of $\delta_l(kr_m)$ in the neighborhood of $kr_m = 0$ is of importance for the very

low temperature limit of the transport coefficients. All phase shifts with $l > 1$ go to zero for zero energy.

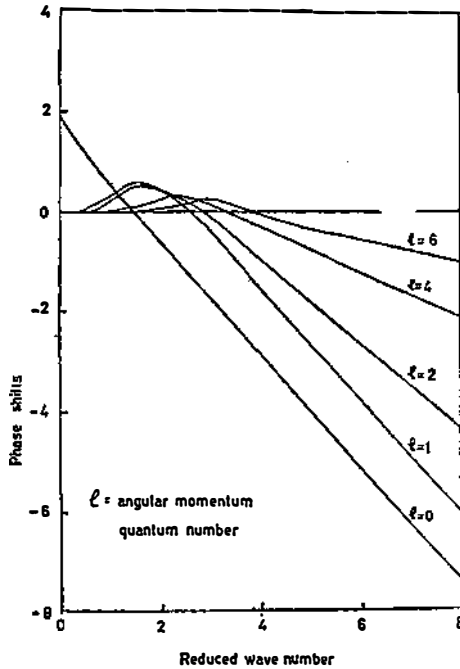


Fig. 1. Phase shifts δ_l for the relative motion of two hydrogen molecules as functions of kr_m .

3. Cross sections effective in transport properties

All transport properties are given as explicit functions of the cross sections $\sigma^{(n)}$ ($n = 1, 2$). They are expressed in terms of the phase shifts $\delta_l(k)$ as follows

$$\sigma^{(1)} = \frac{4\pi}{k^2} \sum_{l=0,1,2,\dots} (l+1) \sin^2(\delta_{l+1} - \delta_l), \quad (5)$$

$$\sigma^{(2)} = \frac{4\pi}{k^2} \sum_{l=0,1,2,\dots} \frac{(l+1)(l+2)}{(2l+3)} \sin^2(\delta_{l+2} - \delta_l). \quad (6)$$

$\sigma^{(1)}$ and $\sigma^{(2)}$ are called diffusion and viscosity cross sections, respectively²³. Expressions (5) and (6) hold only when the two colliding molecules are not in the same state for example for a para-ortho collision.

For the collision of two identical molecules we should use wave functions of proper symmetry²⁴. Since inelastic collisions are excluded and hydrogen molecules consist of an even number of elementary particles, they follow Bose-Einstein

statistics. Consequently the total wave functions describing two hydrogen molecules should be symmetric with respect to the two molecules.

For the cases that only symmetrical or antisymmetrical spatial wave functions are allowed, the corresponding cross sections are respectively

$$\sigma_s^{(1)} = \frac{8\pi}{k^2} \sum_{l=0,2,\dots} (2l+1) \sin^2 \delta_l(k) \quad (7)$$

$$\sigma_a^{(1)} = \frac{8\pi}{k^2} \sum_{l=1,3,\dots} (2l+1) \sin^2 \delta_l(k) \quad (8)$$

$$\sigma_s^{(2)} = \frac{8\pi}{k^2} \sum_{l=0,2,\dots} \frac{(l+1)(l+2)}{(2l+3)} \sin^2 (\delta_{l+2} - \delta_l) \quad (9)$$

$$\sigma_a^{(2)} = \frac{8\pi}{k^2} \sum_{l=1,3,\dots} \frac{(l+1)(l+2)}{(2l+3)} \sin^2 (\delta_{l+2} - \delta_l). \quad (10)$$

For pure para-hydrogen where the molecules have no degeneracy, only symmetric spatial wave functions are allowed and we have for all cross sections^{1,2,3)}

$$\sigma_{pH_2}^{(n)} = \sigma_s^{(n)} \quad (n = 1, 2). \quad (11)$$

Ortho-hydrogen molecules can be in 9 almost degenerate states corresponding to 3 different values of the z -component of the total nuclear spin $s = 1$ and the three different z -values of the rotational quantum number $J = 1$. Therefore, on collision, there are $9^2 = 81$ possible internal states for the system of 2 colliding ortho-molecules. Of these, 45 are to be described by a wave function symmetrical and 36 antisymmetrical in the internal coordinates of the two molecules. Thus there is a 5 : 4 chance on collision that the internal wave function is symmetric or antisymmetric in the two molecules¹⁾. As the total wave function, which also includes the relative motion of the two molecules must be symmetrical in all coordinates, it follows that also the wave function for the relative motion has a 5 : 4 chance to be symmetric or antisymmetric, respectively¹⁾.

Thus the cross sections for ortho-hydrogen are

$$\sigma_{oH_2}^{(n)} = \frac{5}{9} \sigma_s^{(n)} + \frac{4}{9} \sigma_a^{(n)} \quad (n = 1, 2). \quad (12)$$

The para-ortho-hydrogen mixtures should be treated as binary mixtures since the conversion rate between para- and ortho-hydrogen at low densities and temperatures is extremely slow. The mixture formulae which contain cross sections obey Boltzmann statistics, i. e. allowing all scattering waves.

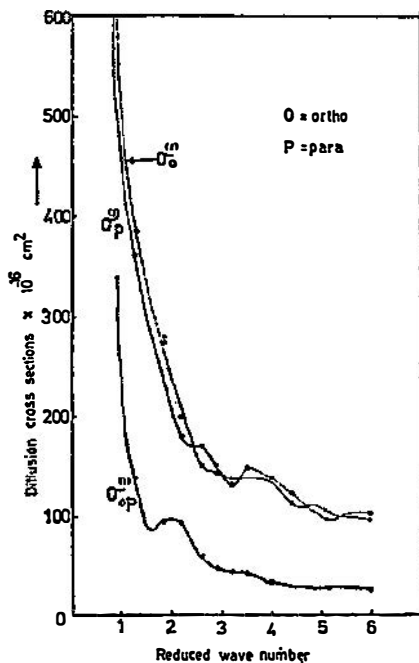


Fig. 2. The variation of diffusion cross sections $\sigma_{diff}^{(1)}$ with kr_m .

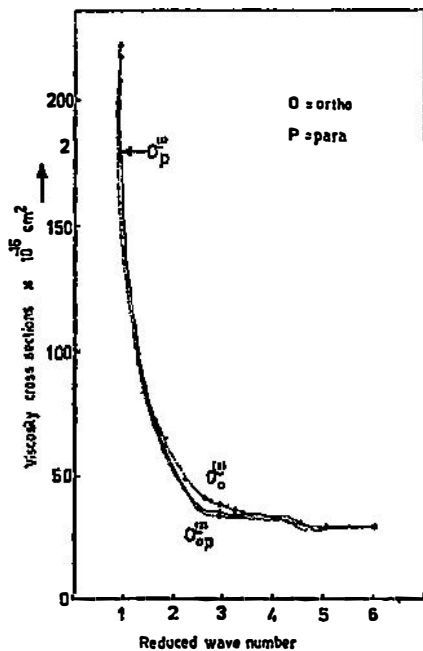


Fig. 3. The variation of viscosity cross sections $\sigma_{visc}^{(2)}$ with kr_m .

The cross sections $\sigma_{qq'}^{(1)}$ and $\sigma_{qq'}^{(2)}$ (q and q' stand for para P or ortho O hydrogen) are plotted in Figs. 2 and 3 as functions of kr_m .

The collision integrals $\Omega(n, t)$ which occur in the final formulae for the transport quantities are defined as follows

$$\Omega_{qq'}^{(n,t)} = (KT/2\pi\mu)^{1/2} \int_0^\infty e^{-\gamma^2} \gamma^{2t+3} \sigma_{qq'}^{(n)} d\gamma \quad (13)$$

where μ is the reduced mass of the molecules and in quantum theory $\gamma^2 = \hbar^2 k^2 / 2\mu KT$. The (n, t) values needed in our calculations are (1, 1), (1, 2), (1, 3) and (2, 2). For the calculations of the para-ortho-hydrogen mixture, the following combinations of the collision integrals $\Omega_{qq'}^{(n,t)}$ are needed^{2,3)}

$$\begin{aligned} A_{qq'} &= \Omega_{qq'}^{(2,2)} / 5 \Omega_{qq'}^{(1,1)} \\ B_{qq'} &= (5 \Omega_{qq'}^{(1,2)} - \Omega_{qq'}^{(1,3)}) / 5 \Omega_{qq'}^{(1,1)} \\ C_{qq'} &= 2 \Omega_{qq'}^{(1,2)} / 5 \Omega_{qq'}^{(1,1)}. \end{aligned} \quad (14)$$

4. Results and discussion

4.1. The viscosity and heat conductivity

The coefficients of viscosity and heat conductivity for pure para- and pure ortho-hydrogen are calculated using the following expressions in first approximation

$$[\eta_q]_1 = 5KT/8 \Omega_q^{(2,2)}, \quad (15)$$

$$[\lambda_q]_1 = \frac{5}{2} [\eta_q]_1 C_v \quad (16)$$

where q stands for para- or ortho-hydrogen and C_v is the specific heat. The expressions for the viscosity and heat conductivity of a mixture of para- and ortho-hydrogen in the first order approximation are

$$\frac{1}{[\eta_{mix}]_1} = \frac{x_p^2 \frac{H_p}{[\eta_p]_1} + 2x_p x_o \frac{H_{po}}{[\eta_{po}]_1} + x_o^2 \frac{H_o}{[\eta_o]_1}}{x_p^2 H_p + 2x_p x_o G_{po} + x_o^2 H_o} \quad (17)$$

$$\frac{1}{[\lambda_{mix}]_1} = \frac{x_p^2 \frac{L_p}{[\lambda_p]_1} + 2x_p x_o \frac{L_{po}}{[\lambda_{po}]_1} + x_o^2 \frac{L_o}{[\lambda_o]_1}}{x_p^2 L_p + 2x_p x_o M_{po} + x_o^2 L_o} \quad (18)$$

where

$$H_p = H_o = 1 + \frac{3}{2} A_{po} \tag{19a}$$

$$H_{po} = 1 + \frac{3}{2} \frac{[\eta_{po}]_1^2}{[\eta_p]_1 [\eta_o]_1} \tag{19b}$$

$$G_{po} = 1 + \frac{3}{2} A_{po} \left\{ \frac{[\eta_{po}]_1}{[\eta_p]_1} + \frac{[\eta_{po}]_1}{[\eta_o]_1} - 1 \right\} \tag{19c}$$

$$L_p = L_o = 1 + \frac{2}{3} A_{po} - \frac{1}{12} (4 B_{po} + 1) \tag{19d}$$

$$L_{po} = 1 + \frac{2}{3} A_{po} \frac{[\lambda_{po}]_1^2}{[\lambda_p]_1 [\lambda_o]_1} - \frac{1}{12} (4 B_{po} + 1) \tag{19e}$$

$$M_{po} = 1 + \frac{2}{3} A_{po} \left\{ \frac{[\lambda_{po}]_1}{[\lambda_p]_1} + \frac{[\lambda_{po}]_1}{[\lambda_o]_1} - 1 \right\} - \frac{1}{12} (4 B_{po} + 1). \tag{19f}$$

The expressions $[\eta_{po}]_1$ and $[\lambda_{po}]_1$ are given by

$$[\eta_{po}]_1 = 5KT/8 \Omega_{po}^{(2,2)}; [\lambda_{po}]_1 = \frac{5}{7} C_v [\eta_{po}]_1. \tag{20}$$

x_p and x_o may take the values (3/4, 1/4), (1/2, 1/2) and (1/4, 3/4). The case for which $x_p = 1/4$ and $x_o = 3/4$ is called normal hydrogen (nH₂).

In Table 1 we give the values of $[\eta_q]$ and $[\lambda_q]_1$ ($q = p, o$) calculated from equations (15) and (16), and the difference $[\eta_o]_1 - [\eta_p]_1$. In the temperature range considered it is clear to see that the viscosity of ortho-hydrogen is smaller than those of para-hydrogen. Such a result agrees with the experimental measurements of Becker and Stehl¹⁶.

TABLE 1.

Temperature (K)	Viscosity (10^{-7} kg m ⁻¹ s ⁻¹)			Heat conductivity (10^{-3} J m ⁻¹ s ⁻¹ K ⁻¹)	
	$[\eta_p]_1$	$[\eta_o]_1$	$[\eta_o]_1 - [\eta_p]_1$	$[\lambda_p]_1$	$[\lambda_o]_1$
1.85	0.49645	0.48182	-0.0146	0.76701	0.74440
3.70	1.37020	1.35340	-0.0168	2.11696	2.09100
7.40	3.33330	3.32655	-0.0067	5.14994	5.13952
11.10	5.80111	5.65935	-0.1417	8.96270	8.74370
14.80	8.09000	7.96491	-0.1251	12.49990	12.30578
18.50	10.54420	10.51345	-0.0307	16.29070	16.24328
22.20	12.51774	12.48122	-0.0365	19.33905	19.28348

Viscosity and heat conductivity of ortho- and para-hydrogen.

Tables 2 and 3 contain the differences $[\eta_{mtx}]_1 - [\eta_p]_1$ and $[\lambda_{mtx}]_1 - [\lambda_p]_1$ for various concentrations x_p and x_o , and the viscosity and heat conductivity differences between normal and para-hydrogen relative to that of para-hydrogen, respectively. The relative viscosity difference not only changes sign from that characteristic of the experimental range $T > 10$ K but magnitude as well. This is primarily a quantum effect due to the differing symmetry restrictions obeyed by ortho- and para-hydrogen.

TABLE 2.

T/K	$[\eta_{mtx}]_1 - [\eta_p]_1$			$(\eta_{nH_2} - \eta_p)/\eta_p$
	$x_p = 3/4$ $x_o = 1/4$	$x_p = 1/2$ $x_o = 1/2$	$x_p = 1/4$ (nH ₂) $x_o = 3/4$	
	(10 ⁻⁷ kg m ⁻¹ s ⁻¹)			
1.85	0.00360	0.00290	0.00310	0.00624
3.70	0.07840	0.02680	0.04260	0.03109
7.40	0.02600	0.03359	0.02260	0.00678
11.10	-0.09660	-0.08570	-0.06710	-0.01157
14.80	-0.02500	-0.09500	-0.03130	-0.00387
18.40	-0.02310	-0.03140	-0.02460	-0.00233
22.20	-0.07800	-0.10930	-0.09530	-0.00761

Viscosity differences for various para-ortho concentrations.

TABLE 3.

T/K	$[\lambda_{mtx}]_1 - [\lambda_p]_1$			$(\lambda_{nH_2} - \lambda_p)/\lambda_p$
	$x_p = 3/4$ $x_o = 1/4$	$x_p = 1/2$ $x_o = 1/2$	$x_p = 1/4$ nH ₂ $x_o = 3/4$	
	(10 ⁻³ J m ⁻¹ s ⁻¹ K ⁻¹)			
1.85	0.00538	0.00529	0.00549	0.00716
3.70	0.019320	0.02168	0.02004	0.00947
7.40	0.037450	0.03628	0.03486	0.00677
11.10	-0.031290	-0.03902	-0.04127	-0.00460
14.80	-0.04491	-0.04177	-0.04655	-0.00372
18.50	-0.03770	-0.03882	-0.03809	-0.00234
22.20	-0.13452	-0.15674	-0.14645	-0.00757

Heat conductivity differences for various para-ortho concentrations.

Fig. 4 shows that there exists good agreement between our calculated values of η_{nH_2} and the experimental values^{1,6)}. Fig. 5 compares our results for the heat conductivity of normal hydrogen with available experimental and theoretical results. There is a remarkable agreement with the calculations of Cohen et al.¹⁾.

The calculations of viscosity differences of ortho-hydrogen-para-hydrogen mixtures at low temperatures show that the collision integrals definitely depend on the colliding pair and thus on the internal structure of the molecules. Three effects can

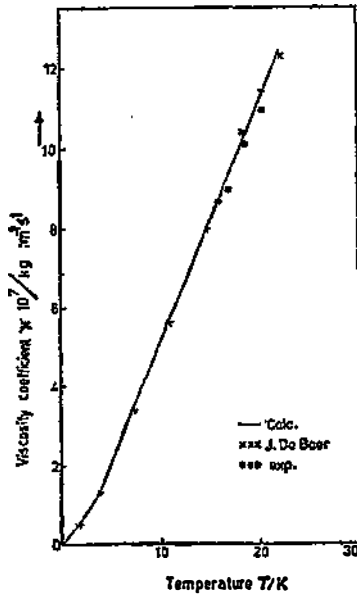


Fig. 4. Viscosity of normal hydrogen gas compared with available experimental and theoretical data.

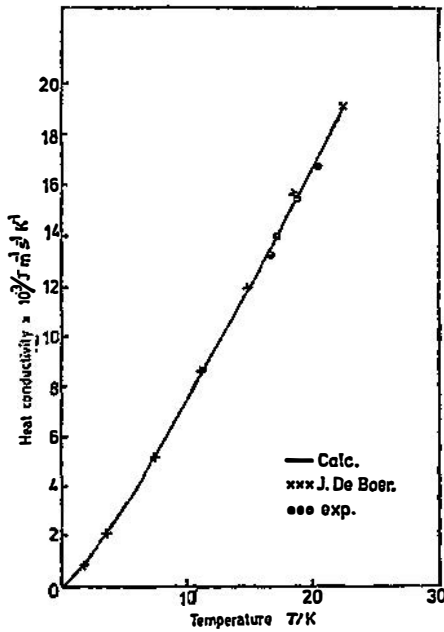


Fig. 5. Thermal conductivity of normal hydrogen gas compared with available experimental and theoretical data.

produce these differences. The first is that the types of collision allowed are governed by the statistics obeyed by the colliding pair. Second, ortho-hydrogen, in the $f = 1$ state, is stretched by centrifugal forces and thus is a little larger and a little more polarizable than para-hydrogen. Third, at low temperatures, ortho-hydrogen in the $f = 1$ state can undergo reorienting collisions whereas para-hydrogen in the $f = 0$ state cannot.

4.2. Mutual and self-diffusion

The coefficients of mutual and self-diffusion in first-order are given respectively by

$$[D_{p-oH_2}]_1 = 3 KT/8 nm \Omega^{(1,1)} \tag{21}$$

and

$$[D_q]_1 = 3 KT/8 n_q m_q \Omega_q^{(1,1)} \tag{22}$$

where n is the total number density of para- and ortho-hydrogen and q stands for para-hydrogen or ortho-hydrogen, respectively. m is the mass of the molecule.

TABLE 4.

T*	$[D_{p-oH_2}]_1^* n^*$	$[D_{pH_2}]_1^* n^*$	$[D_{oH_2}]_1^* n^*$	T/K	$[D_{p-oH_2}]_1^{nm}$	$[D_{pH_2}]_1^{nm}$	$[D_{oH_2}]_1^{nm}$
					(10 ⁻⁷ kg m ⁻¹ s ⁻¹)		
0.05	0.00303	0.00170	0.00171	1.85	0.57210	0.24400	0.29540
0.10	0.01020	0.00438	0.00412	3.70	1.68050	0.75700	0.71240
0.20	0.02338	0.00800	0.00827	7.40	4.04240	1.38310	1.43060
0.30	0.04578	0.01519	0.01380	11.10	7.11420	2.62660	2.38537
0.40	0.05655	0.01900	0.02204	14.80	9.77600	3.24290	3.21152
0.50	0.07160	0.02354	0.02422	18.50	12.64600	4.02600	4.23268
0.60	0.08410	0.02816	0.02902	22.20	15.53933	4.86850	4.99810

Mutual and self diffusion coefficients for hydrogen.

The three types of H₂ diffusion are given in Table 4 as functions of T together with the reduced values $[D]_1^* n^* = [D]_1 n r_m^2 (2\mu/\epsilon)^{1/2}$ as functions of the reduced temperature T^* ($T^* = KT/\epsilon$). The self-diffusion values are plotted against T in Fig. 6 and compared with the theoretical results of Cohen et al.¹⁾

Another manifestation of the internal structure in hydrogen is the observed separation of ortho- and para-hydrogen in a thermal gradient. In an earlier attempt¹⁰⁾ the thermal diffusion ratio for a para-ortho-hydrogen mixture was approximated by

$$[f_T]_1 = 5 (C_{po} - 1) \frac{x_p x_o}{6 [\lambda_{po}]_1} \cdot \frac{S_p x_p - S_o x_o}{x_p \frac{L_p}{[\lambda_p]_1} + 2 x_p x_o \frac{[\lambda_{po}]_1}{L_{po}} + x_o \frac{L_o}{[\lambda_o]_1}} \tag{23}$$

where

$$S_q = [\lambda_{po}]_1 / [\lambda_q] - 1, (q = p, o). \tag{24}$$

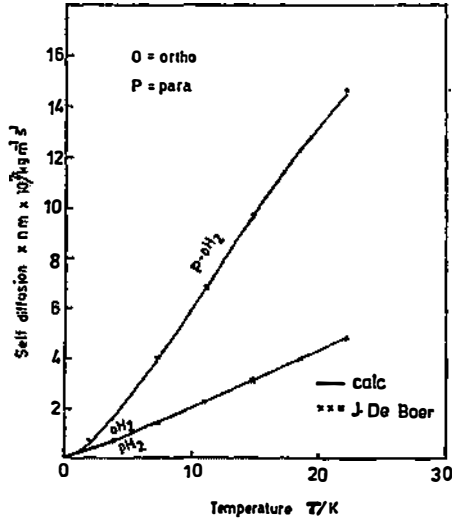


Fig. 6. Variation of self diffusion coefficients for different types of H₂ with temperature.

In Table 5 numerical values for the thermal diffusion factor $[\beta]_1 = [f_T]_1 / X_p X_o$ for different concentrations can be found as functions of temperature T . In the temperature region of our calculations, the zeros of $[\beta]_1$ lie between $T = 3.7$ K and $T = 7.4$ K

TABLE 5.

T/K	$x_p \rightarrow 1$ $x_o \rightarrow 0$	$x_p = 3/4$ $x_o = 1/4$	$x_p = 1/2,$ $x_o = 1/2^i$	$x_p = 1/4$ $x_o = 3/4$	$x_p \rightarrow 0$ $x_o \rightarrow 1$
1.85	-12.872	-9.950	-6.511	-2.526	+1.739
3.7	-8.308	-6.138	-3.872	-1.500	+1.000
7.4	+1.791	+1.322	+0.810	+0.303	-0.203
11.1	+0.900	+0.700	+0.388	+0.200	-0.097
14.8	+0.288	+0.193	+0.137	+0.054	-0.031
18.5	+0.101	+0.068	+0.043	+0.018	-0.009
22.2	+0.034	+0.023	+0.020	+0.007	-0.003

Thermal diffusion factor $[\beta]_1 \times 10^3$.

The existence of thermal diffusion in para- and ortho-hydrogen mixtures is entirely due to quantum effects. For in classical theory, two gases having the same mass and the same potential field would never show thermal diffusion.

The temperature range 50—150 K is generally of interest for processes occurring in intergalactic space, but the range below 25 K is generally of more interest for galactic and intergalactic clouds. When we compare our results obtained in Table 5 with those obtained by Monchick and Schaefer⁹⁾ in the temperature range 50—150 K, we note that, although $[\beta]$ for $T < 25$ K is orders of magnitudes larger than it is for higher temperatures, it oscillates rapidly and so may not be easy to measure.

5. Conclusions

It may be concluded that the modified Buckingham potential fairly successfully predicts integral scattering and transport properties over the range of low temperatures taken. This result is very surprising and seems to indicate that this model is very near the truth at this temperature region, or that the transport phenomena are not sensitive to the actual fields of force between molecules in collisions when they are properly treated on a wave mechanical theory. Also the success of the modified Buckingham potential may be attributed to the fact that it approximates the repulsive contribution to the potential by an exponential term, and the energy at the spurious maximum $U(r_{max})$, is ordinarily sufficiently large that it leads to no difficulties.

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KVANTNA TRANSPORTNA SVOJSTVA PLINOVITOG PARA- I ORTO-VODIKA NA NISKIM TEMPERATURAMA

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UDK 539.19

Originalni znanstveni rad

Istražuje se viskoznost, termička vodljivost i koeficijent difuzije para- i orto-vodika kao i njihovih mješavina, metodom kvantne mehanike. Za vodikov potencijal uzima se Buckingham-ova funkcija u granicama od 1,85 K do 22,2 K. Račun je napravljen za više vrijednosti para-orto koncentracija. Rezultati se uspoređuju s postojećim teorijskim i eksperimentalnim rezultatima i slaganje je dosta dobro. Računi pokazuju da je viskozitet i termička vodljivost orto-vodika manja od para-vodika, što je slaganje s mjerenjima Beckera i Stehla. Faktor termičke difuzije orto- i para-vodika je izračunat za različite koncentracije.