THERMODYNAMIC EQUILIBRIUM IN A "LITHIUM HYDRIDE-HYDROGEN" SYSTEM CONTAINING ISOTOPIC IMPURITIES

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Thermodynamic equilibrium between gaseous hydrogen and crystalline lithium hydride is investigated experimentally for a low concentration of the isotope D or of the isotope H and at temperatures between 230 and 670°C. A 30—40% deviation of the isotope separation coefficient from the classical value of unity can be attributed to quantum effects in the gaseous and condensed phases. An approximate method for calculating the crystal contribution to the isotope separation effect is considered. The experimental values of α are in satisfactory agreement with the values obtained theoretically in[14] and by the approximate method in the present investigation.

THE physical properties of real crystals, i.e., crystals containing defects, are now under intensive study. In particular, quite detailed theoretical studies have been made of the influence of small concentrations of isotopic substitutional defects on the dynamics of the crystal lattice, on the absorption of light, on the electric conductivity, on the specific heat, etc. However, the influence of isotopic substitutional defects on the properties of crystals has not yet been sufficiently well investigated. This is due, primarily, to the fact that as a rule, the isotopes differ little in mass, and consequently it is difficult to measure their influence on the properties of the crystal.

From the experimental point of view, definite interest attaches to the study of the thermodynamic equilibrium between a crystal with isotopic defects and the gas phase. The quantity measured in this case, namely the isotope separation coefficient, is characteristic only of a lattice containing impurity atoms, unlike the other properties of the crystal (for example the specific heat, thermal conductivity, or electric conductivity), which are possessed both by crystals with defects and by crystals without defects.

A theory of thermodynamic equilibrium of a system consisting of a gas and a crystal with defects was recently constructed, with allowance for the singularities of the dynamics of the defective lattice[1], and a connection was established between the isotope separation coefficients and the change of the distribution function of the crystal frequencies caused by defects whose masses differ arbitrarily from those of the host atoms. In this connection, an interesting object of study should be a crystal containing hydrogen isotopes, for in this case the relative difference in the masses of the isotopes is maximal. There are published data on the temperature dependence of the separation coefficient of the isotopes H and D in the "gaseous hydrogen—uranium hydride" system[2]. However, uranium hydride is a very difficult crystal to calculate, and this complicates the comparison of the experimental results with the theory. In[3], the coefficient for the separation of the isotopes H and D was obtained for the "gaseous hydrogen—lithium hydride" system at a temperature 200°C. This investi-

gation, together with studies of the dissociation products of hydrides and deuterides of sodium, potassium[4], rubidium, and cesium[5], points to the possibility of experimentally investigating the thermodynamic equilibrium for "alkali metal hydrides—gaseous hydrogen" systems in a wide temperature interval.

We have undertaken such a study of the thermodynamic equilibrium of gaseous hydrogen with crystalline lithium hydride for both limiting cases—low concentration of the isotope D, and low concentration of the isotope H in the system. A part of the present paper was reported at the conference on localized oscillations in solids[6].

1. MEASUREMENT OF THE EQUILIBRIUM DISTRIBUTION OF THE ISOTOPES H AND D BETWEEN THE CRYSTALLINE LITHIUM HYDRIDE AND THE GASEOUS HYDROGEN

The distribution of the isotopes in the two phases in the state of thermodynamic equilibrium is customarily characterized by a separation coefficient defined by the relation

$$a = \frac{c_1}{1-c_1} \Big/ \frac{c_2}{1-c_2}, \tag{1}$$

where c_1 and c_2 are the relative atomic concentrations of one of the isotopes in phases 1 and 2 in the state of equilibrium of the system.

The experimental setup for the measurement of the coefficient of separation of H and D between the gaseous hydrogen and the crystalline lithium hydride is shown in Fig. 1.

The isotopic equilibrium of the phases was established in a reaction cell consisting of a test tube 1 and a glass bulb 9. The lithium hydride 3 was placed in a crucible 2 made of Armco iron. The hydrogen occupied the entire volume of the reaction cell, up to the valve 10. The volume of the reaction cell was about 1800 cm³. Since only the lower part of the reaction cell was heated by the oven 4, the crucible was covered with a glass cover fixed with an opening in the bottom, in order to make the phase-balancing process isothermal. The tem-
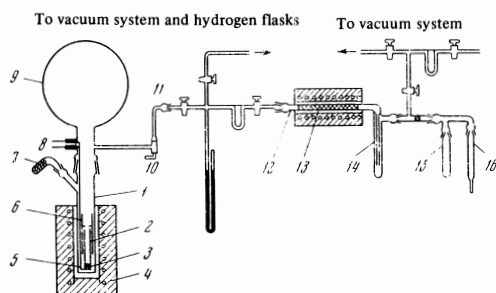
FIG. 1. Overall view of the setup.

perature of the hot zone of the cell was determined by a thermocouple 8, placed in cavity 5 in the thick bottom of the crucible 2.

The isotopic composition of the hydrogen in the gaseous and condensed phases was determined by a temperature-float method from the density of the water [7,8]. The hydrogen gas was converted into water in the tube 12 by means of copper oxide 13 heated to 600°C. To obtain the correct results, all the hydrogen was converted into water, and measures were adopted to exclude the effects of the "memory" of the tube with the copper oxide. The water vapor produced by the reaction between the hydrogen and the copper oxide was frozen out in a liquid-nitrogen-cooled test tube 14. For purification, the obtained water was redistilled from test tube 14 into test tubes 15 and 16 in succession. The water density was determined directly in test tube 16 with the aid of a quartz float calibrated against standard water. The density of the standard water was determined by a pycnometric method [8].

The reaction between the lithium hydride and lead [9] was used to extract the hydrogen from the lithium hydride, so as to determine the isotopic composition of the solid phase. As shown by test experiments aimed at studying the action exerted on the lithium hydride by a stoichiometric amount of lead (relative to lithium), the entire hydrogen was extracted in gaseous form from the lithium hydride at a temperature of 500°C and above. Granulated lead for the decomposition operation was placed in a bent test tube 7. The lithium hydride was decomposed by the lead at 600°C. The relative error in the

determination of the deuterium concentration in the gaseous hydrogen and in the lithium hydride by the temperature-float method was approximately 0.3% at a deuterium content 1—2 at.% in the investigated sample, and approximately 0.02% at a deuterium content 97—98 at.% in the sample.

The experiments were performed in the following sequence. In a chamber filled with dry CO_2, approximately 1.5 g of Li^7H or Li^7D was placed in the reaction cell in crucible 2, in the form of powder with grains not larger than 0.26 mm, and about 30 g of lead was placed in test tube 7. After loading, the reaction cell was connected to the remaining part of the setup through the ground-glass joint 11, and was evacuated to 10^{-2} mm Hg. The gaseous hydrogen was then admitted into the reaction cell. The initial hydrogen was obtained by electrolysis, and contained 3—4 at.% of deuterium in experiments with a small total concentration of deuterium in the system, and 96—97% in experiments with a large total deuterium concentration in the system. The hydrogen pressure in the reaction cell usually was produced in a range 630—650 mm Hg, producing practically as much hydrogen gas as that contained in the lithium hydride. After the admission of the gas, the cell was heated to the temperature of the experiment. The duration of isotopic balancing of the phases was different for each temperature, and was determined in special experiments. After the phases were balanced, an isotopic analysis of the composition of the gaseous hydrogen and of the lithium hydride was made. The gaseous phase was sampled for the analysis at the experimental temperature. The conditions and the results of the experiments are listed in Tables I and II.

2. DISCUSSION OF RESULTS

The experimental values of the separation coefficient of the isotopes H and D in the systems "$Li^7 H : D$—mixture of H_2, HD, and D_2 gases" and "$Li^7 D : H$—mixture of D_2, HD, H_2 gases" listed in Tables I and II, show that α greatly exceeds unity in the entire temperature interval (by 30—40%). As is well known, in the classical limit of high temperatures, the isotope separation coefficient is equal to unity. Its deviation from this limiting case is due to quantum effects in one or both phases.

Table I. Conditions and results of measurements of α in the system "$Li^7H:D$ crystal—mixture of H_2, HD, D_2 gases"

Experiment number	T, °C	Grain dimension, mm	Duration of phase contact, hr	Deuterium concentration c_1 in the gas phase, at.%	Deuterium concentration c_2 in the lithium hydride, at.%	α
1	230	≤0.05	7000	1.949	1.437	1.363
2	310	≤0.13	1037	2.233	1.672	1.343
3	314	0.13—0.26	1445	1.815	1.358	1.343
4	303	≤0.13	800	1.680	1.248	1.352
5	296	0.05—0.13	2100	2.016	1.501	1.350
6	390	0.13—0.26	185	1.717	1.298	1.328
7	398	0.13—0.26	340	1.687	1.280	1.323
8	404	0.13—0.26	570	1.774	1.346	1.324
9	500	0.13—0.26	170	1.616	1.242	1.306
10	500	0.05—0.13	70	2.004	1.560	1.290
11	501	0.13—0.26	110	1.752	1.354	1.299
12	617	≤0.13	91	2.098	1.652	1.276
13	615	≤0.13	115	2.098	1.640	1.285
14	598	0.13—0.26	84	1.813	1.415	1.286
15	600	0.13—0.26	24	1.779	1.392	1.283
16	602	0.13—0.26	45	1.683	1.327	1.273
17	665	0.13—0.26	46	1.872	1.482	1.268
18	670	0.13—0.26	48	1.890	1.486	1.277

Table II. Conditions and results of measurements of α in the
system "Li^{7}D:H crystal—mixture of D$_2$, HD, H$_2$ gases"

Experiment number	T, °C	Grain dimension, mm	Duration of phase contact, hr	Deuterium concentration c_1 in the gas phase, at.%	Deuterium concentration c_2 in the lithium hydride, at.%	α
1	320	0.05—0.13	810	98.606	98.040	1.414
2	316	⩽0.05	900	98.390	97.712	1.431
3	412	0.05—0.13	263	97.987	97.276	1.363
4	515	0.13—0.26	135	98.654	98.236	1.316
5	518	0.05—0.13	120	98.544	98.100	1.311
6	630	0.13—0.26	55	97.857	97.238	1.297

The fact that in our case α differs greatly from unity indicates that the temperature region in which the experimental measurements were made is a quantum region. The quantum effects can be due to the gas phase, since the frequency of oscillations of the molecules H$_2$, HD, and D$_2$ are equal, in energy units, to 8.6×10^{-13}, 7.5×10^{-13}, and 6.1×10^{-13} erg, respectively, i.e., they exceed by almost one order of magnitude the value of kT for the investigated temperature interval (for temperatures 500—1000°K the values of kT correspond to $(0.7-1.4) \times 10^{-13}$ erg). The contribution of the gas phase to the isotope separation coefficient can be calculated exactly by the statistical method developed by Urey[10], using the known molecular constants of the molecules H$_2$, HD, and D$_2$. However, an attempt to explain the value of α as being due only to quantum effects from the gas phase does not lead to a quantitative agreement with experiment.

In the investigated case, we should expect quantum effects also from the crystalline phase, since the melting temperature, say, of LiH (T$_m$ = 961°K[11]) is lower than the Debye temperature (Θ_{LiH} = 1380°K[12]). The classical theory with allowance for quantum corrections[13] shows that the greatest difference between the separation coefficient and unity would occur in the case when the quantum effects are significant in only one of the phases, while the other is described classically. In the presence of quantum corrections from both phases, α may be either larger or smaller than unity, depending on the relative magnitude of these corrections.

We note that in accordance with[1], for a monoatomic crystal which is in equilibrium with a classical monoatomic gas, both in the case of a heavy isotopic defect, such as D is in our case, and in the case of a light defect, α should be smaller than unity if the effects of the separation is due only to the quantum corrections from the solid state. On the other hand, in this case the crystal is in equilibrium with an essentially quantum gas. The quantum corrections from the gas phase, tending to increase α, lead to a value $\alpha > 1$.

Recently, Benedek et al.[14] constructed a theory of thermodynamic equilibrium for a system consisting of a diatomic gas and a crystal, with allowance for the singularities of the dynamics of a diatomic defective crystal. They calculated the isotope separation coefficients for the systems "Li^{7}H : D—H$_2$, HD" and "Li^{7}D : H—D$_2$, HD." The presence in the gas of D$_2$ molecules in the former case and of H$_2$ molecules in the latter case was neglected, since the theory was constructed from small impurity concentrations. The authors presented numerical calculations for two sets of initial data, differing in
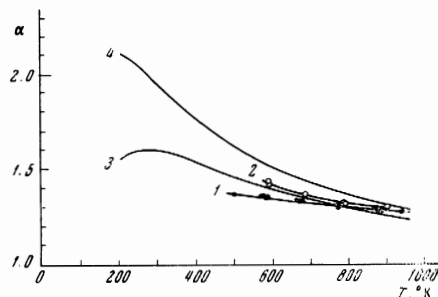

FIG. 2. Comparison of the experimental and theoretically calculated [14] dependence of the separation coefficient on the temperature: 1 and 2—data from Table I and II, 3 and 4—theoretical curves for the systems "Li^{7}H:D—H$_2$, HD" and "Li^{7}D:H—D$_2$, HD."

the value of the ion charge of the Li^{7}H and Li^{7}D crystals, which was assumed for the two crystals to equal ζ/e = 0.70 and ζ/e = 0.85 (ζ—ion charge, e—electron charge). Since in our experiments on the determination of α the relative concentrations of the isotopic impurities H and D do not exceed 2%, it is possible to compare the calculated and the experimental data.

Figure 2 shows the numerical values of the separation coefficients[14] (curve 3 for the system "Li^{7}H : D—H$_2$, HD," curve 4 for the system "Li^{7}D : H—D$_2$, HD"), and also the experimental data Table I (curve 1) and Table II (curve 2). The theoretical curves 3 and 4 shown in Fig. 2 pertain to the case ζ/e = 0.70, since at this value of the ion charge the values of α, calculated in the classical limit of high temperatures, give a smaller deviation from unity, and furthermore in the same direction, than in the case ζ/e = 0.85. As seen from Fig. 2, the agreement between the theoretical and experimental data is perfectly satisfactory.

3. APPROXIMATE CALCULATION OF THE CONTRIBUTION OF THE LITHIUM HYDRIDE CRYSTALS, CONTAINING ISOTOPIC DEFECTS, TO THE ISOTOPE SEPARATION EFFECT

Knowledge of the frequency spectrum of a perfect crystal and of a crystal containing isotopic defects as shown in[1,14], is important for the determination of the contribution of the crystalline phase to the value of the separation coefficient. The x-ray and neutron diffraction experimental methods developed to date for the determination of the vibrational spectra of the crystals make it possible to obtain quantitative information only on the frequency distribution functions of perfect crystals. The problem of theoretically determining the frequency spectrum of perfect and imperfect crystals, even if the phys-

ical constants needed for the calculation are known, is exceedingly complicated and laborious. It is therefore of interest to consider the problem of the contribution of defective crystals, particularly lithium hydride crystals, to the effect of isotope separation approximately, using few initial data.

The spectra of the lithium hydride crystals were recently determined experimentally[15,16] for pure LiH and LiD crystals, and theoretically[12,14] for pure LiH and LiD crystals and for LiH:D and LiD:H crystals, containing isotopic defects. A comparison of the vibrational spectra of the crystals reveals a number of their singularities.

First, the vibrational spectra of LiH and LiD differ little in the acoustic region. There is even a smaller difference between the acoustic branches of the spectra of the LiH:D and LiD:H crystals and the corresponding spectra of perfect LiH and LiD crystals. In the optical region, to the contrary, the spectra of LiH and LiD differ greatly. The small difference of the acoustic vibrations of the crystals may be connected with the collective character of the motion of the ions making up the cell, at least in the long-wave part of the acoustic branch of the spectrum. In the long-wave part of the optical branch, the positive Li^+ ions and the negative H^- and D^- ions move in opposite directions, so that their mass center in the cell remains fixed. As a result of the appreciable relative difference between the masses of the ions of opposite polarity, the displacement of the light negative ions with frequencies of the optical branches is much larger than the displacement of the positive ions. Accordingly, when H^- is replaced in the lattice by D^-, the spectra of the LiH and LiD crystals in the optical region change appreciably.

Second, the frequency distribution functions of the LiH and LiD crystals have clearly pronounced maxima in the optical branch, corresponding to transverse oscillations ω_t and ω_l.

The foregoing singularities of the vibrational motion of the lithium hydride crystals make it possible to consider the following crystal model with which to take into account the role of the crystalline phase in the isotope separation effect.

1. The relatively heavy ions of lithium are rigidly fixed at the lattice sites.

2. Only the hydrogen ions oscillate at the optical frequencies.

3. The spectrum of the optical oscillations is described with the aid of suitably normalized δ-functions at the frequencies corresponding to the maxima of the peaks of the frequency distribution functions of real crystals in the optical region.

The physical picture of such a crystal model consists in the following: It is assumed that the crystal, say LiH, consists of dipole molecules Li-H, each of which is characterized by one vibrational frequency. The dipole-dipole interaction leads to collectivization of the vibrations of the molecules making up the crystals, and to the appearance of a difference in the frequencies of the transverse and longitudinal optical branches[17] (we neglect the dispersion, i.e., the dependence of the oscillation frequency ω on the wave vector).

Thus, the vibrational spectrum of the crystal is represented in the form of three optical branches with-

out dispersion, two transverse ones of equal frequency and one longitudinal one. The frequencies of these branches do not depend on the wave vector. To each of the N values of the wave vector (N—number of unit cells in the crystal) there correspond two identical transverse oscillation frequencies ω_t and one longitudinal-oscillation frequency ω_l. There are thus altogether 3N frequencies in the crystal.

We represent the frequency distribution function of the perfect crystal in the form

$$G(\omega^2) = 2N\delta(\omega^2 - \omega_t^2) + N\delta(\omega^2 - \omega_l^2). \tag{2}$$

When one of the atoms is replaced by its isotope, the vibrational spectrum of the crystal becomes distorted. The new resultant frequencies, which do not coincide with the previous one, can be obtained from the equation (see[18,19])

$$\left(1 - \frac{\varepsilon\omega^2}{3N} \int \frac{G(\Omega)d\Omega^2}{\omega^2 - \Omega^2}\right)^3 = 0, \tag{3}$$

where

$$\varepsilon = (M_I - M_{II})/M_I, \quad M_I \text{ and } M_{II}$$

are the masses of the negative ions of the main lattice and of the negative ions of the impurity. Substituting $G(\omega^2)$ from (2) in (3), we obtain

$$\left\{1 - \frac{\varepsilon\omega^2}{3}\left(\frac{2}{\omega^2 - \omega_t^2} + \frac{1}{\omega^2 - \omega_l^2}\right)\right\}^3 = 0. \tag{4}$$

Equation (4) has two triply-degenerate roots, which we denote by ω_{1L} and ω_{2L}. The frequency distribution functions of a crystal with one impurity atom, with allowance for the produced frequencies, can be represented in the form

$$G_1(\omega^2) = (2N - 3)\delta(\omega^2 - \omega_t^2) + (N - 3)\delta(\omega^2 - \omega_l^2) + 3\delta(\omega^2 - \omega_{1L}^2) + 3\delta(\omega^2 - \omega_{2L}^2). \tag{5}$$

If the number of impurity atoms entering the crystal is not one but N_{II}, with $N_{II} \ll N$, then in the approximation linear in the impurity concentration (i.e., when the impurity atoms do not interact with one another), the frequency distribution function of the defective crystal takes the form

$$G_{N_{II}}(\omega^2) = (2N - 3N_{II})\delta(\omega^2 - \omega_t^2) + (N - 3N_{II})\delta(\omega^2 - \omega_l^2) + 3N_{II}\delta(\omega^2 - \omega_{1L}^2) + 3N_{II}\delta(\omega^2 - \omega_{2L}^2). \tag{6}$$

Now, using the results of[1,14] and expression (6) for $G_{N_{II}}(\omega^2)$, we can obtain the following expression for the isotope separation coefficient: for the system "LiH:D—mixture of H_2 and HD gases" (owing to the small concentration of D in the system, the presence of D_2 molecules in the gas is neglected)

$$\alpha_I = \left(\frac{c_D}{c_H}\right)_{gas} \Big/ \left(\frac{c_D}{c_H}\right)_{cryst} = e^{\mu'/kT}\frac{Z_{HD}}{Z_{H_2}}, \tag{7}$$

for the system "LiD:H—mixture of D_2 and HD gases" we have

$$\alpha_2 = \left(\frac{c_D}{c_H}\right)_{gas} \Big/ \left(\frac{c_D}{c_H}\right)_{cryst} = e^{-\mu'/kT}\frac{Z_{D_2}}{Z_{HD}}, \tag{8}$$

where

$$\mu' = 3kT\ln\left\{\frac{S(\omega_{1L})S(\omega_{2L})}{S(\omega_t)S(\omega_l)}\right\}, \quad S(\omega) = \sh\frac{\hbar\omega}{2kT}, \tag{9}$$

and Z_{H_2}, Z_{HD}, and Z_{D_2} are the partition functions of the molecules H_2, HD, and D_2 (without symmetry numbers).

The spectrum of the natural frequencies of the Li^{7}H crystal was measured experimentally (by the neutron scattering method) by Brockhause et al.[15] and by Cheroplekov et al.[16] According to the data of[15], which deviate only slightly from the data of[16], the maxima of the vibration spectrum of Li^{7}H in the optical region correspond to values $\omega_t = 800$ cm^{-1} and $\omega_l = 1060$ cm^{-1}. The frequencies ω_t and ω_l for the Li^{7}D crystal can be determined in the considered model from the relation

$$\frac{(\omega_l)_{\text{Li}^7\text{H}}}{(\omega_l)_{\text{Li}^7\text{D}}} = \frac{(\omega_t)_{\text{Li}^7\text{H}}}{(\omega_t)_{\text{Li}^7\text{D}}} = \left(\frac{M_{D^-}}{M_{H^-}}\right)^{1/2} \tag{10}$$

(where M_{H^-} and M_{D^-} are the masses of the H$^-$ and D$^-$ ions), since in this model the heavy lithium ions are rigidly secured at the lattice sites, and only the hydrogen ions vibrate. The local oscillation frequencies ω_{1L} and ω_{2L} of the crystals Li^{7}H:D and Li^{7}D:H were calculated by means of formulas (4). The calculated frequencies are listed in table III.

The ratio of the partition functions Z_{HD}/Z_{H_2} and Z_{D_2}/Z_{HD} were calculated from the formula (see[10,13])

$$\frac{Z_1}{Z_2} = \left(\frac{M_1}{M_2}\right)^{3/2} \frac{I_1}{I_2} \left(1 + \frac{\sigma_1 - \sigma_2}{3}\right) \frac{S(\omega_2)}{S(\omega_1)} \tag{11}$$

for the values of the hydrogen molecule constants listed in Table IV.

Table III.

Crystal	Oscillation frequencies, cm^{-1}			
	ω_t	ω_l	ω_{tL}	ω_{2L}
Li^{7}H : D	800 [15]	1060 [15]	598	1003
Li^{7}D : H	560	750	644	932

Table IV.

Molecule	$M \cdot 10^{24}$, g	ω_e, cm^{-1}	$\omega_e x_e$, cm^{-1}	$I \cdot 10^{41}$, g $-$ cm^2
H$_2$	3.3473	4396.6	118.0	4.6013
HD	5.0177	3812.3	90.9	6.1323
D$_2$	6.6885	3118.5	64.1	9.1988

In Table IV, the data for the masses M of the molecules, the oscillation frequencies ω_e of the molecules, and the anharmonicity constants of the oscillations $\omega_c x_c$ are taken from the handbook[20], and the data for the molecule moments of inertia I are taken from the book by Herzberg[21] (in formula (11), $\omega = \omega_e - \omega_e x_e/2$, and $\sigma = h^2/8\pi^2 IkT$).

The values of the separation coefficient α_1 and α_2, calculated from formulas (7) and (8) using the data of Tables III and IV, are shown in Fig. 3 (curves 3 and 4, respectively). The experimental data are represented in Fig. 3 by curves 1 (Table I) and 2 (Table II). It is seen from Fig. 3 that the calculated values of the separation coefficients are smaller than the corresponding experimental values of α. However, the temperature variation of the curves is the same, and the discrepancies between the absolute values are small (within 5%).
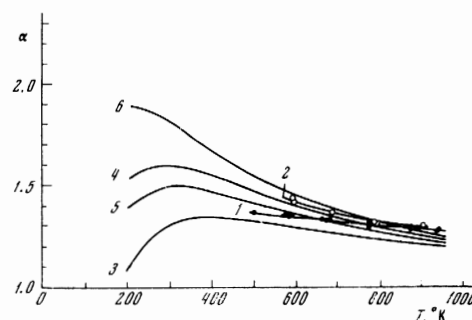

FIG. 3. Comparison of experimental temperature dependence of the separation coefficient with the value calculated from formulas (7) and (8): 1 and 2—data from tables I and II, 3 and 4— calculated curves of α_1 and α_2 at frequencies ω_t and ω_l of the Li^{7}H crystal spectrum obtained by neutron diffraction [15]; 5 and 6— calculated curves of α_1 and α_2 at the frequencies ω_t and ω_l of the theoretically calculated spectra of the Li^{7}H and Li^{7}D crystals [1,14].

Figure 3 shows also the values of α_1 and α_2 (curves 5 and 6), calculated from formulas (7) and (8) and values of $\omega_t = 760$ cm^{-1} and $\omega_l = 994$ cm^{-1} for the Li^{7}H crystal and $\omega_t = 503$ cm^{-1} and $\omega_l = 712$ cm^{-1} for the Li^{7}D crystal, corresponding to the maxima of the frequency distribution functions in the optical region of the theoretically calculated vibrational spectra[12,13]. The frequencies ω_{1L} and ω_{2L}, calculated from (4), are 538 cm^{-1} and 937 cm^{-1} for Li^{7}H:D and 581 and 872 cm^{-1} for Li^{7}D:H. Curves 5 and 6 of Fig. 3 lie somewhat higher than the corresponding curves 3 and 4, obtained for the values of ω_t and ω_l of the experimental spectra of Li^{7}H and Li^{7}D. This is connected with the lower frequencies of the theoretical vibrational spectra. Comparing now curves 5 and 6 of Fig. 3 with curves 3 and 4 of Fig. 2, we see that an approximate allowance for the contribution of the crystal to the isotope separation affect results in a small deviation from the values of α obtained when exact account is taken of the contribution of the crystals. We can therefore conclude that the model of the lithium hydride crystals, in which it is assumed that at the relatively heavy Li ions are rigidly secured at the lattice sites, and the H ions vibrate with frequencies corresponding to the maxima of the distribution functions of the crystal frequencies in the optical branch, describes satisfactorily the isotope separation effect due to the crystal.

The use of this model is expected to yield better agreement with experiment in calculations of the isotope separation effects for systems including H and hydrides of alkali and alkali-earth metals heavier than Li.

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