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STRUCTURAL AND THERMODYNAMIC ASPECTS OF ELECTRON DIFFRACTION BY LITHIUM FLUORIDE DIMERS

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UDC 539.27

Electron-diffraction and spectral data for Li_2F_2 have been combined to derive the equilibrium parameters, force field in the harmonic approximation, and vibrational frequencies inactive in the IR spectrum. The proportions of the molecular forms in the saturated vapor have been derived for 1360 ± 50 K, and the enthalpy and entropy have been determined for the reactions $Li_2F_2 \rightleftarrows 2LiF$ and $3Li_2F_2 \rightleftarrows 2Li_3F_3$.

The present study continues research on lithium fluoride vapor by electron diffraction [1] and is concerned with determining the parameters in the equilibrium configuration, the force field for Li_2F_2, and the enthalpy and entropy in $Li_2F_2 \rightleftarrows 2LiF$ and $3Li_2F_2 \rightleftarrows 2Li_3F_3$ on the basis of electron-diffraction data.

The compositions of alkali fluoride vapors have been examined in some detail, and various methods have shown that they are variously associated. The composition of saturated lithium fluoride vapor has several times been determined [1-5]. These data were recorded under various conditions and are not comparable, but in all cases, there were considerable amounts of dimer (31-62 mole %), and the trimer levels were about 4-15 mole % [1-5].

A planar rhombic structure with D_{2h} symmetry is preferable for alkali fluoride dimers; this has been confirmed by experiment [1, 6] and from calculations [7-12].

Li_2F_2 with symmetry D_{2h} has six normal vibrational frequencies, three of which ($2A_g$, B_{1g}) a active in Raman scattering and three (B_{1u}, B_{2u}, B_{3u}) in the IR. The IR spectra of matrix-isolated lithium fluoride vapor have several times been recorded [13-19] and indicate all three allowed vibrational frequencies for the dimer. The Raman spectra of the alkali fluorides have not been examined. A complete set of vibrational frequencies for Li_2F_2 has been derived by ab initio calculation [11, 12]. An attempt has been made [18] to estimate the unmeasured vibrational frequencies for Li_2F_2 from the ν_4, ν_5, and ν_6 measured in the IR spectrum.

Two D_{3h} configurations have been proposed for Li_3F_3: regular hexagonal [9] and distorted with an FLiF angle of 123.8° [12]. It follows from [12] that $r_e(Li{-}F)_{tr} = r_e(Li{-}F)_d$ –

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TABLE 1. Parameters in the Effective r_g Configuration (Å) of Li_2F_2 and Optimal Vapor Composition (1360 K)

Parameter		$r_\alpha(Li{-}F)_{tr}=r_\alpha(LiF)_d-0{,}03$		$r_\alpha(Li{-}F)_{tr}=r_\alpha(Li{-}F)_d$	
		configuration		configuration	
		regular	distorted	regular	distorted
		Li_3F_3		Li_3F_3	
Li — F	r_g	1,768(5/9)*	1,762(5/13)	1,764(6/18)	1,754(6/18)
	l	0,112(5/7)	0,117(5/6)	0,115(5/7)	0,120(5/8)
Li ... Li	r_g	2,19(8/19)	2,19(8/13)	2,21(9/17)	2,18(10/20)
	l	0,11(5/5)	0,14(5/5)	0,15(5/5)	0,18(7/7)
F ... F	r_g	2,664(8/9)	2,671(8/8)	2,68(1/1)	2,68(1/1)
	l	0,145(8/13)	0,149(8/14)	0,146(8/17)	0,154(8/18)
Optimal vapor composition, mole %	X_M	59^{+5}_{-7}	58^{+6}_{-12}	55^{+5}_{-9}	52^{+9}_{-13}
	X_d	36^{+7}_{-5}	40^{+12}_{-6}	37^{+9}_{-5}	43^{+13}_{-9}
	X_{tr}	5^{+3}_{-2}	5 ± 2	5 ± 2	5 ± 3
R_f, %		3,39	3,45	3,49	3,58

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*The total errors are given in parentheses: on the left, without allowance for the inaccuracy in the vapor composition for the internuclear distances $\sigma = \sqrt{\sigma_{sc}^2 + (2.5\,\sigma_{\ell s})^2}$, while to the right they are given with allowance for the inaccuracy in the composition for the internuclear distances $\sigma = \sqrt{\sigma_{sc}^2 + (2.5\sigma_{sc})^2 + (\Delta r)^2}$, and the amplitudes $\sigma = \sqrt{(2.5\sigma_{sc})^2 + (\Delta\ell)^2}$.

0.031 Å, and four of the 12 frequencies of normal vibration for Li_3F_3, have been measured [18], while the others have been estimated [20].

STRUCTURE ANALYSIS IN TERMS OF EFFECTIVE MOLECULAR PARAMETERS

Our initial data were provided by electron-diffraction patterns for lithium fluoride vapor [1]. The photometry and subsequent processing were on the traditional methods. The total scattering intensity curve was recorded for the angular range s = 2.0-16.8 $Å^{-1}$ which subsequently was reduced to 13.6 $Å^{-1}$ because of large errors in the far region. The reduced molecular component of the scattering intensity $sM_{exp}(s)$ was isolated by a graphical procedure.

The complicated vapor composition means that all molecular forms must be considered in constructing the theoretical analog of the observed sM(s). The theoretical function was written as

$$sM_{th}(s) = \alpha\cdot sM_M(s) + \beta\cdot sM_{tr}(s) + (1-\alpha-\beta)\cdot sM_d(s), \tag{1}$$

in which $sM_M(s)$, $sM_d(s)$, $sM_{tr}(s)$ are functions for the reduced intensity for the monomer, dimer, and trimer correspondingly, while α, β, and $1-\alpha-\beta$ are coefficients related to the concentrations of the corresponding forms.

In [1, 11, 12, 21] it is shown that the compounds have similar internuclear distances. Those distances and the corresponding vibration amplitudes cannot be determined simultaneously and independently from a least-squares analysis of $sM_{exp}(s)$ because of the strong correlation between them. The parameters for a monomer are known [21], while the trimer is present in only small amounts, so we determine the parameters only for Li_2F_2.

There are differences between this structure analysis and [1]. In the latter, the parameters for LiF and Li_3F_3 and the Li...Li term for Li_2F_2 were fixed. The $r_a(Li...Li)_d$ was taken as 2.11 Å, with $\ell(Li...Li)_d$ = 0.18 Å. The parameters for Li_3F_3 were calculated from a regular hexagonal D_{3h} structure and equality of $r_a(Li{-}F)$ and $\ell(Li{-}F)$ in the dimer and trimer.

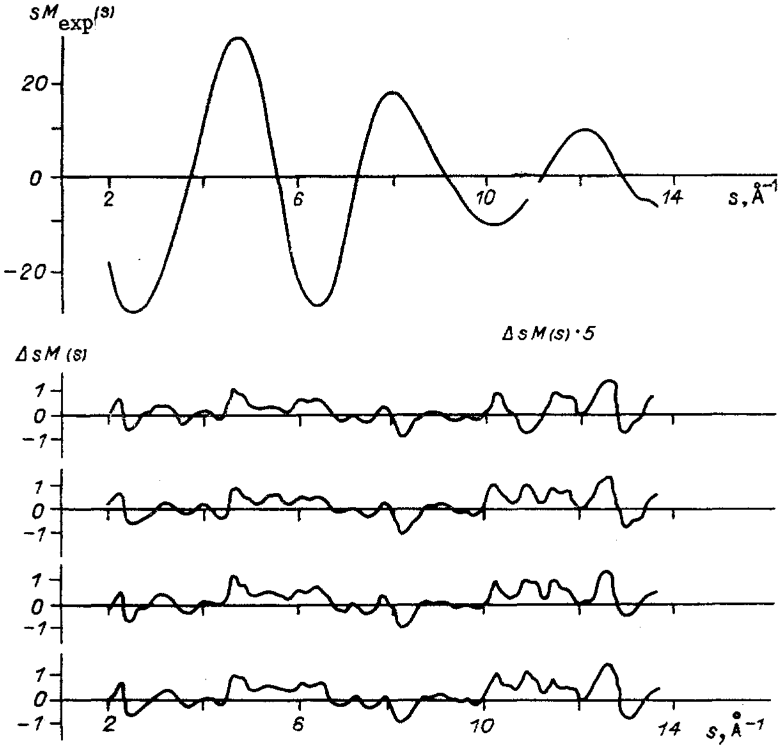

Fig. 1. Experimental curve for the molecular component of the scattering intensity $sM_{exp}(s)$ and curves for the difference $\Delta sM(s)$, corresponding to various forms of calculation based on different features in the Li_3F_3 structure.

In the present case, all parameters for the dimer were independent, while the vibration amplitudes and the corrections to the internuclear distances for the perpendicular vibrations in Li_3F_3 were calculated on the NORCRD program [22] with the [18, 20] data.

We also attempted to distinguish how the two suggested [9, 12] configurations for Li_3F_3 (regular and distorted D_{3h}) influenced the parameters for the dimer. In the regular Li_3F_3 structure, the bond angles were taken as 124 and 116° correspondingly [12]. The structural analysis was also performed in two forms: in the first, with $r_\alpha(Li-F)_{tr} = r_\alpha(Li-F)_d - 0.03$ Å as implied by [12], while in the second, $r_\alpha(Li-F)_{tr} = r_\alpha(Li-F)_d$.

The net method was used to refine the vapor composition over lithium fluoride. Table 1 gives the optimum composition, errors on the Hamilton test for 95% fiducial probability [23]. Table 1 also gives the parameters of the effective r_g configuration for Li_2F_2 derived in various forms of least-squares analysis for the observed sM(s). Figure 1 shows sM_{exp} (s) and ΔsM(s) corresponding to these forms.

One cannot give preference to any of the data sets. The choice criteria can be based on the discrepancy factors for the observed and theoretical sM(s) curves as well as anomalies in the parameters. The Li_2F_2 structure parameters and the R_f discrepancy factors in Table 1 indicate that the observed discrepancies are not significant.

The methods of determining the errors in the Li_2F_2 structure parameters need to be considered in more detail. The traditional approach to error estimation is based on the covariance matrix, but that is not really correct here because of the complicated vapor composition. We corrected for the correlation between the Li_2F_2 structure parameters and the concentrations of the coexisting forms by introducing additional components Δr and Δℓ equal to the differences in the corresponding parameters between the minima in the functional surfaces and the points separated in accordance with the vapor composition from the minima by amounts defined by the statistical criterion [23] (Fig. 2).

The skewness in the section of the optimized functional with respect to the form concentrations is due to the correlation between the distances, the amplitudes, and the vapor

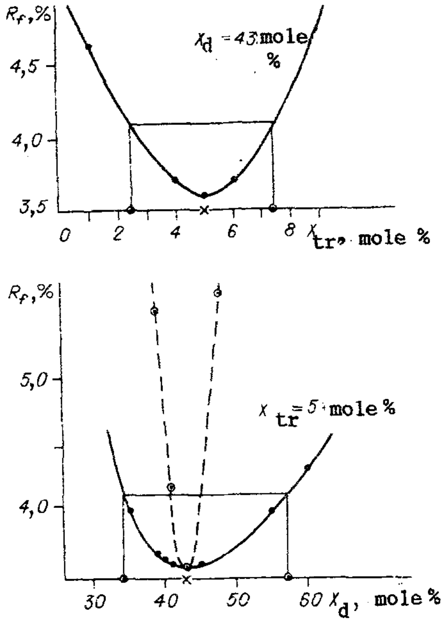

Fig. 2. Changes in discrepancy between the observed and theoretical sM(s) curves on refining the vapor composition (the dashed line shows the section corresponding to fixed values for the distances and amplitudes) with allowance for the distorted Li_3F_3 configuration and $r_\alpha(Li-F)_{tr} = r_\alpha(Li-F)_d$.

TABLE 2. Force Fields (mdyn/Å) and Equilibrium Structure Parameters for Li_2F_2 and Form Concentrations in the Saturated Vapor of Lithium Fluoride at 1360 K

Parameter	$r_\alpha(Li-F)_{tr}=r_\alpha(Li-F)_d-0{,}03$		$r_\alpha(Li-F)_{tr}=r_\alpha(Li-F)_d$	
	configuration		configuration	
	regular	distorted	regular	distorted
	Li_3F_3		Li_3F_3	
$F_1(A_g)$	1,69(17)*	1,80(18)	1,91(19)	1,89(19)
$F_{12}(A_g)$	0,01	0,0	0,0	0,0
$F_2(A_g)$	0,16(2)	0,17(2)	0,17(2)	0,17(2)
$F_3(B_{1g})$	1,58(16)	1,93(19)	1,73(17)	1,75(18)
$F_4(B_{1u})$**	0,135	0,135	0,135	0,135
$F_5(B_{2u})$**	1,06	1,06	1,06	1,06
$F_6(B_{3u})$**	1,25	1,25	1,25	1,25
$r_e^h(Li-F)_d$***, Å	1,737±0,009	1,74±0,01	1,74±0,02	1,74±0,02
FLiF angle, deg	102±1	102±1	102±2	102±2
X_M,	53	54	55	55
X_d, mole %	42	41	40	40
X_{tr}****,	5	5	5	5

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*In parentheses we give the errors calculated from $\sigma = 0.1\ F_i$.

**F_i calculated from the vibration frequencies [18] corrected for the matrix shift (see Table 3).

***The errors quoted for r_e^h and the FLiF angle have been transferred from the traditional form of structure analysis with correction for the inaccuracy in the vapor composition.

****X_{tr} transferred from the traditional form.

TABLE 3. Normal Vibrational Frequencies of Li_2F_2, cm^{-1}

Frequency	$r_\alpha(\mathrm{Li{-}F})_{\mathrm{Tp}} = r_\alpha(\mathrm{Li{-}F})_{Д} - 0,03$		$r_\alpha(\mathrm{Li{-}F})_{\mathrm{Tp}} = r_\alpha(\mathrm{Li{-}F})_{Д}$		*ab initio* calcn.		IR + calculation [18]
	configuration		configuration		[11]	[12]	
	regular	distorted	regular	distorted			
	Li_3F_3		Li_3F_3				
$\nu_1(A_g)$	731(39)	758(40)	778(40)	775(40)	700	691	(560)
$\nu_2(A_g)$	297(18)	305(18)	306(18)	306(19)	370	382	(280)
$\nu_3(B_{1g})$	761(37)	841(40)	796(40)	801(42)	593	589	(490)
$\nu_4(B_{1u})$	300 *	300 *	300 *	300 *	311	331	287
$\nu_5(B_{2u})$	654 *	654 *	654 *	654 *	661	658	641
$\nu_6(B_{3u})$	575 *	575 *	575 *	575 *	606	617	553

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*Transferred from [18] with correction for the matrix shift.

composition. With the section corresponding to fixed values for the distances and amplitudes, the skewness vanishes, and the formal error in determining the form concentrations is reduced.

This shows that the method can provide accurate information on the vapor composition in a system containing two or three forms in comparable amounts.

The structure parameters do not conflict with a planar or near-planar rhombic structure for Li_2F_2.

STRUCTURE ANALYSIS IN TERMS OF THE POTENTIAL-FUNCTION PARAMETERS FOR Li_2F_2

We determined the equilibrium parameters and force field for Li_2F_2 in the harmonic approximation via the [24] method, in which sM(s) is parameterized into force constants F_{ij} and equilibrium internuclear distances r_e^h.

This case differs somewhat from that described in [24]. The complicated vapor composition means that the theoretical sM(s) should incorporate all components, see (1). In the first part, at this stage we determined only the parameters of the dimer and the vapor composition, in which the $sM_m(s)$ and $sM_{tr}(s)$ components were calculated from the traditional formulas by the use of the effective r_g parameters.

Table 1 shows that the parameters for the Li...Li term have been determined with large errors, so the main contributions to sM(s) come from four vibrational parameters: $\langle\Delta z^2(\mathrm{Li{-}F})\rangle$, $\langle\Delta z^2(\mathrm{F...F})\rangle$, $U(\mathrm{Li{-}F})$ and $U(\mathrm{F...F})$. Then the electron-diffraction data alone give values for not more than four force constants, while the complete force field for an M_2X_2 molecule (D_{2h}) contains six. Therefore, we used the measured vibrational frequencies $\nu_4(B_{1u})$ and $\nu_6(B_{3u})$ [18] corrected for the matrix shift, which enabled us to derive the force constants and the vibrational frequencies inactive in the IR for Li_2F_2, as well as $r_e^h(\mathrm{Li{-}F})$ and the FLiF angle (Tables 2 and 3).

The estimator for the errors in the diagonal force constants was $\sigma = 0.1\ F_i$. The errors for the structural parameters were transferred from traditional least-squares analysis with correction for the inaccuracy in determining the vapor composition. The errors in the vibrational frequencies were calculated from the corresponding values for the force constants.

DISCUSSION

Structure. There is formal agreement between the structural and vibrational characteristics of Li_2F_2 and also the concentrations of the molecular forms derived in the four forms of calculation, which differ in the features assumed for the Li_3F_3 structure. Then our results can be compared with published ones from the values obtained on the assumption of a regular structure for Li_3F_3 (FLiF = 120°) together with $r_\alpha(\mathrm{Li{-}F})_{tr} = r_\alpha(\mathrm{Li{-}F})_d - 0.03$ Å, since that form gives the best fit between the observed and theoretical sM(s).

The $r_e^h(\mathrm{Li{-}F})_d$ from [25] is a good estimate for the equilibrium distance r_e. It has been shown [25] that $r_e^h \approx r_\alpha = r_e + \langle\Delta z(1)\rangle + \langle\Delta z(2)\rangle$, where $\langle\Delta z(1)\rangle$ is the anharmonic term and $\langle\Delta z(2)\rangle$

TABLE 4. Enthalpies and Entropies of Reactions in Lithium Fluoride Vapor

Reaction	Thermodynamic functions	$r_\alpha(\mathrm{Li-F})_{tr} = r_\alpha(\mathrm{Li-F})_d - 00{,}3$		$r_\alpha(\mathrm{Li-F})_{tr} = r_\alpha(\mathrm{Li-F})_d$	[33]
		D_{3h} configuration		regular and distorted configuration D_{3h}	
		regular	distorted		
		Li_3F_3		Li_3F_3	
$Li_2F_2 \rightleftarrows 2LiF$	$\Delta_r H°(0)$, kJ/mole	244,4±8,5	248,3±8,5	246,1±8,8	249,5±9,1
	$\Delta_r S°(298{,}15)$, J/mole·K	139,8	140,4	140,4	138,6
$3Li_2F_2 \rightleftarrows 2Li_3F_3$	$\Delta_r H°(0)$, kJ/mole	−213±15	−205±15	−208±15	−243±20
	$\Delta_r S°(298{,}15)$, J/mole·K	−148,3	−146,7	−146,7	−152,0

the curvilinear harmonic one. The $\langle \Delta z(2) \rangle$ term balances out much of $\langle \Delta z(1) \rangle$, particularly at high temperature, i.e., $\langle \Delta z(2) \rangle \approx \langle \Delta z(1) \rangle$, so $r_\alpha \approx r_e^h$ tends to approximate to r_e.

The result r_e^h(Li–F) = 1.74 ± 0.01 Å for Li_2F_2 agrees well with r_e(Li–F) = 1.73 Å [8] and r_e(Li–F) = 1.75 Å [11].

According to [11, 26], the kinematic and dynamic anharmonicities in the out-of-plane vibrations for Li_2X_2 are small, so the estimate for the equilibrium FLiF angle can be recommended as that found from the potential method, which agrees well with the FLiF = 100.1° found in ab initio calculations [11].

Vibrational Frequencies. Our frequencies are compared with published ones in Table 3. $\nu_1(A_g)$ and $\nu_3(B_{1g})$ should be taken as overestimates, which is due to the short sM(s) from experiment, which along with the complicated vapor composition makes it difficult to determine $\langle \Delta z^2(\mathrm{Li-F}) \rangle_T$ reliably because of the correlation with the graphically defined background line. A similar case has been considered in [27]. The parallel mean-square vibration amplitude $\langle \Delta z^2(\mathrm{Li-F}) \rangle_T$ can be represented as in [28]: $\langle \Delta z^2(\mathrm{Li-F}) \rangle_T = \frac{1}{4}[\Sigma_1(A_g) + \Sigma_3(B_{1g}) + \Sigma_5(B_{2u}) + \Sigma_6(B_{3u})]$, while $\Sigma_3(B_{1g})$, $\Sigma_5(B_{2u})$, $\Sigma_6(B_{3u})$ are defined by $\Sigma_i = G_i \cdot \delta_i$, in which G_i is an element in the kinematic-coefficient matrix [28, 29] and δ_i the frequency parameter. The $\Sigma_1(A_g)$ appearing in the second-order block was calculated from $\Sigma_1(A_g) = a \cdot G_1(A_g) + b \cdot F_2(A_g)$, in which a and b are related to $\nu_1(A_g)$ and $\nu_2(A_g)$.

During the least-squares analysis, $\Sigma_5(B_{2u})$ and $\Sigma_6(B_{3u})$ were not varied, so the error in determining $\langle \Delta z^2(\mathrm{Li-F}) \rangle_T$ includes the errors in $\Sigma_1(A_g)$ and $\Sigma_3(B_{1g})$, and in turn, $\Sigma_3(B_{1g})$ is related to $\nu_3(B_{1g})$, and $\Sigma_1(A_g)$ to $\nu_1(A_g)$ and $\nu_2(Ag)$. However, $\nu_2(Ag)$ is determined quite reliably from $\langle \Delta z^2(F...F) \rangle_T$, which is much less sensitive to the background line. Then the overestimated $\nu_1(Ag)$ and $\nu_3(B_{1g})$ may be related to underestimated (Li–F) vibration amplitudes.

Vapor Composition and Thermodynamics. We used electron diffraction as an analytical method for determining the relative form concentrations in the saturated vapor. The results may be compared with those from a previous electron-diffraction study [1], where the recommendations were $X_m = 30^{+15}_{-30}$, $X_d = 60^{+30}_{-15}$, $X_{tr} = 10 \pm 5$ mole %. The differences are evidently due to the simplified estimation of the fixed molecular parameters in [1]. On the other hand, our vapor composition agrees well with that calculated from the temperature dependence of the form concentrations derived [30] by classifying the published thermodynamic characteristic. The data may also be compared with the [31] research in the 1950s by the visual method. As r_{eff} (Li–F) = 1.68 Å from [31], we used r_g(Li–F) for the monomer, dimer, and trimer with X_{tr} = 5 mole % from the present study to get X_m = 63, X_d = 32 mole %.

These concentrations, structure parameters, and vibrational frequencies for Li_2F_2 were used to calculate the enthalpies and entropies of $Li_2F_2 \rightleftarrows 2LiF$ and $3Li_2F_2 \rightleftarrows 2Li_3F_3$. The saturation vapor pressure needed to calculate the K_X to K_P was taken from [32], while the lacking information for the monomer and trimer was taken from [33].

Table 4 compares the $\Delta_rH_0(0)$ and Δ_rS^0 (298.15) with the currently most reliable [33] data. The errors in the reaction enthalpies have been determined with allowance for the uncertainties in the vapor composition, temperature, and vibrational frequencies.

The enthalpies and entropies found from the diffraction data agree well with the [33] values derived from methods used traditionally to obtain them, where the errors are quite small. Vapor electron diffraction with correct diffusion experiments and correct structure analysis can thus provide useful thermodynamic information even when the vapor contains three molecular forms.

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