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Study of Low Frequency Molecular Motions in HF , KHF_2 , KH_2F_3 and NaH_2F_3^*

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Abstract

The spectra of KHF_2 , KH_2F_3 , NaH_2F_3 , liquid and solid HF were measured between 1200 and 30 cm^{-1} by the inelastic scattering of "cold neutrons" (0.005 e.v.). The spectrum of KHF_2 is in agreement with previous infrared measurements and shows a peak at 147 mV corresponding to a deformation frequency ν_2 of the F-H-F group and a broad peak at 13 mV due to a libration of this group. The observed spectra for KH_2F_3 , NaH_2F_3 solid and liquid HF were compared with that for KHF_2 considering the known results that the F-F distance increases, the position of the H atom between the two fluorines becomes more asymmetrical, and the strength of the hydrogen bond decreases in going from the HF_2^- ion to H_2F_3^- ion to HF . In this comparison the known structure of the H_2F_3^- ion is considered as being intermediate between that of HF_2^- and the zig-zag hydrogen bonded chains in solid HF . As a result, the lines observed at 112 mV and 67 mV in the H_2F_3^- spectra and in HF respectively are associated with the deformation frequency ν_2 of the H-F-H group in these compounds. In addition the spectra of H_2F_3^- ions show a peak at a 15 mV attributed to a libration of the group. Both H_2F_3^- and HF show peaks at 8 and 7 mV

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respectively attributed to a rotational motion of one F-H-F unit around the F-F bond. The observed spectrum of HF liquid, showing a high degree of association is also discussed with respect to these motions.

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INTRODUCTION

Previous diffraction studies have shown that the solid phase of HF consists of "zig-zag", quasi-infinite, hydrogen-bonded chains,¹ which are planar and have only weak interactions between one another. Indeed, polymeric association as high as six molecular units can exist even in the gaseous phase.² While little information is available on the structure of the liquid phase measurements of the average molecular weight as a function of temperature³ indicate that considerable association exists in this phase and the amount of association decreases with increasing temperature.

The study of low frequency motions in the liquid and solid phases of HF are of interest for several reasons: a) no disordered solid phase is known to exist despite the small dispersion forces between chains;¹ b) there are large associated units in the liquid;³ c) there is a very large temperature difference, 121°, between the melting and the boiling points over which one can study the motions in the liquid phase.² d) In addition, there is a scarcity of information about the different possible low frequency molecular motions occurring in both phases of HF.

In the present work, the low energy spectra of the solid and liquid phases of HF have been studied by inelastic neutron scattering. A comparison was made with the observed spectra of HF_2^- and H_2F_3^- ions. The HF_2^- ion in KHF_2 has been studied extensively by thermodynamical methods,⁴ infrared,⁵ Raman spectroscopy,⁶ and N. M. R.⁷ and the structure of KH_2F_3 was recently determined by x-ray analysis. $\text{HF}_2^{-(9)}$ and $\text{H}_2\text{F}_3^{-(8)}$ ions have structures which are similar to the units from which the long zig-zag chains in the solid phase of HF is composed. However, the strength of the

hydrogen bond decreases¹⁰ and F-F distance increases as one goes from HF_2^- to H_2F_3^- to HF. A partial summary of available data on the three phases of HF, on KHF_2 and KH_2F_3 is given in Table I.

In the present experiment, the energy of the incident neutrons (0.005 e.v.) is small compared to the thermal energy (kT) of the sample and only those neutrons are observed which have gained energy in a single scattering event. Therefore the observed peaks represent transitions between adjacent levels populated by thermal excitation. As the neutron scattering cross section of hydrogen (20 barns free atom cross section) is large relative to that of F (~ 4 barns) and is mostly incoherent, the neutron spectra represent the low frequency motions of the units in which the hydrogen atoms are bound.

EXPERIMENTAL APPARATUS

The present experiment utilized the cold-neutron facility at the Brookhaven National Laboratory research Reactor, which has been described extensively in the literature.¹¹ The neutron beam incident on the scatterer is produced by filtration through 8 inches of refrigerated beryllium. No Bragg (elastic) scattering can occur for the low-energy (-0.005 e.v.) incident neutrons, and the neutrons which are scattered at 90° by the sample are those which have gained energy or have been elastically scattered by the sample. The energy spectrum of the scattered neutrons was determined by chopper time-of-flight technique.

The liquid and the polycrystalline samples were contained in an aluminum sample holder which was shielded by cadmium so that neutrons could only be scattered off the samples. The effective thickness of the polycrystalline or liquid material was sufficiently small (1 mm)

so that multiple scattering was negligible.

The sample was cooled by a flow of cold gas boiled off from liquid nitrogen through coils in contact with the sample holder. By regulation of the nitrogen flow the sample could be maintained at any desired temperature within $\pm 2^\circ\text{K}$ between 294° and 90°K as determined by copper-constantan thermocouples in contact with the sample.

RESULTS

The spectra of neutrons gaining energy were obtained for HF liquid at $T = 219^\circ\text{K}$ (I) and 280°K (II) and for HF solid at 153°K . The results are shown in Fig. I. The energy spectra for the liquid and solid phases of HF have a similar structure with two peaks at 67 and 7 mV referred to as (A) and (D) respectively. A shoulder of low relative intensity (peak B) appears at 26 mV in the spectrum of the solid phase of HF and is not seen in the liquid phases. The change in intensity with temperature of peak A can be accounted for by a Boltzmann population factor. Peak D broadens with increasing temperature in the liquid phase retaining the position of its maximum: becoming very flat at 280°K (10° below the gaseous phase). The peaks observed above channel 140 represent the Bragg "cut-offs" in the beryllium filter and are due to elastically scattered neutrons. Fig. II shows the observed spectra for KH_2F_3 and NaH_2F_3^* at $T = 293^\circ\text{K}$. A sharp peak A" at 112mV is cation independent. Low intensity peaks (B") occur at 50 and 45 mV respectively in NaH_2F_3 and KH_2F_3 showing a small cation dependence. The spectra of both samples show maxima at about 15 mV(C") and 8mV(D") which appear to correspond to two partially resolved broad peaks at these energies. Despite the poor resolution, the positions of these

*These compounds are very hygroscopic and analyses for water before and after the spectra were taken showed no significant traces of H_2O .

peaks show no strong cation dependence while their intensities do vary with the cations.

Fig. III shows the spectra obtained for polycrystalline KHF_2 at 293°K which is similar in certain respects to the spectra described above. There is a sharp peak (A') at 147 mV, a weak maximum at about 75 mV, and a broad symmetrical peak at 13 mV. A spectrum of KHF_2 taken at 393°K shows that peak A' and B' do not shift in energy with increasing temperature but their intensities increase according to a Boltzmann population factor. At 393°K peak (C') appears to broaden slightly towards high energy while the energy position of its maximum does not shift appreciably.

Table II lists the energy positions of these peaks for the four compounds in both mV and wave number.

DISCUSSION

Any interpretation of the above spectra should take into account:

- a) results of infrared⁵ and neutron diffraction data on KHF_2 ⁽⁹⁾ and x-ray data on KH_2F_3 .⁸
- b) Similarities in the observed spectra of the four compounds in view of the fact that HF_2^- and H_2F_3^- ions have structures similar to the units that compose the zig-zag chains in solid HF.

Infrared data of KHF_2 has shown the fundamental ν_2 of the HF_2^- ion to be at 1200 cm^{-1} ⁽⁵⁾. This agrees with the sharp peak (A') seen at $1180 \pm 20 \text{ cm}^{-1}$ in the present spectrum. This motion corresponding to ν_2 is shown in Fig. IV. Raman⁶ and infrared⁵ lines observed at about 600 cm^{-1} are identified as a symmetric fundamental vibration ν_1 of the HF_2^- ion where the two fluorine ions move in opposite phase along the molecular axis whence the hydrogen atom at the center remains at rest.

This line may be associated in the neutron spectrum with the very weak peak (B') at 600 cm^{-1} . Such a vibration which involves motions of the fluorine atoms can only give rise to a very weak peak in the neutron spectrum because of the different magnitudes of hydrogen and fluorine scattering cross sections. Low frequency Raman⁶ lines observed at 136 , 100 and 90 cm^{-1} were attributed to librational motion of the HF_2^- ion and vibration of the K^+ ion. The motion of the K^+ ion would not be seen in the present experiment due to the relative magnitude of its scattering cross section but the low energy peak (C') occurs at 13 mV (104 cm^{-1}) in good agreement with these Raman data. Also a neutron diffraction study of the crystal structure by Levy and Peterson⁹ has shown an asymmetry in the fluorine displacement. The mean ($2.7\text{\AA}$) displacement in a plane perpendicular to the axis of the bifluorine ion, suggests rotatory oscillations of the $[\text{HF}_2^-]$ with a mean amplitude of 14° . Infrared⁵ data shows a line at 1450 cm^{-1} attributed to the fundamental frequency ν_3 of the HF_2^- unit. This line is not observed due to the low probability of excitation of this motion at the temperature of the sample in this experiment and the decrease in resolution with increasing energy. Fig. IV shows a schematic representation of the motions associated with ν_1, ν_2, ν_3 and the librational motions of the HF_2^- ion.

In view of the similar type of forces in HF_2^- , H_2F_3^- , and HF , peak A' ascribed to ν_2 in the HF_2^- ion may be closely related to peak A'' in H_2F_3^- ion and peak A in HF although the latter two peaks occur at lower frequency because of weaker forces between the fluorine atoms. It is seen in Table I that the F-F distance increases from 2.26 to $2.49\text{\AA}$, the position of the hydrogen between the two fluorines becomes more asymmetric and the

strength of the H bond decreases in going from $[\text{HF}_2^-]$ to $[\text{H}_2\text{F}_3^-]$ to HF; a shift in frequency from 147 mV (or peak A') in HF_2^- to 112 mV in $[\text{H}_2\text{F}_3^-]$ (peak A'') and finally to 66 mV in solid HF (peak A) may thus be due to increase in F-F distance and weakening of the H bond. This shift is quite pronounced but not unusual. As a comparison we can take a calculation by Reid¹² of low frequency vibrations for the O-H---O system. Reid shows that these frequencies vary between 850 cm^{-1} and 110 cm^{-1} as the O---O equilibrium distance varies from 2.43 to $2.74\text{\AA}$. No calculation exists for the similar F-H---F system. Fig. V shows the variation of this frequency with the oxygen-oxygen distances as calculated by Reid together with experimental points for H_2O and KH_2PO_4 . In addition the frequencies of peak A, A', A'' are also plotted as a function of F-F distance.

An infrared study of KHF_2 ⁽¹³⁾ has shown that ν_2 is shifted to a lower frequency by 26 cm^{-1} in aqueous solution compared with the crystalline form where ordering effects and interaction with neighboring K^+ ions restrict the motion and in fact increase the bending force constant. However, such shifts of the order of 30 cm^{-1} are nearly within the resolution of the present experiment for the energies of peaks A, A', A''. Also the observed peaks A'' in KH_2F_3 and NaH_2F_3 are cation independent, and a similar behavior could account for the nearly constant energy of peak A in HF for both the solid and liquid phases.

NaH_2F_3 and KH_2F_3 show relatively weak peaks B'' at 50 and 45 mV respectively. It was noted above that a very weak peak appears at 75 mV in KHF_2 and was attributed to the frequency ν_1 seen in Raman data and involving only the motions of the F atoms in HF_2^- ion. In view of the

increased F-F distance and despite the increased hydrogen to fluorine ratio in H_2F_3^- compared to HF_2^- one might expect the frequency ν_1 in H_2F_3^- ion to occur at lower frequency and show a more intense peak in the spectrum of scattered neutrons due to an increase cooperation between fluorine atoms involved in this motion. While peak B'' is consistent with this behavior, the small cation dependence is not explained at the present time. The shoulder (B) in solid HF at about 27mV might also be attributed to a ν_1 type vibration of the fluorine. Such a definite assignment is precluded as this peak is not well resolved in solid HF and does not appear in the spectra of the liquid phase.

Both NaH_2F_3 and KH_2F_3 show peaks C'' and D'' at 15 and 8 mV respectively. These differ by about 2 mV from the position of peak C' in KHF_2 and peak D in solid and liquid phases of HF. As the H_2F_3^- ion has a structure intermediate between that of HF_2^- and the zig-zag chain in solid HF the possible correspondence between C and C' and D'' and D, respectively, should be considered. Peak C'' may then be associated with librational motion of the H_2F_3^- ion as shown in Fig. VI.

To interpret peaks D'' and D in H_2F_3^- and HF respectively one should consider two fundamental differences for a F-H--F unit in solid or liquid HF and in KHF_2 . In HF solid and liquid unlike in KHF_2 the F-H--F unit is bound in a chain and the proton is not symmetrically located between the two fluorines. Previous investigations indicate that for such an asymmetric position of a proton in certain solids containing strong hydrogen bonds there can occur a splitting of vibrational levels due to tunneling of the proton between two minima of potential. This splitting is of the order of $100\text{--}160\text{ cm}^{-1}$ in the case of the OH--O system.^{14,15} Estimates of the magnitude of such splitting for HF can be obtained from

the work of Glocker and Evans¹⁶ on KHF_2 and is about 55 cm^{-1} . Thus it is possible that the peak at 53 cm^{-1} in solid and liquid HF might be associated with direct transitions between a split oscillator level, but difficulties in calculating an accurate magnitude of this splitting and in verifying that such an effect actually takes place preclude such a definite assignment.

It may also be possible that peak D in HF results from a libration of one link $\text{FH}\cdots\text{F}$ of the chain (probably at the end of the chain), as illustrated in Fig. VII. This libration may be considered as occurring on the surface of a cone of 120° angle with its apex at the F atom, so that the bond angle of the zig-zag chain is preserved. In HF as the temperature rises the amplitude of the libration would increase and several adjacent links may start to librate. When the amplitude of the libration becomes sufficiently large the chain could break in parts of various lengths. Thus in the liquid state the chains are shorter than in the solid and translational as well as librational motions can occur which would symmetrically broaden peak D. In like manner, peak D" in H_2F_3 might be associated with a similar type libration as shown in Fig. VI, but the choice between tunneling effect or such libration is further complicated in this case by the lack of knowledge of the position of the proton between the two fluorines.

CONCLUSION

The spectra of scattered neutrons from liquid and solid phases of HF emphasize the high degree of association that exist through the liquid phase of HF. It is known from x-ray and neutron diffraction data that HF_2^- and H_2F_3^- units are similar to the units composing the zig-zag

chains in HF, although there is an increase in the F-F distance and a decrease in the strength of the hydrogen bond as we proceed to HF_2^- to H_2F_3^- to HF. While the low frequency spectrum of HF_2^- has been previously investigated and interpreted on the basis of Raman spectroscopy, there are no known similar measurements for HF and H_2F_3^- in the frequency range covered by the present experiment. A comparison of the low frequency spectra of HF_2^- , H_2F_3^- and HF, together with the already known interpretation of the Raman spectrum of HF_2^- suggests a tentative explanation of the low frequency spectra of the H_2F_3^- ion and HF which would take into account the high degree of association of liquid HF and the different structural features of the F-H---F units in these three compounds. Figs. VI and VII illustrate schematically the motions tentatively assigned to the peaks observed in the neutron spectra of HF and H_2F_3^- ion.

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FIGURE CAPTIONS

Figure I. Inelastic spectra of 0.005 e.v. incident neutrons scattered at 90° angle by HF in the solid phase and at two different temperatures in the liquid phase. The lower scale in abscissa represents times-of-flight and the upper one is an energy scale. The ordinates are neutron intensity in arbitrary units. The peak at channel 153 corresponds to elastic scattering of the incident neutrons and shows the principal Bragg cut-off in the Beryllium filter. Another peak around channel 142 is due to a secondary cut-off in Be at 0.006 ev. The arrows indicate the energy gain of incident neutrons that correspond to the peaks.

Figure II. Inelastic spectra of 0.005 e.v. incident neutrons scattered at 90° angles from polycrystalline samples of KH_2F_3 and NaH_2F_3 at $T = 293^\circ\text{K}$. The lower scale of the abscissa represents times-of-flight and the corresponding energies are shown on the upper scale. The ordinate represents intensity in arbitrary units. The arrows indicate the energy gains of the neutron with respect to the incident energy that correspond to the peaks. The positions of the low frequency peaks in HF and KHF_2 are also shown for comparison.

Figure III. The spectrum of neutrons inelastically scattered from polycrystalline KHF_2 at a 90° angle. The abscissa shows both neutron energy and time-of-flight while the ordinate is the neutron intensity in arbitrary units. The arrows indicate the energy gain of the scattered neutrons in 10^{-3} electron volts.

Figure IV. A schematic representation of the motions ascribed to the peaks observed in the spectrum of scattered neutrons from KHF_2 .

Figure V. Variation of the low frequency vibration of the hydrogen bond with oxygen-oxygen distance in compounds containing O-H--O bonds. The ordinate is the O-O separations in Å units while the abscissa is the frequency of the vibration. The results of the theory of Reid are given together with measured points for H_2O and KH_2PO_4 . The frequencies of peaks A and A' and A'' from the neutron spectra of the present experiment are also plotted as a function of F-F distance for comparison.

Figure VI. A schematic representation of the motions tentatively associated with the peaks observed in the spectra of KH_2F_3 and NaH_2F_3 .

Figure VII. A schematic representation of the motions tentatively associated with the peaks observed in the spectra of the liquid and solid phases of HF.

FIGURE 1

FIGURE 2

FIGURE 3

$$\nu_1 (\simeq 600 \text{ cm}^{-1})$$

$$\nu_3 (\simeq 1450 \text{ cm}^{-1})$$

$$\nu_1^2 \sim \frac{f}{m_F}$$

$$\nu_3^2 \simeq \frac{f}{m_F} \frac{m_H + 2m_F}{m_H}$$

(PEAK B')

(NOT OBSERVED)

$$\nu_2 (\simeq 1200 \text{ cm}^{-1})$$

$$\nu_2^2 \sim \frac{2d}{m_F} \frac{m_H + 2m_F}{m_H}$$

ν (OBLIQUE PROJECTION)

(PEAK A')

FUNDAMENTAL VIBRATION OF THE HF_2^- ION

OBLIQUE VIEW

LIBRATION
(PEAK C')

HF_2^- ION

FIGURE 4

FIGURE 5

PEAK (A'')

PEAK (B'')

PEAK (C'')

PEAK (D'')

H_2F_3^- ION

FIGURE 6

LIQUID AND SOLID HF

$T = -120^\circ\text{C}$

$\theta = 90^\circ$

FIGURE 7

TABLE I

Compounds	Structural Data	Physical Constants Degree of Association
HF gas	F-F distance = $2.55\text{\AA}$ F-H distance = $1.00 \pm 0.06\text{\AA}$ F-F-F bond angle $140^\circ \pm 5$	Polymeric units (e) at P = 740 mm Hg, T = 88°C HF P = 740 mm Hg, T = 30°C $(\text{HF})_2$ P = 745 mm Hg, T = 20°C $80\%(\text{HF})_6$
HF liquid		Boiling pt. + 19°C (f) Apparent molecular weight varies from 47.7 to 87.4 as T varies from 289°K to 234°K (g)
HF solid	F-F distance $2.49\text{\AA}$ F-F-F bond angle 120° Orthorhombic crystals	Melting pt. - 102°C (f) Antiparallel coplanar zig-zag chains (b)
H_2F_3^-	F-F distance = $2.33\text{\AA}$ F-F-F bond angle = 130° and 139° F-H distance unknown Orthorhombic crystals	Units (c)
HF_2^-	F-F distance = $2.26\text{\AA}$ F-H distance = $1.13\text{\AA}$ Tetragonal crystals	Units (d)

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TABLE II
Comparison of the Positions of the Peaks
in HF, KHF₂, NaH₂F₃, KH₂F₃
Observed in the Present Experiment

Compounds	Solid HF		NaH ₂ F ₃ KH ₂ F ₃		KHF ₂	
	meV	cm ⁻¹	meV	cm ⁻¹	meV	cm ⁻¹
Peaks A, A'', A'	67 ± 2	535 ± 16	112 ± 4	896 ± 32	147 ± 5	1176 ± 40
Peaks B, B'', B'	32 ± 2	260 ± 16	45 ± 2 (K) 50 ± 2 (Na)	364 ± 16 390 ± 16	75 ± 3	600 ± 24
Peaks C', C''			14 ± 1	117 ± 8	13 ± 1	104 ± 8
Peaks D, D''	7 ± 1	53 ± 8	8 ± 1	65 ± 8		