The vibrational spectra and conformation of 1,2-dicyanotetrafluoroethane

J. E. GUSTAVSEN, P. KLAEBOE, C. J. NIELSEN and DAVID L. POWELL* Department of Chemistry, University of Oslo, Oslo 3, Norway

(Received 16 January 1978)

Abstract—Infrared spectra of 1,2-dicyanotetrafluoroethane have been recorded in the vapour, glassy solid, and crystalline solid states. Raman spectra have been recorded of the liquid and the crystalline solid. The *trans* form is shown to exist alone in the crystal, while *trans* and *gauche* forms co-exist in the vapour, liquid and in the amorphous solid with the *trans* conformer dominating.

Complete vibrational assignments are proposed for the *trans* and for the *gauche* conformers. The latter in particular places heavy reliance upon the normal coordinate calculations.

INTRODUCTION

Although 1,2-dicyanotetrafluoroethane has been known for many years, no structural studies of any sort have been performed upon it with the exception of a survey i.r. spectrum of the vapour published more than 20 years ago [1]. The fairly simple nature of this spectrum, consisting as it does of only four intense bands above 650 cm^{-1} , was sufficient to convince us that the compound exists mostly in the *trans* conformation in the vapour phase, a conclusion which proved correct.

Earlier results on related compounds of the general formula CX_2Y — CX_2Y give some indication of the possibilities to be expected in this case. The crystal of 1,1,2,2-tetrafluoroethane is *trans*; in the vapour phase the energy difference is about 1170 cal/mole with the *trans* conformer being the more stable [2,3]. Approximately the same situation prevails with 1,1,2,2-tetrafluorodichloroethane; the stable form in the crystal is the *trans* and this conformer is more stable by about 500 cal/mole in the vapour [4].

In 1,2-dicyanoethane, the more stable form in the crystal is the *gauche*, although both forms may exist above -43.7° C [5,6], but the dominant conformer in the vapour is the *trans* [7]. 1,2-Diiodotetrafluoroethane crystallizes in the *trans* form [8,9], and this conformer is measured to be 1835 cal/mole more stable than the *gauche* in the vapour phase. Finally, 1,1,2,2-tetra-cyanoethane and 1,2-dichlorotetracyanoethane both exist as *trans* conformers in the crystalline state and, surprisingly, no definite evidence was found for any *gauche* conformers in acetonitrile solution [10].

EXPERIMENTAL

1.2-dicyanotetrafluoroethane used in this study was prepared from 1.1,2.2-tetrafluorosuccinamide. obtained from PCR, Inc., by dehydration with P_2O_5 [11]. The product was fractionated by bulb to bulb distillation on a vacuum line. No impurity peaks were detected in a gas chromatogram and its i.r. spectrum agreed with that published earlier [1].

Infrared spectra were recorded of the vapour and of the unannealed and annealed solid at liquid nitrogen temperature on a Perkin-Elmer Model 225 spectrometer. Far i.r. spectra of the vapour and benzene solution were obtained with a fast scan Bruker Model 114C Fourier transform spectrometer using 6, 12 and 23 μ m beam splitters over the range 350-30 cm⁻¹.

Raman spectra were obtained on a modified [12] Cary Model 81 Raman spectrometer, using the 4880 and 5145 Å lines from an argon ion laser for excitation. The liquid sample was studied in a sealed glass tube and polarization data were obtained. Raman spectra were recorded of the unannealed and annealed solids deposited from the vapour on a copper block at liquid nitrogen temperature.

INTERPRETATION

The Raman spectra of the liquid and the crystalline solid are shown in Figs 1 and 2 respectively, while the wavenumbers of the observed i.r. and Raman bands are listed in Table 1. As apparent from these data, a number of i.r. and Raman bands present in the vapour and liquid states and partly in the glassy solids disappear in the crystal spectra. Moreover, with some exceptions the vanishing bands coincide in i.r. and Raman. The i.r. or Raman bands remaining in the crystalline solid have in most cases no counterparts in the other medium. Therefore, it seems certain that the present molecule crystallizes in the *trans* conformer of C_{2h} symmetry. However, the exceptions observed make this experimental evidence somewhat more uncertain than in most other 1.2-disubstituted ethanes.

The most notable discrepancies from the mutual exclusion rule are the bands around 1260 cm^{-1} (strong in i.r. and very strong in Raman), 1165 cm^{-1} (strong in i.r. and Raman), 734 cm^{-1} (very strong in Raman, very weak in i.r.), 495 cm^{-1} (very weak in i.r. and very strong in Raman), 469 cm^{-1} (very weak in i.r. and very strong in Raman). All these bands remain in the

^{*}On leave from the College of Wooster, Wooster, Ohio 44691, U. S. A., 1976–1977.



Fig. 1. Raman spectrum of liquid 1,2-dicyanotetrafluoroethane.



Fig. 2. Raman spectrum of crystalline (annealed) 1,2-dicyanotetrafluoroethane at -180° C.

crystalline solid in one or both spectra. They have been explained as (1) coinciding *trans* and *gauche* fundamentals: 1260, 469 and 190 cm⁻¹; (2) accidentally degenerate *trans* fundamentals: 1165 cm⁻¹ and (3) degeneracy between a Raman active *trans* fundamental and a *trans* i.r. active combination band: 495 cm⁻¹. Other irregularities include apparent i.r. or Raman *gauche* bands with no counterparts in the other spectrum: 605, 280 and 158 cm⁻¹. Since *gauche* is the less abundant conformer in the vapour and liquid states, the missing bands do not severely disturb our assignments.

The i.r. and Raman bands vanishing in the crystalline state are generally considerably weaker than those remaining in the crystal. Exceptions are the very strong i.r. band at 1007 cm⁻¹ (with a very weak Raman counterpart) and a very strong Raman band at 713 cm⁻¹ (having a weak i.r. counterpart) vanishing in the crystal spectra. These two bands are attributed to the C—C(N) stretching mode (b) and central C—C stretch (a), respectively. The corresponding *trans* modes 987 (b_u) and 734 cm⁻¹ (a_g) are of still higher intensities. As a rough estimate the *trans-gauche* ratio can be evaluated to ca. 70:30 in the vapour and 80:20 in the liquid state at room temperature.

One of our goals is the assignment, as far as is possible, of the non-dominant conformer. It is in the liquid phase that the equilibrium will lie furthest toward the *gauche*, as the polar, or *gauche*, form is stabilized in this phase.

Because of the inconvenient boiling point of this compound (5°C), obtaining i.r. spectra of the liquid phase would be an awkward matter, although we obtained far i.r. spectra in benzene solution using vacuum tight liquid cells. Fortunately, a convenient substitute, the spectrum of the glassy solid obtained when the sample was first deposited is available.

Infrared			Ran	nan	Interpretation		
Vapour	Amorph. solid - 180°	Cryst. solid - 180°	Liquid	Cryst. solid - 180°	Trans	Gauche	
2345 w §	2343 s	*	2340 vw, P	*			
	2331 w	*	2329 vw. D	*			
2269 s, br	2276 s	2276 s	2266 vs, P	2270 vs	$v_1(a_g), v_{18}(b_u)$	$v_1(a), v_{14}(b)$	
0010	2271 m	2222	2220 D	2218	trant		
2213 w		2223 W	2220 m, P	2210 W	trans		
2161 W			2131 vw, D				
13/3 W	1381 vw	1379 w			trans		
1361 w	1220	1277			trans		
1343 W	1339 W	1327 VW			trans		
	1290 III 1272 m	1200 III 1271 m			trans		
1250 c b-	12/2 11	1271 III *			L1 66763	$v_{1,s}(b)$	
1239 5, 01	1200 3		1258 vs D	1248 s	$v_{a}(a)$	13(0)	
	1252 11	*	1200 43, 12	12403	(2(ug)	aauche	
	1232 w 1227 m	*				aauche	
	1257 11	1234 vw	1235 vw	1234 vw	trans	0	
1223 m	1223 m	*	1223 vw. P	*		$v_2(a)$	
1225 111	1225 m 1206 w	1207 m	1220		trans	4 ()	
1189 yys) -	1200 **						
1182 yvs	1185 s	1184 s			$v_{19}(b_u)$		
			1170 w, P	1173 vw	trans		
			1166 s, D?	1168 s	$v_{\mathbf{q}}(b_{\mathbf{r}})$		
1173 vs)	11/2 -	1164			v (a)		
1164 vs	1103 \$	1104 VS			v13(a _m)		
)	1152 w	1152 vw	1152 m, P	*		$v_3(a)$	
	1143 m	*	1143 w	*		$v_{16}(b)$	
	1132 vw	*				gauche	
1120 vw	1113 w	*	1120 vw	*		$v_4(a)$	
1102 vw	1097 w	1097 w			trans		
			1095 w, P	1086 s	$v_3(a_g)$		
1084 vw	1078 w	1081 w			trans		
1049 vw	1057 vw	1060 w			trans		
1011 s	1001		1005	*		» (b)	
1007 vs C	1001 s	-	1003 vw, D			V17(D)	
1001 s J							
992 S	094 110	086 10			v. (h)		
967 VS A:	704 VS	700 VS			· 20(0 a)		
980 \$)	974 m	*	973 vw			aauche	
970 5)	274 m		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			5	
964 s (961 vs	964 vs			$v_4 + v_{22}(D_{\rm H}) \Gamma {\rm K}$		
	952 m	950 m			trans		
834 w	839 w	844 w			trans		
	815 w	818 w		815 vw	trans		
738 w	732 vw	732 vw			trans		
			734 vs. P	731 vs	$v_4(a_g)$		
720 vw{	711 w	*	713 vs. P	•		$v_5(a)$	
709 w {						-	
676 W	(80		(72 D				
671 m C	6/0 m	+	672 VW, D			V18(D)	
00/WJ	662 11	663 w			trans		
	656 w	656 w			trans		
656 w)	020 #	000 H			•• •••		
650 m > A	649 s	648 s			$v_{21}(b_{\mu})$		
646 w							
			623 m, D	622 w	$v_{10}(b_{g})$		
617 vw	612 w	615 w			trans		
			605 m, P	*		$v_6(a)$	
	572 vw	*	574 vw, D) *		gauche	
576 w)					·· (-)		
571 w C	557 m	557 m			$v_{14}(a_{\mu})$		
204 W)	5 2 2	*	572 D	*		۷ (b)	
	343 W	•	108 ve D	500 ve	$v_{a}(a)$	-19(0)	
			-70 V3, F	200 13	· 5(**g)		

495 vw

497 vw

trans

,

Table 1. Infrared an	d Raman spectra	l data† for 1,2-di	cyanotetrafluoroethane
----------------------	-----------------	--------------------	------------------------

Infrared		Raman				Interpretation
Vapour	Amorph. solid - 180°	Cryst. solid - 180°	C Liquid	ʻryst. solid — 180°	Trans	Gauche
480 m, br	484 w 474 s	475 s) 472 s(487 w, D	*	$v_{22}(b_{u})$	v ₂₀ (b)
	469 vw	*	469 m, P 453 w, P	469 m *	$v_6(a_g)$	v ₇ (a)
$\begin{array}{c} 438 \text{ m} \\ 432 \text{ m} \\ 427 \text{ w} \end{array} \right\} C$	436 w	*	430 vw	*		$v_8(a), v_{21}(b)$
427 w) 364 w, br	414 vw 380 vw	411 vw *	420 m, D 382 m, P 356 s, P	420 w * 352 s	$v_{11}(b_g)$ trans $v_7(a_g)$	v ₉ (a)
$ \begin{array}{c} 329 \text{ m} \\ 324 \text{ s} \\ 320 \text{ m} \end{array} \right\} A $	328 vs 325 vs	333 vs 327 vs			v ₂₃ (b _u)	
255			313 vw 280 m, P	*		gauche v ₁₀ (a)
250 m C' 250 m C' 245 w	? 252‡ m	265 w			$v_{15}(a_u)$	
238 vw C 193 s	244 ‡ vw	*	255 m, D	* 194 m		$v_{22}(b)$
186 s <i>}C</i> 178 s <i>}</i>	189 ‡ s		190 vs, D	188 s	$v_{12}(b_g), v_{16}(a_u)$	$v_{11}(a), v_{23}(b)$
145			158 vs, D?	175 s 158 m	lati v ₈ (a _g)	lice
145 m 139 m C	144‡ m		148 m	*		$v_{24}(b)$
111 m)			117 m, P	*		$v_{12}(a)$
106 m A $102 m$	118‡ w				$v_{24}(b_u)$	
63 vw			60 vw	81 m	lattice $v_{17}(a_u)$	v ₁₃ (a)
				$ \begin{array}{c} 52 w \\ 48 w \\ 40 w \end{array} $	lattice	

Table 1 (contd.)

†Bands in the regions 5000-2350 and $2150-1400 \text{ cm}^{-1}$ were omitted.

Abbreviations; s, strong; m, medium; w, weak; v, very; br, broad; A. B and C denote vapour contours; P, polarized; D, depolarized; FR, Fermi resonance; asterisks denote bands disappearing in the crystal.

The 1086 cm⁻¹ band was strong in some crystalline spectra, weak in others.

 \ddagger Bands observed in C₆H₆ solution.

Several bands which disappear upon annealing are observed only there. Furthermore, this spectrum provides a link between the spectra of the vapour and of the crystalline solid in helping to decide the correspondence between the bands in the different phases. In the Raman, spectra were essentially identical just after deposition and after annealing. Fortunately this extra check is not as necessary here as the Raman spectrum of the liquid was obtained without difficulty.

In the *trans* form the vibrations divide into $8a_g + 5a_u + 4b_g + 7b_u$ with the *gerade* modes Raman active, the a_g modes polarized, and the *ungerade* modes i.r. active. In the *gauche* form the division is 13a + 11b with all modes active in both effects and the *a* modes polarized.

Assuming the following bond distances: C-C, 1.54;

C—C(N), 1.48; C—F, 1.358 and C=N, 1.148 Å, tetrahedral angles and a dihedral angle of 60° for the gauche conformer, the following rotational constants were calculated (MHz): 2119, 1124 and 998 (trans) and 1603, 1337 and 1080 (gauche). In the trans conformer the b_u modes should have A/B hybrid contours and the a_u modes C-type contours. The PR separations were calculated [13] to be 10, 8 and 15 cm⁻¹ for the A, B and C bands, respectively. In the gauche conformer, the a modes should have B-contours and the b modes A/Chybrid contours. With a κ -value close to zero, the A, B and C type bands of the gauche comformer should have similar appearances with PR separations calculated [13, 14] between 7 and 10 cm⁻¹. However, some characteristic bands with C contours were observed for this conformer at 1007, 671, 432, 238 and 139 cm⁻¹ and assigned as b fundamentals.

The fundamental frequencies assigned for the *trans* and *gauche* comformers are listed in Table 2, together with the calculated frequencies.

Trans conformer

In the Raman spectrum of the *trans* conformer, five bands higher in frequency than about 700 cm⁻¹ are expected, involving symmetric stretching of the C \equiv N, the C--C(N) and the C--F linkages, the stretching of the central C--C bond, and an asymmetric C--F stretch. The first four of these should be a_g , the latter b_g . Bands at 2266 and 734 cm⁻¹ are obviously two of the a_g modes, while those at 1258 and 1166 cm⁻¹ clearly represent two more. Both the latter bands appear depolarized so that from the spectra alone a decision cannot be made on which is which.

The calculations indicate that the two C—F stretches of species a_g and b_g should lie close together with the a_g mode at slightly higher wave number. We have tentatively assigned the most intense band at 1258 cm⁻¹ to v_2 (a_g) and the 1166 cm⁻¹ band to v_9 (b_g).

Candidates for the fifth fundamental are a weak shoulder at 1170 cm^{-1} and a weak band at 1095 cm⁻¹

which appears as a strong peak at 1086 cm^{-1} in one of the annealed, crystalline samples (but appeared weak in others). The latter band was selected as v_3 (a_g) in good agreement with the calculated value.

Assignment of the remaining seven Raman active fundamentals is quite easy with the aid of the polarization data except for the two lowest fundamentals, v_8 and v_{12} . The very strong bands at 190 and 158 cm⁻¹ both appear depolarized as is common for low frequency modes of this type. Again, we have followed the results of the normal coordinate analysis and assigned the two bands as v_{12} and v_8 , respectively. The strong band which appears at 175 cm⁻¹ in the spectrum of the solid has no counterpart in the liquid and hence is assumed due to a crystal effect.

In assigning the i.r. active fundamentals of the *trans* conformer, the apparent first step is to pick out the a_u modes which should be recognizable by their prominent Q branches. However, the obvious Q branches appearing in the spectrum of the vapour, all disappear in the spectrum of the crystal and are therefore attributed to the gauche conformer. Our explanation of this difficulty is that the calculated values for the intermediate moment of inertia I_B is only about 12% less than the largest moment of inertia I_c and the molecule therefore

 Table 2. Observed (obs.) and calculated (calc.) fundamentals (cm⁻¹) for the trans and gauche conformers of 1,2-dicyanotetrafluoroethane

Trans			Gauche				
Species and no.	Obs.*	Calc.	Approx motion†	Species and no.	Obs.†	Calc.	Approx motion [†]
$a_a v_1$	2266	2266	CN str	<i>a v</i> ₁	2269	2268	CN str
v ₂	1258	1256	CF str	v ₂	1223	1211	CF str
v3	1095	1112	CC(N) str	v3	1152	1168	CF str
vz	734	735	CC str	V.	1120	1104	CC(N) str
V.s	498	482	CF, scissor	Ve	714	713	CC str
v ₆	469	463	CCC bend	V ₆	605 §	613	CF ₂ scissor
v7	356	349	CCF bend	v 7	4691	476	CCF bend
v ₈	158	164	CCN bend	v ₈	432	446	CCC roch
b _a v ₉	1166	1158	CF str	v ₉	364	377	CCF bend
v ₁₀	623	586	CCF bend	V10	280 §	278	CCF bend
v ₁₁	420	406	CCF bend	v11	186	194	CCN bend
v ₁₂	190	189	CCN bend	v ₁₂	117§	117	CCN bend
				v ₁₃	63	66	torsion
$a_{u}v_{13}$	1169	1170	CF str	b v14	2269	2267	CN str
v ₁₄	571	574	CCF bend	v ₁₅	1259	1255	CF str
v ₁₅	250	248	CCF bend	v ₁₆	1143‡	1160	CF str
v ₁₆	186	182	CCN bend	v ₁₇	1007	995	CC str
v ₁₇	63	66	torsion	v18	671	658	CF ₂ scissor
				v ₁₉	523‡	550	CCF bend '
<i>b</i> _w v ₁₈	2269	2268	CN str	v ₂₀	484‡	474	CCF bend
v ₁₉	1185	1196	CF str	v ₂₁	432	433	CCC bend
v ₂₀	9 87	975	CC(N) str	v ₂₂	238	266	CCF bend
v ₂₁	650	636	CF ₂ scissor	v23	186	199	CCN bend
v ₂₂	480	472	CCF bend	V24	139	152	CCN bend
v ₂₃	324	343	CCC bend				
v ₂₄	106	119	CCN bend				

*The trans fundamentals of species a_g and b_g are from Raman liquid, the a_u and b_u fundamentals are i.r. vapour values.

[†]The gauche fundamentals are from i.r. vapour except when noted.

‡Infrared liquid values.

§Raman liquid values.

approaches an accidental symmetric top.

The very strong i.r. band at 1185 cm^{-1} has *B*-contour and is assigned as v_{19} , whereas the neighbouring band at 1169 cm⁻¹ with smoothed out contours was assigned as v_{13} , both connected with C—F stretches. The band at 987 cm⁻¹ was assigned as v_{20} because it looks most nearly like a type *A*-band and the calculations strongly favour a b_{μ} mode in this region.

Heavy reliance was placed upon the normal coordinate calculations in assigning the remaining eight modes as none of them with the possible exception of the band at 186 cm^{-1} seem to be type C. The three lowest bands are also assigned, in the absence of a far i.r. spectrum of the solid, without definite proof that they do indeed belong to the *trans* conformer.

Gauche conformer

Since the *gauche* conformer is less abundant than the *trans*, the i.r. and Raman bands are obviously weaker and therefore more difficult to identify. On the other hand the *gauche* bands are active both in i.r. and in Raman and disappear in the crystalline state.

Coinciding i.r. and Raman bands which disappear in the crystal spectra are situated on both sides of the *trans* $C \equiv N$ stretching modes around 2266 cm⁻¹. However, the $C \equiv N$ stretch is a typical group frequency negligibly affected by conformational differences. We believe shifts of 60 cm⁻¹ or more between the *trans* and gauche $C \equiv N$ stretches as highly unlikely, and therefore consider $v_1(a)$ and $v_{14}(b)$ to overlap the corresponding *trans* modes.

The four C—F stretching modes were assigned to the bands at 1259 (b), 1223 (a), 1152(a) and 1143 cm⁻¹ (b), while the two very intense *gauche* bands at 1007 (b) and 714 cm⁻¹ (a) have been discussed before. Weak i.r. and Raman bands around 1120 cm⁻¹ were tentatively attributed to the remaining C—C stretch (v_4) of which the corresponding *trans* fundamental at 1095 cm⁻¹ was very weak.

The vapour bands with C-contours at 671, 432, 238 and 139 cm⁻¹ were as mentioned previously assigned as the *b*-fundamentals v_{18} , v_{21} , v_{22} and v_{24} , respectively. The *b*-modes v_{19} and v_{20} were assigned to i.r. and depolarized Raman bands around 523 and 484 cm⁻¹. Since no other candidates were available, the remaining *b* fundamental v_{23} was considered coinciding with the *trans* fundamental of species b_a at 190 cm⁻¹.

The gauche fundamentals of species a have generally diffuse vapour contours but sometimes distinct, polarized Raman bands. Thus, the polarized Raman bands at 605, 453, 382, 280 and 117 cm⁻¹ were assigned as v_6 , v_7 , v_9 , v_{10} and v_{12} , respectively. Much more uncertain are our attributions of the remaining a-modes v_8 , v_{11} and v_{13} . With no available candidates for these fundamentals in the expected regions they were tentatively considered to overlap with other fundamentals, viz: 432 cm⁻¹ (overlapping v_{21}), 189 cm⁻¹ (overlapping v_{23} as the trans a_g modes v_{12} and v_{16}) and 63 cm⁻¹ (overlapping a trans a_u mode).

Various i.r. and a few Raman bands were observed

which have not been considered as fundamentals. They can readily be considered as combination bands or overtones, often with alternative explanations, and have therefore not been included but are denoted *trans* or *gauche* in Table 1.

Normal coordinate calculations

Detailed knowledge about the harmonic force constants cannot be obtained for 1,2-dicyanotetrafluoroethane from the present information. Also the ambiguities in the assignments suggest using force constant calculations as a tool for obtaining more reliable assignments rather than finding a unique set of force constants of general physical significance.

An initial set of valence force constants common for the two conformers was adopted from halogenated malononitriles [15] and from 1,2-dibromotetrafluoroethane [16]. A number of different approximations regarding the number of interaction terms, relations between these etc. were tried, but it was found that the large number of bend-bend interactions presented for 1,2-dibromotetrafluoroethane [16] had little influence on the predicted spectrum. After a few iterations, a final force field common to both conformers, consisting of ten diagonal and nine different interaction constants (Table 3), was found to reproduce the assigned fundamentals with reasonably small deviations. The calculated frequencies together with the assignments adopted for both conformers are shown in Table 2.

 Table 3. Proposed valence force constants for trans and gauche 1,2 dicyanotetrafluoroethane

Force constant	Value*	Force constant	Value*
Stretch		Stretch/stretch	
Kcc	4.25	FCFCF	0.70
KCCAN	5,40	FCFCC	0.50
KCF	6.40	FCECCINI	0.85
KCN	17.70	F _{CC,CC(N)}	0.10
Bend		Stretch/bend	
HECE	1.40	FCC.CCC	0.48
Hree	1.09	FCCNVCCC	0.48
HECCOL	1.14	F _{CC/FCC}	0.50
Hecc	1.50	FCC(N)/FCC(N)	0.50
HCCN	0.21	F _{CF/FCF}	0.40
H.t	0.25	FCF/FCC	0.72
		F _{CF/FCC(N)}	0.90

*Units for stretching and stretch/stretch interaction constants are mdyn/Å, for bending constants units are mdyn $Å/rad^2$, and stretch/bend interaction constants have units of mdyn/rad.

Torsion coordinate defined as the C-C-C-C torsion.

Acknowledgements—We are grateful to K. RUZICKA for synthesizing and purifying the compound. Financial support was provided by the Norwegian Research Council for Science and the Humanities.

REFERENCES

 D. G. WEIBLEN, The infrared spectra of fluorocarbons and related compounds, In: *Fluorine Chemistry* J. H. SIMONS, Ed.) Academic Press, New York (1954).

- [2] P. KLAEBOE and J. R. NIELSEN, J. Chem. Phys. 32, 899 (1960).
- [3] D. E. BROWN and B. BEAGLEY, J. Mol. Struct. 38, 167 (1977).
- [4] R. E. KAGARISE, J. Chem. Phys. 26, 380 (1957).
- [5] W. E. FITZGERALD and G. J. JANZ, J. Mol. Spectrosc. 1, 49 (1957).
- [6] T. FUJIYAMA, T. TOKUMARU and T. SHIMANOUCHI, Spectrochim. Acta 20, 415 (1964).
- [7] L. FERNHOLT and K. KVESETH, Acta Chem. Scand. 33A (1979) in press.
- [8] G. SERBOLI and B. MINASSO, Spectrochim. Acta 24A, 1813 (1968).
- [9] D. L. POWELL, J. E. GUSTAVSEN, P. KLAEBOE and C. J. NIELSEN, J. Raman Spectrosc. 7, 111 (1978).

- [10] D. L. POWELL, T. R. DYKE, C. HEBREW, C. T. VAN BUREN and P. KLAEBOE, Acta Chem. Scand. 27, 613 (1973).
- [11] B. C. BISHOP, J. B. HYNES and A. L. BIGELOW, J. Am. Chem. Soc. 85, 1606 (1963).
- [12] B. GILBERT and G. DUYCKAERTS, Spectrochim. Acta 26A, 2197 (1970).
- [13] W. A. SETH-PAUL and H. DEMEYER, J. Mol. Struct. 3, 403 (1969).
- [14] T. VEDA and T. SHIMANOUCHI, J. Mol. Spectrosc. 28, 358 (1968).
- [15] S. BJØRKLUND, E. AUGDAHL, D. H. CHRISTENSEN and G. O. SØRENSEN, Spectrochim. Acta 32A, 1021 (1976).
- [16] H. F. SHURVELL, F. CAHILL, V. DEVARAJAN and D. W. JAMES. Can. J. Chem. 54, 2220 (1976).