Acta Chemica Scandinavica A 34 (1980) 515–522

The Vibrational Spectra of Tetrafluorosuccinic Anhydride

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The IR spectra (4000–200 cm^{-1}) of tetrafluorosuccinic anhydride as a vapour, liquid and dissolved in CS_2 were recorded. Additional spectra from the vapour were obtained in the region 400–30 cm^{-1}. Raman spectra of the liquid were recorded, and semiquantitative polarization ratios were measured. The fundamental frequencies were tentatively assigned in terms of C_2 symmetry based upon Raman polarization data and vapour band contours.

The IR spectra of succinic anhydride as a solid and dissolved in various solvents were recorded between 4000 and 30 cm^{-1}. Raman spectra of the solid were also recorded. The fundamental frequencies were assigned in terms of C_{2v} symmetry and compared to those of tetrafluorosuccinic anhydride.

Force fields were derived by the overlay technique for succinic and tetrafluorosuccinic anhydride.

We have for some time been interested in the vibrational spectra of five-membered, unsaturated cyclic molecules, and have earlier reported our results for maleimide,[1] *N*-deuterio[1] and *N*-chloro[2] maleimide, succinimide[3] and *N*-deuterio,[3] *N*-chloro, *N*-bromo and *N*-iodo succinimide.[4] These studies have now been extended to include succinic anhydrides. In the present paper we shall report our results for tetrafluorosuccinic anhydride (FSA). Various authors[5–7] have discussed the IR and Raman spectra of succinic anhydrides, but to our knowledge no IR or Raman data have been reported for FSA.

In the present work we have recorded IR spectra of FSA as a vapour, liquid and dissolved in CS_2. Raman spectra were obtained from the neat liquid. Unfortunately we were not able to record spectra of FSA in the solid state since the sample seemed to polymerize upon crystallization.

As an aid to the assignments normal coordinate analyses of FSA were carried out. The data were fitted together with the frequencies from the solution state of succinic anhydride (SA). As the earlier IR data for SA in the solution are rather incomplete, we have also recorded IR spectra of SA dissolved in CCl_4, CS_2 and CH_2Cl_2.

EXPERIMENTAL

The sample of FSA was a commercial product from the K&K laboratories. No impurities were detected by gas chromatography. SA was a commercial product from Fluka AG and was purified by repeated sublimation on a cold finger.

Raman spectra of the pure liquid FSA were recorded with a Cary Model 81 spectrometer, modified for perpendicular illumination. The 5145 Å line of an argon ion laser was used for excitation. IR spectra were recorded on a Perkin-Elmer Model 225 spectrometer in the region 5000–200 cm^{-1}. Far IR spectra were recorded of the vapour (FSA) with an RIIC interferometer FS-520, equipped with a light pipe gas cell of optical path *ca.* 6 m. FIR spectra (400–30 cm^{-1}) of SA as a polyethylene pellet and dissolved in C_6H_6 were recorded using a Perkin-Elmer, Hitachi model FIS-3 spectrometer.

RESULTS

FSA has recently been studied by electron diffraction.[8] In contrast to SA[9] it was found to have a non-planar ring skeleton although planarity was found for the O=C–O–C=O group. Hence the spectra of FSA will be interpreted in terms of C_2 symmetry, while SA is considered to possess C_{2v} symmetry.

The 27 fundamentals of SA will accordingly divide themselves into the symmetry species: $9\,a_1+8\,b_2+5\,a_2+5\,b_1$. The a_1 and b_2 fundamentals represent in-plane, the a_2 and b_1 out-of-plane modes. All the fundamentals are active in the Raman effect while those of species a_2 are forbidden in the infrared spectra.

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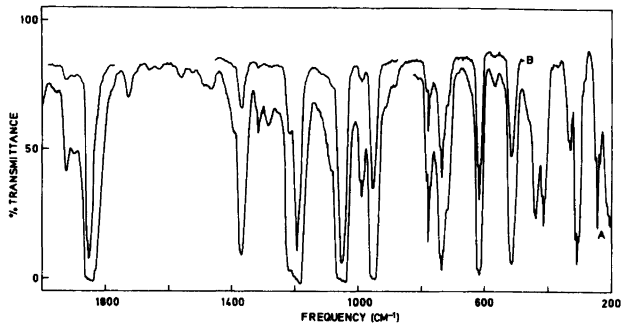

Fig. 1. The infrared spectrum of tetrafluorosuccinic anhydride as a vapour. Path length, 10 cm. Pressure, A, 100 Torr; B, 25 Torr.

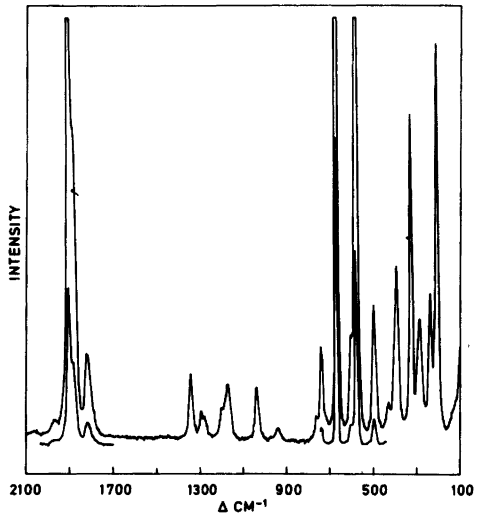

Fig. 2. The Raman spectrum of tetrafluorosuccinic anhydride as a neat liquid.

For FSA all the fundamentals are active both in the Raman and in the IR spectra, and the 27 fundamentals will divide themselves into the symmetry species: 14 $a+13$ b. The a species correspond to a_1+a_2 and the b species to b_1+b_2 for SA.

From the structural parameters[8] of FSA the following moments of inertia are obtained (10^{-40} g cm^2): $I_A = 331.7$, $I_B = 412.7$ and $I_C = 545.8$. The following PR separations (cm^{-1}) were calculated[10] at 300 K: 10 for A, 11 for B and 14 for C-bands. The $Q-Q$ separation for the B-bands should be 2.5 cm^{-1}. Vibrations belonging to species a give rise to B-bands in the IR vapour spectra, while vibrations of species b give A/C hybride bands. Thus, the IR vapour band contours and the Raman polarization measurements offered reasonable good criteria for the assignments of most of the fundamentals for FSA.

Spectral interpretations. As an illustration the IR vapour spectrum of FSA is shown in Fig. 1, whereas a Raman spectrum of the liquid appears in Fig. 2.

Table 1. Infrared[a] and Raman spectral data for tetrafluorosuccinic anhydride (FSA).

Infrared		Raman	Assignments	
Vapour	Liquid	Liquid		
2005 m[b]	1997 m		$\nu_{14}+\nu_{15}$	b
		1987 vw P	$\nu_{15}+\nu_{27}$	a
1955 w	1955 w sh		$\nu_4+\nu_{20}$	b
1923 s	1923 m	1925 s P	ν_1	a
1899 m	1903 m	1903 m P	$\nu_{16}+\nu_{22}$	a
	1887 w sh		$\nu_3+\nu_7$	a
1858 s sh 1852 s A/C 1847 sh	1840 vs	1840 m D	ν_{15}	b

Table 1. Continued.

1830 s sh		~1815 s sh	1812 vw sh	$\nu_9+\nu_{16}$	b
1770 w sh				$\nu_2+\nu_{23}$	b
1732 sh		1740 w sh		$\nu_6+\nu_{19}$	b
1728 m		1723 m		$\nu_3+\nu_9$	a
1487 m		1484 w		$\nu_4+\nu_{24}$	b
1466 m		1462 w		$2\times\nu_{21}$	a
1395 m sh		1390 m sh		$\nu_7+\nu_{21}$	b
1369 s		1361 s	1361 m P	ν_2	a
1347 w sh				$\nu_{18}+\nu_{24}$	a
1323 w sh 1317 m 1310 w sh	A/C	1313 m	1314 w D	ν_{16}	b
1303 w		1300 w		$\nu_4+\nu_{27}$	b
1293 vw sh 1285 w 1277 vw sh	A/C	1283 w		$\nu_{12}+\nu_{19}$	b
1250 vw				$\nu_5+\nu_{26}$	b
1218 s	B	1217 s	1217 w P	ν_3	a
1199 sh 1194 s 1187 sh	A/C	~1180 vs	1189 m P	ν_4,ν_{17}	a,b
1131 vw		1129 w		$\nu_9+\nu_{22}$	b
1115 vw		1112 w		$\nu_7+\nu_{10}$	a
1086 m 1079 m	B	~1085 m sh		$\nu_{20}+\nu_{24}$	a
1053 vs		~1052 s sh	1054 m P	ν_5	a
1048 s 1044 sh		1035 s		ν_{18}	b
993 m 989 m 983 sh	A/C	991 s		$\nu_6+\nu_{25}$	b
954 s		~960 s sh	957 w D	ν_{19}	b
951 s		950 s		$\nu_9+\nu_{10}$	a
919 vw sh 912 w 905 vw sh	A/C	912 w sh		$\nu_{12}+\nu_{22}$	b
884 w sh				$\nu_7+\nu_{26}$	b
835 vw				$\nu_{10}+\nu_{23}$	b
807 vw				$\nu_7+\nu_{27}$	b
783 m 778 s 770 m sh	A/C	776 m	777 w D	ν_{20}	b
742 s sh 735 s 728 s sh	A/C	~745 w sh 732 s	747 s P 728 vw sh	ν_6 ν_{21}	a b
717 m sh				$\nu_8+\nu_{27}$	b
682 vw		683 w	683 s P	ν_7	a
620 s sh 616 s 611 s sh		619 s 593 w sh	618 w 593 s P	ν_{22} ν_8	b a
567 w				$2\times\nu_{13}$	a
544 vw sh		544 vw sh		$\nu_{12}+\nu_{25}$	b
521 sh 518 sh 514 s	B	509 s	509 m P	ν_9	a
460 w sh				$\nu_{13}+\nu_{14}$	a

Table 1. Continued.

~442 s sh, 437 s } B	439 m	440 w P	ν_{10}	a
418 m sh, 413 s, 408 m sh } A/C	403 m	403 m D	ν_{23}	b
385 vw			$\nu_{14}+\nu_{26}$	b
370 vw			$\nu_{25}+\nu_{27}$	a
335 m, 329 m } B	337 m	337 s P	ν_{11}	a
311.5 s, 306.5 s, 301.5 s } A/C		305 w sh P	ν_{12}	a
		291 m D	ν_{24}	b
290 vw sh, 283 vw sh } B			ν_{13}	a
249 s, 242.5 s, 236 s } A/C		248 w D	ν_{25}	b
214.5 m, 204 s } A/C		217 s D	ν_{26}	b
180 vw			ν_{14}	a
135 sh, 129 m, 125 sh } A/C		140 vw	ν_{27}	b

[a] Weak infrared bands in the regions 4000 – 2000 cm^{-1} and 1700 – 1500 cm^{-1} are omitted. [b] w, weak; m, medium; s, strong; v, very; sh, shoulder; P, polarized; D, depolarized; A, B and C, vapour band contours.

Table 2. Observed and calculated fundamental frequencies[a] for tetrafluorosuccinic anhydride (FSA).

Species and No.		Obs.	Calc.	PED[b]
a	ν_1	1923	1923	82s[c]
	ν_2	1369	1362	46d
	ν_3	1218	1233	$541_2+421_1+18\phi_2$
	ν_4	1189	1174	65a
	ν_5	1053	1061	69r+36d
	ν_6	747	756	321_2+271_1
	ν_7	682	674	$45\pi+25\tau_2$
	ν_8	593	607	$23\beta+22\alpha$
	ν_9	514	552	37θ
	ν_{10}	440	445	$54\tau_2+32\psi_2+17\psi_1$
	ν_{11}	332	345	$29\eta+24\xi$
	ν_{12}	305	309	$27\phi_2+24d+15\theta$
	ν_{13}	285	271	$90\phi_2+79\phi_1$
	ν_{14}	180	166	$48\psi_2+38\tau_1+36\psi_1$
b	ν_{15}	1852	1851	85s
	ν_{16}	1317	1297	$40r+341_1+16\varepsilon$
	ν_{17}	1194	1190	611_2+251_1
	ν_{18}	1048	1059	$71a+16\xi$
	ν_{19}	954	959	261_1+251_2+21a
	ν_{20}	778	792	27η
	ν_{21}	735	703	35θ
	ν_{22}	616	622	68π
	ν_{23}	413	409	$19\xi+15r$

Table 2. Continued.

ν_{24}	306	327	$21\psi_1+18\varepsilon+15\theta$
ν_{25}	242	238	$43\tau_1+27\tau_3+18\psi_1+18\psi_2$
ν_{26}	204	204	$75\psi_2+69\psi_1+15\phi_1$
ν_{27}	129	144	$102\phi_2+71\phi_1+22\tau_3+17\varepsilon$

[a] When possible, frequencies are taken from the vapour phase data. [b] The potential energy distribution defined as $X_{ik}=100F_{ii}L_{ik}^2/\lambda_k$. [c] For meaning of symbols, see Fig. 3. Terms below 15 are neglected.

Table 3. Observed and calculated fundamental frequencies[a] for succinic anhydride (SA).

Species and No.		Obs.	Calc.	PED[b]
a_1	ν_1	2953	2965	981[c]
	ν_2	1872	1876	80s
	ν_3	1432	1447	$57\theta+16$d
	ν_4	1268	1288	$30\psi+23$d$+20$a
	ν_5	1197	1169	53a$+35$r$+16$d
	ν_6	999	991	22r$+15\phi$
	ν_7	813	807	50r$+38$d$+15\phi$
	ν_8	620	607	$27\alpha+25\beta$
	ν_9	407	395	$36\eta+33\xi+17$a
a_2	ν_{10}	2975	2977	991
	ν_{11}	1225	1239	$60\psi+36\tau_2$
	ν_{12}	1005	1012	92ϕ
	ν_{13}	652	637	$70\pi+20\tau_2$
	ν_{14}	279	251	$29\tau_2+25\psi+17\tau_1+15\pi$
b_1	ν_{15}	2985	2971	991
	ν_{16}	1160	1132	$55\psi+41\phi$
	ν_{17}	813	832	$51\phi+32\psi$
	ν_{18}	528	551	81π
	ν_{19}	135	158	$77\tau_3+17\tau_1$
b_2	ν_{20}	2945	2960	991
	ν_{21}	1796	1802	84s
	ν_{22}	1414	1400	74θ
	ν_{23}	1292	1289	$50\phi+23\psi+21$r
	ν_{24}	1047	1072	64a$+40$r$+16\xi$
	ν_{25}	906	924	32a$+19$r
	ν_{26}	645	659	$42\varepsilon+19$a$+19\eta$
	ν_{27}	559	559	$38\xi+22\eta+19$r

[a] When possible frequencies are taken from solution. [b] The potential energy distribution defined as $X_{ik}=F_{ii}L_{ik}^2/\lambda_k$. [c] For meaning of symbols, see Fig. 3. $l=l_1=l_2$, $\phi=\phi_1=\phi_2$, $\psi=\psi_1=\psi_2$. Terms below 15 are neglected.

The observed IR and Raman frequencies are listed in Table 1, while the assigned fundamentals are given in Table 2 (FSA) and Table 3 (SA) together with the calculated frequencies and the potential energy distribution (PED) among the valence coordinates.

Our assignments of the fundamentals of the in-plane modes (a_1 and b_2) of SA agree with those previously noted.[5] No complete analyses of the out-of-plane vibrations are reported. We have interpreted the fundamentals of species a_2 and b_1 by comparing the spectra with those of the succinimides.[3,4] The CH_2 rock fundamental ν_{12} of species a_2 is assigned to a weak band at 1005 cm^{-1} only observed in the IR spectra of the solid SA. Similar weak bands at about the same frequency are also observed for all the succinimides,[3,4] and we suggest that these

bands should be taken as the CH_2 rock frequency rather than that previously indicated at *ca.* 920 cm^{-1}.[4]

It is well-known from the maleimides,[1,2] succinimides,[3,4] maleic[11-13] and succinic[5,6] anhydrides that the C=O stretching of species a_1 is invariably at higher frequency than the b_2 mode. The same rule applies to FSA, and ν_1 (*a*) is found at 1923 cm^{-1} *ca.* 70 cm^{-1} higher than ν_{15} (*b*) at 1852 cm^{-1}. A similar frequency splitting is also observed for SA where the two fundamentals are found at *ca.* 50 cm^{-1} lower than for FSA, at 1872 cm^{-1} (a_1) and 1796 cm^{-1} (b_2). As was earlier discussed for the succinimides,[4] the C=O stretching vibration of species b_2 shows significantly larger frequency shifts upon solution than the symmetric vibration (a_1). This is also valid for FSA, and the vapour band at 1852 cm^{-1} is shifted towards 1840 cm^{-1} in CS_2 solution, while the corresponding shift for the vapour band at 1923 cm^{-1} is only 4 cm^{-1}.

Several very strong bands in the IR spectra of FSA are observed between 1400 and 700 cm^{-1}. Eight fundamentals involving C–C, C–O and C–F streching are to be expected in this region. The C–O stretching vibrations are observed at slightly higher frequencies for SA than for FSA. The symmetric mode (*a*) is found at 1197 and 1189 cm^{-1}, and the asymmetric (*b*) at 1047 and 1035 cm^{-1} for SA in solution and liquid FSA, respectively. As indicated by the PED of Tables 2 and 3, the C–O stretchings are well-localized vibrations although for SA they are somewhat mixed with the C–C stretchings.

From Table 2 four fundamentals, ν_3 (1218), ν_6 (747), ν_{17} (1194) and ν_{19} (954 cm^{-1}), can be interpreted as almost pure C–F stretching vibrations with only small mixings with the C–C stretchings. The four vibrations assigned to C–F stretching correspond to either relatively strong bands in the IR spectra of the vapour or to polarized Raman bands. This is in agreement with a non-planar structure of FSA as was also found from the electron diffraction investigation.[8] If the molecule possessed C_{2v} symmetry, only three of the four C–F stretchings should give IR active vibrations, and only one should give a polarized Raman band.

The ring and C=O in-plane bending vibrations will be expected in the region 800–400 cm^{-1}. For FSA two additional FCF bending vibrations at 735 and 514 cm^{-1} are complicating this spectral area. For all the similar five-membered rings investigated[1-6,11-13] a characteristic, usually weak IR and strong Raman band is observed in the narrow frequency region 600–650 cm^{-1}. This band has been assigned to an in-plane ring bending, mostly involving the C–O–C part of the molecule. The corresponding bands of FSA and SA (ν_8) are observed at 593 cm^{-1} and at 620 cm^{-1}, respectively.

The symmetric C=O in-plane bending vibration was observed at *ca.* 400–420 cm^{-1} for maleimide,[1] maleic anhydride,[11] succinimide,[3] SA and their deuterated species.[1,3,5,11] For FSA this mode is situated at 332 cm^{-1}. A considerable frequency shift for this vibration was also noticed for the halogenated maleimides,[2] succinimides[4] and maleic anhydrides.[12,13] This shift can, except for FSA, be explained by a coupling between the C=O in-plane bending and the N–X or C–X stretching vibrations. For FSA a mixing with the FCF bending vibration at 514 cm^{-1} could explain the low frequency of the symmetric C=O bending vibration although such a mixing is not calculated by the PED (Table 2).

The far IR spectra of FSA are quite different from those of SA due to the many CCF bending vibrations in this region. All bands below 350 cm^{-1} (FSA) are considered to be fundamentals (Table 1). The IR vapour band contours and the Raman polarization data make the assignments in this spectral area rather straight-forward.

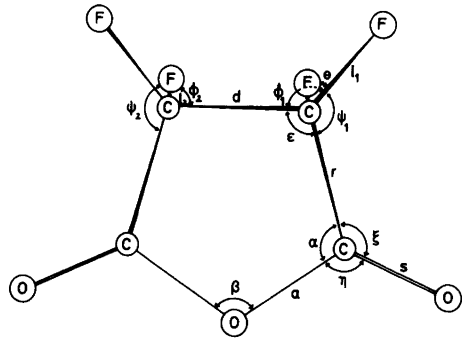

Fig. 3. Internal coordinates for tetrafluorosuccinic anhydride. The following coordinates are not shown on the figure: π the bending of C'=0 relative to the plane formed by the atoms C—C'—0. τ_1; the normalized sum of the two torsions around the C–O bond. τ_2; the normalized sum of the nine torsions around the $(F_2)C-C(F_2)$ bond. τ_3; the normalized sum of the six torsions around the $(O)C-C(F_2)$ bond.

Table 4. Valence force constants for succinic anhydride (SA) and tetrafluorosuccinic anhydride (FSA).

Force type	Constants		
	Symbol[a]	Value[b]	
		FSA	SA
Stretch	K_a	5.68	–[c]
	K_s	12.6	11.8
	$K_r = K_d$	5.0	–
	K_1	5.5	4.8
Bend	$H_\eta = H_\xi$	0.92	–
	$H_\psi = H_\phi$	1.07	0.57
	H_θ	1.85	0.5
	$H_\alpha = H_\beta = H_\varepsilon$	1.33	–
Outo	π	0.44	–
Torsion	τ_1	0.06	–
	τ_2	0.69	0.11
	τ_3	0.06	0.013
Stretch-stretch	$F_{a,a}$	1.3	–
	$F_{a,s}$	0.71	–
	$F_{r,1} = F_{d,1}$[d]	0.3	0
	F_{l_1,l_2}[d]	0.3	0.1
	$F_{s,s}$	0.15	–
Stretch-bend	$F_{a,\alpha} = F_{a,\beta} = F_{r,\alpha} = F_{r,\varepsilon} = F_{d,\varepsilon}$	0.56	–
	$F_{a,\eta} = F_{r,\xi}$	0.31	–
	$F_{1,\psi} = F_{1,\phi}$[d]	0.23	0
	$F_{r,\psi} = F_{d,\phi}$[d]	0.23	0.03
	$F_{1,\theta}$[d]	1.13	0
Bend-bend	$F_{\psi_1,\psi_2} = F_{\phi_1,\phi_2}$[d]	0.6	–0.03
	$F_{\tau,\psi} = F_{\varepsilon,\phi}$	0.3	0
	$F_{\phi_1,\phi_1} = F_{\phi_2,\phi_2}$	0	–0.06

[a] For meaning of symbols, see Fig. 3. Unnumbered indices, l, ψ and ϕ mean $F_l = F_{l_1} = F_{l_2}$ *etc.* [b] In units of mdyn Å^{-1} (stretch constants), mdyn rad^{-1} (stretch – bend interaction) and mdyn Å rad^{-2} (bending and torsion constants). [c] The force constant is the same as for FSA. [d] Interaction between adjacent coordinates.

NORMAL COORDINATE ANALYSES

We wanted to use force constant calculations as a tool for obtaining more reliable assignments. Because of the similarity in the structure of FSA and SA, it was possible to construct an almost common force field for the two compounds. Except for the force constants directly involving the CF_2 or CH_2 groups, only the C=O stretching force constant is different for FSA and SA. A considerably larger value for this constant had to be used for FSA than for SA in order to reproduce the much higher C=O stretching frequencies for FSA.

We have strictly limited the number of independent force constants, and the final force fields contain 31 parameters given in Table 4. The symbols are defined in Fig. 3. For FSA we have used frequencies from the vapour phase in the calculations whereas for SA we have used data from solution since no vapour phase data were available for this compound. Hence, the transferability of the force constants are somewhat uncertain since both FSA and SA show considerable frequency shifts when passing from one phase to the other. However, considering the approximations used, the fit between the observed and calculated frequencies is satisfactory.

Only a few normal coordinate analyses are reported for molecules containing CF_2 groups,[14-20] and our final force constants seem to be of reasonable magnitudes compared to them. C–F stretching force constants are previously found from 4.288 for $CH_3CF_2CH_3$[17] to 6.40 mdyn/Å for $N{=}C{-}CF_2{-}CF_2{-}C{=}N$[20], and our value of 5.5 mdyn/Å can therefore be considered as very normal for a

C – F stretching. The CCF bending force constant is almost always found to be *ca.* 1.1 mdyn Å/rad^2 in agreement with the value of 1.07, suitable for FSA. The FCF bending force constant varies from 1.40 (CF_2Br—CF_2Br)[14] to 2.331 mdyn Å/rad^2 ($CH_3CF_2CH_3$),[17] a value of 1.85 thus being very reasonable. Quite different interaction force constants are used for the CF_2 groups.[14-20] Especially the C – C stretching/CCF bending interaction force constant seems to be indeterminable. We have therefore chosen to set this interaction ($F_{r,\psi}$,$F_{d,\phi}$) constant equal to the CF/CCF interactions ($F_{1,\psi}$, $F_{1,\phi}$).

The observed and calculated fundamental frequencies are given in Tables 2 (FSA) and 3 (SA) together with the potential energy distribution among the valence coordinates.

Acknowledgements. The author is grateful to P. Klæboe and to C. J. Nielsen for helpful discussions and to the late K. Ružička for the preparative work. Financial support from the Norwegian Research Council for Science and the Humanities is acknowledged.

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Received March 7, 1980.