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Microwave Spectrum of Ethyl Isothiocyanate

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The microwave spectrum of ethyl isothiocyanate, CH_3CH_2NCS, has been obtained in the frequency region from 8.5 to 35 GHz. The spectrum identified is attributed to the *cis* configuration, namely, the methyl group eclipses the isothiocyanato group. The rotational constants for the ground vibrational state obtained are $A=14194\pm10$, $B=1799.27\pm0.02$ and $C=1612.14\pm0.02$ MHz. The dipole moment of this rotamer is $\mu_{\text{total}}=3.33\pm0.03$ D ($\mu_a=3.33\pm0.03$ D, $\mu_b=0.07\pm0.02$ D). Two sets of vibrational satellites were observed and assigned to the modes of C–N torsion (58 ± 30 cm^{-1}) and CNC bending (107 ± 30 cm^{-1}).

Recently microwave spectroscopy has been increasingly applied to the study of the rotational isomerism of molecules. Most of these studies have, however, been made on the rotational isomerism about a C–C single bond, and less attention has been paid to that about single carbon-heteroatom bonds. It is interesting, therefore, to study the rotational isomerism of mono-substituted ethanes, having, for example, thiocyanato (–SCN), isothiocyanato (–NCS), selenocyanato (–SeCN), isoselenocyanato (–NCSe) groups, *etc.* Kniseley *et al.*[1] have investigated the structure of ethyl isothiocyanate using infrared spectroscopy and concluded that the molecule existed in two rotameric forms, presumably *trans* and *gauche.* They observed two absorption bands at 2199 and 2154 cm^{-1} at liquid nitrogen temperature and assigned them to the NCS asymmetric stretching vibration in the *gauche* and *trans* configurations. Bjørseth and Marstokk[2] have studied the microwave spectrum of ethyl thiocyanate, CH_3CH_2SCN, and determined that the molecule exists in a single rotameric form, probably *gauche,* in gas phase, which is more stable than the *trans* form by at least 0.8 kcal·mol^{-1}.

In this paper, the spectrum of ethyl isothiocyanate in a configuration characterized by predominant absorption lines, the *cis* form, is reported and the structure and dipole moment are discussed.

Experimental

The sample of ethyl isothiocyanate was obtained commercially and purified by distillation *in vacuo.* The rotational spectrum was obtained in the frequency region from 8.5 to 35 GHz with a conventional 100-kHz sinusoidal- and square-wave Stark modulation spectrometer. The waveguide cell was cooled with dry ice in order to enhance the intensity of the absorption lines. Transition frequencies were measured with a Hewlett-Packard Model 5245 L frequency counter.

Results and Discussion

Spectrum and Assignment for the Vibrational Ground State. The observed spectrum was considerably dense in appearance, consisting of a large number of absorption lines. This feature may be ascribed to the various rotational isomers and their vibrationally-excited states. Four rotational isomers may be considered for the ethyl isothiocyanate molecule, namely, the *cis*, *gauche*, *skew*, and *trans* forms, as shown in Fig. 1. The moments of inertia calculated from the assumed structure of these isomers indicate that all are nearly prolate symmetric top molecules (the value of the asymmetric parameter of Ray are in the region from −0.998 to −0.974). A large a-component of the dipole moment is expected for these molecules because the –N=C=S group, having a large moment, lies close to the a-axis. Consequently, strong a-type R-branch absorption lines with $K_{-1}=0$ and 1 are expected. In the vicinity of the $K_{-1}=0$ line, absorption lines for K_{-1} equal to or larger than two should appear and a large Stark effect should be observed.

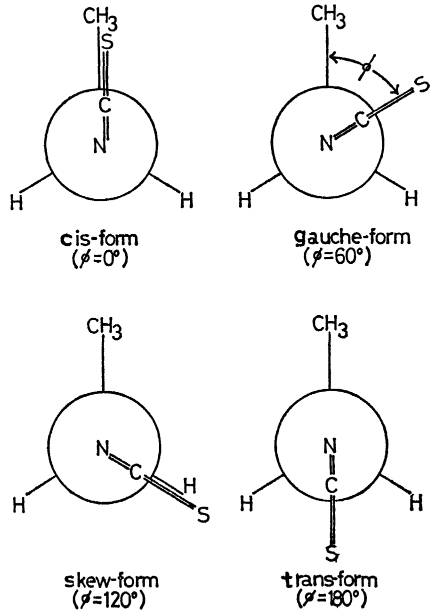

Fig. 1. Model of rotational isomers of ethyl isothiocyanate.
ϕ: dihedral angle.

The $J=4\leftarrow3$ transitions with $K_{-1}=0$ and 1 in the ground vibrational state were first observed and identified from their Stark effects. With the preliminary values of the rotational constants fitted to only the low-J transition frequencies, the high-J transition frequencies were predicted from the rigid rotor Hamiltonian. As the values of J and K_{-1} increase, the difference between the observed and calculated transition frequencies was found to become larger, in particular, for lines with values of K_{-1} larger than one as shown in Fig. 2 (obsd and calcd-I). This difference is probably attributable to the centrifugal distortion effect.

The preliminarily determined rotational constants

TABLE 1. ASSIGNED ROTATIONAL TRANSITIONS OF ETHYL ISOTHIOCYANATE (in MHz)

Transition	Ground state		Set-I CN torsion		Set-II CNC bend	
	ν_{obsd}[a]	$\Delta\nu$[b]	ν_{obsd}[a]	$\Delta\nu$[b]	ν_{obsd}[a]	$\Delta\nu$[b]
$4_{04} \leftarrow 3_{03}$	13548.86	0.30	13372.96	0.02	13303.99	−0.16
$4_{14} \leftarrow 3_{13}$	13228.17	0.16	13083.72	0.38	13016.68	−0.17
$4_{13} \leftarrow 3_{12}$	13896.66	0.21	13684.15	−0.07	13612.25	0.20
$4_{23} \leftarrow 3_{22}$	13565.29	0.13	13387.15	0.60	13317.82	0.39
$4_{22} \leftarrow 3_{21}$	13581.70	−0.18	13399.53	0.10	13329.25	−0.44
$4_{32} \leftarrow 3_{31}$	13570.90[c]	−0.35	13392.97[c]	0.50	13323.59[c]	0.31
$4_{31} \leftarrow 3_{30}$		−0.41		0.52		0.27
$5_{05} \leftarrow 4_{04}$	16922.53	−0.36	16706.15	0.10	16620.58	−0.01
$5_{15} \leftarrow 4_{14}$	16531.28	−0.37	16351.54	0.08	16267.93	−0.46
$5_{14} \leftarrow 4_{13}$	17367.34	0.27	17102.61	0.14	17012.65	0.35
$5_{24} \leftarrow 4_{23}$	16954.38	0.31	16730.86	−0.38	16645.02	0.19
$5_{23} \leftarrow 4_{22}$	16987.16	−0.32	16757.56	0.17	16669.29	−0.05
$5_{33} \leftarrow 4_{32}$	16965.41	0.13	16741.61[c]	0.61	16655.38[c]	0.59
$5_{32} \leftarrow 4_{31}$		0.13		0.46		0.46
$5_{42} \leftarrow 4_{41}$	16966.01	0.07	16742.38[c]	−0.51	16657.90	0.22
$5_{41} \leftarrow 4_{40}$		0.07		−0.51		0.22
$6_{06} \leftarrow 5_{05}$	20289.00	0.23	20032.51	0.03	19930.22	−0.44
$6_{16} \leftarrow 5_{15}$	19833.38	0.26	19617.81	0.01	19517.92	−0.26
$6_{15} \leftarrow 5_{14}$	20835.55	0.25	20518.88	0.08	20410.85	0.17
$6_{25} \leftarrow 5_{24}$	20341.28	−0.11	20074.74	0.10	19970.84	−0.10
$6_{24} \leftarrow 5_{23}$	20399.96	0.18	20120.62	0.27	20013.42	−0.36
$6_{31} \leftarrow 5_{33}$	20360.18[c]	0.12	20090.26[c]	−0.18	19987.17[c]	0.44
$6_{33} \leftarrow 5_{32}$		0.46		−0.58		0.09
$6_{43} \leftarrow 5_{42}$	20360.18	0.24	20092.20	0.22	19989.82	0.32
$6_{42} \leftarrow 5_{41}$		0.24		0.22		0.32
$6_{52} \leftarrow 5_{51}$	20363.38[c]	0.96	20096.24	0.18	19995.06	−0.01
$6_{51} \leftarrow 5_{50}$		0.96		0.18		−0.01
$7_{07} \leftarrow 6_{06}$	23644.20	−0.41	23350.87	−0.08	23233.23	0.06
$7_{17} \leftarrow 6_{16}$	23131.36	−0.67	22882.10	0.03	22765.92	0.02
$7_{16} \leftarrow 6_{15}$	24300.36	−0.24	23933.41	0.61	23806.91	0.13
$7_{26} \leftarrow 6_{25}$	23726.66	−0.16	23416.69	0.20	23295.36	−0.13
$7_{25} \leftarrow 6_{24}$	23820.11	0.13	23489.42	−0.04	23363.86	−0.04
$7_{35} \leftarrow 6_{34}$	23756.18	0.50	23441.10[c]	0.60	23319.83[c]	0.69
$7_{34} \leftarrow 6_{33}$	23756.18[c]	−0.81		−0.30		−0.11
$7_{41} \leftarrow 6_{43}$	23754.20	−0.16	24441.10	−0.25	23321.82	0.34
$7_{43} \leftarrow 6_{42}$		−0.16		−0.25		0.34
$7_{53} \leftarrow 6_{52}$	23756.18	−0.45	23446.06	0.45	23327.87	0.38
$7_{52} \leftarrow 6_{51}$		−0.45		0.45		0.38
$7_{62} \leftarrow 6_{61}$	23760.85	−0.21	23452.15	0.02	23336.49	0.43
$7_{61} \leftarrow 6_{60}$		−0.21		0.02		0.43
$8_{08} \leftarrow 7_{07}$	26988.64	−0.30	26660.09	−0.17	26526.74	−0.21
$8_{18} \leftarrow 7_{17}$	26427.64	−0.06	26144.04	0.09	26526.74	−0.21
$8_{17} \leftarrow 7_{16}$	27762.21	−0.21	27343.51	−0.50	26011.15	−0.12
$8_{27} \leftarrow 7_{26}$	27109.90	−0.13	26756.13	−0.38	26617.96	−0.27
$8_{26} \leftarrow 7_{25}$	27249.39	0.20	26865.88	0.24	26720.48	−0.06
$8_{36} \leftarrow 7_{35}$	27152.48	0.27	26791.32	0.10	26653.54[c]	1.47
$8_{35} \leftarrow 7_{34}$	27155.54[c]	0.69		0.10		−0.12
$8_{45} \leftarrow 7_{44}$	27149.30	−0.03	26791.32	0.27	26653.54	−0.11
$8_{44} \leftarrow 7_{43}$		−0.03		0.27		−0.12
$8_{54} \leftarrow 7_{53}$	27151.21	0.14	26795.38	0.12	26660.18[c]	0.28
$8_{53} \leftarrow 7_{52}$		0.14		0.12		0.28
$8_{63} \leftarrow 7_{62}$	27155.54	−0.16	26803.15[c]	0.79	26669.54	0.16
$8_{62} \leftarrow 7_{61}$		−0.16		0.79		0.16
$8_{72} \leftarrow 7_{71}$	27162.20	−0.07	26812.02	0.41	26680.80	−0.58
$8_{71} \leftarrow 7_{70}$		−0.07		0.41		−0.58
$9_{09} \leftarrow 8_{08}$	30320.20	−0.30	29959.09	−0.22	29810.67	−0.27
$9_{19} \leftarrow 8_{18}$	29720.92	0.11	29403.74	0.56	29254.56	0.55

Table 1. (Continued)

Transition	Ground state		Set-I CN torsion		Set-II CNC bend	
	ν_{obsd}[a]	$\Delta\nu$[b]	ν_{obsd}[a]	$\Delta\nu$[b]	ν_{obsd}[a]	$\Delta\nu$[b]
$9_{18} \leftarrow 8_{17}$	31219.69	−0.43	30751.20[c]	−0.78	30589.92	−0.47
$9_{28} \leftarrow 8_{27}$	30490.44	−0.27	30093.88[c]	0.79	29939.10	0.22
$9_{27} \leftarrow 8_{26}$	30688.71	0.38	30249.67	0.01	30084.29	−0.15
$9_{37} \leftarrow 8_{36}$	30550.10	0.41	30142.54	−0.18	29986.37[c]	0.85
$9_{36} \leftarrow 8_{35}$	30554.58	0.06	30145.20[c]	−0.70	29988.42	−0.01
$9_{46} \leftarrow 8_{45}$ $9_{45} \leftarrow 8_{44}$	30545.08	0.24 0.24	30141.09	0.01 0.01	29986.37	0.35 0.35
$9_{55} \leftarrow 8_{54}$ $9_{54} \leftarrow 8_{53}$	30545.68	−0.07 −0.07	30145.20	0.19 0.19	29992.87[c]	0.59 0.59
$9_{64} \leftarrow 8_{63}$ $9_{63} \leftarrow 8_{62}$	30550.10	−0.30 −0.30	30152.80	0.24 0.24	30002.89	0.36 0.36
$9_{73} \leftarrow 8_{72}$ $9_{72} \leftarrow 8_{71}$	30557.46	−0.02 −0.02	30162.83	0.12 0.12	30015.49	−0.30 −0.30
$9_{82} \leftarrow 8_{81}$ $9_{81} \leftarrow 8_{80}$	30566.30	−0.14 −0.14	30175.09	0.03 0.03	30030.86[c]	−0.82 −0.82
$10_{010} \leftarrow 9_{09}$	33637.99	−0.26	33246.63	−0.55	33084.52	0.29
$10_{110} \leftarrow 9_{19}$	33010.42	0.33	34158.35[c]	2.15	32494.95[c]	1.09
$10_{19} \leftarrow 9_{18}$	34672.84	−0.24	32660.27	0.76	33975.66[c]	−1.31
$10_{29} \leftarrow 9_{28}$	33868.42	−0.12	33429.77	−0.33	33257.35	0.14
$10_{28} \leftarrow 9_{27}$	34138.34	0.28	33641.88	−0.27	33456.24	0.04
$10_{38} \leftarrow 9_{37}$	33948.09	−0.01	33494.60	−0.12	33319.31	−0.17
$10_{37} \leftarrow 9_{36}$	33956.62	0.26	33500.05	−0.30	33324.83	0.36
$10_{47} \leftarrow 9_{46}$ $10_{46} \leftarrow 9_{45}$	33940.88	−0.13 −0.23	33491.39	−0.16 −0.22	33319.31[c]	0.69 0.69
$10_{56} \leftarrow 9_{55}$ $10_{55} \leftarrow 9_{54}$	33940.88	0.14 0.14	33494.60	−0.28 −0.28	33324.83	0.21 0.21
$10_{65} \leftarrow 9_{64}$ $10_{64} \leftarrow 9_{63}$	33945.42	0.21 0.21	33502.69	−0.04 −0.04	33335.92	0.43 0.43
$10_{74} \leftarrow 9_{73}$ $10_{73} \leftarrow 9_{72}$	33952.81	0.16 0.16	33513.58	−0.10 −0.10	33349.22[c]	−0.73 −0.73
$10_{83} \leftarrow 9_{82}$ $10_{82} \leftarrow 9_{81}$	33962.46	0.11 0.11	33526.82	−0.38 −0.38	33349.22[c]	0.62 0.62
$10_{92} \leftarrow 9_{91}$ $10_{91} \leftarrow 9_{90}$	33973.78	−0.18 −0.18	33542.86	−0.14 −0.14	33388.36[c]	0.71 0.71

a) Experimental uncertainty: ±0.20 MHz. b) $\Delta\nu = \nu_{\mathrm{obsd}} - \nu_{\mathrm{calcd}}$. c) Not included in the least-squares fitting.

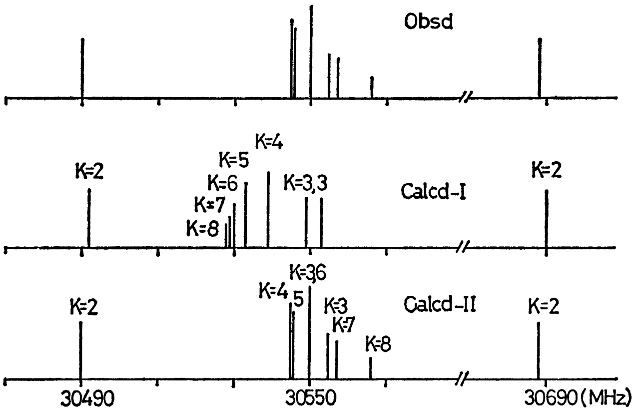

Fig. 2. Observed and calculated $J=9\leftarrow 8$ transition of ethyl isothiocyanate (ground vibrational state). Calcd-I: calculated with the rigid rotor model; Calcd-II: calculated using Eq. (1), the centrifugal distortion effect included.

suggest that the molecule studied was a nearly symmetric top. Therefore, the observed transition frequencies given in Table 1 were fitted to the following equations:

$$E = E_{\mathrm{r}} + E_{\mathrm{d}} \tag{1}$$

$$E_{\mathrm{d}} = -D_J J^2(J+1)^2 - D_{JK} J(J+1)K^2 - D_K K^4 \tag{2}$$

where E_{r} is the energy for a nearly symmetric rigid rotor molecule and E_{d} the correction for the first-order centrifugal distortion effect.

The rotational and centrifugal distortion constants were obtained by the least-squares method as given in Table 2. The observed and calculated transition frequencies are in good agreement, as is shown in the column of Table 1 with the heading "ground state". As shown in Fig. 2, the transitions with K_{-1} larger than four appear at higher frequencies as their K_{-1} increase, (obsd and calcd-II), in contrast with the rigid rotor spectrum (calcd-I). This is because of the negative value of D_{JK}.

Conformation of the Molecule. For the ground vibrational state, the value of $\Delta(I_{\mathrm{a}}+I_{\mathrm{b}}-I_{\mathrm{c}})$ is 6.159

TABLE 2. ROTATIONAL CONSTANTS AND MOMENTS OF INERTIA[a] FOR ETHYL ISOTHIOCYANATE

	Ground State	Set-I C-N torsion	Set-II CNC bend
A(MHz)	14194±10	14599±10	15215±15
B(MHz)	1779.27 ±0.02	1748.42 ±0.02	1739.03 ±0.02
C(MHz)	1612.14 ±0.02	1598.18 ±0.02	1590.22 ±0.02
D_J(kHz)	1.58 ±0.02	1.70 ±0.02	2.31 ±0.02
D_{JK}(kHz)	−36.9 ±0.2	−48.6 ±0.2	−61.6 ±0.2
I_a(amu·Å^2)	35.605±0.025	34.617±0.024	33.215±0.033
I_b(amu·Å^2)	284.035±0.003	289.047±0.003	290.608±0.003
I_c(amu·Å^2)	313.481±0.004	316.219±0.004	317.803±0.004
Δ(amu·Å^2)[b]	6.159±0.032	7.445±0.031	6.020±0.040
Δ'(amu·Å^2)[c]	0.084±0.032	−1.202±0.031	0.222±0.040

a) Conversion factor$=5.05376\times10^5$ MHz·amu·Å^2. b)$\Delta=I_a+I_b-I_c$. c) $\Delta'=I_c-I_b-I_a+8m_Hc_H^2$.

amu·Å^2, as calculated from the moments of inertia given in Table 2. If the molecule studied in this work has a plane of symmetry, there are four hydrogen atoms out of this plane. Consequently, the following relation is valid if the molecule is rigid:

$$8m_Hc_H^2 = I_a + I_b - I_c \qquad (3)$$

where m_H is the mass of one hydrogen atom and c_H is its distance from the plane of symmetry. There are two possible configurations for the molecule having a plane of symmetry, namely, the *cis* and *trans* forms. Using the assumed structural parameters given in Table 3, the value of $8\,m_Hc_H{}^2$ for the two forms was calculated to be 6.345 amu·Å^2. This is in good agreement with the value determined experimentally. This result suggests that the configurations of the molecule are the forms having plane symmetry, namely, the *cis* or *trans* form. Moreover, comparing the rotational constants determined experimentally with those calculated from the assumed structures given in Table 4, the preferred configuration is clearly the *cis* form shown in Fig. 3. Ethyl isothiocyanate molecules are in the *cis* conformation in the gas phase as one of the possible rotational isomers. This result is consistent with the fact that propionaldehyde,[3] 1-butene,[4] propionic acid,[5] and propionyl fluoride[6] exist in the *cis* and *skew* forms as rotational isomers, rather than in the *trans* form, with respect to the methyl group and the C=O or C=C double bond.

Three structural parameters, $r_{C_\alpha-N}$, $\angle C_\beta C_\alpha N$ and $\angle C_\alpha NC$, of the ethyl isothiocyanate molecule in the ground vibrational state were obtained from the observed rotational constants, A, B, and C, fixing the remaining structural parameters to the values assumed in Table 3. The results obtained are $r_{C_\alpha-N}=1.454$ Å,

TABLE 3. ASSUMED STRUCTURAL PARAMETERS[a]

Distances	Angles
C-H : 1.091Å	$\angle$HCH : 108.8°
C_β-C_α : 1.522Å	$\angle HC_\beta C_\alpha$: 109.6°
C_α-N : 1.437Å	$\angle C_\beta C_\alpha H$: 110.6°
N=C : 1.210Å	$\angle C_\beta C_\alpha N$: 109.5°
C=S : 1.550Å	$\angle C_\alpha NC$: 147.5°

a) Carbon atoms at the α- and β-positions are denoted as C_α and C_β, respectively. The structural parameters are taken from mono-substituted ethanes CH_3CH_2X (X=F[9], Cl[10], Br[11], I[12], OH[13], NC[14]) for the ethyl group and from methyl isothiocyanate[15] for the isothiocyanato group.

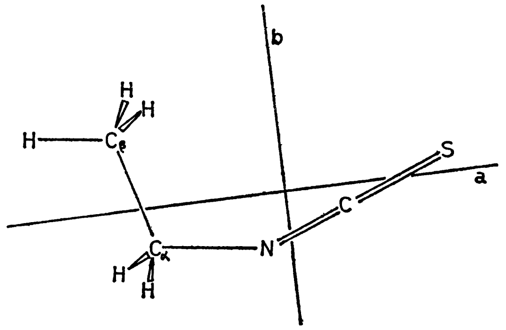

Fig. 3. Configuration of the predominant rotamer, *cis*-ethyl isothiocyanate. The c principal axis is perpendicular to the plane of paper.

TABLE 4. OBSERVED AND PREDICTED ROTATIONAL CONSTANTS

	Obsd	Calcd			
		cis	*gauche*	*skew*	*trans*
A(MHz)	14194	14197.29	15558.54	24035.91	33364.61
B(MHz)	1779.27	1778.77	1694.55	1494.95	1427.60
C(MHz)	1612.14	1612.73	1569.60	1451.58	1392.96
κ	−0.973433	−0.973611	−0.982135	−0.996159	−0.997833
Δ(amu·Å^2)[a]	6.159	6.345	8.740	10.925	6.343
ϕ(°)[b]		0	60	120	180

a) $\Delta=I_a+I_b-I_c$. b) ϕ: dihedral angle about the C-N bond, see Fig. 1.

$\angle C_\beta C_\alpha N=109.6°$ and $\angle C_\alpha NC=151.0°$.

An attempt was made to assign the microwave spectrum of the other rotamers which would give rather weak absorption lines, but it was unsuccessful. This may be partly because of the overlap of the lines of the vibrationally-excited states of the *cis* form with those of the *skew* or the *trans* form.

Vibrational Satellites. Satellite lines were observed around each rotational transition of the ground vibrational state. They spread from 300 to 500 MHz and have essentially the same Stark effect behavior and K series pattern as the corresponding ground state transitions. Evidently, these satellites are due to molecules in the vibrationally-excited states for which the effective moments of inertia are different from those for the ground states. Figure 4 illustrates the typical satellite pattern of the a-type transitions of $J=4\leftarrow3$. Two sets (set-I and set-II) of vibrationally-excited lines were assigned as shown in Table 1. The effective rotational constants obtained for two vibrationally-excited states are given in Table 2.

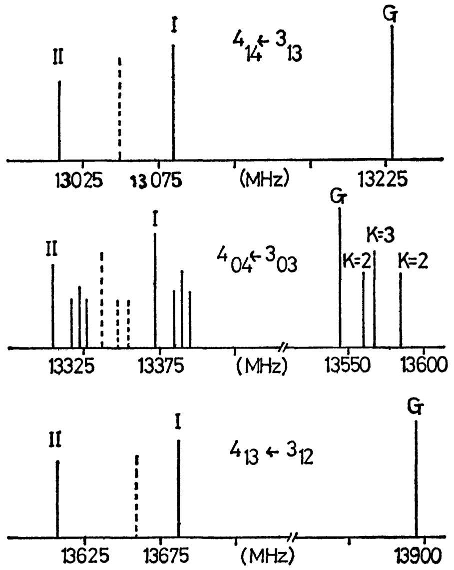

Fig. 4. Observed spectrum of $J=4\leftarrow3$ transitions showing vibrational excited satellite lines, I and II; dotted lines are unassigned lines.

Table 5. Far-infrared spectrum (cm^{-1})

CH_3NCS[a]	CH_3CH_2NCS	Assignment
(100)[b]	70(w)	C–N torsion
180.0	130(s)	CNC bend
	225(w)	C–C torsion
	380(s)	CCN bend (in-plane)[c]
440.0	450(m)	NCS bend (out-of-plane)[c]
569.0	540(s)	NCS bend (in-plane)[c]

Abbreviations: s, strong; m, medium; w, weak.
a) Ref. 15. b) Postulated value. c) Ref. 1.

Measurements of the relative intensities of the satellites with respect to the ground state line yielded vibrational frequencies 58±30 cm^{-1} for set-I and 107±30 cm^{-1} for set-II. Bands were observed at 70, 130 and 225 cm^{-1} in the far-infrared spectrum of ethyl isothiocyanate in the gas phase. Referring to Kniseley's assignment of the infrared spectrum[1] and to the study of methyl isothiocyanate,[15] these bands were assigned to the C–N torsion, CNC bending and C–C torsion modes, respectively, as shown in Table 5. Therefore, the vibrational satellite corresponding to 58 and 107 cm^{-1} can be ascribed to excited states of the C–N torsion and CNC bending modes, respectively. These assignments are supported by the fact that $\Delta'(I_c-I_b-I_a+8m_Hc_H^2)$ for set-I (out-of-plane vibration) has a negative value while the value of Δ' for set-II (in-plane vibration) is larger than that of the ground state[16] as shown in Table 2.

Dipole Moment. From the Stark coefficients of the transitions $4_{04}\leftarrow3_{03}$, $4_{14}\leftarrow3_{13}$, and $4_{13}\leftarrow3_{12}$, the dipole moment of the molecule was determined for both the ground and excited vibrational states. The second-order Stark coefficients determined for the eight Stark component lines and the dipole moment obtained are shown in Table 6. The electric field strength in the absorption cell was calibrated using

Table 6. Stark coefficients ($\Delta\nu/E^2$[MHz/(V/cm)^2]$\times10^{-5}$) and dipole moments

Transition	M	Ground state		Set-I CN torsion		Set-II CNC bend	
		Obsd	Calcd	Obsd	Calcd	Obsd	Calcd
$4_{13}\leftarrow3_{12}$	0	−0.440	−0.455	−0.476	−0.476	−0.485	−0.514
	1	−1.68	−1.74	−1.95	−1.97	−2.07	−2.14
$4_{04}\leftarrow3_{03}$	0	−0.758	−0.749	−0.809	−0.790	−0.881	−0.840
	1	−0.446	−0.452	−0.467	−0.478	−0.514	−0.504
	2	0.442	0.441	0.454	0.456	0.508	0.501
	3	1.91	1.93	2.06	2.01	2.27	2.18
$4_{14}\leftarrow3_{13}$	0	−0.441	−0.472	−0.396	−0.493	−0.515	−0.517
	1	1.34	1.30	1.44	1.52	1.62	1.66
μ_a(D)		3.33±0.03		3.38±0.03		3.50±0.05	
μ_b(D)		0.07±0.02		0.05±0.02		0.04±0.02	
μ_c(D)		0 (assumed)		0 (assumed)		0 (assumed)	
μ_{total}(D)		3.33±0.03		3.38±0.03		3.50±0.05	

the value of the dipole moment of OCS, 0.71521 D.7) The dipole moment determined for the ground state was $\mu_{\text{total}}=3.33\pm0.03$ D, with $\mu_a=3.33\pm0.03$ D and $\mu_b=0.07\pm0.02$ D. The μ_c component was assumed to be zero because of the plane symmetry as discussed above. The total dipole moment μ_{total} is compared with the value of 3.31 D obtained from dielectric constant measurements in a benzene solution.8)

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