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Microwave Spectrum of the Ethylmethyl Ether Molecule

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Abstract: We have observed rotational transitions of ethylmethyl ether ($CH_3CH_2OCH_3$) in the 24-110 GHz frequency range. We newly assigned the transitions of four Q-branch series for J=1-38 with Ka=0-5 and six R-branch series of b-type transitions for J=7-37 with Ka=0-3. All these assigned transitions were observed to be split into two or four components due to the internal rotations of the methyl groups. We analyzed the averaged frequencies of the split components on the basis of the Watson *A*-reduced Hamiltonian, neglecting the effect of the internal rotations. A total of 122 transitions were fitted to eight molecular parameters to a 1 s standard deviation of 24 kHz. The parameters *A*, *B*, *C* and D_J were improved, and D_{JK}, D_k, d_J and d_K were determined for the first time.

Keywords: Ethylmethyl ether, spectroscopy, microwave.

Introduction

The ethylmethyl ether molecule ($CH_3CH_2OCH_3$) has internal rotations of two CH_3 groups of threefold symmetry. The molecular structure is shown in Figure 1. This molecule is a slightly asymmetric top molecule and has the dipole moment components along principal inertia a- and b-axis. Since the component along a-axis is so small that the transitions assigned so far are all b-type transitions. The first microwave spectra of this molecule and its isotopic species were observed in the frequency range from

8.5 to 34 GHz by Hayashi and Kuwada, and molecular parameters *A, B, C* and D_J and components of dipole moment in the ground state were reported. They also reported the potential barrier heights 2554 and 3294 cal/mol for OCH_3 and CH_3C groups, respectively [1].

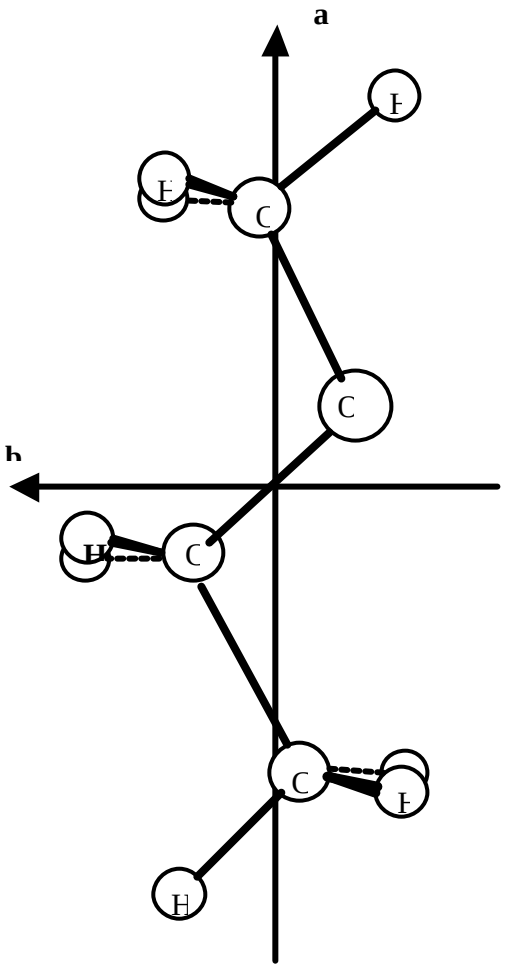


Figure 1. Molecular Structure of $C_2H_5OCH_3$

In this study, we have observed rotational transitions in the 24-110 GHz frequency range and newly assigned 111 transitions according to the prediction from the molecular parameters determined by Hayashi *et al.* A rotational transition split into two or four components due to the internal rotation of the two methyl groups: a transition split into two components due to the internal rotation of OCH_3 group, and each component further splits into two components due to the internal rotation of CH_3C group. However, for lower J transitions these latter splitting are too small to be observed with a conventional microwave spectrometer. We analyzed the averaged frequencies of the split components on the basis of the Watson *A*-reduced Hamiltonian [2], neglecting the effect of the internal rotations. A total of 122 transitions including 11 transitions observed by Hayashi [1] were fitted to the Hamiltonian with a 1σ standard deviation of 24 kHz.

Experimental

The block diagram of spectrometer is shown in Figure 2. [3] The fundamental microwave source is a microwave synthesizer (HP83642A) operating in the frequency range from 2 to 40 GHz. In the frequency range from 40 to 110 GHz, millimeter-wave source modules (Hewlett Packard, HP83556A, HP83557A and HP8358A) were used. In the measurement above 40 GHz, the source frequency was modulated by small amplitude of a 50 kHz sinusoidal-wave, and the detected microwave signal was demodulated by a lock-in amplifier operated in the 2f mode. The second derivative of an absorption line shape was recorded on a personal computer. In the measurement below 40 GHz, the square-wave Stark modulation at 100 kHz was used to prevent distortion of baselines. The accuracy of observed frequencies is estimated to be better than 70 kHz for the Stark modulation measurements and better than 50 kHz for the source modulation measurements. The observation was made at room temperature.

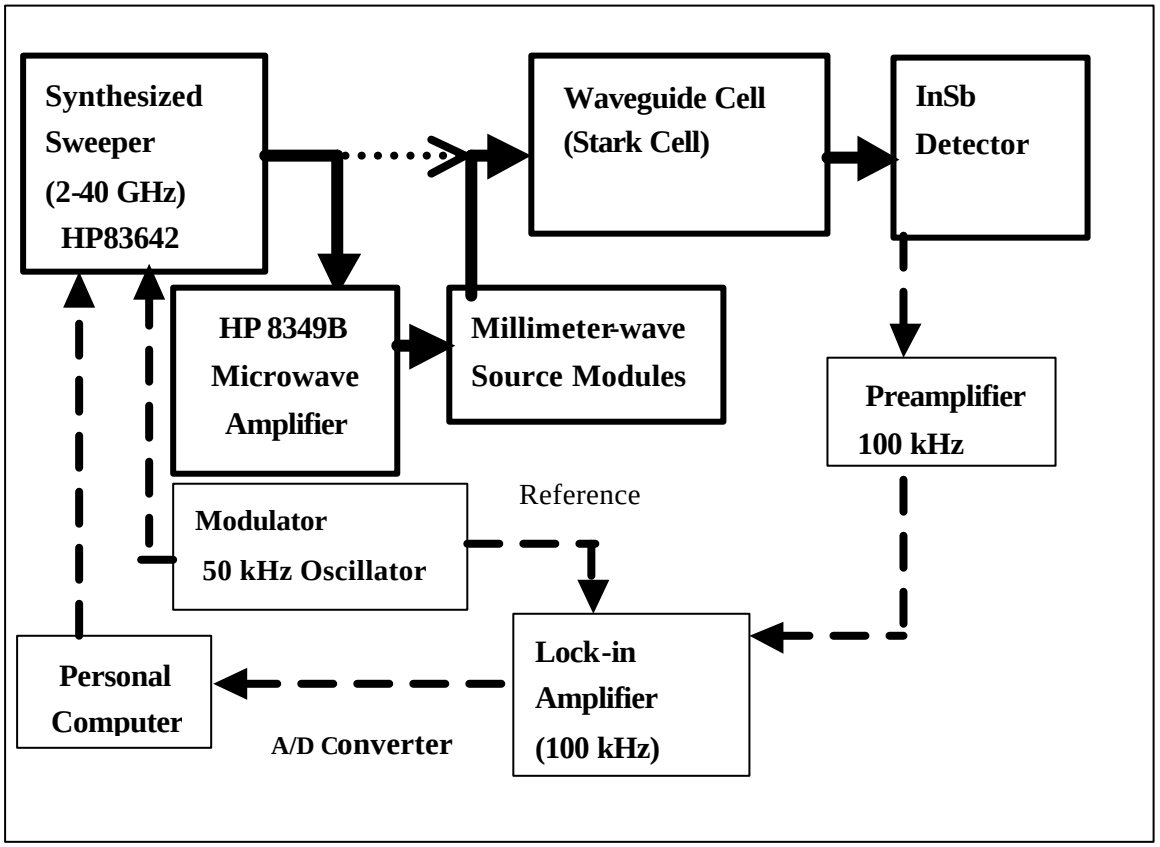


Figure 2. Block diagram of Millimeter-wave-Spectrometer.

Observed Spectrum and analysis

Transitions of Q-branch series for Ka=1 ← 0, 2 ← 1, and 3 ← 2 and those of R-branch series for Ka=1 ← 0, 0 ← 1, 1 ← 2, 2 ← 3, 3 ← 4 and 4 ← 5 were assigned.

(a) Q-branch transition

$J_{1\ J-1} \leftarrow J_{0\ J}$ series: The absorption line for the $26_{1\ 25} \leftarrow 26_{0\ 26}$ transitio n is shown in Figure 3 as a typical rotational line. All the lines belonging to this series show doublet structures due to the internal rotation of the -OCH_3 group. Separations of the components in this series are from 0.36 to 1.03 MHz, which increase with J. The assignment to this series was made with the help of calculated frequencies using the rotational constants reported by Hayashi *et al.* To find the successive J transitions in the Q-branch series, we used the power series expansion of J (J+1). We assigned the transitions of this series with J=1 to 29.

Q-branch series transitions $J_{2\ J-2} \leftarrow J_{1\ J-1}$ with J = 7 to 9, with 12 to 16, and with J=21 to 37, $J_{2\ J-1} \leftarrow J_{1J}$ with J =7 and 12 to 22, and $J_{3\ J-3} \leftarrow J_{2\ J-2}$ with J = 21 to 30 were assigned. Absorption lines for $20_{2\ 19} \leftarrow 20_{1\ 20}$ and $30_{2\ 27} \leftarrow 30_{2\ 28}$ are shown in Figures 4 and 5, respectively. Transitions belonging to $J_{2\ J-2} \leftarrow J_{1\ J-1}$ series show the doublet structures and those belonging to $J_{2\ J-1} \leftarrow J_{1\ J}$, and $J_{3\ J-3} \leftarrow J_{2\ J-2}$ series show the quartet structures due to the internal rotations of the two methyl groups.

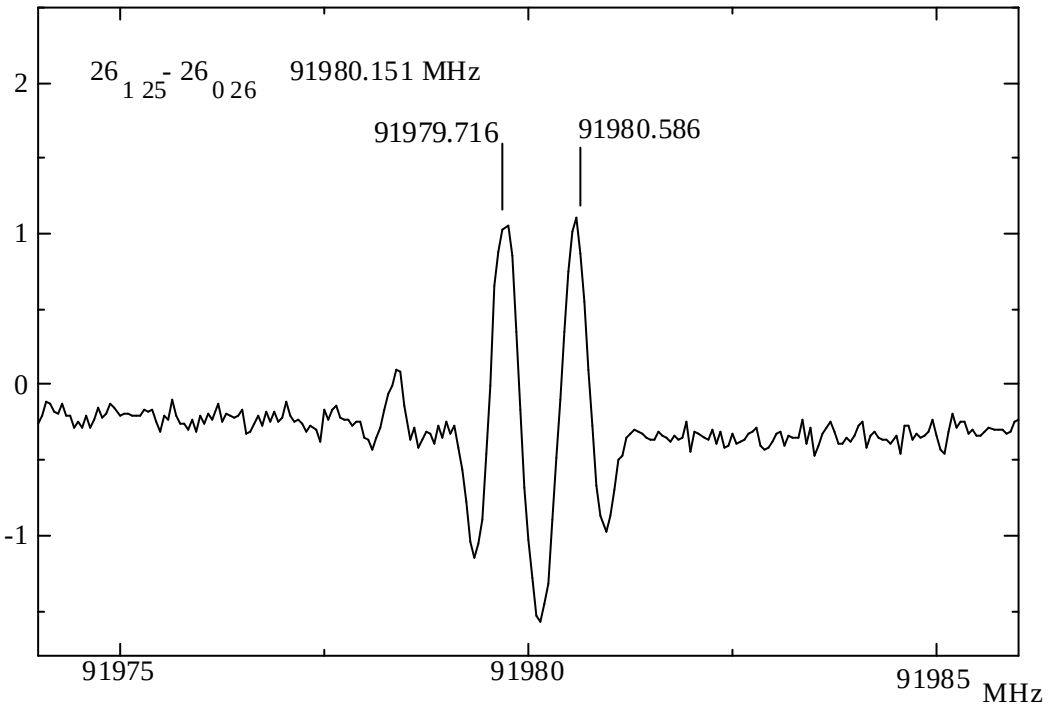


Figure 3. Absorption line for the $26_{1\ 25} \leftarrow 26_{0\ 26}$ transition.

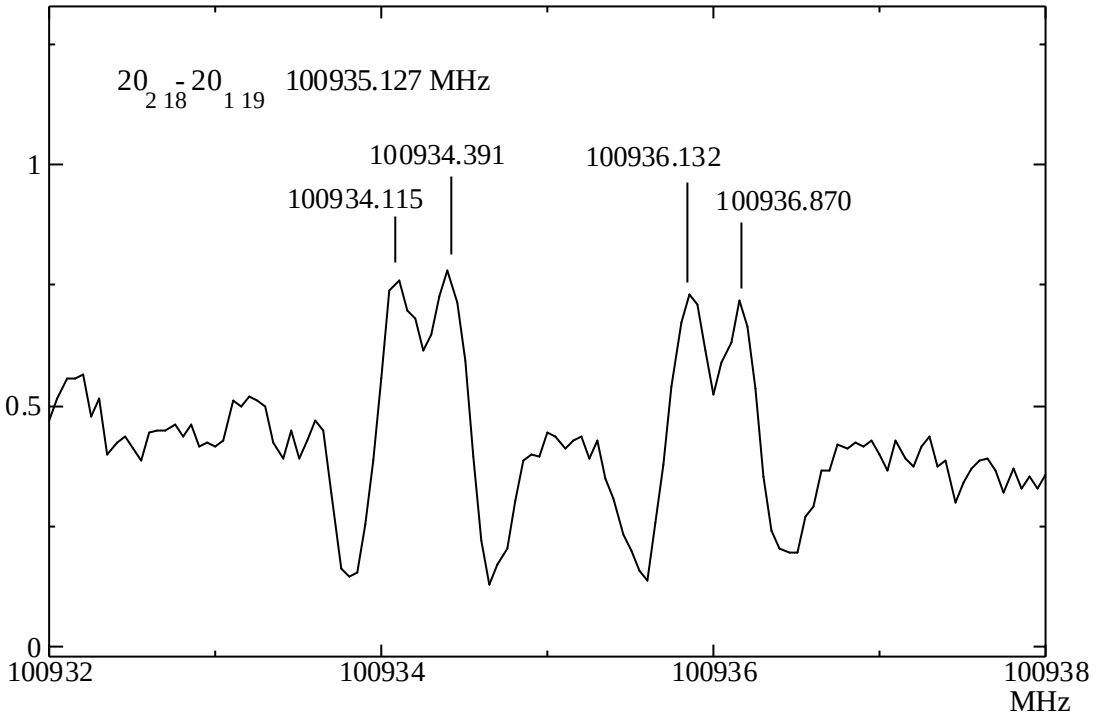


Figure 4. Absorption line for the $20_{2\ 19} \leftarrow 20_{1\ 20}$ transition.

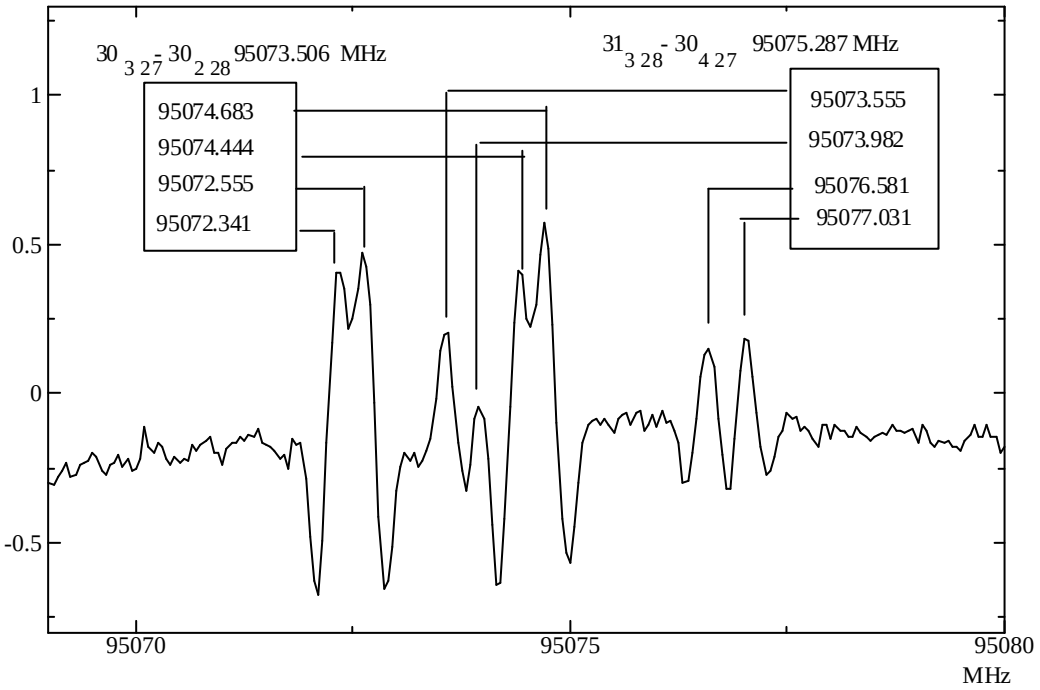


Figure 5. Absorption lines for the $30_{3\ 27} \leftarrow 30_{2\ 28}$ and $31_{3\ 28} \leftarrow 30_{4\ 27}$ transitions.

(b) R-branch transition

The absorption line for $9_{1\ 9} \leftarrow 8_{0\ 8}$ is shown in Figure 6 and that for $31_{3\ 28} \leftarrow 30_{4\ 27}$ is included in Figure 5. The R-branch series transitions $(J+1)_{1\ J+1} \leftarrow J_{0\ J}$ with J = 1 to 10, $(J+1)_{0\ J+1} \leftarrow J_{1\ J}$ with J = 5 to 14, $(J+1)_{1\ J} \leftarrow J_{2\ J-1}$ with J = 10 to 18, $(J+1)_{2\ J-1} \leftarrow J_{3\ J-2}$ with J = 18, 21, 22, 23, and 24, $(J+1)_{3\ J-2} \leftarrow J_{4\ J-3}$ with J =25 to 31, and $(J+1)_{4\ J-3} \leftarrow J_{5\ J-4}$ with J = 34 to 38 were assigned. Transitions belonging to $(J+1)_{1\ J+1} \leftarrow J_{0\ J}$, $(J+1)_{0\ J+1} \leftarrow J_{1\ J}$, and $(J+1)_{1\ J} \leftarrow J_{2\ J-1}$ series show the doublet structures and those belonging to $(J+1)_{2\ J-1} \leftarrow J_{3\ J-2}$, $(J+1)_{3\ J-2} \leftarrow J_{4\ J-3}$, and $(J+1)_{4\ J-3} \leftarrow J_{5\ J-4}$ series show the quartet structures.

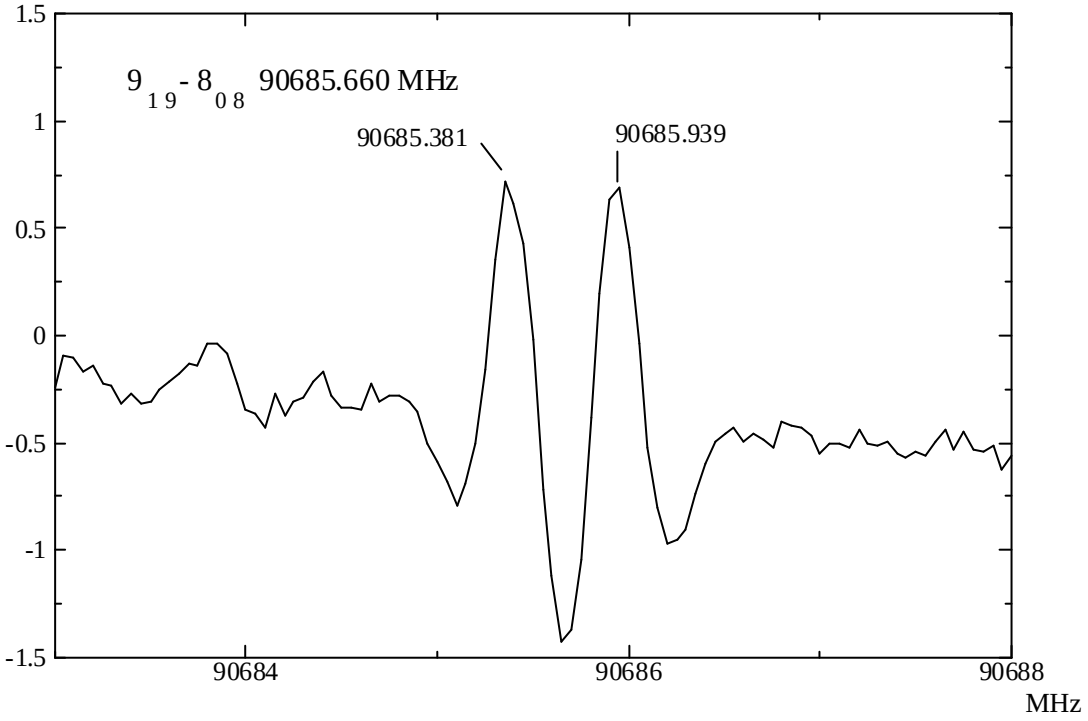


Figure 6. Absorption line for the $9_{1\ 9} \leftarrow 8_{0\ 8}$ transition.

(c) Rotational Constant

A total of 322 lines have been observed and listed in Table 1. 122 b-type transitions in total were assigned. In this study, we obtained the average of frequencies of split components as the transition frequencies. The 122 transition frequencies are also listed in Table 1. We fitted these frequencies to determine the rotational constants using the Watson A-reduced Hamiltonian.

$$\mathbf{H} = \frac{1}{2}(B+C)\,\mathbf{P^2} + \left[A - \frac{1}{2}(B+C)\right] P_a^2 + \frac{1}{2}(B-C)(P_b^2 - P_c^2)$$

$$- D_J\,(\mathbf{P^2})^2 - D_{JK}\,\mathbf{P^2}\,P_a^{\,2} - D_K P_a^4 - 2d_J\,\mathbf{P^2}\,(P_b^2 - P_c^2) - d_K\left[P_a^2(P_b^2 - P_c^2) + (P_b^2 - P_c^2)P_a^2\right],$$

where **P** is total angular momentum with components P_a, P_b and P_c along the a-, b- and c-axis, respectively.

Table 1. Observed frequencies of Methylethyl Ether. (MHz)

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
(1) Q-branch transition									
(a) $J_{1\ J-1} \leftarrow J_{0\ J}$ series.									
1	1	0	1	0	1	24100.391	24100.572	24100.621	-0.049
						24100.753			
2	1	1	2	0	2	24370.963	24371.207	24371.192	0.015
						24371.451			
3	1	2	3	0	3	24781.024	24781.266	24781.260	0.006
						24781.508			
4	1	3	4	0	4	25335.610	25335.853	25335.856	-0.003
						25336.096			
5	1	4	5	0	5	26041.543	26041.661	26041.638	0.023
						26041.779			
6	1	5	6	0	6	26906.707	26906.893	26906.834	0.059
						26907.078			
7	1	6	7	0	7	27940.930	27941.173	27941.138	0.035
						27941.415			
8	1	7	8	0	8	29155.356	29155.644	29155.562	0.082
						29155.931			
9	1	8	9	0	9	30562.021	30562.251	30562.211	0.040
						30562.480			
10	1	9	10	0	10	32173.777	32174.020	32173.987	0.033
						32174.263			
11	1	10	11	0	11	34003.959	34004.270	34004.200	0.070
						34004.581			
12	1	11	12	0	12	36065.858	36066.118	36066.090	0.028
						36066.378			
13	1	12	13	0	13	38372.022	38372.292	38372.271	0.021
						38372.562			
14	1	13	14	0	14	40933.710	40934.145	40934.126	0.019
						40934.580			
15	1	14	15	0	15	43760.760	43761.165	43761.174	-0.009
						43761.570			
16	1	15	16	0	16	46860.100	46860.495	46860.474	0.021
						46860.890			
17	1	16	17	0	17	50235.686	50236.100	50236.094	0.006
						50236.513			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
18	1	17	18	0	18	53888.277	53888.715	53888.703	0.012
						53889.152			
19	1	18	19	0	19	57814.889	57815.312	57815.310	0.002
						57815.734			
20	1	19	20	0	20	62008.831	62009.174	62009.169	0.005
						62009.517			
21	1	20	21	0	21	66459.481	66459.856	66459.850	0.006
						66460.231			
22	1	21	22	0	22	71153.089	71153.445	71153.457	-0.012
						71153.820			
23	1	22	23	0	23	76072.572	76072.955	76072.978	-0.023
						76073.337			
24	1	23	24	0	24	81198.339	81198.757	81198.738	0.019
						81199.174			
25	1	24	25	0	25	86508.462	86508.913	86508.923	-0.010
						86509.364			
26	1	25	26	0	26	91979.716	91980.151	91980.167	-0.016
						91980.586			
27	1	26	27	0	27	97587.703	97588.155	97588.165	-0.010
						97588.606			
28	1	27	28	0	28	103307.822	103308.307	103308.312	-0.005
						103308.791			
29	1	28	29	0	29	109115.821	109116.335	109116.321	0.014
						109116.848			
(b) $J_{2\,J-2} \leftarrow J_{1\,J-1}$.									
7	2	5	7	1	6	68455.322	68456.087	68456.067	0.020
						68456.852			
8	2	6	8	1	7	67589.252	67590.039	67590.000	0.039
						67590.826			
9	2	7	9	1	8	66676.621	66677.398	66677.468	-0.070
						66678.174			
12	2	10	12	1	11	63879.656	63880.380	63880.416	-0.036
						63881.104			
13	2	11	13	1	12	63007.562	63008.290	63008.323	-0.033
						63009.017			
14	2	12	14	1	13	62207.641	62208.391	62208.389	0.002
						62209.140			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
15	2	13	15	1	14	61505.288	61506.020	61506.015	0.005
						61506.752			
16	2	14	16	1	15	60925.333	60926.037	60926.050	-0.013
						60926.740			
21	2	19	21	1	20	60649.185	60649.798	60649.791	0.007
						60650.410			
22	2	20	22	1	21	61255.456	61256.041	61256.053	-0.012
						61256.626			
23	2	21	23	1	22	62120.858	62121.436	62121.460	-0.024
						62122.014			
24	2	22	24	1	23	63259.303	63259.878	63259.873	0.005
						63260.453			
25	2	23	25	1	24	64683.379	64683.927	64683.916	0.011
						64684.475			
26	2	24	26	1	25	66404.416	66404.943	66404.937	0.006
						66405.470			
27	2	25	27	1	26	68432.372	68432.858	68432.873	-0.015
						68433.343			
28	2	26	28	1	27	70775.554	70776.018	70776.025	-0.007
						70776.482			
29	2	27	29	1	28	73440.285	73440.730	73440.750	-0.020
						73441.174			
30	2	28	30	1	29	76430.674	76431.100	76431.117	-0.017
						76431.525			
31	2	29	31	1	30	79748.116	79748.521	79748.533	-0.012
						79748.925			
32	2	30	32	1	31	83391.012	83391.401	83391.415	-0.014
						83391.789			
33	2	31	33	1	32	87354.527	87354.902	87354.908	-0.006
						87355.277			
34	2	32	34	1	33	91630.373	91630.736	91630.720	0.016
						91631.098			
35	2	33	35	1	34	96206.714	96207.068	96207.061	0.007
						96207.421			
36	2	34	36	1	35	101068.384	101068.734	101068.726	0.008
						101069.084			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
37	2	35	37	1	36	106196.973	106197.321	106197.301	0.020
						106197.668			
(c) $J_{2\,J-1} \leftarrow J_{1\,J}$									
7	2	6	7	1	7	75681.685	75682.676	75682.685	-0.009
						75681.958			
						75683.395			
						75683.667			
12	2	11	12	1	12	82536.046	82536.998	82537.012	-0.014
						82536.284			
						82537.646			
						82538.015			
13	2	12	13	1	13	84333.665	84334.639	84334.650	-0.011
						84333.921			
						84335.399			
						84335.570			
14	2	13	14	1	14	86275.083	86276.064	86276.070	-0.006
						86275.332			
						86276.791			
						86277.050			
15	2	14	15	1	15	88360.471	88361.486	88361.510	-0.024
						88360.754			
						88362.238			
						88362.480			
16	2	15	16	1	16	90589.942	90590.948	90590.922	0.026
						90590.244			
						90591.696			
						90591.911			
17	2	16	17	1	17	92962.950	92963.905	92963.930	-0.025
						92963.165			
						92964.625			
						92964.881			
18	2	17	18	1	18	95478.826	95479.816	95479.791	0.025
						95479.086			
						95480.548			
						95480.802			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
19	2	18	19	1	19	98136.344	98137.339	98137.372	-0.033
						98136.599			
						98138.074			
						98138.337			
20	2	19	20	1	20	100934.115	100935.127	100935.122	0.005
						100934.391			
						100935.870			
						100936.132			
21	2	20	21	1	21	103870.000	103871.039	103871.058	-0.019
						103870.324			
						103871.793			
						103872.038			
22	2	21	22	1	22	106941.696	106942.751	106942.757	-0.006
						106942.005			
						106943.485			
						106943.816			
(d) $J_{3\,J-3} \leftarrow J_{2\,J-2}$									
21	3	18	21	2	19	109216.845	109218.259	109218.246	0.013
						109217.248			
						109219.266			
						109219.675			
22	3	19	22	2	20	107655.357	107656.756	107656.741	0.015
						107655.748			
						107657.764			
						107658.154			
23	3	20	23	2	21	106030.312	106031.693	106031.690	0.003
						106030.685			
						106032.695			
						106033.081			
24	3	21	24	2	22	104364.899	104366.268	104366.268	0.000
						104365.276			
						104367.265			
						104367.633			
25	3	22	25	2	23	102684.844	102686.188	102686.187	0.001
						102685.202			
						102687.175			
						102687.531			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
26	3	23	26	2	24	101017.829	101019.152	101019.156	-0.004
						101018.179			
						101020.124			
						101020.474			
27	3	24	27	2	25	99393.033	99394.324	99394.316	0.008
						99393.333			
						99395.329			
						99395.602			
28	3	25	28	2	26	97840.436	97841.662	97841.647	0.015
						97840.701			
						97842.601			
						97842.911			
29	3	26	29	2	27	96390.259	96391.406	96391.396	0.010
						96390.460			
						96392.321			
						96392.582			
30	3	27	30	2	28	95072.341	95073.506	95073.518	-0.012
						95072.555			
						95074.444			
						95074.683			
(2) R-branch transitions									
(a) $(J+1)_{1\ J+1} \leftarrow J_{0\ J}$									
2	1	2	1	0	1	39664.870	39665.110	39665.143	-0.033
						39665.350			
3	1	3	2	0	2	47313.703	47314.044	47314.057	-0.013
						47314.384			
4	1	4	3	0	3	54832.064	54832.409	54832.453	-0.044
						54832.753			
5	1	5	4	0	4	62224.580	62224.865	62224.872	-0.007
						62225.150			
6	1	6	5	0	5	69497.300	69497.587	69497.582	0.005
						69497.874			
7	1	7	6	0	6	76658.282	76658.569	76658.570	-0.001
						76658.855			
8	1	8	7	0	7	83717.232	83717.510	83717.507	0.003
						83717.788			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
9	1	9	8	0	8	90685.381	90685.660	90685.668	-0.008
						90685.939			
10	1	10	9	0	9	97575.563	97575.831	97575.803	0.028
						97576.099			
11	1	11	10	0	10	104401.662	104401.933	104401.925	0.008
						104402.203			
(b) $(J+1)_{0\ J+1} \leftarrow J_{1\ J}$									
6	0	6	5	1	5	26206.237	26206.479	26206.514	-0.035
						26206.720			
7	0	7	6	1	6	34953.242	34953.498	34953.503	-0.005
						34953.753			
8	0	8	7	1	7	43783.052	43783.323	43783.315	0.008
						43783.595			
9	0	9	8	1	8	52682.093	52682.390	52682.397	-0.007
						52682.686			
10	0	10	9	1	9	61635.779	61636.037	61636.021	0.016
						61636.294			
11	0	11	10	1	10	70628.302	70628.567	70628.569	-0.002
						70628.831			
12	0	12	11	1	11	79643.660	79643.913	79643.910	0.003
						79644.165			
13	0	13	12	1	12	88665.588	88665.833	88665.836	-0.003
						88666.078			
14	0	14	13	1	13	97678.312	97678.552	97678.549	0.003
						97678.792			
15	0	15	14	1	14	106666.948	106667.175	106667.171	0.004
						106667.402			
(c) $(J+1)_{1\ J} \leftarrow J_{2\ J-1}$									
11	1	10	10	2	9	25260.962	25261.775	25261.822	-0.047
						25262.587			
12	1	11	11	2	10	34826.535	34827.289	34827.328	-0.039
						34828.043			
13	1	12	12	2	11	44500.354	44501.061	44501.095	-0.034
						44501.768			
14	1	13	13	2	12	54277.305	54278.044	54278.025	0.019
						54278.782			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
15	1	14	14	2	13	64151.563	64152.285	64152.275	0.010
						64153.007			
16	1	15	15	2	14	74116.549	74117.276	74117.178	0.098
						74118.002			
17	1	16	16	2	15	84164.426	84165.146	84165.170	-0.024
						84165.865			
18	1	17	17	2	16	94287.001	94287.716	94287.718	-0.002
						94288.431			
19	1	18	18	2	17	104474.574	104475.263	104475.274	-0.011
						104475.951			
(d) $(J+1)_{2\ J-1} \leftarrow J_{3\ J-2}$									
19	2	17	18	3	16	41939.196	41940.599	41940.573	0.026
						41939.562			
						41941.617			
						41942.022			
22	2	20	21	3	19	71703.719	71705.157	71705.170	-0.013
						71704.122			
						71706.175			
						71706.613			
23	2	21	22	3	20	81973.114	81974.524	81974.526	-0.002
						81973.490			
						81975.550			
						81975.943			
24	2	22	23	3	21	92407.276	92408.703	92408.705	-0.002
						92407.691			
						92409.705			
						92410.141			
25	2	23	24	3	22	102998.435	102999.828	102999.814	0.014
						102998.776			
						103000.849			
						103001.251			
(e) $(J+1)_{3\ J-2} \leftarrow J_{4\ J-3}$									
26	3	23	25	4	22	47419.843	47421.609	47421.596	0.013
						47420.295			
						47422.928			
						47423.369			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
27	3	24	26	4	23	56601.309	56603.066	56603.049	0.017
						56601.766			
						56604.362			
						56604.827			
28	3	25	27	4	24	65945.742	65947.471	65947.480	-0.009
						65946.172			
						65948.759			
						65949.209			
29	3	26	28	4	25	75465.481	75467.221	75467.219	0.002
						75465.927			
						75468.512			
						75468.962			
30	3	27	29	4	26	85171.613	85173.342	85173.352	-0.010
						85172.054			
						85174.629			
						85175.071			
31	3	28	30	4	27	95073.555	95075.287	95075.311	-0.024
						95073.982			
						95076.581			
						95077.031			
32	3	29	31	4	28	105178.779	105180.513	105180.519	-0.006
						105179.233			
						105181.802			
						105182.238			
(f) $(J+1)_{4\ J-3} \leftarrow J_{5\ J-4}$									
35	4	31	34	5	30	72014.287	72016.208	72016.219	-0.011
						72014.879			
						72017.601			
						72018.066			
36	4	32	35	5	31	80953.050	80954.830	80954.823	0.007
						80953.504			
						80956.143			
						80956.623			
37	4	33	36	5	32	90009.917	90011.705	90011.707	-0.002
						90010.384			
						90013.027			
						90013.490			

Table 1. Continued

J'	Ka'	Kc'	J''	Ka''	Kc''	obs.	average	calc.*	ave.-calc
38	4	34	37	5	33	99197.885	99199.656	99199.648	0.008
						99198.340			
						99200.972			
						99201.428			
39	4	35	38	5	34	108530.180	108531.940	108531.936	0.004
						108530.636			
						108533.247			
						108533.696			

* Frequencies were calculated with the molecular parameters in Table 2.

The determined rotational constants are listed in Table 2. *A*, *B*, *C* and D_J were refined and D_{JK}, D_K, d_J and d_K were determined for the first time.

Table 2. Molecular parameters of Ethylmethyl Ether

Parameter	Value(MHz)	
A-(B+C)/2	23966.5365(83)	
(B+C)/2	4025.2902(12)	
(B-C)/2	134.15358(12)	
D_J	0.9734(12)	$\times 10^{-3}$
D_{JK}	-0.2476(18)	$\times 10^{-2}$
D_K	0.7514(70)	$\times 10^{-1}$
d_J	0.87151(81)	$\times 10^{-4}$
d_K	-0.934(27)	$\times 10^{-3}$

. . 0.024 MHz

* The numbers in parentheses are 1σ uncertainties in units of the last quoted digits.

Conclusions

The potential barrier heights for the CH_3 torsions are relatively high, and the torsional splittings are small in the ground state. The average frequencies of these split components were determined as transition frequencies. These frequencies were fitted to the asymmetric rotor Hamiltonian with 8 molecular parameters with a 1σ standard deviation of 24 kHz.

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