The Rotational Spectrum of (^{17}O)Ketene

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The rotational spectrum of $H_2CC^{17}O$ in the ground vibrational state has been investigated between 20 and 330 GHz. From 82 *R*-branch transitions a set of rotational constants and several centrifugal distortion constants could be derived, employing the Watson *S*-reduction formalism. The obtained rotational constants in MHz are: A = 282071.6(223), B = 10013.4764(28), C = 9655.9118(24). The nuclear quadrupole coupling structure of the $J'_{Ka'Kc'} \leftarrow J_{KaKc} = 1_{01} \leftarrow 0_{00}$ line has been recorded by means of molecular beam Fourier transform microwave spectroscopy allowing the determination of the nuclear quadrupole constant $\chi_{aa} = -1.534(54)$ MHz (without considering the spin-rotation interaction). A recalculation of the r_s-structure has also been carried out, using the constants of the new isotopomer. The result agrees with the values reported by East et al. in 1995. This is, to our knowledge, the first reported investigation of the $H_2CC^{17}O$ rotational spectrum.

Key words: Rotational Spectra; Structure; Ketene; Isotopomer.

Introduction

The microwave and millimeter-wave spectra of ketene and its isotopomers have been the subject of a large number of studies since the beginning of microwave spectroscopy.

Several reviews have appeared, summarizing much of the work (see, e. g., [1]), but new measurements continue to be made. The spectrum, particularly that of the normal isotopomer in the ground and first excited vibrational states, has been subject of increasingly refined analyses in order to understand the different interactions which connect the states up to 1000 cm^{-1} [2 - 5]. Spectra of isotopomers with D, ^{13}C and ^{18}O have been investigated in [6, 7].

A knowledge of the rotational spectrum of the various isotopomers of ketene could not only be of interest for refined structural analyses, but also because ketene has been found to be present in several interstellar clouds [8 - 19]. Molecules containing Oxygen-17 and Oxygen-18, as for instance CO, have been detected in interstellar clouds, allowing the determination of the ^{18}O/^{17}O ratio which can give important information about star life and development [20 - 25].

Nothing is known until now, to our knowledge, about the ketene isotopomer with ^{17}O, and therefore this paper reports an investigation of the spectrum of $H_2CC^{17}O$, considering also a determination of the nuclear quadrupole coupling constant related to this nucleus.

Experimental

Ketene has been obtained by vacuum pyrolysis of acetic anhydride, $(CH_3CO)_2O$, at 800 °C. The by-product of the pyrolysis, acetic acid, was held back in a cold trap at –80 °C, and the ketene was collected in a second cold trap held at liquid nitrogen temperature.

The spectra of the ^{17}O isotopomer have been recorded in natural concentration with a millimeter / submillimeter-wave (MMW / SubMMW) spectrometer [5] at high frequencies and with a molecular beam Fourier transform microwave (MBFTMW) spectrometer [26] at low frequencies. The MMW / SubMMW spectrometer is of the type operating in source modulation mode and second derivative presentation of the absorption lines. The sources in the range 40 - 550 GHz were phase-locked against a frequency synthesizer (PTS 500) which was controlled by a 10 MHz frequency standard provided by a GPS receiver. The free-space absorption cell consisted of a 10 cm diameter glass tube, 2.40 m in length, capped

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Table 1. Constants of $H_2C_2{}^{17}O$ determined for different maximum values of the K_a quantum number using the Watson S-reduced formalism . The fit with $K_a \leq 7$ is considered to be the "best" one (see text).

Parameter	Fit with 62 lines up to K_a = 5	Fit with 72 lines up to K_a = 6	**Fit with 82 lines up to K_a = 7**	Fit with 92 lines up to K_a = 8	Fit with 102 lines up to K_a = 9	Unit
A	282113(31)	282111(24)	**282072(22)**	282369(125)	280097(1084)	MHz
B	10013.4750(27)	10013.4752(27)	**10013.4764(28)**	10013.4555(166)	10013.6381(1516)	MHz
C	9655.9111(23)	9655.9112(23)	**9655.9118(24)**	9655.9049(144)	9655.9533(1330)	MHz
D_J	3.1050(24)	3.1053(22)	**3.1056(22)**	3.0868(124)	3.2476(1097)	kHz
D_{JK}	455.11(32)	455.20(20)	**455.69(14)**	450.72(60)	482.81(416)	kHz
D_K	22.84*	22.84*	**22.84***	22.84*	22.84*	MHz
d_1	−135.8(26)	−135.8(26)	**−136.1(28)**	−128.2(166)	−203.9(1530)	Hz
d_2	−49.81(110)	−49.86(98)	**−50.97(97)**	−42.82(575)	−104.16(5218)	Hz
H_J	−2.04*	−2.04*	**−2.04***	−2.04*	−2.04*	mHz
H_{JK}	1.87(61)	2.05(40)	**2.36(29)**	−4.01(129)	37.25(894)	Hz
H_{KJ}	−546.3(234)	−540.4(91)	**−509.4(45)**	−711.7(145)	318.8(782)	Hz
H_K	5.23*	5.23*	**5.23***	5.23*	5.23*	KHz
L_{JJKK}	−38.1(244)	−29.7(115)	**−18.2(62)**	−184.4(211)	654.1(1171)	mHz
L_{JKKK}	2.831(551)	2.893(142)	**3.376(50)**	1.498(121)	9.052(508)	Hz
σ_{Fit}	26.5	27.3	**28.6**	173.2	1596.7	kHz

* Not determinable. Value fixed to that of the main isotopomer H_2CCO as given in [27].

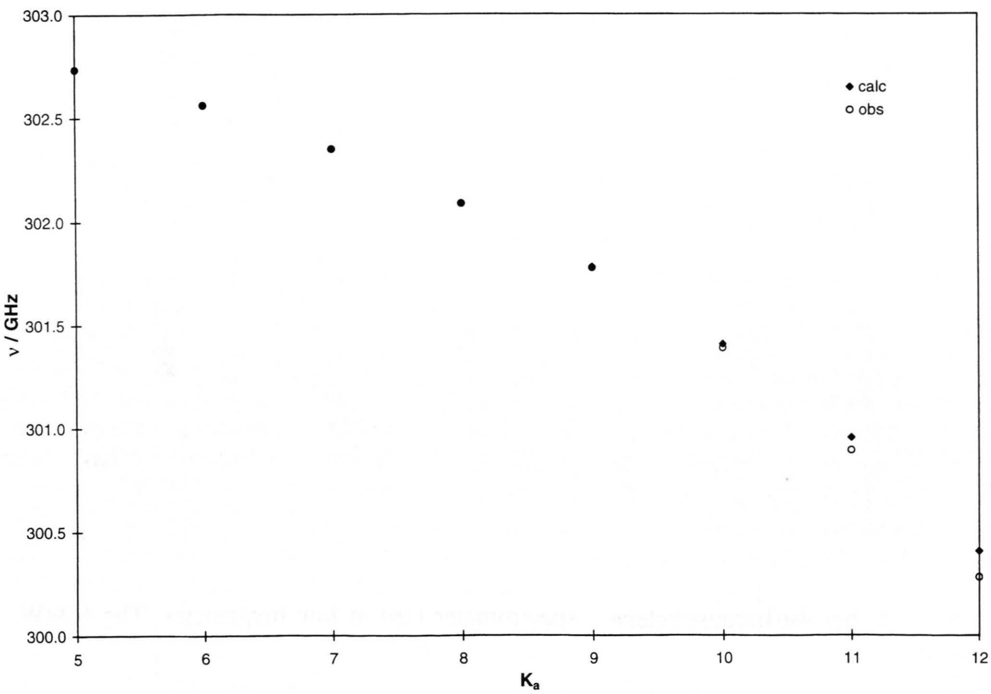

Fig. 1. Plot of line frequencies belonging to different K_a values of the rotational transition $J' \leftarrow J$ = 15 ← 14 (normal isotopomer). The calculated values have been obtained with the parameters resulting from the line fit, considering K_a values up to 7, which gives an acceptable value of the standard deviation. Observed values show in fact already a displacement with respect to the calculated ones for $K_a \geq 8$. This displacement is in this figure only seen for $K_a \geq 10$ because of the unfavorable coordinate scale (See text).

at the ends with Teflon windows and provided externally with teflon collimating lenses. Low-noise detection was achieved by a liquid helium cooled InSb bolometer ("Putley-detector").

Table 2a. Observed and calculated transition frequencies of (^{17}O)ketene.

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}/GHz	ν_{calc}/GHz	o-c/kHz
1	0	1	0	0	0	19.669374	19.669377	–3
4	0	4	3	0	3	78.673261	78.673234	24
4	1	3	3	1	2	79.387501	79.387498	3
4	1	4	3	1	3	77.957323	77.957311	12
5	0	5	4	0	4	98.338318	98.338342	–24
5	1	4	4	1	3	99.233120	99.233126	–6
5	1	5	4	1	4	97.445407	97.445443	–39
5	2	3	4	2	2	98.333311	98.333320	–9
5	2	4	4	2	3	98.326320	98.326323	–3
5	3	2	4	3	1	98.305149	98.305164	–15
5	3	3	4	3	2	98.305149	98.305161	–12
12	0	12	11	0	11	235.910502	235.910499	3
12	1	12	11	1	11	233.831345	233.831354	–6
12	2	11	11	2	10	235.951825	235.951789	36
12	4	8	11	4	7	235.840527	235.840494	36
12	4	9	11	4	8	235.840527	235.840494	36
12	5	7	11	5	6	235.734248	235.734281	–33
12	5	8	11	5	7	235.734248	235.734281	–33
12	6	6	11	6	5	235.602231	235.602201	30
12	6	7	11	6	6	235.602231	235.602201	30
12	7	5	11	7	4	235.440334	235.440334	0
12	7	6	11	7	5	235.440334	235.440334	0
12	8	4	11	8	3	235.244911	235.243817	1091*
12	8	5	11	8	4	235.244911	235.243817	1091*
12	9	3	11	9	2	235.003003	235.006193	–3190*
12	9	4	11	9	3	235.003003	235.006193	–3190*
13	0	13	12	0	12	255.546629	255.546629	3
13	1	12	12	1	11	257.954049	257.954070	–21
13	1	13	12	1	12	253.308777	253.308756	21
13	2	11	12	2	10	255.734515	255.734527	–9
13	2	12	12	2	11	255.607298	255.607295	3
13	3	10	12	3	9	255.584283	255.584364	–81
13	3	11	12	3	10	255.583821	255.583731	90
13	4	9	12	4	8	255.491161	255.491152	9
13	4	10	12	4	9	255.491161	255.491152	9
13	5	8	12	5	7	255.375639	255.375648	–9
13	5	9	12	5	8	255.375639	255.375648	–9
13	6	7	12	6	6	255.232377	255.232362	15
13	6	8	12	6	6	255.232377	255.232362	15
13	7	6	12	7	5	255.056939	255.056927	12
13	7	7	12	7	6	255.056939	255.056927	12
13	8	5	12	8	4	254.845705	254.844023	1682*
13	8	6	12	8	5	254.845705	254.844023	1682*
13	9	4	12	9	3	254.580212	254.586642	–6431*
13	9	5	12	9	4	254.580212	254.586642	–6431*
14	0	14	13	0	13	275.177219	275.177234	–15
14	1	13	13	1	12	277.786121	277.786124	0

The accuracy of the frequency measurements carried out at room temperature and at a pressure of 1 to 3 Pa is supposed to be, in this particular case, ±25 kHz.

The MBFTMW measurements were performed at the frequency of the $J'_{K_{a'}K_{c'}} \leftarrow J_{K_aK_c} = 1_{01} \leftarrow 0_{00}$ line at 19.6 GHz with the setup described in [26].

Table 2a (continued).

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}/GHz	ν_{calc}/GHz	o-c/kHz
14	1	14	13	1	13	272.784119	272.784128	–9
14	2	12	13	2	11	275.420090	275.420081	9
14	2	13	13	2	12	275.261089	275.261086	0
14	3	11	13	3	10	275.242975	275.242924	48
14	3	12	13	3	11	275.241986	275.242004	–18
14	4	10	13	4	9	275.141157	275.141160	–3
14	4	11	13	4	10	275.141157	275.141157	0
14	5	9	13	5	8	275.016242	275.016257	–15
14	5	10	13	5	9	275.016242	275.016257	–15
14	6	8	13	6	7	274.861696	274.861717	–21
14	6	9	13	6	8	274.861696	274.861717	–21
14	7	7	13	7	6	274.672671	274.672692	–21
14	7	8	13	7	7	274.672671	274.672692	–21
14	8	6	13	8	5	274.445713	274.443402	2311*
14	8	7	13	8	6	274.445713	274.443402	2311*
14	9	5	13	9	4	274.155895	274.166277	–10382*
14	9	6	13	9	5	274.155895	274.166277	–10382*
15	0	15	14	0	14	294.801897	294.801900	–3
15	1	14	14	1	13	297.615794	297.615806	–12
15	2	13	14	2	12	295.108660	295.108648	12
15	2	14	14	2	13	294.913036	294.913033	3
15	3	12	14	3	11	294.901170	294.901113	54
15	3	13	14	3	12	294.899821	294.899806	12
15	4	11	14	4	10	294.790466	294.790466	0
15	4	12	14	4	11	294.790466	294.790463	3
15	5	10	14	5	9	294.656006	294.656051	–45
15	5	11	14	5	10	294.656006	294.656051	–45
15	6	9	14	6	8	294.490188	294.490206	–15
15	6	10	14	6	9	294.490188	294.490206	–15
15	7	8	14	7	7	294.287576	294.287567	6
15	7	9	14	7	8	294.287576	294.287567	6
15	8	7	14	8	6	294.045020	294.041890	3130*
15	8	8	14	8	7	294.045020	294.041890	3130*
15	9	6	14	9	5	293.729950	293.745033	–15080*
15	9	7	14	9	6	293.729950	293.745033	–15080*
16	0	16	15	0	15	314.420252	314.420216	36
16	1	15	15	1	14	317.442931	317.442943	–12
16	1	16	15	1	15	311.728140	311.728179	–39
16	2	14	15	2	13	314.800425	314.800434	–9
16	2	15	15	2	14	314.562984	314.563002	–18
16	3	13	15	3	12	314.558954	314.558909	45
16	3	14	15	3	13	314.557072	314.557102	–30
16	4	12	15	4	11	314.438995	314.439019	–24
16	4	13	15	4	12	314.438995	314.439013	–18
16	5	11	15	5	10	314.294966	314.294969	–3
16	5	12	15	5	11	314.294966	314.294969	–3
16	6	10	15	6	9	314.117828	314.117762	66
16	6	11	15	6	10	314.117828	314.117762	66
16	7	9	15	7	8	313.901480	313.901492	–12
16	7	10	15	7	9	313.901480	313.901492	–12
16	8	8	15	8	7	313.643364	313.639422	3942*
16	8	9	15	8	8	313.643364	313.639422	3942*
16	9	7	15	9	6	313.302230	313.322844	–20614*
16	9	8	15	9	7	313.302230	313.322844	–20614*
17	1	17	16	1	16	331.196563	331.196560	3

* Not included in the fit because of the K_a value larger than 7 (see text).

Table 2b. Correlation matrix of the fit.

	A	B	C	D_J	D_{JK}	d_1	d_2	H_{JK}	H_{KJ}	L_{JJKK}	L_{JKKK}
A	100	−9.9	2.5	9.6	−24.2	8.6	59.3	10.3	−40.8	9	−49.9
B	−9.9	100	−74.9	49.8	35.1	−91.9	−4.3	32.4	23.5	25.5	9.4
C	2.5	−74.9	100	15.3	11.9	88.1	2	11.8	7.9	9.9	2.5
D_J	9.6	49.8	15.3	100	55.7	−23.6	8.6	68.7	25.8	55	−6.2
D_{JK}	−24.2	35.1	11.9	55.7	100	−15	−13.7	83.3	87.5	80.4	47.1
d_1	8.6	−91.9	88.1	−23.6	−15	100	4	−14.4	−9.5	−11	−3.4
d_2	59.3	−4.3	2	8.6	−13.7	4	100	7.1	−24.5	5.9	−30.3
H_{JK}	10.3	32.4	11.8	68.7	83.3	−14.4	7.1	100	50.1	96	−5
H_{KJ}	−40.8	23.5	7.9	25.8	87.5	−9.5	−24.5	50.1	100	53.2	81.5
L_{JJKK}	9	25.5	9.9	55	80.4	−11	5.9	96	53.2	100	−4.1
L_{JKKK}	−49.9	9.4	2.5	−6.2	47.1	−3.4	−30.3	−5	81.5	−4.1	100

A pyrex vessel, containing the pyrolysis products, was filled with argon up to atmospheric pressure at room temperature and connected directly to the valve for the beam generation. The accuracy for this type of measurements is estimated to be ±2 kHz.

Results

The rotational spectrum of $H_2C_2{}^{17}O$ was predicted from structural calculations based on the rotational constants of H_2C_2O [27] and its ^{13}C, ^{18}O and HD isotopic species [6, 7]. Firstly, we could assign the K_a = 3 doublets at high frequencies, followed by additional lines with K_a = odd which are, because of the spin statistics, three times stronger than the lines with K_a = even. Through successive fits it was possible to assign all lines up to K_a = 7, which revealed no relevant deviation from the predicted absorption frequencies: The lines have always been found within an interval of a few 100 kHz with respect to the calculated ones, as far as the value of K_a was limited to $K_a \leq 7$. For higher K_a values the well-known effect of interactions with the lowest vibrational excited states through the centrifugal distortion [28] got more and more evident.

We have performed different fits, changing the maximum value of the K_a quantum number from 5 up to 9. As can be seen from Table 1, the standard error of the fit does not change very much up to a maximum K_a value of 7, but it increases significantly when lines with K_a = 8 and 9 are included in the fit. In Fig. 1 we report a plot of the frequencies for given values of K_a of the transition line $J' \leftarrow J$, 15 ← 14, comparing the experimental absorption frequencies with the calculated ones (the latter obtained using the parameters of the fit up to K_a = 7). The data used for the best fit (with K_a limited to a value of 7) are given in Table 2.

The fit of the measured frequencies has been made using Watson's S-reduced Hamiltonian in the I^r axis representation, because the molecule is a prolate top with asymmetry parameter $\kappa = -0.9974$. As was to be expected, the value obtained for the constant A (Table 3) is almost identical with the value obtained for the main isotopomer and the two ^{13}C species, though in the present case the error of the fit seems to be too optimistic. The values of the constants B and C are in the range limited by the values of the normal and the ^{18}O isotopomer [7]. The D_K, H_J, and H_K centrifugal distortion constants were fixed to the values obtained for the normal isotopomer [27]. The addition of the two octic constants L_{JJKK} and L_{JKKK} to the pool of determinable centrifugal distortion constants led to a better result of the fit (in comparison with that obtained by limiting the constants to sextic order).

The quadrupole hyperfine structure of the $1_{01} \leftarrow 0_{00}$ transition due to the nuclear spin I = 5/2 of ^{17}O was observed experimentally by means of a MBFTMW spectrometer at the frequency predicted by the high frequency lines fit. Unfortunately, only the quadrupole constant χ_{aa} could be determined by the three possible hyperfine components (Table 5) – due to the lack of experimental possibilities we could not investigate frequencies higher than 26 GHz.

Structure Determination

We have used the acquisition of the additional set of rotational constants as an opportunity to carry out a new calculation to confirm the molecular structure of ketene. We have chosen to limit the calculations to the r_0 and r_s structure; the results are presented in Table 4, where they are compared to the r_e equilibrium structure from [1].

Table 3. Rotational constants, principal moments of inertia, and inertial defects of the investigated isotopomers.

	H_2CCO^a	$H_2CC^{17}O^b$	$H_2CC^{18}O^c$	$H_2{}^{13}CCO^c$	$H_2C^{13}CO^c$	$DHCCO^d$	D_2CCO^d
$A^{(S)}$	282101.185(409)	282072(22)	287350(910)	282112(334)	282334(521)	194305(38)	141537(12)
$B^{(S)}$	10293.32117(80)	10013.476(3)	9761.2368(33)	9960.9659(79)	10293.6209(58)	9647.0664(13)	9120.8296(14)
$C^{(S)}$	9915.90548(82)	9655.9118(24)	9421.1236(33)	9607.1276(84)	9916.2046(57)	9174.6457(13)	8552.7008(16)
I_a	1.7914813(27)	1.79167(14)	1.7588(55)	1.7914(21)	1.7900(33)	2.60096(51)	3.57065(30)
I_b	49.0977597(43)	50.469888(15)	51.774075(17)	50.735944(40)	49.096330(28)	52.386807(7)	55.409325(8)
I_c	50.9665013(42)	52.338818(14)	53.643178(17)	52.604590(43)	50.964964(28)	55.084308(8)	59.089991(11)
Δ	0.077260	0.077263	0.110346	0.077233	0.078630	0.096543	0.110016

The coefficient 505379 MHz·amu·Å^2 has been used for the conversion. $\kappa = -0.9974$. [a] [27]; [b] this work; [c] [7]; [d] [6]. Data refitted to S-reduced Hamiltonian [7].

Table 4a. Structure data for ketene from the sets of rotational constants given in Table 3.

Distance, Angle	r_0 [a]	r_0 [b]	r_s-Fit[c]	r_s [d]	r_e [e]	Unit
CO	116.3(38)	[116.1]	116.15(131)	116.19(4)	116.030(29)	pm
CC	131.5(40)	131.66(12)	131.42(259)	131.38(4)	131.212(30)	pm
CH	107.6(7)	107.62(25)	107.93(64)	107.954(104)	107.576(7)	pm
HCH	122.27(71)	[122.1]	122.11(121)	122.127(62)	121.781(12)	°

[a] *MWSTRGEOM* program [35, 36] written by V. Typke was used. Correlation matrix a) (see below). [b] Because of the high correlation coefficients CO/CC and CH/HCH, CO and HCH were fixed to the values of the r_s-fit. Correlation Matrix b) (see below). [c] r_s-fit program *RSSTR* written by V. Typke [30, 31, 33] was used. Center of mass condition has been used, and out-of-plane coordinates have been fixed to zero. Correlation Matrix c) (see below). [d] Kraitchman's [32] substitution structure. Program *RU233* by H. D. Rudolph [29] was used. Because of the imaginary value of the carbonyl-C-coordinate, the first moment conditions have been used which lead to a real value of x_C = 2.09(4) pm. For the distance C-O the newly determined data of the ^{17}O isotopomer were used. Errors given in parentheses reflect the uncertainty of constants. [e] Equilibrium structure (I; 1s-ABC) [1].

Correlation Matrix a)					Correlation Matrix b)			Correlation Matrix c)				
	C-O	C-C	C-H	HCH		C-C	C-H		C-O	C-C	C-H	HCH
C-O	1				C-C	1		C-O	1			
C-C	−1	1			C-H	−0.071	1	C-C	−0.968	1		
C-H	0.928	−0.938	1					C-H	−0.014	0.000	1	
HCH	0.928	−0.938	1	1				HCH	0.009	0.000	−0.643	1

a) r_s-Structure

For the determination of the r_s structure we made use of two programs: *RU233* written by Rudolph [29] and *RSSTR* (r_s-fit) written by Typke [30, 31].

The program *RU233* is a traditional one based on Kraitchman's equations [32], which uses the tensor of the planar inertial moments of an isotopomer expressed as function of the principal planar moments of the parent molecule and the cartesian coordinates of the atom substituted into this isotopomer. These equations must be separately applied to the parent molecule and to monosubstituted isotopomers to obtain a substitution structure which can be complete or partial, depending on the number of investigated isotopomers. *RU233* provides the possibility to use additional substituted isotopomers which are considered as daughters of the monosubstituted ones, so that, starting from a parent molecule, one obtains the sequence mother – daughter – grand daughter. The advantage of this method is an improved determination of small coordinates (but larger than 12 pm) [33] for atoms near to the center of mass or a principal axis of the molecule.

Table 4b. Substitution coordinates for ketene. Values given in pm.

Atom	a	b
O	118.2805(31)	0
C (carbonyl)	2.09(4)	0
C (methylene)	129.2938(419)	0
H	181.6181(75)	94.4260(144)

In the r_s-fit program *RSSTR*, on the other hand, Typke has shown how the system of separate equa-

Table 5. Hyperfine structure of the $J'_{K_a' K_c'} \leftarrow J_{K_a K_c} = 1_{01} \leftarrow 0_{00}$ transition of (^{17}O)ketene, calculated according to the method described by Bragg and Golden [37]. Spin-rotation interactions could not be considered due to lack of additional information. – Value of the quadrupole coupling constant: $\chi_{aa} = -1.534(54)$ MHz.

J'	K_a'	K_c'	J	K_a	K_c	F'	F	ν_{exp} / MHz	ν_{calc} / MHz	e-c / kHz
1	0	1	0	0	0	3/2	5/2	19669.595	19669.586	8.2
1	0	1	0	0	0	5/2	5/2	19669.131	19669.118	12.5
1	0	1	0	0	0	7/2	5/2	19669.439	19669.446	7.0

tions, like that obtained by application of Kraichman's method to a data set of different isotopomers, can be linearized and arranged into a least squares system to obtain an r_s structure from an iterative fit to the planar moments for a sufficiently large data set of substituted isotopomers. When the number of equations equals the number of coordinates to be determined, the resulting structure is identical with the result from Kraitchman's separate equations of monosubstituted isotopomers.

The program *RSSTR* provides the possibility of introducing the first and second moment conditions as constraints into the least squares formalism for a better determination of very small coordinates. In the case of a bad convergence of the r_s-fit – always when the Kraichman's equations would give an *imaginary* coordinate if the substituted atom is on a plane of symmetry – it is possible to avoid the complication by fixing to zero the out of plane coordinate of the substituted atom known to lie on a symmetry plane of the molecule. Both possibilities have been used in the case of ketene because of the planarity of the molecule and the position of the carbon atom of the C=O group which is very near to the center of mass of the molecule and therefore difficult to determine (even with an "oversized" data set).

The results of the application of these two programs are shown in Table 4a (Columns 3, 4) and in Table 4b for the coordinates of the pure substitution method.

b) r_0-Structure

For this type of structure [33, 34] we used the *MWSTRGEOM* program (version 2.3) written by Typke [35, 36]. It performs a non linear weighted fit of bond lengths, bond angles, and dihedral angles to measured rotational constants. Using the rotational constants listed in Table 3, structural parameters have been obtained with only indicative character because of the high correlation coefficients which connect some of the fitted parameters with each other (Column 1, Table 4a). Constraining two parameters, as it is shown in Table 4a (Column 2), to values obtained through the r_s-fit method, one gets values for the other two parameters which differ only slightly from those of the r_s-fit structure.

The oversized substitution data set considered here seems indeed not to be sufficient for the determination of a reasonable r_0 or r_s structure without being forced to use the first moment conditions which are, strictly speaking, valid only for the equilibrium structure. Rotational constants of more multisubstituted isotopomers seem to be necessary to give a reliable structure of this molecule based on experimental data.

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