Millimeter Wave Spectrum and Centrifugal Distortion Analysis of Difluorochloromethane CHF_2Cl in the Ground State

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Z. Naturforsch. **45a**, 1165–1168 (1990); received July 2, 1990

The rotational spectra of $\text{CHF}_2^{35}\text{Cl}$ and $\text{CHF}_2^{37}\text{Cl}$ (CFC22) in the vibrational ground state between 42 and 214 GHz are reported. A centrifugal distortion analysis up to the sixth order is carried out.

1. Introduction

The need of getting precise rotational parameters of CFC22 has been stated sufficiently [1, 2]. Cramb et al. [1] give a survey over the previous microwave researches on CFC22. Until now the rotational constants, the quartic centrifugal distortion constants of both isotopomers [1, 2] and two of a set of seven sextic centrifugal distortion constants of the ^{35}Cl -isotopomere [3] are known. To yield the missing constants of sixth order for both isotopomers, rotational transitions up to $J=35$ with frequencies up to 213 GHz were measured. The central frequency of each quadrupole line pattern was calculated using the chlorine nuclear quadrupole coupling constants of [1].

2. Experimental

Commercially available CFC22 from J.T. Baker, PF 1661, D-6080 Groß-Gerau, was used without further purification. The spectrometer we used is described in detail in [4]. The radiation of a PLL-stabilized and phasemodulated klystron is frequency-multiplied by a point-contact harmonic generator and fed to a free-space-cell, filled with the gas under a pressure of about 1–2 Pa at a temperature between +25 and –50 °C. The microwave source is swept by a personal computer (PC) via a special interface. The absorption signal is detected by a Schottky-barrier-diode or a helium cooled InSb-bolometer. After amplification by a PAR-preamplifier and a lock-in-amplifier the signal is transferred to the PC by an A/D-converter. Data handling and recording follows

in real time, the recorded spectrum is displayed simultaneously during the averaging.

Taking into account the width of the frequency steps, multiplied by the harmonic numbers of the two phase locked loops and the klystron, the spectrometer limits the resolution of a line centre to about 6 kHz.

3. Theoretical

We used the rotational and centrifugal distortion constants of [1] to predict the spectrum in the investigated range, beginning at 42 GHz. With the program HT1NQ (Author Herberich) [5] we calculated the splitting, caused by the chlorine nuclear quadrupole coupling and obtained the unperturbed frequencies. The transition frequencies were fitted together with the microwave results of [1] to Watson's S-reduced effective Hamiltonian in the I-r representation including quartic and sextic terms [6]:

$$\begin{aligned} H = & AJ_Z^2 + BJ_X^2 + CJ_Y^2 - D_J J^4 - D_{JK} J^2 J_Z^2 - D_K J_Z^4 \\ & + d_1 J^2 (J_+^2 + J_-^2) + d_2 (J_+^4 + J_-^4) + H_J J^6 \\ & + H_{JK} J^4 J_Z^2 + H_{KJ} J^2 J_Z^4 + H_K J_Z^6 + h_1 J^4 (J_+^2 + J_-^2) \\ & + h_2 J^2 (J_+^4 + J_-^4) + h_3 (J_+^6 + J_-^6), \end{aligned} \quad (1)$$

where

$$J^2 = J_X^2 + J_Y^2 + J_Z^2, \quad J_+ = J_X + iJ_Y, \quad J_- = J_X - iJ_Y.$$

For the fitting we used the program ZFAP6 (Author: Typke) [7].

4. Results and Discussion

CFC22 is an asymmetric top molecule with an asymmetry parameter of nearly –0.6. The millimeter-wave spectrum shows pretty strong lines in agreement with the presence of a dipole moment component

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Table 1. Rotational transition frequencies of $\text{CHF}_2^{35}\text{Cl}$. Frequencies in GHz, differences in kHz. Lines labeled with * have been measured in [1].

N	J	K _P	K _O	J'	K' _P	K' _O	ν_{calc}	ν_{obs}	$\nu_{\text{calc-obs}}$	N	J	K _P	K _O	J'	K' _P	K' _O	ν_{calc}	ν_{obs}	$\nu_{\text{calc-obs}}$
1*	1	1	0	0	0	0	15.095929	15.095983	-54	62	8	8	1	7	7	1	157.722150	157.722140	10
2*	2	1	1	1	0	1	24.818345	24.818354	-09	63	11	6	6	10	5	6	158.778129	158.778113	16
3*	3	3	0	3	2	2	30.405627	30.405675	-48	64	12	5	8	11	4	8	156.709622	156.709587	35
4*	3	3	1	3	2	1	29.294788	29.294778	10	65	13	5	8	12	4	8	157.019613	157.019499	114
5*	3	1	2	2	0	2	35.288185	35.288224	-39	66	23	14	10	23	13	10	160.043635	160.043648	-13
6*	4	3	2	4	2	2	27.906059	27.906008	51	67	28	14	15	28	13	15	157.030094	157.030077	17
7*	4	2	2	4	1	4	28.300967	28.300928	39	68	29	14	16	29	13	16	156.166077	156.166193	-116
8*	5	3	3	5	2	3	25.629541	25.629461	80	69	19	16	4	19	15	4	185.807435	185.807495	-60
9*	5	1	4	4	2	2	29.058776	29.058735	41	70	20	16	5	20	15	5	185.634080	185.634092	-12
10*	6	2	4	5	3	2	27.716955	27.716971	-16	71	21	16	6	21	15	6	185.433750	185.433741	9
11*	6	1	5	5	2	3	36.234634	36.234590	44	72	22	16	7	22	15	7	185.203578	185.203519	59
12*	7	2	5	6	3	3	38.633591	38.633603	-12	73	19	16	4	19	15	4	185.807435	185.807495	-60
13*	7	1	6	6	2	4	41.455947	41.455901	46	74	10	9	1	9	8	1	186.620281	186.620327	-46
14*	8	4	5	8	3	5	35.210170	35.210198	-28	75	10	9	2	9	8	2	186.620281	186.620327	-46
15*	8	2	7	7	3	5	28.324143	28.324068	75	76	15	6	9	14	5	9	186.825106	186.825088	18
16*	8	3	5	7	4	3	32.758028	32.757984	44	77	16	4	12	15	3	12	187.139802	187.139796	6
17*	9	4	6	9	3	6	31.198210	31.198256	-46	78	15	5	11	14	4	11	187.240815	187.240846	-31
18*	9	3	6	8	4	4	44.823205	44.823177	28	79	15	4	12	14	3	12	187.278373	187.278311	62
19*	10	3	7	9	4	5	56.845085	56.845069	16	80	13	7	7	12	6	7	187.531402	187.531427	-25
20*	10	4	7	9	5	5	32.346384	32.346369	15	81	23	16	8	23	15	8	184.940486	184.940443	43
21*	11	5	7	10	6	5	29.470228	29.470283	-55	82	24	16	9	24	15	9	184.641162	184.641048	114
22*	12	5	8	11	6	6	38.685291	38.685320	-29	83	25	16	10	25	15	10	184.302033	184.301902	131
23*	13	6	8	12	7	6	35.087658	35.087663	-05	84	14	6	9	13	5	9	184.299664	184.299681	-17
24*	14	5	10	14	4	10	28.334865	28.334881	-16	85	27	16	12	27	15	12	183.488558	183.488622	-64
25*	15	7	9	14	8	7	40.573084	40.573111	-27	86	28	16	13	28	15	13	183.005432	183.005320	112
26*	15	8	8	14	9	6	27.225015	27.225015	-55	87	11	8	4	10	7	4	183.001184	183.001216	-32
27*	18	6	13	18	5	13	28.625564	28.625576	-12	88	11	8	3	10	7	3	183.000670	183.000777	-107
28*	19	7	13	19	6	13	52.283354	52.283420	-66	89	30	16	15	30	15	15	181.861208	181.861116	92
29*	20	7	14	20	6	14	44.326081	44.326082	-01	90	16	5	11	15	4	11	181.502209	181.502230	-21
30*	20	12	9	19	13	7	21.171529	21.171526	03	91	14	6	8	13	5	8	180.533678	180.533702	-24
31*	21	12	9	20	13	7	30.242704	30.242668	36	92	12	7	6	11	6	6	179.234294	179.234318	-24
32*	22	7	16	22	6	16	27.667389	27.667375	14	93	12	7	5	11	6	5	179.174479	179.174499	-20
33*	23	8	16	23	7	16	53.184317	53.184274	43	94	9	9	0	8	8	0	178.182708	178.182696	12
34*	24	8	17	24	7	17	43.892915	43.892894	21	95	9	9	1	8	8	1	178.182708	178.182696	12
35*	25	15	10	24	16	8	28.037950	28.037855	95	96	14	5	10	13	4	10	176.492599	176.492618	-19
36*	25	8	18	25	7	18	34.549053	34.549035	18	97	14	2	12	13	1	12	176.488955	176.488913	42
37*	26	8	19	26	7	19	25.797448	25.797495	-47	98	16	1	15	15	0	15	206.360613	206.360597	16
38*	27	17	11	26	18	9	20.616274	20.616326	-52	99	18	6	12	17	5	12	206.446853	206.446933	-80
39*	28	17	12	27	18	10	29.608916	29.608865	51	100	30	18	13	30	17	13	207.356881	207.356919	-38
40*	30	19	12	29	20	10	22.202188	22.202228	-40	101	29	18	12	29	17	12	207.767966	207.767996	-30
41	3	3	0	2	2	0	55.286354	55.286324	30	102	21	18	4	21	17	4	209.826597	209.826532	65
42	3	2	1	2	1	1	42.313109	42.313096	13	103	20	18	3	20	17	3	209.968208	209.968233	-25
43	3	2	2	2	1	2	45.287402	45.287394	08	104	35	18	18	35	17	18	204.557149	204.557129	20
44	3	3	1	2	2	1	55.487658	55.487610	48	105	34	18	17	34	17	17	205.230446	205.230444	02
45	4	1	3	3	0	3	46.698445	46.698453	-08	106	32	18	15	32	17	15	206.397996	206.397934	62
46	4	2	2	3	1	2	50.581395	50.581393	02	107	31	18	14	31	17	14	206.901461	206.901573	-112
47	4	2	3	3	1	3	55.640824	55.640818	06	108	28	18	11	28	17	11	208.138149	208.138221	-72
48	7	5	3	7	4	3	53.262133	53.262110	23	109	27	18	10	27	17	10	208.470616	208.470664	-48
49	8	5	4	8	4	4	52.419210	52.419199	11	110	26	18	9	26	17	9	208.768332	208.768337	-05
50	14	6	9	14	5	9	54.871925	54.871920	05	111	25	18	8	25	17	8	209.034064	209.034054	10
51	11	5	7	11	4	7	44.954626	44.954619	07	112	24	18	7	24	17	7	209.270401	209.270378	23
52	10	5	6	10	4	6	48.526363	48.526365	-02	113	22	18	5	22	17	5	209.664457	209.664486	-29
53	8	4	5	7	3	5	110.593677	110.593624	53	114	17	5	13	16	4	13	210.444113	210.444026	87
54	7	5	2	6	4	2	113.117160	113.117150	10	115	16	7	9	15	6	9	210.403451	210.403523	-72
55	7	5	3	6	4	3	113.197380	113.197371	09	116	17	3	14	16	2	14	211.669736	211.669845	-109
56	13	10	4	13	9	4	113.623929	113.623890	39	117	13	9	5	12	8	5	211.870552	211.870520	32
57	12	10	3	12	9	3	113.829234	113.829155	79	118	17	4	14	16	3	14	212.979695	212.979733	-38
58	11	10	2	11	9	2	113.990423	113.990461	-38	119	14	8	7	13	7	7	208.061703	208.061730	-27
59	14	4	10	13	3	10	159.612176	159.612232	-56	120	14	8	6	13	7	6	208.035423	208.035328	95
60	24	14	11	24	13	11	159.584798	159.584824	-26	121	18	5	13	17	4	13	205.488337	205.488296	41
61	8	8	0	7	7	0	157.722149	157.722140	09	122	15	7	9	14	6	9	204.079044	204.079037	07

along the c -axis of about 1.5 Debye. Several lines over 200 GHz are visible with quadrupole splitting in video mode. The dipole moment component along the a -axis is of the order of magnitude of 0.1 Debye [1], it was not yet possible to assign a -type transitions. This is an aim of the current work, eventually applying Fourier-Transform-Techniques.

The constants of the ^{35}Cl -isotopomere listed in Table 3 show a very good correspondence up to the fourth order with the ones of [3]. The differences are smaller than the given uncertainties.

The obtained sextic constants of both isotopomeres do not correspond in sign and magnitude, except the H_K 's, which are connected with J_z only. A lack of transitions with higher J -quantum numbers as well as the limitation to c -type transitions may cause this disagreement.

Further, the sextic constants do not agree with the ones of [3]. The discrepancies arise from the correlation of the sextic constants considering the fact that the sextic constants except H_J and H_K in the fit of [3] are fixed to zero.

Table 2. Rotational transition frequencies of CHF₂³⁷Cl. Frequencies in GHz, differences in kHz. Lines labeled with * have been measured in [1].

N	J	K _P	K _O	J'	K _P '	K _O '	V _{calc}	V _{obs}	V _{calc-obs}
1*	1	1	0	0	0	0	14.950972	14.950940	32
2*	2	2	1	1	1	1	35.418484	35.418510	-26
3*	2	2	0	1	1	0	34.332734	34.332780	-46
4*	3	2	1	3	1	3	23.417647	23.417650	-03
5*	3	1	2	2	0	2	34.525464	34.525480	-16
6*	4	3	2	4	2	2	28.689175	28.689190	-15
7*	4	3	1	4	2	3	31.550855	31.550870	-15
8*	5	3	2	5	2	4	32.889416	32.889380	36
9*	5	1	4	4	2	2	27.651369	27.651350	19
10*	6	1	5	5	2	3	34.936986	34.937010	-24
11*	8	4	5	8	3	5	36.843671	36.843600	71
12*	9	4	6	9	3	6	33.169866	33.169880	-14
13*	10	4	7	10	3	7	28.699770	28.699760	10
14*	13	6	7	12	7	5	30.621838	30.621820	18
15*	14	5	10	14	4	10	31.976047	31.976040	07
16*	16	8	9	15	9	7	30.524774	30.524830	-56
17*	18	6	13	18	5	13	33.826528	33.826570	-42
18*	19	6	14	19	5	14	26.586871	26.586930	-59
19*	20	7	14	20	6	14	50.789127	50.789150	-23
20*	20	6	15	20	5	15	19.806693	19.806750	-57
21*	21	12	10	20	13	8	22.240810	22.240805	05
22*	22	7	16	22	6	16	34.480935	34.480900	35
23*	23	13	10	22	14	8	26.833294	26.833300	-06
24*	24	13	12	23	14	10	35.700134	35.700090	44
25*	24	14	11	23	15	9	22.619465	22.619480	-15
26*	24	7	18	24	6	18	19.265076	19.265070	06
27*	26	15	12	25	16	10	27.205012	27.205020	-08
28*	26	8	19	26	7	19	34.145781	34.145710	71
29*	27	16	11	26	17	9	23.009856	23.009900	-44
30*	28	16	13	27	17	11	31.796773	31.796790	-17
31*	29	17	13	28	18	11	27.589847	27.589816	31
32*	30	18	13	29	19	11	23.408726	23.408720	06
33*	30	9	22	30	8	22	33.017144	33.017170	-26
34	9	5	5	9	4	5	52.452928	52.452942	-14
35	8	5	4	8	4	4	53.690958	53.690985	-27
36	7	5	3	7	4	3	54.400287	54.400267	20
37	6	5	2	6	4	2	54.793765	54.793709	56
38	4	2	3	3	1	3	54.889327	54.889288	39
39	5	5	1	5	4	1	55.007431	55.007482	-51
40	3	3	0	2	2	0	55.179354	55.179276	78
41	3	3	1	2	2	1	55.359239	55.359255	-16
42	14	6	9	14	5	9	58.014731	58.014657	74
43	12	5	8	12	4	8	43.113058	43.113027	31
44	3	2	2	2	1	2	44.852453	44.852557	-14
45	4	1	3	3	0	3	45.550038	45.550059	-21
46	4	2	2	3	1	2	49.923509	49.923511	-02
47	10	5	6	10	4	6	50.414101	50.414096	05
48	9	4	5	8	3	5	113.437498	113.437480	18
49	9	2	8	8	1	8	112.727604	112.727616	-12
50	9	3	7	8	2	7	112.728299	112.728322	-23
51	17	10	8	17	9	8	114.574082	114.574086	-04
52	16	10	7	16	9	7	114.991642	114.991703	-61
53	15	10	6	15	9	6	115.335800	115.335796	04

N	J	K _P	K _O	J'	K _P '	K _O '	V _{calc}	V _{obs}	V _{calc-obs}
54	18	10	9	18	9	9	114.070227	114.070214	13
55	13	4	10	12	3	10	159.399488	159.399452	36
56	11	6	6	10	5	6	157.517004	157.517051	-47
57	13	2	11	12	1	11	158.666236	158.666211	25
58	14	4	10	13	3	10	155.262341	155.262324	17
59	29	14	16	29	13	16	159.962878	159.962905	-27
60	30	16	15	30	15	15	185.889259	185.889269	-10
61	13	7	7	12	6	7	186.068104	186.068089	15
62	10	9	1	9	8	1	186.263963	186.263963	00
63	10	9	2	9	8	2	186.263964	186.263963	01
64	29	16	14	29	15	14	186.419583	186.419541	42
65	28	16	13	28	15	13	186.895285	186.895301	-16
66	27	16	12	27	15	12	187.320996	187.320998	-02
67	17	5	12	16	4	12	187.657105	187.657120	-15
68	26	16	11	26	15	11	187.700947	187.700911	36
69	25	16	10	25	15	10	188.039029	188.039036	-07
70	24	16	9	24	15	9	188.338830	188.338833	-03
71	22	16	7	22	15	7	188.836640	188.836654	-14
72	21	16	6	21	15	6	189.040608	189.040663	-55
73	19	16	4	19	15	4	189.372084	189.372120	-36
74	18	16	3	18	15	3	189.504435	189.504416	19
75	13	7	6	12	6	6	185.951451	185.951430	21
76	15	4	12	14	3	12	182.971752	182.971777	-25
77	9	9	0	8	8	0	178.054296	178.054335	-39
78	9	9	1	8	8	1	178.054297	178.054335	-38
79	12	7	6	11	6	6	177.990439	177.990486	-47
80	15	3	12	14	2	12	177.964148	177.964195	-47
81	12	7	5	11	6	5	177.949541	177.949535	06
82	16	5	11	15	4	11	177.693936	177.693893	43
83	18	15	4	18	14	4	177.131129	177.131113	16
84	19	15	5	19	14	5	176.970816	176.970791	25
85	20	15	6	20	14	6	176.784136	176.784107	29
86	21	15	7	21	14	7	176.568146	176.568142	04
87	22	15	8	22	14	8	176.319677	176.319707	-30
88	14	2	13	13	1	13	176.241463	176.241421	42
89	14	1	13	13	0	13	176.181004	176.181029	-25
90	23	15	9	23	14	9	176.035313	176.035318	-05
91	11	10	1	10	9	1	206.720095	206.720054	41
92	11	10	2	10	9	2	206.720095	206.720054	41
93	14	8	7	13	7	7	206.599269	206.599345	-76
94	14	8	6	13	7	6	206.582496	206.582473	23
95	35	18	18	35	17	18	209.191123	209.191083	40
96	34	18	17	34	17	17	209.781966	209.781992	-26
97	33	18	16	33	17	16	210.319870	210.319899	-29
98	32	18	15	32	17	15	210.808825	210.808833	-08
99	17	5	13	16	4	13	205.786999	205.787030	-31
100	16	7	9	15	6	9	208.757287	208.757274	13
101	17	6	12	16	5	12	209.014941	209.014883	58
102	13	9	4	12	8	4	210.837498	210.837462	36
103	29	18	12	29	17	12	212.017346	212.017311	35
104	28	18	11	28	17	11	212.344581	212.344583	-02
105	19	5	14	18	4	14	212.394121	212.394107	14

Table 3. Rotational parameters of CHF₂³⁵Cl. Standard deviations of the fitting procedure are given in parenthesis as uncertainties in the last digits.

	this work	[3]	
A	10.2347070(13)	10.2347085(21)	GHz
B	4.8612454(1)	4.8612511(15)	GHz
C	3.5074515(15)	3.5074583(47)	GHz
D _J	1.297(38)	1.3320(33)	kHz
D _{JK}	6.261(85)	6.177(16)	kHz
D _K	3.55(12)	3.693(16)	kHz
d ₁	-0.445(24)	-0.4410(33)	kHz
d ₂	-0.1374(53)	-0.1361(25)	kHz
H _J	0.0188(30)	0.681(36)	Hz
H _{JK}	-0.0601(72)	0.0	(fixed) Hz
H _{KJ}	0.175(18)	0.0	(fixed) Hz
H _K	-0.059(27)	5.87(14)	Hz
h ₁	-0.0041(24)	0.0	(fixed) Hz
h ₂	0.004915 (fixed)	0.0	(fixed) Hz
h ₃	-0.00302(96)	0.0	(fixed) Hz
rms error of the fit	52	5400	kHz

Table 4. Rotational parameters of CHF₂³⁷Cl. Standard deviations of the fitting procedure are given in parenthesis as uncertainties in the last digits.

A	10.233858(1)	GHz
B	4.7171362(8)	GHz
C	3.4318556(11)	GHz
D _J	1.2264(27)	kHz
D _{JK}	5.9627(65)	kHz
D _K	3.864(10)	kHz
d ₁	-0.4134(18)	kHz
d ₂	-0.12663(87)	kHz
H _J	-0.0201(37)	Hz
H _{JK}	0.0347(79)	Hz
H _{KJ}	-0.01687 (fixed)	Hz
H _K	-0.058(20)	Hz
h ₁	0.0369(58)	Hz
h ₂	-0.0282(42)	Hz
h ₃	0.00108255 (fixed)	Hz
rms error of the fit	52	kHz

Table 5. Correlation matrices for $\text{CHF}_2^{35}\text{Cl}$ and $\text{CHF}_2^{37}\text{Cl}$.

A	1.000																		
B	.609	1.000																	
C	.209	.125	1.000																
D _J	.489	.490	.754	1.000															
D _{JK}	-.048	-.122	-.437	-.719	1.000														
D _K	.514	.321	.230	.682	-.798	1.000													
d ₁	-.073	-.398	.765	.543	-.519	.249	1.000												
d ₂	.140	.225	-.390	-.275	.190	-.001	-.604	1.000											
H _J	.484	.384	.638	.877	-.623	.636	.508	-.147	1.000										
H _{JK}	-.054	.049	-.224	-.281	.368	-.292	-.313	-.030	-.651	1.000									
H _{KJ}	-.006	-.144	-.137	-.313	.459	-.375	-.128	.135	.073	-.630	1.000								
H _K	.388	.321	.224	.613	-.718	.861	.204	-.051	.396	.159	-.772	1.000							
h ₁	-.008	.305	-.545	-.392	.393	-.223	-.759	.244	-.631	.659	-.206	-.038	1.000						
h ₃	.039	.098	-.176	-.088	-.005	.050	-.167	.040	.201	-.398	.239	-.066	-.384	1.000					

A	1.000																		
B	.508	1.000																	
C	.154	.484	1.000																
D _J	.436	.651	.725	1.000															
D _{JK}	-.059	-.194	-.332	-.724	1.000														
D _K	.527	.240	.082	.643	-.800	1.000													
d ₁	-.046	-.124	.540	.588	-.671	.421	1.000												
d ₂	.058	.064	-.306	-.493	.597	-.400	-.891	1.000											
H _J	.347	.421	.454	.861	-.806	.750	.710	-.731	1.000										
H _{JK}	-.152	-.209	-.286	-.707	.904	-.781	-.731	.756	-.940	1.000									
H _K	.552	.304	.143	.679	-.740	.961	.456	-.472	.827	-.817	1.000								
h ₁	-.120	-.103	-.270	-.583	.702	-.589	-.789	.867	-.896	.923	-.678	1.000							
h ₂	.122	.128	.198	.540	-.664	.572	.719	-.850	.878	-.906	.667	-.992	1.000						

Acknowledgements

We wish to thank the members of the laboratory for discussions, the Deutsche Forschungsgemeinschaft

for a grant (R.S.) and research funds. Further we wish to thank the workshop of the Institute of Physical Chemistry, which has provided us with the construction of necessary microwave parts.

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