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

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The rotational spectra of $CHF_2{}^{35}Cl$ and $CHF_2{}^{37}Cl$ (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 isotopomeres [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 isotopomeres, 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]:

$$\begin{aligned} H = {} & A J_Z^2 + B J_X^2 + C J_Y^2 - D_J J^4 - D_{JK} J^2 J_Z^2 - D_K J_Z^4 \\ & + d_1 J^2 (J_+^2 + J_-^2) + d_2 (J_+^4 + J_-^4) + H_J J^6 \\ & + H_{JK} J^4 J_Z^2 + H_{KJ} J^2 J_Z^4 + H_K J_Z^6 + h_1 J^4 (J_+^2 + J_-^2) \\ & + h_2 J^2 (J_+^4 + J_-^4) + h_3 (J_+^6 + J_-^6), \end{aligned} \tag{1}$$

where

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

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 $CHF_2{}^{35}Cl$. 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}	$\nu_{calc-obs}$
1*	1	1	0	0	0	0	15.095929	15.095983	-54
2*	2	1	1	1	0	1	24.818345	24.818354	-09
3*	3	3	0	3	2	2	30.405627	30.405675	-48
4*	3	3	1	3	2	1	29.294788	29.294778	10
5*	3	1	2	2	0	2	35.288185	35.288224	-39
6*	4	3	2	4	2	2	27.906059	27.906008	51
7*	4	2	2	4	1	4	28.300967	28.300928	39
8*	5	3	3	5	2	3	25.629541	25.629461	80
9*	5	1	4	4	2	2	29.058776	29.058735	41
10*	6	2	4	5	3	2	27.716955	27.716971	-16
11*	6	1	5	5	2	3	36.234634	36.234590	44
12*	7	2	5	6	3	3	38.633591	38.633603	-12
13*	7	1	6	6	2	4	41.455947	41.455901	46
14*	8	4	5	8	3	5	35.210170	35.210198	-28
15*	8	2	7	7	3	5	28.324143	28.324068	75
16*	8	3	5	7	4	3	32.758028	32.757984	44
17*	9	4	6	9	3	6	31.198210	31.198256	-46
18*	9	3	6	8	4	4	44.823205	44.823177	28
19*	10	3	7	9	4	5	56.845085	56.845069	16
20*	10	4	7	9	5	5	32.346384	32.346369	15
21*	11	5	7	10	6	5	29.470228	29.470283	-55
22*	12	5	8	11	6	6	38.685291	38.685320	-29
23*	13	6	8	12	7	6	35.087658	35.087663	-05
24*	14	5	10	14	4	10	28.334865	28.334881	-16
25*	15	7	9	14	8	7	40.573084	40.573111	-27
26*	15	8	8	14	9	6	27.224960	27.225015	-55
27*	18	6	13	18	5	13	28.625564	28.625576	-12
28*	19	7	13	19	6	13	52.283354	52.283420	-66
29*	20	7	14	20	6	14	44.326081	44.326082	-01
30*	20	12	9	19	13	7	21.171529	21.171526	03
31*	21	12	9	20	13	7	30.242704	30.242668	36
32*	22	7	16	22	6	16	27.667389	27.667375	14
33*	23	8	16	23	7	16	53.184317	53.184274	43
34*	24	8	17	24	7	17	43.892915	43.892894	21
35*	25	15	10	24	16	8	28.037950	28.037855	95
36*	25	8	18	25	7	18	34.549053	34.549035	18
37*	26	8	19	26	7	19	25.797448	25.797495	-47
38*	27	17	11	26	18	9	20.616274	20.616326	-52
39*	28	17	12	27	18	10	29.608916	29.608865	51
40*	30	19	12	29	20	10	22.202188	22.202228	-40
41	3	3	0	2	2	0	55.286354	55.286324	30
42	3	2	1	2	1	1	42.313109	42.313096	13
43	3	2	2	2	1	2	45.287402	45.287394	08
44	3	3	1	2	2	1	55.487658	55.487610	48
45	4	1	3	3	0	3	46.698445	46.698453	-08
46	4	2	2	3	1	2	50.581395	50.581393	02
47	4	2	3	3	1	3	55.640824	55.640818	06
48	7	5	3	7	4	3	53.262133	53.262110	23
49	8	5	4	8	4	4	52.419210	52.419199	11
50	14	6	9	14	5	9	54.871925	54.871920	05
51	11	5	7	11	4	7	44.954626	44.954619	07
52	10	5	6	10	4	6	48.526363	48.526365	-02
53	8	4	5	7	3	5	110.593677	110.593624	53
54	7	5	2	6	4	2	113.117160	113.117150	10
55	7	5	3	6	4	3	113.197380	113.197371	09
56	13	10	4	13	9	4	113.623929	113.623890	39
57	12	10	3	12	9	3	113.829234	113.829155	79
58	11	10	2	11	9	2	113.990423	113.990461	-38
59	14	4	10	13	3	10	159.612176	159.612232	-56
60	24	14	11	24	13	11	159.584798	159.584824	-26
61	8	8	0	7	7	0	157.722149	157.722140	09
62	8	8	1	7	7	1	157.722150	157.722140	10
63	11	6	6	10	5	6	158.778129	158.778113	16
64	12	5	8	11	4	8	156.709622	156.709587	35
65	13	5	8	12	4	8	157.019613	157.019499	114
66	23	14	10	23	13	10	160.043635	160.043648	-13
67	28	14	15	28	13	15	157.030094	157.030077	17
68	29	14	16	29	13	16	156.166077	156.166193	-116
69	19	16	4	19	15	4	185.807435	185.807495	-60
70	20	16	5	20	15	5	185.634080	185.634092	-12
71	21	16	6	21	15	6	185.433750	185.433741	09
72	22	16	7	22	15	7	185.203578	185.203519	59
73	19	16	4	19	15	4	185.807435	185.807495	-60
74	10	9	1	9	8	1	186.620281	186.620327	-46
75	10	9	2	9	8	2	186.620281	186.620327	-46
76	15	6	9	14	5	9	186.825106	186.825088	18
77	16	4	12	15	3	12	187.139802	187.139796	06
78	15	5	11	14	4	11	187.240815	187.240846	-31
79	15	4	12	14	3	12	187.278373	187.278311	62
80	13	7	7	12	6	7	187.531402	187.531427	-25
81	23	16	8	23	15	8	184.940486	184.940443	43
82	24	16	9	24	15	9	184.641162	184.641048	114
83	25	16	10	25	15	10	184.302033	184.301902	131
84	14	6	9	13	5	9	184.299664	184.299681	-17
85	27	16	12	27	15	12	183.488558	183.488622	-64
86	28	16	13	28	15	13	183.005432	183.005320	112
87	11	8	4	10	7	4	183.001184	183.001216	-32
88	11	8	3	10	7	3	183.000670	183.000777	-107
89	30	16	15	30	15	15	181.861208	181.861116	92
90	16	5	11	15	4	11	181.502209	181.502230	-21
91	14	6	8	13	5	8	180.533678	180.533702	-24
92	12	7	6	11	6	6	179.234294	179.234318	-24
93	12	7	5	11	6	5	179.174479	179.174499	-20
94	9	9	0	8	8	0	178.182708	178.182696	12
95	9	9	1	8	8	1	178.182708	178.182696	12
96	14	5	10	13	4	10	176.492599	176.492618	-19
97	14	2	12	13	1	12	176.488955	176.488913	42
98	16	1	15	15	0	15	206.360613	206.360597	16
99	18	6	12	17	5	12	206.446853	206.446933	-80
100	30	18	13	30	17	13	207.356881	207.356919	-38
101	29	18	12	29	17	12	207.767966	207.767996	-30
102	21	18	4	21	17	4	209.826597	209.826532	65
103	20	18	3	20	17	3	209.968208	209.968233	-25
104	35	18	18	35	17	18	204.557149	204.557129	20
105	34	18	17	34	17	17	205.230446	205.230444	02
106	32	18	15	32	17	15	206.397996	206.397934	62
107	31	18	14	31	17	14	206.901461	206.901573	-112
108	28	18	11	28	17	11	208.138149	208.138221	-72
109	27	18	10	27	17	10	208.470616	208.470664	-48
110	26	18	9	26	17	9	208.768332	208.768337	-05
111	25	18	8	25	17	8	209.034064	209.034054	10
112	24	18	7	24	17	7	209.270401	209.270378	23
113	22	18	5	22	17	5	209.664457	209.664486	-29
114	17	5	13	16	4	13	210.444113	210.444026	87
115	16	7	9	15	6	9	210.403451	210.403523	-72
116	17	3	14	16	2	14	211.669736	211.669845	-109
117	13	9	5	12	8	5	211.870552	211.870520	32
118	17	4	14	16	3	14	212.979695	212.979733	-38
119	14	8	7	13	7	7	208.061703	208.061730	-27
120	14	8	6	13	7	6	208.035423	208.035328	95
121	18	5	13	17	4	13	205.488337	205.488296	41
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 $CHF_2{}^{37}Cl$. 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}	$\nu_{calc-obs}$
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	54.793675	54.793709	-34
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	44.852543	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
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 $CHF_2{}^{35}Cl$. 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 $CHF_2{}^{37}Cl$. 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 $CHF_2{}^{35}Cl$ and $CHF_2{}^{37}Cl$.

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

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[1] D. T. Cramb, Y. Bos, H. M. Jemsson, H. M. Gerry, and C. J. Marsden, J. Mol. Struct. **190,** 387 (1988).
[2] A. Amrein, D. Luckhaus, F. Merkt, and M. Quack, Chem. Phys. Lett. **152,** 275 (1988).
[3] D. Luckhaus and M. Quack, Molec. Phys. **68,** No. 3, 745 (1989).
[4] J. Doose, A. Guarnieri, W. Neustock, R. Schwarz, F. Winther, and F. Hegelund, Z. Naturforsch. **44a,** 538 (1989).
[5] M. Stolze, D. Hübner, and D. H. Sutter, Z. Naturforsch. **36a,** 886 (1981).
[6] J. K. G. Watson, Vibrational Spectra and Structure, vol. 6 (J. R. Durig, ed.), Elsevier, Amsterdam 1978.
[7] V. Typke, J. Mol. Spectrosc. **63,** 170 (1976).
[8] D. B. McLay and C. R. Mann, Can. J. Phys. **40,** 40 (1962).