Pure Rotational Spectroscopy of Sodium Chloride, NaCl, up to 930 GHz

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The pure rotational spectra of both isotopomers of NaCl, i. e. ^{23}Na^{35}Cl and ^{23}Na^{37}Cl, have been recorded in high resolution with the Cologne terahertz spectrometer. A total of 189 new rotational lines have been measured in the frequency region between 200 and 930 GHz. Twenty nine of these transitions are assigned for Na^{35}Cl to the vibrational ground state with $J \leq 72$, and 102 lines arise from vibrationally excited states up to the 5th vibrational state: $v = 5$. For Na^{37}Cl a total of 58 rotational lines with $J \leq 76$ and $v \leq 4$ could be detected. The newly measured lines were fitted together with the published microwave and millimeter-wave transitions to obtain a refined and extended set of molecular parameters: Na^{35}Cl: B_0 = 6513.04908(41) MHz, D_0 = 9.338978(141) kHz, H_0 = –1.0433(144) mHz and Na^{37}Cl: B_0 = 6373.74158(66) MHz, D_0 = 8.943327(185) kHz, H_0 = –0.9623(162) mHz.

From the experimental data the equilibrium constants B_e, α, γ, D_e, β, δ, H_e and ε are calculated as well. The refined parameters for both isotopomers allow precise frequency predictions to be made far into the terahertz region. Thus this new and highly precise data set for NaCl is intended to support future astrophysical observations.

Key words: Rotational Spectroscopy; Sodium Chloride; NaCl; BWO; THz-Spectroscopy.

Introduction

The first few low frequency rotational transitions ($J = 2 \leftarrow 1$, $v \leq 3$ at $\sim$ 26 GHz) of NaCl were measured by Honig et al. in 1954 [1]. These authors recorded with moderate accuracy ($\sim$ 1 MHz) four lines for Na^{35}Cl and three of the less abundant Na^{37}Cl in different vibrationally exited states with $v \leq 3$. Ten years later Clouser and Gordy [2] investigated the pure rotational spectra of the four alkali chlorides, i. e. NaCl, KCl, RbCl, and CsCl in the 0.96 mm to 3 mm wavelength range. The availability of this enlarged wavelength region just barely touching the sub-millimeter part of the electromagnetic spectrum clearly states the technical progress which was achieved during these 10 years. It is, therefore, not only of pure historic interest to quickly look at the highest frequency line at 312 GHz presented in the work of Clouser and Gordy. It is of interest to compare the "extremely weak line" judged from its appearance with the signal to noise ratio obtained with the Cologne terahertz spectrometer: it is the rotational transition $J = 24 \leftarrow 23$ measured at 312109.74 $\pm$ 0.15 MHz for which we present in Fig. 1 (left side) a scanned-in version of the original line profile as published by Clouser and Gordy, whereas Fig. 1 (right side) shows the same transition recorded and signal averaged with the techniques of the year 2000. The difference in the signal to noise ratio reflects mainly the difference in the submillimeter power level of the two sources: harmonic generation of a klystron in 1964 and a fundamental mode backward wave oscillator (BWO) in 2000.

Clouser and Gordy covered the frequency range from 104 GHz to 312 GHz which corresponds to the rotational transitions from $J = 8 \leftarrow 7$ to $J = 24 \leftarrow 23$. They recorded and analyzed for Na^{35}Cl a total of 13 lines for the three vibrational states v = 0, 1, 2 and for Na^{37}Cl six transitions (v = 0 and 1) were assigned. Dunham's solution for the diatomic molecule was applied in interpretation of the data. The six Dunham constants, Y_{01}, α_e, γ_e, D_e, β_e, and H_e were calculated directly from the measurements. The predictions of line positions for high J transitions, which are based on these medium J measurements, are reliable only to the millimeter wavelength range.

Sodium Chloride and Astrophysics

In 1987 Cernicharo and Guèlin [3] reported the detection of the three metal halides NaCl, AlCl, and KCl

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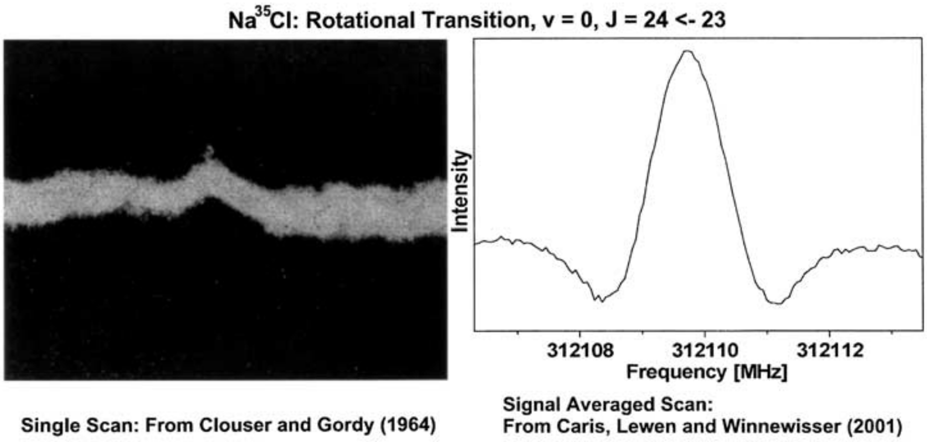

Single Scan: From Clouser and Gordy (1964)

Signal Averaged Scan:
From Caris, Lewen and Winnewisser (2001)

Fig. 1. Comparison between two recordings of the same rotational transition $J = 24 \leftarrow 23$, $v = 0$ of NaCl recorded in two different years: in 1964 and recently in 2001. There exists a fantastic difference in the intensities between the two lines displayed on the left and on the right side of the figures. *Left:* The 1964 single scan has been photographed from a cathode ray oscilloscope. (Clouser and Gordy, 1964). *Right:* The recent frequency averaged recording gives an impression of the gain in sensitivity since 1964.

in the warm, inner and dense circumstellar envelope of the late type star IRC+10216. The NaCl rotational lines were observed in the frequency-region between 90 and 170 GHz with the IRAM 30 m telescope. The circumstellar spectra display a plethora of different molecular species aside from NaCl. Among the large number of circumstellar transitions found in this survey work, six lines were assigned to the ground vibrational state of Na^{35}Cl. In addition one circumstellar line matches the rest-frequency position at 101961.9 MHz of the $J = 7 \leftarrow 6$ transition for Na^{37}Cl. The relatively high interstellar abundance of sodium and chlorine, i. e. the 15th and 20th abundance, lend encouraging motivation to continue the search towards hotter and even denser core regions as well as to check in other sources with the aim to find NaCl's probable interstellar distribution as well. A similar reasoning will apply to all the other circumstellar alkalides.

Concerning the millimeter-, sub-millimeter and adjoining far infrared region, two missions are planned for investigating interstellar space: the air-borne SOFIA mission (Stratospheric Observatory For Infrared Astronomy) with its planned maiden-flight by 2004, and the space mission Herschel to be launched by 2007. The planned airplane mission SOFIA calls for a converted jumbo-jet carrying a 3 m radiotelescope on board at an altitude of about 15 km, and it will conduct in part interstellar observations with most of the intervening atmosphere removed. In 2007 Herschel will be launched and will place a 3 m telescope into space. With all the various heterodyne high resolution receivers on board, Herschel will cover most of the submillimeter wavelengths far into the terahertz region. Both missions will require significant spectroscopic input on atomic and molecular line positions occurring at high frequencies, specifically in the terahertz region, which has been notoriously difficult to work in for both, the laboratory spectroscopists and the astrophysicists. This development emphasizes the very strong demand for highly accurate laboratory spectroscopic data throughout the terahertz domain. We try to provide some of these data and linepositions in the terahertz region.

Along these lines we have started some time ago a program to provide highly accurate and very reliable spectroscopic data which are made available worldwide via the Cologne Database for Molecular Spectroscopy, CDMS, which can be accessed free of charge via http://www.ph1.uni-koeln.de/vorhersagen/ or alternatively via the short-cut http://www.cdms.de [4]).

In this work we provide precise data for both isotopomers. Predictions up to 2 THz will be very reliable.

Experimental

Under normal temperature and pressure conditions, NaCl is a white solid with extremely low vapor

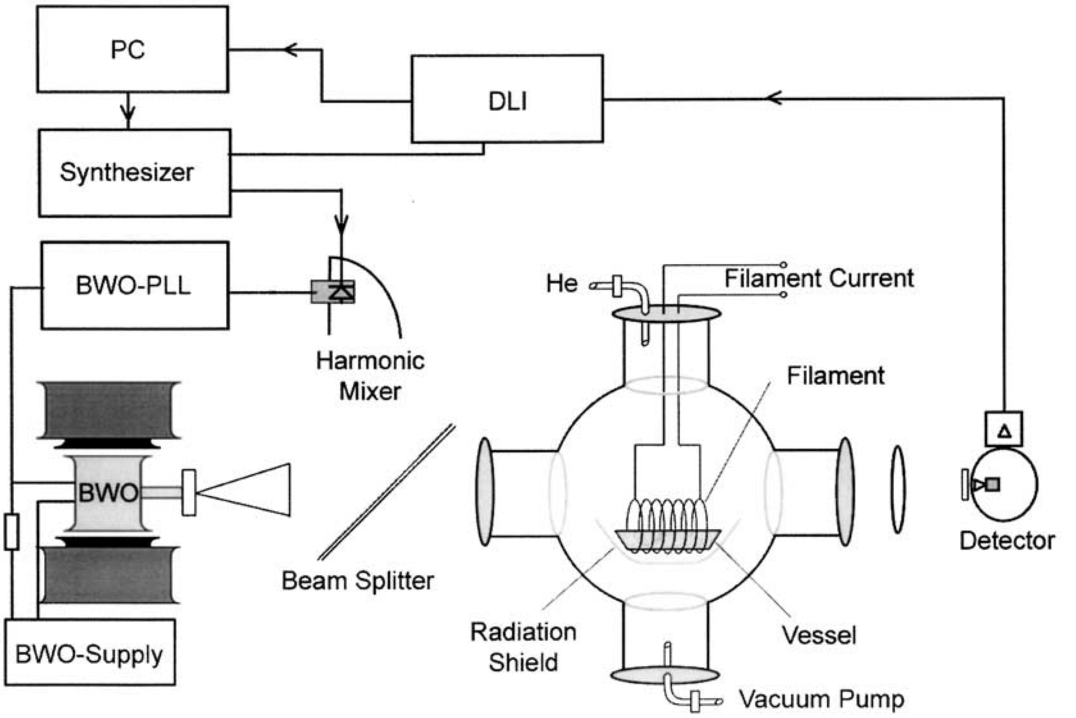

Fig. 2. Schematic diagram of the Cologne THz-Spectrometer: The key element is a backward wave oscillator (BWO) which is installed inside of an electromagnet. A part of the BWO radiation is reflected to the harmonic mixer, where the BWO frequency is downconverted by mixing with a harmonic of the synthesizer. The obtained intermediate frequency is analyzed in phase to lock with the PLL unit the BWO frequency. The main part of the BWO radiation passes the evaporation cell and is focused with the aid of a PTFE lens into the detector. The detector signal is processed with a Digital Lock-In amplifier (DLI) and transmitted to a PC, which controls the spectrometer.

Table 1. Physical Parameters of Sodium Chloride.

Melting Point (1 atm)	801 °C
Boiling Point (1 atm)	1413 °C
Isotopic Ratio ^{35}Cl to ^{37}Cl	75.8 : 24.2 = 3.1
Dipole moment [a]	8.97 D
Mass ^{23}Na [b]	22.9897677 amu
Mass ^{35}Cl [b]	34.968852721 amu
Mass ^{37}Cl [b]	36.96590262 amu
First Excited Mode ^{35}Cl [c]	361.15111(18) cm^{-1}
First Excited Mode ^{37}Cl [c]	357.29437(49) cm^{-1}

[a] Mizoguchi *et al.* [7], [b] Audi *et al.* [8], [c] Ram *et al.* [9].

pressure. In Table 1 we summarize the most important physical parameters of sodium chloride necessary for this work. To obtain NaCl-vapor in measurable amounts, low total pressures and high temperatures ($\sim$ 1000 K) are required. The temperature range needed to evaporate NaCl or any other alkali chloride, asks for special experimental arrangements. For this purpose we have constructed a special heater system, which heats a small ceramic evaporation vessel, a ca. 5 cm long hollow container used to hold the salt. The entire heating system is encircled by the heater filament. In addition there exists a radiation shield, surrounding the filament to protect the absorption-cell against the thermal radiation and reflect it towards the vessel. This construction is positioned at the center of the spherical cell (see Fig. 2), which offers the advantage of easily positioning the heater very tightly beneath the test beam but with sufficient distance to the walls of the glass-sphere. Operational conditions of the sample cell were provided by applying helium as buffer gas, in order to reduce the decay of NaCl molecules on the cell walls. The partial pressure of helium within the cell was controlled to be 100 µbar, to maintain a maximum in intensity and to keep the line-shape of most lines as narrow as possible. The NaCl content of the vessel allowed 3 - 4 hours of continuous measurements.

Table 2. Rotational Frequencies of $Na^{35}Cl$.

ν	$J' \leftarrow J''$		Obs. [MHz]	O-C [kHz]	ν	$J' \leftarrow J''$		Obs. [MHz]	O-C [kHz]	ν	$J' \leftarrow J''$		Obs. [MHz]	O-C [kHz]
0	19	18	247239.733(100)	106	0	20	19	260223.111(100)	13	0	21	20	273202.096(100)	12
0	22	21	286176.346(100)	–17	0	23	22	299145.700(100)	–10	0	24	23	312109.739(150)	–160
0	25	24	325068.287(200)	–421	0	34	33	441418.821(40)	5	0	35	34	454311.490(40)	19
0	36	35	467196.294(30)	17	0	37	36	480073.021(30)	14	0	38	37	492941.452(30)	13
0	39	38	505801.357(30)	11	0	40	39	518652.473(30)	–31	0	41	40	531494.680(30)	–9
0	42	41	544327.670(30)	–6	0	45	44	582769.201(30)	1	0	46	45	595563.164(30)	19
0	47	46	608346.775(30)	6	0	48	47	621119.831(30)	–14	0	53	52	684819.143(30)	5
0	54	53	697524.218(30)	14	0	55	54	710217.159(30)	12	0	58	57	748220.984(30)	0
0	60	59	773492.141(30)	11	0	61	60	786107.620(30)	18	0	66	65	848975.006(30)	62
0	70	69	899003.259(30)	9	0	72	71	923923.925(30)	14	1	19	18	245401.085(100)	109
1	20	19	258287.544(150)	–197	1	21	20	271170.104(100)	72	1	22	21	284047.408(150)	–218
1	23	22	296920.373(100)	75	1	24	23	309787.633(150)	–192	1	34	33	438130.892(30)	23
1	35	34	450927.034(30)	10	1	36	35	463715.363(30)	16	1	37	36	476495.624(30)	11
1	38	37	489267.615(40)	16	1	39	38	502031.096(30)	15	1	40	39	514785.834(30)	0
1	41	40	527531.621(30)	–13	1	42	41	540268.177(30)	–79	1	45	44	578420.754(30)	–66
1	46	45	591118.464(30)	–28	1	47	46	603805.866(40)	0	1	48	47	616482.701(30)	–15
1	54	53	692310.253(30)	–15	1	55	54	704907.159(30)	–14	1	57	56	730063.792(30)	–7
1	60	59	767702.403(30)	–9	1	61	60	780222.012(30)	–18	1	67	66	855044.800(30)	–32
1	71	70	904629.296(30)	–37	1	73	72	929326.938(30)	–30	2	19	18	243574.269(150)	201
2	21	20	269151.033(200)	71	2	22	21	281932.365(100)	–126	2	23	22	294709.205(100)	96
2	24	23	307480.381(100)	–214	2	34	33	434864.025(40)	31	2	35	34	447564.310(30)	37
2	36	35	460256.765(40)	26	2	37	36	472941.194(30)	27	2	38	37	485617.372(40)	38
2	39	38	498285.042(40)	25	2	40	39	510944.018(30)	27	2	41	40	523594.019(30)	–15
2	42	41	536234.888(30)	–33	2	46	45	586702.444(30)	1	2	47	46	599294.222(30)	24
2	48	47	611875.413(30)	–42	2	49	48	624445.973(30)	–17	2	54	53	687129.996(30)	–8
2	55	54	699631.508(30)	1	2	56	55	712120.721(30)	1	2	61	60	774374.595(30)	–4
2	62	61	786785.369(30)	1	2	67	66	848626.842(30)	1	2	72	71	910093.743(30)	–39
3	22	21	279830.768(200)	–191	3	23	22	292512.229(100)	85	3	24	23	305188.210(100)	1
3	37	36	469409.694(30)	25	3	38	37	481990.670(30)	27	3	39	38	494563.165(30)	11
3	40	39	507126.995(30)	18	3	41	40	519681.871(30)	–20	3	42	41	532227.650(40)	–21
3	46	45	582314.950(30)	–48	3	47	46	594811.794(50)	29	3	48	47	607298.018(30)	–42
3	49	48	619773.587(50)	–73	3	55	54	694390.169(30)	20	3	56	55	706784.655(30)	28
3	58	57	731535.947(30)	34	3	61	60	768565.333(30)	22	3	62	61	780881.558(30)	17
3	68	67	854480.784(30)	1	3	72	71	903246.608(30)	20	3	74	73	927534.014(40)	6
4	24	23	302910.671(100)	4	4	38	37	478387.530(40)	3	4	39	38	490865.495(30)	3
4	40	39	503334.805(30)	13	4	41	40	515795.244(40)	40	4	42	41	528246.497(30)	–9
4	43	42	540688.431(30)	–43	4	46	45	577956.141(30)	–16	4	47	46	590358.586(30)	18
4	49	48	615131.824(50)	–6	4	55	54	689183.115(40)	16	4	56	55	701483.519(40)	39
4	57	56	713771.450(50)	40	4	62	61	775016.526(30)	28	4	68	67	848053.216(40)	87
4	69	68	860174.320(40)	64	4	73	72	908503.060(40)	34	5	55	54	684010.358(30)	0
5	56	55	696217.277(30)	–1	5	57	56	708411.774(30)	–6	5	58	57	720593.624(30)	–18
5	59	58	732762.628(30)	–13	5	60	59	744918.542(30)	–13	5	61	60	757061.183(50)	21
5	62	61	769190.220(30)	–19	5	63	62	781305.541(30)	–24	5	69	68	853696.271(40)	4
5	73	72	901653.488(30)	–22	5	75	74	925535.774(50)	–47					

This cell was installed into the Cologne THz-spectrometer designed in 1993 [5] to observe rotational spectra in the millimeter- and submillimeter-wave range (Fig. 2). In this setup Backward Wave Oscillators (BWO) built in Russia are used as radiation source. In a BWO (left of Fig. 2) electrons, accelerated to 5 - 10% of the speed of light, pass a "slow wave structure", where they are slowed down and accelerated periodically. This way electromagnetic radiation is generated. The frequency of the emitted radiation depends on the "slow wave structure" and the speed of the electrons. The latter can be controlled by the accelerating voltage, which amounts to a few kV. These compact BWOs are very precise in frequency and we cover with them bands in between 53 and 1250 GHz. Frequency multiplication has been tested at the spectrometer reaching up to 2.3 THz.

We recorded a large number of new lines of NaCl, which are listed in Tables 2 and 3. The positional accuracy of the center frequency of the lines de-

Table 3. Rotational Frequencies of $Na^{37}Cl$.

ν	$J' \leftarrow J''$		Obs. [MHz]	O-C [kHz]	ν	$J' \leftarrow J''$		Obs. [MHz]	O-C [kHz]	ν	$J' \leftarrow J''$		Obs. [MHz]	O-C [kHz]
0	40	39	507609.238(40)	–8	0	41	40	520180.602(40)	–9	0	42	41	532743.168(40)	1
0	43	42	545296.692(40)	–8	0	46	45	582900.991(40)	–15	0	47	46	595416.289(50)	–3
0	48	47	607921.516(50)	38	0	53	52	670288.366(30)	–1	0	55	54	695156.876(40)	–3
0	56	55	707573.502(30)	–5	0	57	56	719978.096(40)	2	0	58	57	732370.427(30)	1
0	59	58	744750.285(30)	–1	0	60	59	757117.462(30)	4	0	61	60	769471.741(30)	13
0	62	61	781812.897(30)	19	0	68	67	855572.192(30)	13	0	72	71	904455.297(30)	5
0	74	73	928804.730(30)	–2	1	55	54	690015.987(40)	–12	1	56	55	702339.651(30)	–12
1	57	56	714651.301(30)	–15	1	58	57	726950.732(40)	–8	1	59	58	739237.716(30)	–7
1	60	59	751512.039(40)	–8	1	61	60	763773.504(30)	5	1	62	61	776021.858(30)	–3
1	68	67	849225.084(30)	–31	1	73	72	909828.349(40)	–31	2	55	54	684907.979(30)	4
2	56	55	697139.287(30)	0	2	57	56	709358.616(40)	1	2	58	57	721565.740(30)	–5
2	59	58	733760.465(40)	3	2	60	59	745942.550(30)	–2	2	62	61	770267.992(30)	2
2	63	62	782410.919(30)	10	2	69	68	854977.670(40)	–7	2	73	72	903062.859(30)	3
2	75	74	927012.477(30)	–4	3	56	55	691972.374(50)	–3	3	57	56	704099.989(40)	–4
3	58	57	716215.442(30)	2	3	59	58	728318.545(50)	40	3	60	59	740408.976(30)	3
3	62	61	764551.293(30)	29	3	63	62	776602.670(30)	12	3	70	69	860573.747(50)	26
3	74	73	908232.867(50)	–44	3	76	75	931968.576(50)	88	4	56	55	686838.925(40)	–9
4	57	56	698875.439(30)	–9	4	58	57	710899.817(40)	–7	4	59	58	722911.858(30)	8
4	60	59	734911.300(40)	–11	4	63	62	770832.159(40)	–10	4	64	63	782779.226(40)	–9
4	70	69	854167.843(40)	–19										

pends on various factors such as: (i) the line width due to the Doppler broadening (typically 1.8 MHz at 700 GHz), (ii) signal to noise ratio, (iii) baseline variations and (iv) instabilities in the line intensity. Lines below 350 GHz were measured with a Schottky barrier diode detector, operated at room temperature. This device leads to higher noise, and thus an increase in the line uncertainties. Lines above 350 GHz have been measured with a low noise liquid He cooled InSb hot electron bolometer. According to (iv) the line position accuracy is affected by non stationary salt vapor generation. Experimental line shifts are possible if the concentration of evaporated NaCl varies during the scanning of a particular spectrum. All spectra were recorded with ascending and subsequent descending frequency. The time amounted to 40 seconds for each scan direction. Finally both scans were added.

Results and Conclusion

As a demonstration of lines in high excited states we present spectra of the two isotopomers in Figs. 3 and 4, respectively. The lines are recorded in second derivative form, to partly suppress the baseline influence and to improve the signal to noise ratio. The new lines are subjected to a least squares fit, where the previous microwave measurements of Honig et al. [1] and Clouser and Gordy [2] with totally 23 lines were included. The data were fitted with aid of the program of Herb Pickett [6] to the customary energy level expression.

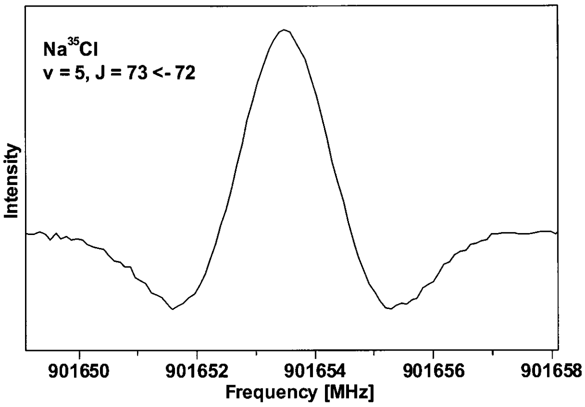

Fig. 3. Rotational Line of $Na^{35}Cl$ ($J = 73 \leftarrow 72$) in vibrationaly excited state ($v = 5$) The total excitation energy of this level is 2863 cm^{-1}.

$$F_{\nu,J} = \left[B_e - \alpha\left(\nu + \frac{1}{2}\right) + \gamma\left(\nu + \frac{1}{2}\right)^2\right] \cdot J(J+1)$$
$$- \left[D_e - \beta\left(\nu + \frac{1}{2}\right) + \delta\left(\nu + \frac{1}{2}\right)^2\right] \cdot J^2(J+1)^2$$
$$+ \left[H_e - \varepsilon\left(\nu + \frac{1}{2}\right)\right] \cdot J^3(J+1)^3.$$

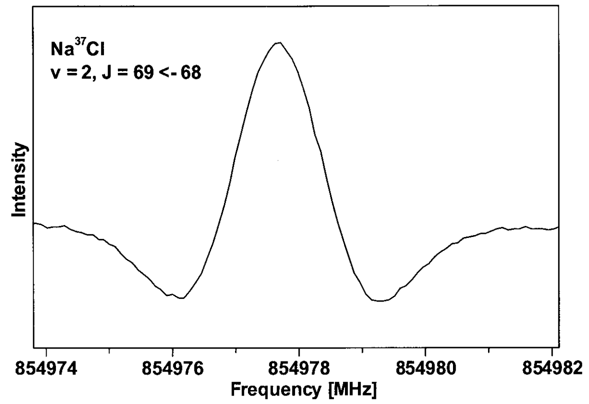

Fig. 4. Rotational Line of Na^{37}Cl (J = 69 ← 68) in vibrationaly excited state (v = 2) The total excitation energy of this level is 1629 cm^{-1}.

The resulting revised molecular parameters, including 2 new parameters (δ and ε) are shown in Table 4 for each isotopomer. Because of the astrophysical relevance, the ground state parameters B_0, D_0 and H_0 are calculated additionally and listed separately in Table 5.

On the basis of the data presented in this paper, the rotational spectrum of both isotopomers of sodium chloride can be predicted up to 2 THz with a high level of confidence for astrophysical investigations. It might be pointed out that it will be not an easy requirement to find in circumstellar sources or in star forming regions, excitation conditions based on collisional pumping excite transitions as high as $J \geq 60$ for a molecule with a permanent electric dipole moment of 9 Debye. It seems more likely that very specific excitation conditions, like e. g. line pumping, can selectively pump certain energy levels to produce an increase in higher level populations. These "unusual" excitation conditions will certainly be confined to the hot-inner cores in star formation regions. They can also be found in the central ring-regions, where the molecules are "in status nascendi" and presumably very hot, i. e. around 1500 K.

Table 4. Equilibrium Rotational Parameters for Na^{35}Cl and Na^{37}Cl.

Rotational Parameters	Na^{35}Cl (MHz)	Na^{37}Cl (MHz)
$B_e \approx Y_{01}$	6537.36521(37)	6397.28111(78)
α	48.709240(210)	47.15252(68)
γ	0.1543160(424)	0.147749(100)
D_e	$9.349225(120)\cdot 10^{-3}$	$8.953116(211)\cdot 10^{-3}$
β	$0.0202776(424)\cdot 10^{-3}$	$0.019324(142)\cdot 10^{-3}$
δ	$-0.2694(560)\cdot 10^{-6}$	$-0.2641(119)\cdot 10^{-6}$
H_e	$-1.0808(123)\cdot 10^{-9}$	$-0.9875(187)\cdot 10^{-9}$
ε	$-0.07922(410)\cdot 10^{-9}$	$-0.0600(110)\cdot 10^{-9}$

Table 5. Rotational Parameters for Na^{35}Cl and Na^{37}Cl in the Ground Vibrational State.

Rotational Constants	Na^{35}Cl (MHz)	Na^{37}Cl (MHz)
B_0	6513.04908(41)	6373.74158(66)
D_0	$9.338978(141) \cdot 10^{-3}$	$8.943327(185)\cdot 10^{-3}$
H_0	$-1.0433(144) \cdot 10^{-9}$	$-0.9623(162) \cdot 10^{-9}$

The predictions will be accessible via the Cologne Database for Molecular Spectroscopy (URL: http//:www.cdms.de) [4]. As often in the past, astronomical observations have triggered a more elaborate and refined molecular analysis, and thus NaCl provides another example of the synergy between molecular spectroscopy and radio astronomy.

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