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High-Resolution Rotational Spectrum, Dunham Coefficients, and Potential Energy Function of NaCl

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Abstract

We report laboratory spectroscopy for the first time of the $J = 1-0$ and $J = 2-1$ lines of Na^{35}Cl and Na^{37}Cl in several vibrational states. The hyperfine structure has been resolved in both transitions for all vibrational levels, which permit us to predict with high accuracy the hyperfine splitting of the rotational transitions of the two isotopologues at higher frequencies. The new data have been merged with all previous works at microwave, millimeter, and infrared wavelengths and fitted to a series of mass-independent Dunham parameters and to a potential energy function. The obtained parameters have been used to compute a new dipole moment function, from which the dipole moment for infrared transitions up to $v = 8$ has been derived. Frequency and intensity predictions are provided for all rovibrational transitions up to $J = 150$ and $v = 8$, from which the ALMA data of evolved stars can be modeled and interpreted.

Keywords

astrochemistry; molecular data; molecular processes; radiative transfer; stars: AGB and post-AGB

1 Introduction

Metal halides were found in the circumstellar envelope of IRC+10216 by Cernicharo & Guelin (1987). Recently, the spatial distribution of some of these species has been analyzed using the ALMA interferometer (Cernicharo et al. 2013; Agúndez et al. 2015; Quintana-Lacaci et al. 2016). The increase of sensitivity provided by ALMA allows us to characterize the excitation mechanisms of the transitions of metal-bearing species in different vibrational states (Quintana-Lacaci et al. 2016). Most of the metal halides found in IRC +10216 have low values for their vibrational frequencies. Hence, vibrational levels could be excited by

collisions near the star, and by infrared photons through the whole envelope. The global view of the pumping mechanism is a mandatory step to derive accurate column densities from the observation of a few rotational lines in different vibrational states. Moreover, the intensities of the rotational lines in the ground state of several species have been found to follow closely the pulsation of the star (Cernicharo et al. 2015). Hence, the modeling of the observations in evolved stars requires a precise knowledge of the Einstein coefficients and frequencies of the rovibrational transitions as done for SiS by Velilla Prieto et al. (2015).

One of the species in which the ALMA data have provided new information is sodium chloride, NaCl (Quintana-Lacaci et al. 2016). The rotational spectrum of the isotopologues of NaCl has been extensively observed in the laboratory up to $J_{\max} = 75$ and $v_{\max} = 5$ (Honig et al. 1954; Clouser & Gordy 1964; Caris et al. 2002; Timp et al. 2012); however, accurate frequencies for the lowest J values are only available for $v = 0$ (Timp et al. 2012). Additionally, hyperfine quadrupole coupling constants have been determined for Na³⁵Cl up to $v = 3$ and $v = 0$ of Na³⁷Cl (Cederberg & Miller 1969) using the molecular-beam electric resonance method. The rovibrational spectrum of the isotopologues of NaCl has also been observed in the laboratory covering up to $J_{\max} = 118$ and $v_{\max} = 8$ (Horiai et al. 1988; Uehara et al. 1989; Ram et al. 1997). As described in the next sections, we have observed in the laboratory the $J = 1-0$ and $J = 2-1$ lines of Na³⁵Cl up to $v = 6$ and of Na³⁷Cl up to $v = 4$. With these new data, together with previous experimental ones (de Leeuw et al. 1970), it is possible to derive a new potential energy function (PEF) and a more accurate dipole moment function (DMF), which allows us to include in our radiative transfer models vibrational transitions up to $v = 8$ if needed. A recent work by Barton et al. (2014) provides line lists for NaCl. Our results provide a more accurate PEF and DMF. Hence, the predicted frequencies and line intensities are more adequate for the interpretation of NaCl data in the millimeter, submillimeter, and infrared domains (Quintana-Lacaci et al. 2016).

2 Line Frequencies and Intensities for NaCl

2.1 Experimental Section

The rotational spectrum of NaCl has been obtained using two different FTMW spectrometers constructed at the University of Valladolid. A solid rod was prepared by pressing the NaCl fine powder mixed with a small amount of commercial binder and was placed in the ablation nozzle (Alonso et al. 2009; Mata et al. 2012). A picosecond Nd:YAG laser (12 mJ per pulse, 20 ps pulse width) was used as a vaporization tool. Then, NaCl neutral molecules were supersonically expanded using the flow of a carrier gas (Ne at backing pressure of 15 bars) into the spectrometer chamber. NaCl was first investigated using a chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer with a laser ablation source (Mata et al. 2012; Bermúdez et al. 2013) operating between 6.0 and 12.0 GHz to sample swiftly the rotational spectra of the different species present in the supersonic expansion. Chirped pulses of 4 μ s directly generated by the 24 Gs s⁻¹ AWG were amplified to about 300W peak power using a traveling wave tube amplifier. The amplified pulse is broadcasted into the vacuum chamber through two microwave horns, interacting with the vaporized molecules in the pulsed jet. Finally, a total of 40,000 free induction decays (4 FID emissions per gas pulse), of 10 μ s length duration, were averaged and digitized using a 50 Gs

s⁻¹ digital oscilloscope. Line widths of the order of 100 kHz FWHM were achieved. The sub-Doppler resolution LA-MB-FTMW spectrometer, described elsewhere (Alonso et al. 2009), operating from 4 to 26 GHz, was used to record the NaCl spectra with the resolution necessary to analyze the hyperfine structure due to the presence of two nuclei with $I = 3/2$ in the molecule. Microwave pulses of 0.3 μ s duration with powers of 140 mW were applied to polarize the molecules in the jet. The free induction decay (FID) was recorded for 100 μ s in the time domain at 40–100 ns sample intervals and then converted to the frequency domain by Fourier transformation. All the transitions appeared as Doppler doublets due to the parallel configuration of the molecular beam and the microwave radiation. The resonance frequency was determined as the arithmetic mean of the two Doppler components. The estimated accuracy of the frequency measurements is greater than 3 kHz. From 10 (in the case of the ground state and the lower vibrational states) to 2500 (for the higher vibrational states) averages were phase-coherently co-added to achieve reasonable signal-to-noise ratios.

2.2 Analysis of the Spectra

The previously reported (Honig et al. 1954; Clouser & Gordy 1964; Caris et al. 2002) spectroscopic constants B_0 and D_0 for the ground vibrational state for sodium chloride were used to predict the positions of the corresponding $J = 1-0$ rotational transition of both Na³⁵Cl and Na³⁷Cl isotopic species covered by our CP-FTMW spectrometer. As can be seen in Figure 1, $J = 1-0$ rotational transitions of both Na³⁵Cl and Na³⁷Cl isotopic species in the ground vibrational state were quickly found near the predicted frequencies around 13 GHz. Furthermore, several lines harmonically related with the former were also observed. They correspond to the vibrationally excited states of both Na³⁵Cl and Na³⁷Cl isotopic species, up to $\nu = 6$ for Na³⁵Cl and $\nu = 4$ for Na³⁷Cl (Figure 1).

Each line was split in a very complex hyperfine structure that follows very much the same hyperfine model in each vibrational state. These hyperfine patterns were accounted for in terms of nuclear quadrupole coupling interaction effects due to the presence of two nuclei with nonzero electric quadrupole moments ($I = 3/2$ for ²³Na, ³⁵Cl, and ³⁷Cl) in NaCl. The interaction at the nuclei of these quadrupole moments with the electric field gradient created by the rest of the molecular charges causes the coupling of the nuclear spin moments to the overall rotational momentum and gives rise to the hyperfine structure. As shown in Figure 1(c), the resolution attained with the CP-FTMW technique is not sufficient to analyze the hyperfine structure. For this reason, in the next step of the investigation NaCl was probed by taking advantage of the sub-Doppler resolution of our LA-MB-FTMW spectrometer. This made it possible to resolve the hyperfine structure of the $J = 1-0$ rotational transition for all the states. Figure 1(d) shows the hyperfine structure of the $J = 1-0$ rotational transition for the Na³⁵Cl isotopic species in the ground vibrational state. The measurements using the LA-MB-FTMW technique were extended up to 26 GHz covering the $J = 2-1$ rotational transition for the ground and all the excited states of both isotopic species.

A total of 400 hyperfine components for the 10 states of both Na³⁵Cl and Na³⁷Cl isotopologues were recorded. The complete list of the measured transition frequencies is given in Tables 1 and 2. All the observed transitions were fit independently for each vibrational state using the SPFIT program of Pickett (1991) with a Hamiltonian of the

following form (Gordy & Cook 1984): $H = H_R + H_Q$, where H_R contains rotational and centrifugal distortion parameters and H_Q the quadrupole coupling interactions. The quadrupole coupling Hamiltonian was set up in the coupled J, F, F_1 basis set, where $I_{\text{Na}} + J = F_1$ and $I_{\text{Cl}} + F_1 = F$ (Foley 1947). The energy levels involved in each transition are thus labeled with the quantum numbers J, F, F_1 . The analysis rendered the accurate rotational constant B_0 , the quartic centrifugal distortion constant D_0 , and the nuclear electric quadrupole coupling constants eQq (for ^{23}Na , ^{35}Cl , and ^{37}Cl) shown in Table 3 for the Na^{35}Cl isotopologues and in Table 4 for the Na^{37}Cl isotopologues. Our values for the quadrupole coupling constants of Na^{35}Cl agree with those reported by Cederberg & Miller (1969); however, the values for the $\nu = 0$ level of Na^{37}Cl do not agree.

2.3 Mass-independent Fit to NaCl

These center frequencies derived from the new measurements, together with all previous infrared (Horiai et al. 1988; Uehara et al. 1989; Ram et al. 1997), microwave (Timp et al. 2012), and millimeter-wave (Honig et al. 1954; Clouser & Gordy 1964; Caris et al. 2002) data found in the literature for the two isotopologues of NaCl, have been combined in a global fit to a mass-independent Dunham's series expansion for the energy levels of a diatomic molecule in a 1 state (Watson 1973, 1980):

$$E_{v,J} = \sum_{kl} \mu^{-(k/2+l)} U_{kl} [1 + m_e \Delta_{kl}^{\text{Na}} / M_{\text{Na}} + m_e \Delta_{kl}^{\text{Cl}} / M_{\text{Cl}}] \left(v + \frac{1}{2}\right)^k [J(J+1)]^l,$$

where U_{kl} are the mass-independent coefficients and Δ_{kl}^i are the Born–Oppenheimer approximation breakdown (BOB) terms. M_{Na} and M_{Cl} are the atomic masses of the corresponding isotope (see Table 3).

The fit has been carried out using a linear least-squares fitting program coupled to the MADEX code (Cernicharo 2012), which allows us to predict the frequencies of the pure rotational and rovibrational lines of the two isotopologues of NaCl from the parameters provided by the fitting routine. The data set contains 1633 experimental frequencies (236 pure rotational lines and 1397 rovibrational lines). Line frequency centers for the $J = 1-0$ and $J = 2-1$ lines of Na^{35}Cl ($\nu = 0-6$) and Na^{37}Cl ($\nu = 0-4$) were derived from the data presented in the previous section. The range of quantum numbers is $J_{\text{max}}(\text{rot}) = 75$, $\nu_{\text{max}}(\text{rot}) = 6$, $J_{\text{max}}(\text{rovib}) = 118$, and $\nu_{\text{max}}(\text{rovib}) = 8$. The lines have been weighted by the square of their estimated reciprocal uncertainty. The whole set of data is provided as supplementary information. The resulting constants are given in Table 5, together with the parameters obtained by fitting all the previous data prior to this work (i.e., including all rotational lines reported up to the work of Timp et al. 2012 and the rovibrational lines used by Ram et al. 1997). The results of the global fits available prior to our work are also given in this Table (Ram et al. 1997; Caris et al. 2004). The parameters with no uncertainty in Table 5 have been fixed to the values derived from the fitted parameters U_{k0} , U_{kl} and the Dunham relations between them and U_{jj} as provided by the code ACET of the Computer Physics Communications library written by Ogilvie (1983).

The BOB term Δ_{10}^{Cl} does not improve the quality of the fit. However, the BOB term Δ_{01}^{Cl} is needed, and accurately derived in the present work, to reproduce the observed frequencies in the global fit. The parameters U_{10} , U_{20} , U_{30} , U_{40} , U_{01} , $_{01}(\text{Cl})$, U_{11} , U_{21} , U_{31} , and U_{02} were included in the fit, providing a weighted standard deviation (wsd) of 0.818. Removing U_{02} from the fit produces a significant degradation of the wsd (1.713 versus 0.818), although its value derived from the Dunham relations differs from the fitted one by less than $4 \times 10^{-4} \text{ cm}^{-1}$ ($-6.000478571 \times 10^{-5} \text{ cm}^{-1}$ versus $-6.00014946(495) \times 10^{-5} \text{ cm}^{-1}$). We have tried to fit U_{02} and $_{02}$ simultaneously. Both parameters are strongly correlated, and we obtain $U_{02} = -6.000585(198) \times 10^{-5}$ and $_{02} = -4.72(214)$. It is rather satisfactory to see that with this fit the value derived for U_{02} differs from the one obtained from the Dunham relations by 7×10^{-10} , which provides consistency to the value derived for $_{02}$ even if it is determined only with a 2σ uncertainty in this fit. Hence, for the final fit we fixed the U_{02} value to the one derived from the Dunham relations, and we fitted $_{02}$. The value derived for this BOB parameter is much more accurate ($_{02} = -3.5545(533)$), and the wsd of the fit is the same. Since the global quality of the fit is the same and all the other parameters do not show significant changes by fitting or not $_{02}$, we give in Table 5 the parameters resulting only from the fit with this BOB parameter (this work). A comparison of the first column with the fourth column (Caris et al. 2004) of Table 5 shows the significant improvement of the rotational parameters U_{01} , U_{11} , U_{21} , and U_{31} and the determination of Δ_{01}^{Cl} and Δ_{02}^{Cl} . The complete list of lines used in the fit, fitted frequencies, observed minus calculated differences, and calculated uncertainties is provided as electronic supplementary information. A complete list of line frequencies, energies, uncertainties, and Einstein coefficients up to $J=200$ and $v=8$ ($v_{\text{max}}=8$) is provided (Tables 6–8).

2.4 Potential Energy and DMFs

The PEF used to describe the internuclear motions of the NaCl isotopologues is the Born–Oppenheimer (BO) potential previously employed by Ram et al. (1997), extended to accommodate Born–Oppenheimer breakdown (BOB) corrections. The effective potential has the form (Campbell et al. 1993; Dulick et al. 1998; Coxon & Hajigeorgiou 2000)

$$V^{\text{eff}}(r) = V^{\text{BO}}(r) + \frac{V_A(r)}{M_A} + \frac{V_B(r)}{M_B} - \frac{\hbar^2}{2\mu} [1 + q(r)] \frac{J(J+1)}{r^2} \quad (1)$$

where M_A and M_B are the sodium and chlorine atomic masses and μ is the reduced mass. The BO potential is given by (Ram et al. 1997)

$$V^{\text{BO}}(r) = D_e \left[\frac{1 - e^{-\beta(r)}}{1 - e^{-\beta(\infty)}} \right]^2 \quad (2)$$

where

$$\beta(r) = z \sum_{i=0}^4 \beta_i z^i, \quad (3)$$

$$\beta(\infty) = \sum_{i=0}^4 \beta_i, \quad (4)$$

and

$$z = \frac{r - r_e}{r + r_e}, \quad (5)$$

and the BOB potential and centrifugal correction terms are represented by the power expansions (Campbell et al. 1993; Dulick et al. 1998; Coxon & Hajigeorgiou 2000)

$$V_A(r) = \sum_{i=1} u_i^A z^i, \quad (6)$$

$$V_B(r) = \sum_{i=1} u_i^B z^i, \quad (7)$$

$$q(r) = M_A^{-1} \sum_{i=1} q_i^A z^i + M_B^{-1} \sum_{i=1} q_i^B z^i. \quad (8)$$

The potential parameters were obtained by nonlinear least-squares fitting to the whole set of 1633 infrared and microwave lines compiled for the two NaCl isotopologues, 1277 for Na³⁵Cl and 356 for Na³⁷Cl (see previous section). The fit was performed by minimizing the χ^2 function with the line position data weighted by the square of the experimental uncertainties, and employing the Levenberg–Marquardt algorithm (Levenberg 1944; Marquardt 1963) for that purpose. The rovibrational energy levels of the isotopologues needed to calculate the line positions required in the fit were computed by solving the radial Schrödinger equation with the HEG variational method (Harris et al. 1965) and with harmonic-type basis functions. The fit was run using as the starting point the BO potential function derived by Ram et al. (1997). In Table 9 we give the values of the potential parameters obtained in the fit, and in Figure 2 we show the resulting potential curve for the parent ²³Na³⁵Cl isotopologue. The reduced χ^2 value decreased from 22.332 to 0.699, with no further significant improvements achieved when adding higher-order BOB parameters.

The unweighted standard deviations for the rotational and rovibrational lines of the isotopologues were 0.0495 MHz and 0.00334 cm⁻¹, respectively.

The frequencies calculated using the PEF can be compared with those obtained from the fit to the mass-independent Dunham parameters (U_{ij}) discussed in the previous section. The differences between both methods never exceed 0.0002 MHz for the pure rotational lines and 0.00015 cm⁻¹ for the rovibrational lines of both isotopologues. Quite recently, Barton et al. (2014) determined a different PEF for NaCl also by fitting to spectroscopic data but employing a smaller number of lines, specifically 1370 in all, 1060 for Na³⁵Cl and 310 for Na³⁷Cl. The equilibrium distance was fixed to the value provided by Ram et al. (1997), and no BOB potential terms were found necessary. The input data in the Barton et al. (2014) fit were reproduced within 0.01 cm⁻¹ and better, so the present potential function is expected to be more accurate. In Tables 10–13 we give the frequencies calculated with our NaCl potential as compared with the experimental frequencies for the rotational and vibrational-rotational transitions of the two isotopologues.

The rovibrational energy levels supported by the BOB potential function fitted for the NaCl isotopologues were used to calculate their internal partition functions up to high temperatures. In this much more computationally demanding case, the variational HEG calculations were carried out using a large particle-in-box basis set of 498 functions with limits $r = [0.9–12]$ Å. We included in the partition sums all the calculated rovibrational levels of the isotopologues up to 34,000 cm⁻¹, thus accounting for nearly the entire bonding domain of the potential curves ($D_e = 34129$ cm⁻¹). Accordingly, the values of the partition functions obtained were safely converged to eight significant figures up to 1500 K and were somewhat less accurate at higher temperatures up to 3000 K. In Table 14 we give the partition functions of the isotopologues for a number of increasing temperatures, along with the values provided by Barton et al. (2014) and those included in the CDMS database (Müller et al. 2005) for comparison. As observed, partition functions calculated in this work practically reproduce the CDMS values and agree well with Barton partition functions up to 500 K. For practical purposes, we fitted the partition functions in the range of temperatures between 500 and 3000 K to the series expansion used by Vidler & Tennyson (2000):

$$\log_{10} Q(T) = \sum_{n=0}^6 a_n [\log_{10} T]^n. \quad (9)$$

The values of the a_n coefficients are given in Table 15. The absolute differences between calculated and fitted partition functions are always smaller than 0.4.

The DMF of NaCl has been previously studied experimentally by Hebert et al. (1968) and de Leeuw et al. (1970) using molecular beam electric resonance, and also by carrying out electronic calculations at different levels of theory (Zeiri & Balint-Kurti 1983; Adamowicz & Bartlett 1988; Pluta 2001; Giese & York 2004; Barton et al. 2014). In order to get accurate transition intensities, we derived in this work an empirical DMF by direct interpolation of the vibrational dipole moments of the NaCl isotopologues measured by de Leeuw et al.

(1970) for $v = 0, 1, 2, 3$ ($^{23}\text{Na}^{35}\text{Cl}$) and $v = 0, 1$ ($^{23}\text{Na}^{37}\text{Cl}$), to the third-order polynomial expansion,

$$\mu(r) = \mu_e + \mu'_e (r - r_e) + \mu''_e (r - r_e)^2 / 2 + \mu'''_e (r - r_e)^3 / 6, \quad (10)$$

with the dipole moment matrix elements being computed using the HEG calculated variational wave functions. We note that since the NaCl potential function contains BOB correction terms, the DMFs thus obtained are isotopologue dependent. Also, since there are fewer experimental dipole moments available for the $^{23}\text{Na}^{37}\text{Cl}$ isotopologue, two instead of four for $^{23}\text{Na}^{35}\text{Cl}$, we calculated the DMF of $^{23}\text{Na}^{37}\text{Cl}$ by readjusting the DMF of $^{23}\text{Na}^{35}\text{Cl}$ to the two experimental vibrational moments of $^{23}\text{Na}^{37}\text{Cl}$, for the two DMFs to have a similar degree of accuracy.

The dipole moment expansion coefficients obtained for the two isotopologues are given in Table 16, along with the corresponding BO rotational constants and harmonic vibrational frequencies. The permanent dipole moment value of $^{23}\text{Na}^{35}\text{Cl}$, $\mu_e = 8.97137$ D, agrees quite well, as expected, with the experimental value determined by de Leeuw et al. (1970) of 8.97141 D. In Figure 3, we compare the empirical DMF determined for $^{23}\text{Na}^{35}\text{Cl}$ with the most recent ab initio DMF computed by Barton et al. (2014). As observed, except for lower internuclear distances below 1.5 Å, which are not expected to have a significant effect on the NaCl rovibrational spectra, the agreement between them is good, with the ab initio function taking slightly higher values than the empirical in the spectroscopic range of internuclear distances between 1.5 and 4 Å.

We finally computed the vibrational matrix elements for the DMFs of the two NaCl isotopologues up to $v = 8$, which values are given in Tables 17 and 18, and from them, the corresponding Einstein coefficients, which values are included in Tables 19 and 20.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1.

(a) Section of the broadband CP-FTMW rotational spectrum of NaCl showing the $J = 1 \leftarrow 0$ rotational transition of both Na^{35}Cl and Na^{37}Cl isotopic species. (b) Detail of the CP-FTMW spectrum showing the less intense vibrational states of Na^{35}Cl and Na^{37}Cl isotopic species. (c) $J = 1 \leftarrow 0$ rotational transition in the ground vibrational state arising from the chirped spectrum. (d) High-resolution LA-MB-FTMW spectrum of the same transition, showing the quadrupole components labeled. Because the molecular beam and the microwave radiation travel parallel to each other, each rotational transition appears as a doublet due to the Doppler effect.

Figure 2.
Potential energy function for NaCl.

Figure 3.
Dipole moment function for NaCl.

Table 1

Measured Frequencies and Residuals (All in MHz) for the Nuclear Quadrupole Coupling Hyperfine Components of Rotational Transitions for Na³⁵Cl

ν	J_u	J_l	$F_{1,u}$	$F_{1,l}$	F_u	F_l	ν	$\nu_{\text{obs}} - \nu_{\text{cal}}$
0	1	0	1.5	1.5	0	1	13023.79786	-0.00005
0	...	...	1.5	1.5	1	2	13024.27114	-0.00077
0	...	...	1.5	1.5	1	0	13024.27114	-0.00093
0	...	...	1.5	1.5	3	3	13024.36323	-0.00059
0	...	...	1.5	1.5	2	1	13025.13322	0.00304
0	...	...	1.5	1.5	2	3	13025.13322	0.00304
0	...	...	2.5	1.5	3	2	13026.06100	-0.00048
0	...	...	2.5	1.5	2	2	13026.06100	-0.00052
0	...	...	2.5	1.5	4	3	13026.62929	0.00186
0	...	...	2.5	1.5	1	1	13027.19242	-0.00093
0	...	...	0.5	1.5	1	2	13027.85048	-0.00056
0	...	...	0.5	1.5	1	0	13027.85048	-0.00073
0	...	...	0.5	1.5	2	1	13028.12337	-0.00135
0	...	...	0.5	1.5	2	3	13028.12337	-0.00135
0	2	1	2.5	0.5	2	1	26048.59622	-0.00070
0	...	...	2.5	2.5	1	1	26049.60731	0.00143
0	...	...	2.5	2.5	3	4	26049.71563	-0.00057

(This table is available in its entirety in machine-readable form.)

Table 2

Measured Frequencies and Residuals (All in MHz) for the Nuclear Quadrupole Coupling Hyperfine Components of Rotational Transitions for Na³⁷Cl

ν	J_u	J_l	$F_{1,u}$	$F_{1,l}$	F_u	F_l	ν	$\nu_{\text{obs}} - \nu_{\text{cal}}$
0	1	0	1.5	1.5	0	1	12745.42316	0.00077
0	...	...	1.5	1.5	1	2	12745.83913	-0.00090
0	...	...	1.5	1.5	1	0	12745.83913	-0.00103
0	...	...	1.5	1.5	3	2	12745.91817	-0.00071
0	...	...	1.5	1.5	3	3	12745.91817	-0.00078
0	...	...	1.5	1.5	2	2	12746.58018	-0.00041
0	...	...	1.5	1.5	2	1	12746.58018	-0.00048
0	...	...	1.5	1.5	2	3	12746.58018	-0.00048
0	...	...	2.5	1.5	3	2	12747.45737	0.00102
0	...	...	2.5	1.5	3	3	12747.45737	0.00095
0	...	...	2.5	1.5	2	2	12747.47145	0.00163
0	...	...	2.5	1.5	4	3	12747.95463	0.00169
0	...	...	2.5	1.5	1	1	12748.43764	-0.00079
0	...	...	0.5	1.5	1	2	12749.07307	-0.00113
0	...	...	0.5	1.5	1	0	12749.07307	-0.00126
0	...	...	0.5	1.5	1	1	12749.07307	-0.00120
0	...	...	0.5	1.5	2	2	12749.30136	-0.00085
0	...	...	0.5	1.5	2	1	12749.30136	-0.00091
0	...	...	0.5	1.5	2	3	12749.30136	-0.00091
0	2	1	2.5	2.5	1	1	25492.63678	0.00141
0	...	...	2.5	2.5	3	4	25492.72126	0.00012

(This table is available in its entirety in machine-readable form.)

Table 3Experimental Spectroscopic Parameters in MHz for the Ground and Excited States of Na³⁵Cl

Parameter	References	$\nu=0$	$\nu=1$	$\nu=2$	$\nu=3$	$\nu=4$	$\nu=5$	$\nu=6$
B_0		6513.04940(33)	6464.64907(33)	6416.55727(29)	6368.77404(33)	6321.29898(29)	6274.13229(24)	6227.27383(49)
$D_0 \times 10^3$		9.333(44)	9.323(44)	9.308(38)	9.288(43)	9.212(40)	9.180(34)	9.243(66)
eQq (Na)	Present	-5.687(15)	-5.608(10)	-5.5461(51)	-5.5076(47)	-5.4356(48)	-5.3680(67)	-5.364(14)
	Cederberg et al.	-5.674(50)	-5.600(20)	-5.538(12)	-5.488(15)			
eQq (Cl)	Present	-5.632(16)	-5.8227(96)	-5.9945(47)	-6.1526(45)	-6.3305(43)	-6.4973(59)	-6.639(11)
	Cederberg et al.	-5.642(50)	-5.832(20)	-6.007(12)	-6.168(15)			
N		46	44	43	40	23	15	12
rms kHz		1.5	1.5	1.3	1.4	1.2	0.9	1.2

Table 4Experimental Spectroscopic Parameters in MHz for the Ground and Excited States of Na³⁷Cl

Parameter	References	$\nu=0$	$\nu=1$	$\nu=2$	$\nu=3$	$\nu=4$
B_0		6373.74124(34)	6326.88506(29)	6280.32470(34)	6234.05998(33)	6188.08922(28)
$D_0 \times 10^3$		8.924(44)	8.939(38)	8.968(44)	8.979(44)	8.815(40)
eQq (Na)	Present	-5.6655(26)	-5.6147(38)	-5.5747(72)	-5.536(11)	-5.549(17)
	Cederberg et al.	-5.6458(10)				
eQq (Cl)	Present	-4.4567(33)	-4.5807(42)	-4.6953(85)	-4.814(12)	-4.878(19)
	Cederberg et al.	-4.4798(10)				
N		54	44	36	21	11
rms kHz		1.6	1.4	1.4	1.1	0.7

Table 5*U_{ij}* Mass-independent Dunham Coefficients for NaCl (in Units of cm⁻¹ amu^(*i/2+j*))

<i>U_{ij}</i>	This Work	All Previous Data	Caris et al. (2004)	Ram et al. (1997)
<i>U</i> ₁₀	1358.20726 (151)	1358.20721(152)	1358.20633(544)	1358.20342(153)
<i>U</i> ₂₀	-24.63629 (283)	-24.63618(284)	-24.63029(833)	-24.63228(283)
<i>U</i> ₃₀	0.030804 (190)	0.30797(192)	0.30100(345)	0.305157(192)
<i>U</i> ₄₀ × 10 ³	-2.798 (415)	-2.787(418)	...	-2.054(420)
<i>U</i> ₀₁	3.024725746 (339)	3.024723997(355)	3.024723941(477)	3.024682410(486)
₀₁ (Cl)	-0.87496 (724)	-0.83774(753)	-0.84558(926)	
<i>U</i> ₁₁ × 10 ²	-8.3934484 (212)	-8.3934386(221)	-8.3933958(324)	-8.3926480(1690)
<i>U</i> ₂₁ × 10 ⁴	9.91229 (320)	9.91019(336)	9.90280(233)	9.8594(107)
<i>U</i> ₃₁ × 10 ⁷	-4.34 (135)	-3.27(143)	...	...
<i>U</i> ₀₂ × 10 ⁵	-6.000478571 (0)	-6.00014997(532)	-6.0000172(623)	-6.0003(0)
₀₂ (Cl)	-3.5545 (533)	...	...	...
<i>U</i> ₁₂ × 10 ⁷	4.826568385 (0)	4.82695158(0)	4.84742(881)	4.8324(0)
<i>U</i> ₂₂ × 10 ⁸	2.714803269 (0)	2.71260512(0)	...	2.5841(0)
<i>U</i> ₃₂ × 10 ⁹	-1.149308265 (0)	-1.15530148(0)	...	-0.2721(0)
<i>U</i> ₀₃ × 10 ¹¹	-9.135631671 (0)	-9.13556517(0)	-9.5863(847)	-9.1179(0)
<i>U</i> ₁₃ × 10 ¹¹	2.620691965 (0)	2.61762507(0)	2.5678(109)	2.5565(0)
<i>U</i> ₂₃ × 10 ¹³	-3.531736550 (0)	-3.25554340(0)	...	-1.5197(0)
<i>U</i> ₀₄ × 10 ¹⁵	-4.856082193 (0)	-4.85548283(0)	...	-4.8462(0)
<i>U</i> ₁₄ × 10 ¹⁶	6.064198217 (0)	6.06016863(0)	...	5.4755(0)
<i>U</i> ₂₄ × 10 ¹⁷	-6.590055738 (0)	-6.82993569(0)	...	3.4469(0)
<i>U</i> ₀₅ × 10 ²⁰	9.299150780 (0)	9.27302690(0)	...	8.7537(0)
<i>U</i> ₁₅ × 10 ²⁰	1.010681105 (0)	1.10449012(0)	...	1.6829(0)
<i>U</i> ₀₆ × 10 ²⁴	4.553780423 (0)	4.54519100(0)	...	4.0752(0)
<i>U</i> ₁₆ × 10 ²⁵	-9.714676585 (0)	-10.24218460(0)	...	1.3648(0)
<i>U</i> ₀₇ × 10 ²⁸	2.068519161 (0)	2.10469022(0)	...	2.1918(0)

Table 6

Observed and Fitted Frequencies (Mass-independent Fit)

Isotopologue	J_u	J_l	ν_u	ν_l	Freq. Obs.	Unc	Freq. Calc.	Cal. Unc.	Units	Obs–Calc	R
Na ³⁵ Cl	1	0	0	0	13026.0615	0.0030	13026.0623	0.0003	MHz	–0.0006	1
Na ³⁵ Cl	1	0	0	0	13026.0633	0.0030	13026.0623	0.0003	MHz	0.0012	2
Na ³⁵ Cl	1	0	1	1	12929.2608	0.0030	12929.2609	0.0003	MHz	–0.0002	1
Na ³⁵ Cl	1	0	2	2	12833.0773	0.0030	12833.0771	0.0002	MHz	0.0001	1
Na ³⁵ Cl	1	0	3	3	12737.5109	0.0030	12737.5105	0.0003	MHz	0.0003	1
Na ³⁵ Cl	1	0	4	4	12642.5611	0.0030	12642.5610	0.0003	MHz	0.0003	1
Na ³⁵ Cl	1	0	5	5	12548.2279	0.0030	12548.2283	0.0005	MHz	0.0001	1
Na ³⁵ Cl	1	0	6	6	12454.5107	0.0030	12454.5122	0.0008	MHz	–0.0005	1
Na ³⁵ Cl	2	1	0	0	26051.8989	0.0030	26051.9004	0.0007	MHz	–0.0012	1
Na ³⁵ Cl	2	1	1	1	25858.2979	0.0030	25858.2983	0.0005	MHz	–0.0005	1

References. (1) This work; (2) Timp et al. 2012; (3) Clouser & Gordy 1964; (4) Caris et al. 2002; (5) Horiai et al. 1988; (6) Uehara et al. 1989; (7) Ram et al. 1997.

(This table is available in its entirety in machine-readable form.)

Table 7

Predicted Frequencies and Intensities for NaCl

J_u	J_l	v_u	v_l	$\nu_{\text{calculated}}$	$\text{Unc}(1\sigma)$	Units	$E_{\text{upp}}(\text{K})$	$A_{ij}(\text{s}^{-1})$
1	0	8	8	12268.92900	0.00200	MHz	4019.5	6.46E-07
1	0	7	7	12361.41300	0.00100	MHz	3534.1	6.52E-07
1	0	6	6	12454.51200	0.00010	MHz	3043.9	6.58E-07
1	0	5	5	12548.22800	0.00010	MHz	2548.9	6.64E-07
1	0	4	4	12642.56100	0.00010	MHz	2049.2	6.70E-07
1	0	3	3	12737.51100	0.00010	MHz	1544.5	6.76E-07
1	0	2	2	12833.07700	0.00010	MHz	1034.9	6.82E-07
1	0	1	1	12929.26100	0.00010	MHz	520.3	6.89E-07
1	0	0	0	13026.06200	0.00010	MHz	0.6	6.95E-07
2	1	8	8	24537.63800	0.00300	MHz	4020.7	6.20E-06

(This table is available in its entirety in machine-readable form.)

Table 8Predicted Frequencies and Intensities for Na³⁷Cl

J_u	J_l	v_u	v_l	$\nu_{\text{calculated}}$	Unc(1 σ)	Units	$E_{\text{upp}}(\text{K})$	$A_{ij}(\text{s}^{-1})$
1	0	8	8	12014.28900	0.00200	MHz	3978.1	6.07E-07
1	0	7	7	12103.86700	0.00100	MHz	3497.5	6.12E-07
1	0	6	6	12194.03500	0.00010	MHz	3012.2	6.17E-07
1	0	5	5	12284.79400	0.00010	MHz	2522.3	6.23E-07
1	0	4	4	12376.14300	0.00010	MHz	2027.6	6.29E-07
1	0	3	3	12468.08200	0.00010	MHz	1528.1	6.34E-07
1	0	2	2	12560.61300	0.00010	MHz	1023.9	6.40E-07
1	0	1	1	12653.73500	0.00010	MHz	514.7	6.46E-07
1	0	0	0	12747.44700	0.00010	MHz	0.6	6.51E-07
2	1	8	8	24028.36700	0.00300	MHz	3979.2	5.82E-06

(This table is available in its entirety in machine-readable form.)

Table 9

Internuclear Potential Energy Parameters for the NaCl Molecule

Parameter	Value	Uncertainty
$D_e(\text{cm}^{-1})$	34120.0	...
$r_e(\text{\AA})$	2.360789166	9.93×10^{-9}
β_0	4.2246415	2.27×10^{-6}
β_1	0.1501821	4.13×10^{-6}
β_2	0.3957719	3.53×10^{-5}
β_3	8.0479335	6.25×10^{-4}
β_4	-5.6559597	3.45×10^{-4}
$q_1^{\text{Na}}(\text{amu})$	0.000969141	7.03×10^{-6}
$q_1^{\text{Cl}}(\text{amu})$	-0.000507845	9.57×10^{-6}
$u_1^{\text{Na}}(\text{cm}^{-1} \text{ amu})$	53.3350	5.40×10^{-3}
$u_1^{\text{Cl}}(\text{cm}^{-1} \text{ amu})$	-137.6536	1.14×10^{-2}
$m(^{23}\text{Na})(\text{amu})$	22.98976928196	...
$m(^{35}\text{Cl})(\text{amu})$	34.968852682	...
$m(^{37}\text{Cl})(\text{amu})$	36.965902602	...

Table 10Comparison between Observed and Calculated Frequencies (in MHz) of Rotational Transitions of Na³⁵Cl

v	J_u	J_l	Observed	Calculated	$\nu_{\text{obs}} - \nu_{\text{cal}}$
0	1	0	13026.0615 ^a	13026.0622	−0.0007
0	2	1	26051.8989 ^a	26051.9003	−0.0014
0	8	7	104189.740 ^b	104189.669	0.071
0	12	11	156248.600 ^b	156248.640	−0.040
0	14	13	182262.890 ^b	182262.883	0.007
0	15	14	195265.390 ^b	195265.409	−0.019
0	17	16	221260.150 ^b	221260.148	0.002
0	18	17	234251.830 ^b	234251.914	−0.084

Notes.^aThis work.^bClouser & Gordy (1964).

(This table is available in its entirety in machine-readable form.)

Table 11Comparison between Observed and Calculated Frequencies (in MHz) of Rotational Transitions of Na³⁷Cl

ν	J_u	J_l	Observed ^a	Calculated	$\nu_{\text{obs}} - \nu_{\text{cal}}$
0	1	0	12747.4468*	12747.4467	0.0001
0	2	1	25494.6794*	25494.6788	0.0006
0	9	8	114701.330**	114701.263	0.067
0	15	14	191091.620**	191091.497	0.123
0	17	16	216531.440**	216531.439	0.001
0	40	39	507609.238	507609.216	0.022
0	41	40	520180.602	520180.581	0.021

Note.

^aFrom Caris et al. (2002) except those marked with an asterisk, which are reported in the present work, and those marked with a double asterisk, which are from Clouser et al. (1964).

(This table is available in its entirety in machine-readable form.)

Table 12

Comparison between Observed and Calculated Frequencies (in cm^{-1}) of Vibrational-rotational Transitions of Na^{35}Cl

$\nu_u - \nu_l$	$J_u - J_l$	Observed	Calculated	Obs-Cal
1-0	1-0	...	361.5828	...
1-0	2-1	...	362.0108	...
1-0	3-2	362.4283	362.4356	-0.0073
1-0	4-3	362.8527	362.8571	-0.0044
1-0	5-4	363.2724	363.2754	-0.0030
1-0	6-5	363.6873	363.6904	-0.0031
1-0	7-6	...	364.1022	...
1-0	8-7	364.5144	364.5106	0.0038

(This table is available in its entirety in machine-readable form.)

Table 13

Comparison between Observed and Calculated Frequencies (in cm^{-1}) of Vibrational-rotational Transitions of Na^{37}Cl

$\nu_u - \nu_l$	$J_u - J_l$	Observed	Calculated	Obs-Cal
1-0	1-0	...	357.7210	...
1-0	2-1	...	358.1400	...
1-0	3-2	...	358.5558	...
1-0	4-3	...	358.9684	...
1-0	5-4	...	359.3780	...
1-0	6-5	359.7674	359.7843	-0.0169
1-0	7-6	360.1705	360.1875	-0.0170

(This table is available in its entirety in machine-readable form.)

Table 14Comparison of Na^{35}Cl and Na^{37}Cl Internal Partition Functions

$T(\text{K})$	Na^{35}Cl			Na^{37}Cl		
	Barton et al. (2014)	Present	CDMS	Barton et al.	Present	CDMS
9.375	30.3338	30.330750	30.3307	...	30.986296	30.9862
18.75	60.3352	60.329972	60.3299	...	61.641247	61.6411
37.5	120.3556	120.34573	120.3455	...	122.96878	122.9685
75	240.6984	240.67745	240.6770	245.9697	245.94916	245.9486
150	496.6455	496.55497	496.5538	508.1159	508.02279	508.0214
225	802.3712	802.11992	802.1167	822.1828	821.92296	821.9190
300	1173.0397	1172.5442	1172.5403	1203.5434	1203.0306	1203.0172
500	2506.9232	2505.3912	2505.0340	2577.6122	2576.0208	...
1000	8161.702	8154.9921	...	8409.530	8402.5860	...
1500	17333.48	17317.348	...	17874.21	17857.514	...
2000	30394.77	30264.287	...	31253.05	31221.509	...
2500	47362.31	47321.903	...	48873.17	48822.063	...
3000	68909.60	68844.495	...	71120.07	71052.957	...

Table 15

Fitting Parameters for the Partition Functions.

	Na^{35}Cl	Na^{37}Cl
a_0	31.97195003	35.92320561
a_1	-60.27247749	-67.83543064
a_2	51.02199242	57.04026152
a_3	-23.34154924	-25.88650231
a_4	6.153399044	6.757279312
a_5	-0.8751871901	-0.9514728014
a_6	0.05216181420	0.05617142531

Note. Fits are valid for temperatures between 500 and 3000 K.

Table 16

Spectroscopic Constants and Dipole Moment Coefficients for the NaCl Isotopologues

Parameter	$^{23}\text{Na}^{35}\text{Cl}$	$^{23}\text{Na}^{37}\text{Cl}$
$B_e(\text{cm}^{-1})$	0.2180641	0.2133912
$B_e(\text{MHz})$	6537.39682	6397.30622
$\omega_e(\text{cm}^{-1})$	364.6894	360.7608
$\mu_e(\text{D})$	8.971368	8.971489
$\mu'_e (\text{D } \text{\AA}^{-1})$	4.277686	4.265881
$\mu''_e (\text{D } \text{\AA}^{-2})$	1.098930	1.098930
$\mu'''_e (\text{D } \text{\AA}^{-3})$	-0.864938	-0.864938

Table 17Calculated Vibrational Dipole Moment Matrix Elements (D) for Na³⁵Cl

v'/v''	0	1	2	3	4	5	6	7	8
0	9.00117	...	...	...	...	...	...	...	...
1	0.24805	9.06016	...	...	...	...	...	...	...
2	-0.10611E-1	0.35237	9.12144	...	...	...	...	...	...
3	0.82081E-3	-0.18452E-1	0.43349	9.18231	...	...	...	...	...
4	0.86767E-4	-0.16468E-2	0.26199E-1	-0.50277	9.24367	...	...	...	...
5	0.11145E-4	-0.19457E-3	0.26120E-2	-0.33955E-1	-0.56459	9.30552	...	...	...
6	0.16367E-5	-0.27381E-4	0.33792E-3	-0.37053E-2	-0.41749E-1	-0.62120	9.36786	...	...
7	0.26468E-6	-0.43468E-5	0.51370E-4	-0.51754E-3	-0.49163E-2	-0.49590E-1	-0.67391	9.43069	...
8	0.45827E-7	-0.75250E-6	0.87239E-5	-0.84113E-4	-0.73378E-3	-0.62372E-2	-0.57483E-1	-0.72358	9.49401

Table 18Calculated Vibrational Dipole Moment Matrix Elements (D) for Na³⁷Cl

v'/v''	0	1	2	3	4	5	6	7	8
0	9.00090	...	...	...	...	...	...	...	...
1	0.24611	9.06005	...	...	...	...	...	...	...
2	0.10434E-1	-0.34972	9.11974	...	...	...	...	...	...
3	0.86730E-3	-0.18114E-1	-0.43038	9.17999	...	...	...	...	...
4	0.98840E-4	-0.17359E-2	-0.25676E-1	-0.49936	9.24078	...	...	...	...
5	-0.13697E-4	0.22096E-3	0.27468E-2	0.33224E-1	0.56101	9.30214	...	...	...
6	0.21789E-5	-0.33521E-4	-0.38259E-3	-0.38872E-2	-0.40783E-1	0.61753	9.36405	...	...
7	0.38473E-6	-0.57572E-5	-0.62647E-4	-0.58419E-3	-0.51456E-2	0.48364E-1	-0.67025	9.42652	...
8	-0.73763E-7	0.10866E-5	0.11498E-4	0.10219E-3	0.82580E-3	-0.65128E-2	0.55971E-1	0.72001	9.48956

Table 19Calculated Vibrational Einstein Coefficients (s^{-1}) for Na^{35}Cl

v'/v''	0	1	2	3	4	5	6	7
1	0.90899	...	...	...	...	...	...	...
2	0.13115E-1	1.78148	...	...	...	...	...	...
3	0.26102E-3	0.38516E-1	2.61850	...	...	...	...	...
4	0.68141E-5	0.10205E-2	0.75409E-1	3.42166	...	...	...	...
5	0.21642E-6	0.33278E-4	0.24934E-2	0.12303	4.19014	...	...	...
6	0.79510E-8	0.12687E-5	0.97494E-4	0.48731E-2	0.18064	4.92670	...	...
7	0.32540E-9	0.54459E-7	0.43373E-5	0.22212E-3	0.83328E-2	0.24754	5.63167	...
8	0.14353E-10	0.25546E-8	0.21305E-6	0.11292E-4	0.43367E-3	0.13026E-1	0.32306	6.30598

Table 20Calculated Vibrational Einstein Coefficients (s^{-1}) for Na^{37}Cl

v'/v''	0	1	2	3	4	5	6	7
1	0.86646	...	...	...	...	...	...	...
2	0.12282E-1	1.69979	...	...	...	...	...	...
3	0.28229E-3	0.35961E-1	2.50102	...	...	...	...	...
4	0.85665E-5	0.10987E-2	0.70195E-1	3.27114	...	...	...	...
5	0.31675E-6	0.41592E-4	0.26724E-2	0.11418	4.01112	...	...	...
6	0.13653E-7	0.18430E-5	0.12115E-3	0.52000E-2	0.16716	4.72189	...	...
7	0.66640E-9	0.92611E-7	0.62542E-5	0.27443E-3	0.88528E-2	0.22839	5.40436	...
8	0.36047E-10	0.51648E-8	0.35886E-6	0.16167E-4	0.53277E-3	0.13779E-1	0.29720	6.05943