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Fourier Transform Infrared Emission Spectroscopy of NaCl and KCl

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The infrared emission spectra of NaCl and KCl have been recorded at high resolution with a Fourier transform spectrometer. A total of 929 lines belonging to 8 vibrational bands, 1–0 to 8–7, for Na^{35}Cl, 252 lines of 1–0, 2–1, and 3–2 bands of Na^{37}Cl, and 355 lines of 1–0, 2–1, 3–2, and 4–3 bands of K^{35}Cl have been measured and combined with the existing microwave and millimeter-wave data to obtain a set of refined molecular constants. The data for Na^{35}Cl and Na^{37}Cl have also been fitted to determine the Dunham Y_{ij} constants and mass-reduced Dunham constants U_{ij}. In one fit all U_{ij}'s were treated as adjustable parameters while in a second fit only U_{i0}'s and U_{i1}'s were allowed to vary freely with the remaining U_{ij} constants determined by the constraints imposed by the Dunham model. In addition, the internuclear potential energy parameters were determined by fitting the entire NaCl data set to the eigenvalues of the Schrödinger equation containing a parameterized potential energy function.

INTRODUCTION

Diatomic alkali halides are high temperature species of fundamental importance. Their low vapor pressures and highly ionic nature present challenges for gas phase experimental studies (*1*). There are many studies of NaCl (*2–9*) and KCl (*2–4, 10–14*) in the near-ultraviolet and microwave regions. NaCl (*2, 3*) and KCl (*10–12*) have a long series of unresolved bands in the near ultraviolet which have been called ''fluctuation bands'' (*15*). These bands arise from transitions between individual vibrational levels of one electronic state and a rather flat portion of the potential curve of the other state. The ground state of these molecules are relatively well characterized experimentally by infrared and microwave studies.

The NaCl and KCl molecules are important species in the combustion of coal. Coal contains substantial amounts of inorganic material that are responsible for slagging and fouling of coal-fired power plants. NaCl and KCl can, in principle, be monitored by the absorption or emission using the vibration–rotation bands.

The low resolution infrared spectra of NaCl and KCl were first observed in absorption by Rice and Klemperer (*4*), who determined the ground state vibrational constants ω_e and $\omega_e x_e$ from band head positions in conjunction with the ground state B values, previously reported by Honig *et al.* (*5*) in a microwave study. The high-resolution infrared vibration–rotation spectra of Na^{35}Cl and Na^{37}Cl have been studied by Horiai *et al.* (*6*) and Uehara *et al.* (*7*) by infrared diode laser spectroscopy. These measurements were used to determine a set of Dunham parameters Y_{ij} for the ground state of NaCl. The potential constants for the ground state were also calculated by Uehara *et al.* (*7*) in a least squares fit using the Dunham equations. In a separate study, Uehara *et al.* (*13*) investigated the infrared emission spectra of KCl at a resolution of 0.1 cm^{-1} and provided a set of Dunham coefficients for the ground electronic state.

Some matrix isolation studies of NaCl and KCl are also available. Martin and Schaber (*8*) observed the infrared spectra of NaCl while Ismail *et al.* (*14*) observed both NaCl and KCl in a solid argon matrix.

Extensive microwave data for NaCl and KCl have been published (*5, 9*). In the initial work of Honig *et al.* (*5*), several alkali halide molecules were investigated and they reported rotational constants and electric dipole moments. In another study, Clouser and Gordy (*9*) measured the millimeter-wave molecular beam absorption spectra of NaCl, KCl, and several other alkali chlorides. In this work they measured a number of pure rotational transitions in several vibrational levels of the ground state and reported improved values for B_e, α_e and γ_e for most of the molecules studied. They also provided indirect estimates for the vibrational constants.

The alkali halides have dissociative UV absorption spectra. Silver *et al.* (*16*) measured the absolute UV dissociation cross sections for gas phase NaCl and Novick *et al.* (*17*) measured the photodetachment spectra of the alkali halide negative ions NaCl$^-$, NaBr$^-$, and NaI$^-$.

The ionic nature of the alkali halide ground states has led to the development of simple potential energy functions such as the Rittner model (*18–20*). There are a number of theoretical calculations of electronic structure and other properties available for NaCl (*21–29*) and KCl (*30–35*). Bounds and Hinchliffe (*23*) performed *ab initio* calculations of the SCF pair potential and polarizability of NaCl and Leasure *et al.* (*26*) calculated the electronic structure. Swaminathan

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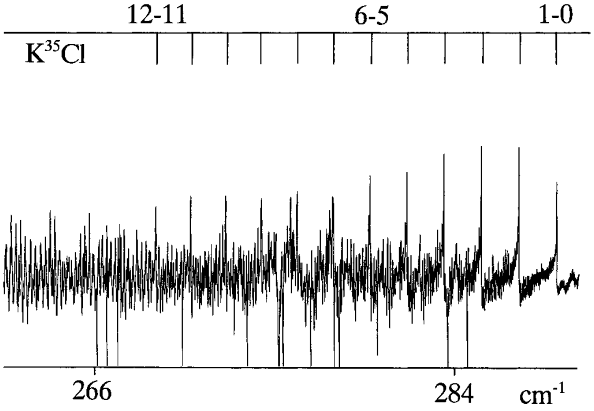

FIG. 1. A compressed portion of infrared bands of KCl marking the band heads in the 1–0 sequence of $K^{35}Cl$.

TABLE 1
The *R* Head Positions (in cm^{-1}) of Vibration–Rotation Bands in the 1–0 Sequence of $K^{35}Cl$

Band v′ - v″	Head Position (cm^{-1})
1 - 0	296.702
2 - 1	294.181
3 - 2	291.680
4 - 3	289.201
5 - 4	286.742
6 - 5	284.303
7 - 6	281.884
8 - 7	279.488
9 - 8	277.110
10 - 9	274.752
11 - 10	272.414
12 - 11	270.012

et al. (*28*) calculated the potential energy of NaCl with large atomic basis sets and extensive configuration interaction. Bounds and Hinchliffe (*32*) studied the polarizability of KCl and Zeiri and Balint-Kurti (*34*) studied the potential energy curves and transition dipole moments of NaCl, KCl, and several other alkali halides.

Some of the alkali halides are also of astrophysical importance. Recently the presence of NaCl and KCl, along with AlCl and AlF, has been established in the carbon star IRC + 10216 by millimeter-wave astronomers (*36*). Normally metals are depleted onto grains in the interstellar medium but this discovery indicates that metal-containing molecules are more abundant in cool circumstellar envelopes. Unfortunately, the infrared spectra of many of the metal halide diatomic molecules have not been investigated at high resolution and their vibrational constants are not precisely known. The high-resolution studies of these molecules are, therefore, particularly important since high-quality spectroscopic parameters are necessary for infrared searches for these molecules.

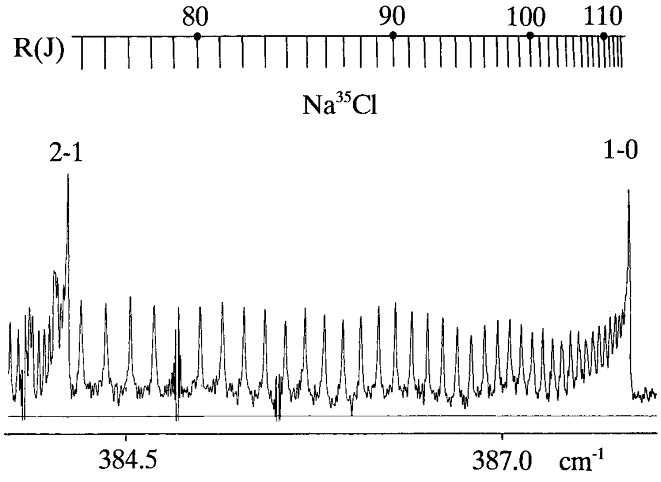

FIG. 2. An expanded portion of the 1–0 band of $Na^{35}Cl$ near the *R* head.

In this paper we report on the observation of vibration–rotation bands of $Na^{35}Cl$, $Na^{37}Cl$, and $K^{35}Cl$. Eight bands, 1–0, 2–1, 3–2, 4–3, 5–4, 6–5, 7–6, and 8–7, for $Na^{35}Cl$, three bands, 1–0, 2–1, and 3–2, for $Na^{37}Cl$, and four bands, 1–0, 2–1, 3–2, and 4–3, for $K^{35}Cl$ have been observed at a resolution of 0.01 cm^{-1}. Analysis of the data has provided improved molecular constants and the Dunham coefficients Y_{ij} for these species. The $Na^{35}Cl$ and $Na^{37}Cl$ data sets have also been fitted together to obtain mass-reduced Dunham constants U_{ij} and the constants of a parameterized potential energy function.

EXPERIMENTAL

The high-resolution emission spectra of $Na^{35}Cl$, $Na^{37}Cl$, and $K^{35}Cl$ were recorded with a Bruker IFS 120HR Fourier transform spectrometer at the University of Waterloo. The molecules were vaporized in an alumina tube furnace by heating NaCl or KCl gradually until the operating temperature of 1000°C was achieved. A 3.5 μm mylar beam splitter and a Si:B detector (NaCl) or a 4 K bolometer (KCl) were used to record the spectra. The cell was pressurized with about 5 Torr of argon to avoid the deposition of the solid material on the KRS-5 windows. The resolution was 0.01 cm^{-1} for both molecules. The final interferograms for NaCl

TABLE 2

Observed Rotational Lines (in cm^{-1}) in the Vibration–Rotation Bands of Na^{35}Cl and Na^{37}Cl

v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C
Na^{35}Cl																	
0	2	0	1	0.8689712a	-264	1	56	0	55	380.1195	13	1	9	0	10	356.6637	16
1	2	1	1	0.8625167a	-231	1	57	0	56	380.3561	-10	1	10	0	11	356.1926	-32
2	2	2	1	0.8561423a	192	1	58	0	57	380.5933	7	1	11	0	12	355.7249	-13
3	2	3	1	0.8497178a	-299	1	59	0	58	380.8261	18	1	12	0	13	355.2537	1
0	8	0	7	3.47539564b	31	1	60	0	59	381.0519	-6	1	13	0	14	354.7737	-41
0	12	0	11	5.21189229b	-1	1	61	0	60	381.2786	16	1	14	0	15	354.2974	-15
0	14	0	13	6.07963560b	16	1	62	0	61	381.4982	4	1	15	0	16	353.8169	1
0	15	0	14	6.51335231b	8	1	63	0	62	381.7140	-10	1	16	0	17	353.3329	12
0	17	0	16	7.38044417b	15	1	64	0	63	381.9296	12	1	17	0	18	352.8412	-23
0	18	0	17	7.81379997b	-14	1	65	0	64	382.1393	10	1	18	0	19	352.3510	-11
0	21	0	20	9.11303913b	-12	1	66	0	65	382.3432	-13	1	19	0	20	351.8582	5
0	24	0	23	10.41086497b	-20	1	67	0	66	382.5482	12	1	20	0	21	351.3605	3
1	14	1	13	6.03443400b	-18	1	68	0	67	382.7475	18	1	21	0	22	350.8618	21
1	15	1	14	6.46492681b	8	1	69	0	68	382.9416	9	1	22	0	23	350.3634	73
1	18	1	17	7.75569711b	17	1	70	0	69	383.1325	3	1	23	0	24	349.8491	-2
1	24	1	23	10.33340939b	12	1	71	0	70	383.3218	20	1	24	0	25	349.3420	24
2	15	2	14	6.41680752b	-24	1	72	0	71	383.5027	-11	1	25	0	26	348.8275	6
1	3	0	2	362.4283	-70	1	73	0	72	383.6837	-3	1	26	0	27	348.3125	14
1	4	0	3	362.8527	-42	1	74	0	73	383.8602	-4	1	27	0	28	347.7903	-20
1	5	0	4	363.2724	-27	1	75	0	74	384.0346	13	1	28	0	29	347.2715	11
1	6	0	5	363.6873	-28	1	76	0	75	384.2024	1	1	29	0	30	346.7440	-16
1	8	0	7	364.5144	40	1	77	0	76	384.3674	-2	1	30	0	31	346.2173	-5
1	9	0	8	364.9176	21	1	78	0	77	384.5289	-3	1	31	0	32	345.6861	-9
1	10	0	9	365.3188	14	1	79	0	78	384.6870	1	1	32	0	33	345.1529	-3
1	11	0	10	365.7155	-5	1	81	0	80	384.9916	5	1	33	0	34	344.6194	30
1	12	0	11	366.1119	6	1	82	0	81	385.1384	8	1	34	0	35	344.0770	3
1	13	0	12	366.5005	-27	1	83	0	82	385.2803	0	1	35	0	36	343.5292	-48
1	14	0	13	366.8955	37	1	84	0	83	385.4198	6	1	36	0	37	342.9910	26
1	15	0	14	367.2807	35	1	85	0	84	385.5546	4	1	37	0	38	342.4364	-34
1	16	0	15	367.6604	13	1	86	0	85	385.6853	-3	1	38	0	39	341.8879	-4
1	17	0	16	368.0428	51	1	87	0	86	385.8123	-8	1	39	0	40	341.3322	-16
1	18	0	17	368.4120	-9	1	88	0	87	385.9356	-11	1	40	0	41	340.7763	-1
1	19	0	18	368.7829	-20	1	89	0	88	386.0555	-11	1	41	0	42	340.2133	-29
1	20	0	19	369.1527	-7	1	90	0	89	386.1726	-1	1	42	0	43	339.6488	-41
1	21	0	20	369.5211	26	1	91	0	90	386.2849	0	1	43	0	44	339.0791	-78
1	22	0	21	369.8813	10	1	92	0	91	386.3923	-9	1	44	0	45	338.5167	-12
1	23	0	22	370.2380	-6	1	93	0	92	386.4972	-6	1	45	0	46	337.9399	-62
1	24	0	23	370.5906	-30	1	94	0	93	386.5986	2	1	46	0	47	337.3622	-92
1	25	0	24	370.9467	15	1	95	0	94	386.6951	-2	1	47	0	48	336.7887	-51
1	26	0	25	371.2934	0	1	96	0	95	386.7886	3	2	3	1	2	358.9248	-19
1	27	0	26	371.6356	-25	1	97	0	96	386.8776	3	2	4	1	3	359.3419	-32
1	28	0	27	371.9798	4	1	98	0	97	386.9643	18	2	5	1	4	359.7587	-15
1	29	0	28	372.3169	-5	1	99	0	98	387.0444	5	2	6	1	5	360.1705	-16
1	30	0	29	372.6519	1	1	100	0	99	387.1219	5	2	8	1	7	360.9890	28
1	31	0	30	372.9817	-11	1	101	0	100	387.1950	-0	2	9	1	8	361.3886	3
1	32	0	31	373.3111	7	1	102	0	101	387.2650	3	2	10	1	9	361.7867	-5
1	33	0	32	373.6320	-25	1	103	0	102	387.3320	15	2	11	1	10	362.1852	24
1	34	0	33	373.9554	3	1	104	0	103	387.3905	-19	2	12	1	11	362.5740	-11
1	35	0	34	374.2739	17	1	105	0	104	387.4499	-5	2	13	1	12	362.9612	-29
1	36	0	35	374.5851	-8	1	106	0	105	387.5034	-11	2	14	1	13	363.3523	26
1	37	0	36	374.8961	0	1	107	0	106	387.5516	-31	2	15	1	14	363.7320	-1
1	38	0	37	375.2052	24	1	108	0	107	387.5996	-13	2	16	1	15	364.1106	-5
1	39	0	38	375.5006	-54	1	109	0	108	387.6400	-31	2	17	1	16	364.4850	-19
1	40	0	39	375.8057	0	1	110	0	109	387.6812	-3	2	18	1	17	364.8553	-40
1	41	0	40	376.1035	16	1	111	0	110	387.7139	-21	2	19	1	18	365.2298	15
1	42	0	41	376.3954	8	1	112	0	111	387.7481	17	2	20	1	19	365.5939	-2
1	43	0	42	376.6846	10	1	113	0	112	387.7742	12	2	21	1	20	365.9572	8
1	44	0	43	376.9689	-3	1	114	0	113	387.7972	17	2	22	1	21	366.3145	-9
1	45	0	44	377.2505	-8	1	115	0	114	387.8164	23	2	23	1	22	366.6693	-17
1	46	0	45	377.5294	-4	1	116	0	115	387.8292	4	2	24	1	23	367.0289	56
1	47	0	46	377.8065	18	1	117	0	116	387.8419	24	2	25	1	24	367.3711	-10
1	48	0	47	378.0710	-51	1	118	0	117	387.8458	-4	2	26	1	25	367.7226	50
1	49	0	48	378.3423	-16	1	1	0	2	360.2810	20	2	27	1	26	368.0618	21
1	50	0	49	378.6085	4	1	2	0	3	359.8413	32	2	28	1	27	368.3975	-9
1	51	0	50	378.8714	26	1	3	0	4	359.3926	-13	2	29	1	28	368.7312	-25
1	52	0	51	379.1249	-10	1	4	0	5	358.9496	30	2	30	1	29	369.0708	53
1	53	0	52	379.3791	-3	1	6	0	7	358.0445	21	2	31	1	30	369.3940	0
1	54	0	53	379.6285	-7	1	7	0	8	357.5864	10	2	32	1	31	369.7237	47
1	55	0	54	379.8749	-6	1	8	0	9	357.1226	-28	2	33	1	32	370.0431	26

TABLE 2—*Continued*

v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C
2	34	1	33	370.3587	1	2	104	1	103	383.6722	-28	3	19	2	18	361.7074	1
2	35	1	34	370.6727	-6	2	105	1	104	383.7317	-4	3	20	2	19	362.0687	-15
2	36	1	35	370.9872	27	2	106	1	105	383.7846	-7	3	21	2	20	362.4283	-15
2	37	1	36	371.2934	12	2	108	1	107	383.8795	-5	3	22	2	21	362.7855	-5
2	38	1	37	371.5964	-1	2	109	1	108	383.9208	-7	3	23	2	22	363.1383	-6
2	39	1	38	371.9009	36	2	110	1	109	383.9585	-6	3	24	2	23	363.4889	5
2	40	1	39	372.1935	-11	2	111	1	110	383.9924	-4	3	25	2	24	363.8348	1
2	41	1	40	372.4877	-7	2	112	1	111	384.0235	10	3	26	2	25	364.1785	11
2	42	1	41	372.7781	-6	2	113	1	112	384.0477	-7	3	27	2	26	364.5144	-25
2	43	1	42	373.0660	6	2	114	1	113	384.0692	-10	3	28	2	27	364.8553	24
2	44	1	43	373.3469	-19	2	115	1	114	384.0880	-2	3	29	2	28	365.1856	-0
2	45	1	44	373.6320	35	2	116	1	115	384.1031	9	3	30	2	29	365.5157	8
2	46	1	45	373.9046	-2	2	117	1	116	384.1154	31	3	31	2	30	365.8411	4
2	47	1	46	374.1809	35	2	2	1	3	356.3523	35	3	32	2	31	366.1594	-38
2	48	1	47	374.4467	1	2	3	1	4	355.9063	-16	3	33	2	32	366.4840	18
2	49	1	48	374.7121	-1	2	4	1	5	355.4658	20	3	34	2	33	366.7982	4
2	50	1	49	374.9738	-5	2	5	1	6	355.0189	23	3	35	2	34	367.1087	-13
2	51	1	50	375.2335	6	2	8	1	9	353.6590	30	3	36	2	35	367.4195	7
2	52	1	51	375.4875	-3	2	9	1	10	353.2014	52	3	37	2	36	367.7226	-15
2	53	1	52	375.7376	-15	2	10	1	11	352.7360	26	3	38	2	37	368.0270	10
2	54	1	53	375.9865	-4	2	11	1	12	352.2694	21	3	39	2	38	368.3235	-8
2	56	1	55	376.4724	7	2	12	1	13	351.7984	3	3	40	2	39	368.6188	-5
2	57	1	56	376.7085	-3	2	13	1	14	351.3278	20	3	41	2	40	368.9102	-6
2	58	1	57	376.9422	1	2	14	1	15	350.8512	8	3	42	2	41	369.1958	-29
2	59	1	58	377.1724	4	2	15	1	16	350.3746	27	3	43	2	42	369.4854	22
2	60	1	59	377.3983	1	2	16	1	17	349.8908	5	3	44	2	43	369.7634	-8
2	61	1	60	377.6204	-3	2	17	1	18	349.4050	-6	3	45	2	44	370.0431	14
2	62	1	61	377.8400	3	2	18	1	19	348.9179	0	3	46	2	45	370.3161	4
2	63	1	62	378.0554	5	2	19	1	20	348.4267	-4	3	47	2	46	370.5906	44
2	64	1	63	378.2666	-0	2	20	1	21	347.9357	24	3	48	2	47	370.8479	-53
2	65	1	64	378.4744	-2	2	21	1	22	347.4379	16	3	49	2	48	371.1160	-7
2	66	1	65	378.6789	-1	2	22	1	23	346.9347	-17	3	50	2	49	371.3762	-4
2	67	1	66	378.8820	24	2	23	1	24	346.4318	-16	3	51	2	50	371.6356	26
2	68	1	67	379.0762	-4	2	24	1	25	345.9290	16	3	52	2	51	371.8904	46
2	69	1	68	379.2711	12	2	25	1	26	345.4174	-11	3	53	2	52	372.1351	0
2	70	1	69	379.4594	-2	2	26	1	27	344.9032	-32	3	54	2	53	372.3817	9
2	71	1	70	379.6397	-59	2	27	1	28	344.3908	-6	3	55	2	54	372.6238	8
2	72	1	71	379.8274	-4	2	28	1	29	343.8727	-6	3	56	2	55	372.8642	27
2	73	1	72	380.0067	3	2	29	1	30	343.3576	52	3	57	2	56	373.0992	26
2	74	1	73	380.1833	20	2	30	1	31	342.8297	14	3	58	2	57	373.3278	-2
2	75	1	74	380.3561	37	2	31	1	32	342.3018	4	3	59	2	58	373.5548	-10
2	76	1	75	380.5197	-1	2	32	1	33	341.7706	-9	3	60	2	59	373.7810	8
2	77	1	76	380.6838	2	2	33	1	34	341.2390	4	3	61	2	60	374.0013	5
2	78	1	77	380.8446	10	2	34	1	35	340.6957	-71	3	62	2	61	374.2193	15
2	79	1	78	380.9992	-7	2	35	1	36	340.1666	25	3	63	2	62	374.4307	-5
2	80	1	79	381.1539	15	2	36	1	37	339.6219	-4	3	64	2	63	374.6410	-1
2	81	1	80	381.3012	0	2	37	1	38	339.0791	13	3	65	2	64	374.8460	-13
2	82	1	81	381.4465	4	2	38	1	39	338.5260	-42	3	66	2	65	375.0487	-11
2	83	1	82	381.5857	-17	2	39	1	40	337.9782	-16	3	67	2	66	375.2491	4
2	84	1	83	381.7259	10	2	40	1	41	337.4265	0	3	68	2	67	375.4446	7
2	85	1	84	381.8577	-9	2	41	1	42	336.8675	-28	3	69	2	68	375.6355	-1
2	86	1	85	381.9896	11	2	42	1	43	336.3154	42	3	70	2	69	375.8221	-14
2	87	1	86	382.1162	15	2	43	1	44	335.7478	-15	3	71	2	70	376.0075	-3
2	88	1	87	382.2368	-2	2	44	1	45	335.1800	-44	3	72	2	71	376.1862	-22
2	89	1	88	382.3546	-10	3	3	2	2	355.4544	13	3	74	2	73	376.5400	14
2	90	1	89	382.4693	-11	3	5	2	4	356.2826	21	3	75	2	74	376.7085	3
2	91	1	90	382.5820	6	3	6	2	5	356.6872	-21	3	76	2	75	376.8741	1
2	92	1	91	382.6879	-6	3	7	2	6	357.0904	-45	3	77	2	76	377.0359	-3
2	93	1	92	382.7924	5	3	8	2	7	357.4990	18	3	78	2	77	377.1940	-7
2	94	1	93	382.8911	-3	3	9	2	8	357.8953	-10	3	79	2	78	377.3497	2
2	95	1	94	382.9879	8	3	10	2	9	358.2932	10	3	80	2	79	377.5002	-3
2	96	1	95	383.0782	-7	3	11	2	10	358.6864	17	3	81	2	80	377.6488	10
2	97	1	96	383.1673	4	3	12	2	11	359.0756	15	3	82	2	81	377.7910	-4
2	98	1	97	383.2495	-16	3	13	2	12	359.4565	-36	3	83	2	82	377.9324	12
2	99	1	98	383.3332	18	3	14	2	13	359.8413	-17	3	84	2	83	378.0710	37
2	100	1	99	383.4073	-6	3	15	2	14	360.2227	3	3	85	2	84	378.1998	1
2	101	1	100	383.4804	-0	3	16	2	15	360.6025	39	3	86	2	85	378.3272	-11
2	102	1	101	383.5473	-18	3	17	2	16	360.9721	6	3	87	2	86	378.4533	2
2	103	1	102	383.6145	5	3	18	2	17	361.3425	15	3	88	2	87	378.5742	-1

TABLE 2—*Continued*

v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C
3	89	2	88	378.6938	22	4	13	3	12	355.9945	32	4	84	3	83	374.4467	3
3	90	2	89	378.8042	-8	4	14	3	13	356.3713	1	4	85	3	84	374.5742	-31
3	91	2	90	378.9146	-3	4	15	3	14	356.7499	22	4	86	3	85	374.7021	-26
3	92	2	91	379.0219	11	4	16	3	15	357.1226	15	4	87	3	86	374.8270	-12
3	93	2	92	379.1249	19	4	17	3	16	357.4883	-28	4	88	3	87	374.9480	-1
3	94	2	93	379.2211	-3	4	18	3	17	357.8537	-41	4	89	3	88	375.0630	-11
3	95	2	94	379.3144	-15	4	19	3	18	358.2185	-28	4	90	3	89	375.1785	21
3	96	2	95	379.4064	-3	4	20	3	19	358.5819	5	4	91	3	90	375.2860	10
3	97	2	96	379.4929	-7	4	21	3	20	358.9390	7	4	92	3	91	375.3895	-3
3	98	2	97	379.5767	-1	4	22	3	21	359.2934	16	4	93	3	92	375.4875	-33
3	99	2	98	379.6521	-39	4	23	3	22	359.6417	-3	4	94	3	93	375.5905	24
3	100	2	99	379.7296	-19	4	24	3	23	359.9902	13	4	95	3	94	375.6793	-22
3	101	2	100	379.8042	11	4	25	3	24	360.3322	-1	4	96	3	95	375.7715	3
3	102	2	101	379.8749	40	4	26	3	25	360.6737	11	4	97	3	96	375.8570	-1
3	103	2	102	379.9333	-15	4	27	3	26	361.0076	-18	4	98	3	97	375.9387	-5
3	104	2	103	379.9955	7	4	28	3	27	361.3425	-3	4	99	3	98	376.0215	41
3	105	2	104	380.0533	22	4	29	3	28	361.6718	-11	4	100	3	99	376.0903	-17
3	106	2	105	380.1033	-1	4	31	3	30	362.3244	15	4	101	3	100	376.1631	5
3	107	2	106	380.1446	-73	4	32	3	31	362.6443	14	4	103	3	102	376.2909	-15
3	108	2	107	380.1968	3	4	33	3	32	362.9612	18	4	104	3	103	376.3536	19
3	109	2	108	380.2367	-5	4	34	3	33	363.2724	-1	4	105	3	104	376.4089	19
3	110	2	109	380.2722	-19	4	35	3	34	363.5850	27	4	106	3	105	376.4611	26
3	111	2	110	380.3014	-56	4	36	3	35	363.8877	-9	4	108	3	107	376.5507	6
3	112	2	111	380.3372	11	4	37	3	36	364.1925	10	4	111	3	110	376.6595	11
3	113	2	112	380.3561	-51	4	38	3	37	364.4936	26	4	112	3	111	376.6846	-21
3	114	2	113	380.3791	-33	4	39	3	38	364.7857	-13	4	113	3	112	376.7085	-28
3	115	2	114	380.3986	-12	4	40	3	39	365.0821	25	4	114	3	113	376.7244	-74
3	116	2	115	380.4129	-3	4	41	3	40	365.3681	-6	4	115	3	114	376.7481	-5
3	117	2	116	380.4254	27	4	42	3	41	365.6558	14	4	116	3	115	376.7606	-8
3	3	2	4	352.4549	-19	4	43	3	42	365.9343	-23	4	117	3	116	376.7725	21
3	5	2	6	351.5728	6	4	44	3	43	366.2161	8	4	3	3	4	349.0375	-28
3	6	2	7	351.1244	-7	4	45	3	44	366.4840	-66	4	4	3	5	348.6060	32
3	7	2	8	350.6754	5	4	46	3	45	366.7615	-9	4	5	3	6	348.1629	6
3	8	2	9	350.2217	1	4	47	3	46	367.0289	-18	4	6	3	7	347.7188	3
3	10	2	11	349.3059	2	4	48	3	47	367.2959	4	4	7	3	8	347.2715	-1
3	11	2	12	348.8431	1	4	49	3	48	367.5543	-25	4	8	3	9	346.8215	-3
3	12	2	13	348.3775	2	4	50	3	49	367.8133	-13	4	9	3	10	346.3662	-25
3	13	2	14	347.9067	-18	4	52	3	51	368.3235	39	4	10	3	11	345.9128	2
3	14	2	15	347.4379	14	4	53	3	52	368.5675	6	4	11	3	12	345.4553	20
3	15	2	16	346.9643	27	4	54	3	53	368.8107	2	4	12	3	13	344.9871	-39
3	16	2	17	346.4844	8	4	55	3	54	369.0491	-16	4	13	3	14	344.5232	-24
3	17	2	18	346.0052	27	4	56	3	55	369.2839	-34	4	14	3	15	344.0558	-14
3	18	2	19	345.5195	12	4	57	3	56	369.5211	7	4	15	3	16	343.5885	27
3	19	2	20	345.0315	4	4	58	3	57	369.7495	-3	4	16	3	17	343.1114	1
3	20	2	21	344.5365	-43	4	59	3	58	369.9747	-10	4	17	3	18	342.6338	1
3	21	2	22	344.0460	-16	4	60	3	59	370.1977	-4	4	18	3	19	342.1510	-20
3	22	2	23	343.5579	66	4	61	3	60	370.4173	4	4	19	3	20	341.6663	-32
3	23	2	24	343.0533	13	4	62	3	61	370.6334	13	4	20	3	21	341.1799	-29
3	24	2	25	342.5530	33	4	63	3	62	370.8479	43	4	21	3	22	340.6957	26
3	25	2	26	342.0441	-4	4	64	3	63	371.0513	-3	4	22	3	23	340.1981	-24
3	26	2	27	341.5320	-41	4	65	3	64	371.2562	2	4	23	3	24	339.7008	-41
3	27	2	28	341.0279	31	4	66	3	65	371.4569	2	4	25	3	26	338.7027	-19
3	28	2	29	340.5125	19	4	67	3	66	371.6522	-17	4	26	3	27	338.1970	-31
3	29	2	30	339.9929	-5	4	68	3	67	371.8478	4	4	28	3	29	337.1873	53
3	30	2	31	339.4731	-1	4	69	3	68	372.0377	3	4	29	3	30	336.6718	31
3	31	2	32	338.9502	0	4	70	3	69	372.2223	-13	4	30	3	31	336.1601	79
3	32	2	33	338.4227	-14	4	71	3	70	372.4085	22	4	31	3	32	335.6320	-10
3	34	2	35	337.3622	-10	4	72	3	71	372.5854	2	5	3	4	2	348.6060	-40
3	35	2	36	336.8319	36	4	73	3	72	372.7574	-32	5	4	4	3	349.0193	1
3	36	2	37	336.2920	13	4	74	3	73	372.9345	22	5	5	4	4	349.4289	39
3	37	2	38	335.7478	-22	4	75	3	74	373.0992	-10	5	6	4	5	349.8327	49
3	38	2	39	335.2043	-22	4	76	3	75	373.2642	-4	5	8	4	7	350.6262	25
4	6	3	5	353.2427	14	4	77	3	76	373.4237	-16	5	9	4	8	351.0187	19
4	7	3	6	353.6448	10	4	78	3	77	373.5822	-0	5	10	4	9	351.4097	30
4	8	3	7	354.0434	2	4	79	3	78	373.7368	13	5	11	4	10	351.7984	50
4	9	3	8	354.4373	-19	4	80	3	79	373.8879	28	5	12	4	11	352.1733	-35
4	10	3	9	354.8301	-20	4	81	3	80	374.0301	-9	5	13	4	12	352.5572	2
4	11	3	10	355.2211	-7	4	82	3	81	374.1718	-13	5	14	4	13	352.9328	-13
4	12	3	11	355.6087	5	4	83	3	82	374.3111	-5	5	15	4	14	353.3051	-27

TABLE 2—*Continued*

v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C
5	16	4	15	353.6786	3	5	87	4	86	371.2393	-2	6	43	5	42	358.9496	5
5	17	4	16	354.0434	-22	5	88	4	87	371.3611	29	6	44	5	43	359.2260	27
5	18	4	17	354.4081	-14	5	89	4	88	371.4730	0	6	45	5	44	359.4992	50
5	19	4	18	354.7737	35	5	90	4	89	371.5845	4	6	46	5	45	359.7674	58
5	20	4	19	355.1257	-19	5	91	4	90	371.6928	13	6	47	5	46	360.0246	-11
5	21	4	20	355.4804	-13	5	92	4	91	371.7937	-14	6	48	5	47	360.2810	-51
5	22	4	21	355.8329	5	5	93	4	92	371.9009	58	6	49	5	48	360.5406	-26
5	23	4	22	356.1760	-40	5	94	4	93	371.9941	29	6	50	5	49	360.7988	20
5	24	4	23	356.5270	28	5	95	4	94	372.0848	12	6	51	5	50	361.0463	-6
5	25	4	24	356.8650	-0	5	96	4	95	372.1731	9	6	52	5	51	361.2972	36
5	27	4	26	357.5350	-18	5	97	4	96	372.2574	3	6	53	5	52	361.5393	26
5	28	4	27	357.8676	-1	5	98	4	97	372.3369	-13	6	54	5	53	361.7750	-14
5	29	4	28	358.1997	45	5	100	4	99	372.4877	-14	6	55	5	54	362.0074	-52
5	30	4	29	358.5272	78	5	101	4	100	372.5582	-6	6	56	5	55	362.2447	-6
5	31	4	30	358.8426	24	5	102	4	101	372.6238	-9	6	57	5	56	362.4751	7
5	32	4	31	359.1586	10	5	103	4	102	372.6870	2	6	58	5	57	362.7022	21
5	33	4	32	359.4704	-13	5	105	4	104	372.7976	-21	6	59	5	58	362.9246	24
5	34	4	33	359.7830	6	5	106	4	105	372.8508	4	6	60	5	59	363.1383	-24
5	35	4	34	360.0888	-9	5	4	4	5	345.2290	50	6	61	5	60	363.3523	-35
5	36	4	35	360.3937	1	5	5	4	6	344.7880	14	6	62	5	61	363.5713	40
5	37	4	36	360.6920	-21	5	6	4	7	344.3452	-10	6	63	5	62	363.7729	-25
5	38	4	37	360.9890	-22	5	7	4	8	343.9017	-10	6	64	5	63	363.9814	17
5	39	4	38	361.2861	13	5	8	4	9	343.4583	22	6	65	5	64	364.1785	-21
5	40	4	39	361.5723	-28	5	9	4	10	343.0078	14	6	66	5	65	364.3776	-3
5	41	4	40	361.8617	-3	5	10	4	11	342.5530	-6	6	67	5	66	364.5692	-25
5	42	4	41	362.1447	-7	5	11	4	12	342.0966	-12	6	68	5	67	364.7664	46
5	43	4	42	362.4283	30	5	12	4	13	341.6350	-39	6	69	5	68	364.9467	-16
5	44	4	43	362.7022	4	5	13	4	14	341.1799	29	6	70	5	69	365.1332	19
5	45	4	44	362.9760	11	5	14	4	15	340.7116	-4	6	71	5	70	365.3060	-47
5	46	4	45	363.2481	36	5	15	4	16	340.2418	-22	6	72	5	71	365.4860	-4
5	47	4	46	363.5113	7	5	16	4	17	339.7751	21	6	73	5	72	365.6558	-28
5	48	4	47	363.7729	-4	5	20	4	21	337.8656	69	6	74	5	73	365.8259	-12
5	49	4	48	364.0344	20	5	21	4	22	337.3760	33	6	75	5	74	365.9987	65
5	50	4	49	364.2877	-4	5	22	4	23	336.8776	-60	6	76	5	75	366.1594	60
5	51	4	50	364.5406	3	5	23	4	24	336.3888	-28	6	77	5	76	366.3145	34
5	52	4	51	364.7857	-33	6	8	5	7	347.2386	1	6	78	5	77	366.4672	21
5	53	4	52	365.0320	-22	6	9	5	8	347.6306	20	6	79	5	78	366.6176	21
5	54	4	53	365.2742	-16	6	10	5	9	348.0166	9	6	80	5	79	366.7615	-8
5	55	4	54	365.5157	17	6	11	5	10	348.4044	50	6	82	5	81	367.0451	2
5	56	4	55	365.7457	-29	6	12	5	11	348.7832	32	6	83	5	82	367.1821	15
5	57	4	56	365.9806	9	6	13	5	12	349.1577	3	6	84	5	83	367.3134	7
5	58	4	57	366.2040	-33	6	14	5	13	349.5288	-27	6	85	5	84	367.4381	-30
5	59	4	58	366.4320	7	6	15	5	14	349.9060	36	6	86	5	85	367.5701	43
5	60	4	59	366.6511	-6	6	16	5	15	350.2729	29	6	87	5	86	367.6886	17
5	61	4	60	366.8672	-15	6	17	5	16	350.6362	17	6	88	5	87	367.8011	-31
5	62	4	61	367.0784	-36	6	18	5	17	351.0043	86	6	89	5	88	367.9191	12
5	63	4	62	367.2959	41	6	19	5	18	351.3605	70	6	90	5	89	368.0270	-8
5	64	4	63	367.4975	-4	6	20	5	19	351.7097	14	6	91	5	90	368.1358	17
5	65	4	64	367.7062	57	6	21	5	20	352.0599	2	6	92	5	91	368.2354	-12
5	66	4	65	367.9014	18	6	22	5	21	352.4090	12	6	93	5	92	368.3373	19
5	67	4	66	368.0971	21	6	23	5	22	352.7519	-7	6	94	5	93	368.4283	-22
5	68	4	67	368.2888	20	6	24	5	23	353.0921	-21	6	95	5	94	368.5200	-18
5	69	4	68	368.4740	-11	6	25	5	24	353.4322	-2	6	96	5	95	368.6058	-36
5	70	4	69	368.6589	-8	6	26	5	25	353.7676	2	6	98	5	97	368.7680	-54
5	71	4	70	368.8404	-2	6	27	5	26	354.0979	-10	6	99	5	98	368.8523	26
5	72	4	71	369.0182	2	6	28	5	27	354.4240	-33	6	100	5	99	368.9234	11
5	73	4	72	369.1958	40	6	29	5	28	354.7562	39	6	101	5	100	368.9918	6
5	74	4	73	369.3649	30	6	30	5	29	355.0767	28	6	102	5	101	369.0616	54
5	75	4	74	369.5373	90	6	31	5	30	355.3910	-12	6	104	5	103	369.1772	22
5	76	4	75	369.6933	22	6	32	5	31	355.7097	25	6	106	5	105	369.2839	52
5	77	4	76	369.8507	4	6	33	5	32	356.0145	-44	6	109	5	108	369.4086	30
5	79	4	78	370.1556	-21	6	34	5	33	356.3238	-33	6	110	5	109	369.4426	23
5	80	4	79	370.3049	-9	6	35	5	34	356.6324	5	6	112	5	111	369.5026	43
5	81	4	80	370.4503	0	6	36	5	35	356.9328	-7	6	113	5	112	369.5211	-5
5	82	4	81	370.5906	-4	6	38	5	37	357.5230	-33	6	114	5	113	369.5373	-37
5	83	4	82	370.7302	20	6	39	5	38	357.8179	2	6	115	5	114	369.5551	-14
5	84	4	83	370.8606	-10	6	40	5	39	358.1063	6	6	117	5	116	369.5781	19
5	85	4	84	370.9872	-41	6	41	5	40	358.3894	-8	7	15	6	14	346.5349	38
5	86	4	85	371.1160	-13	6	42	5	41	358.6731	18	7	16	6	15	346.9023	64

TABLE 2—*Continued*

v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C
7	17	6	16	347.2582	6	7	58	6	57	359.2260	-19	8	36	7	35	350.1175	8
7	18	6	17	347.6194	34	7	59	6	58	359.4421	-61	8	37	7	36	350.4158	56
7	19	6	18	347.9719	6	7	60	6	59	359.6641	-9	8	38	7	37	350.7058	55
7	20	6	19	348.3259	27	7	61	6	60	359.8743	-39	8	39	7	38	350.9881	10
7	21	6	20	348.6725	6	7	62	6	61	360.0888	9	8	40	7	39	351.2687	-17
7	22	6	21	349.0193	19	7	63	6	62	360.2944	3	8	41	7	40	351.5525	20
7	23	6	22	349.3608	13	7	64	6	63	360.4998	30	8	42	7	41	351.8281	9
7	24	6	23	349.6953	-31	7	65	6	64	360.6920	-38	8	43	7	42	352.1026	21
7	25	6	24	350.0313	-28	7	66	6	65	360.8883	-32	8	44	7	43	352.3678	-26
7	26	6	25	350.3634	-31	7	67	6	66	361.0821	-14	8	45	7	44	352.6389	19
7	27	6	26	350.6942	-14	7	68	6	67	361.2675	-45	8	46	7	45	352.8988	-13
7	28	6	27	351.0187	-26	7	69	6	68	361.4579	10	8	47	7	46	353.1544	-54
7	29	6	28	351.3465	28	7	70	6	69	361.6396	13	8	48	7	47	353.4194	32
7	30	6	29	351.6615	-15	7	71	6	70	361.8173	12	8	49	7	48	353.6693	3
7	32	6	31	352.2905	-8	7	73	6	72	362.1649	41	8	50	7	49	353.9187	2
7	33	6	32	352.6029	25	7	74	6	73	362.3244	-35	8	51	7	50	354.1658	12
7	34	6	33	352.9101	38	7	75	6	74	362.4924	11	8	52	7	51	354.4081	8
7	35	6	34	353.2148	60	7	76	6	75	362.6443	-69	8	53	7	52	354.6424	-41
7	36	6	35	353.5106	26	7	77	6	76	362.8088	14	8	54	7	53	354.8861	40
7	37	6	36	353.8030	-7	7	78	6	77	362.9612	12	8	55	7	54	355.1126	-19
7	38	6	37	354.0979	18	7	79	6	78	363.1045	-45	8	56	7	55	355.3394	-39
7	39	6	38	354.3914	62	7	80	6	79	363.2481	-63	8	57	7	56	355.5714	28
7	40	6	39	354.6712	3	7	81	6	80	363.3938	-23	8	58	7	57	355.7849	-56
7	41	6	40	354.9523	-9	7	82	6	81	363.5330	-11	8	59	7	58	356.0145	55
7	42	6	41	355.2323	2	8	20	7	19	344.9735	14	8	60	7	59	356.2242	3
7	43	6	42	355.5098	22	8	21	7	20	345.3165	-17	8	61	7	60	356.4329	-24
7	44	6	43	355.7849	53	8	22	7	21	345.6574	-35	8	62	7	61	356.6466	33
7	45	6	44	356.0606	122	8	23	7	22	345.9947	-58	8	63	7	62	356.8485	8
7	46	6	45	356.3238	102	8	25	7	24	346.6641	-58	8	64	7	63	357.0499	12
7	47	6	46	356.5811	56	8	26	7	25	346.9932	-65	8	66	7	65	357.4388	-12
7	48	6	47	356.8357	18	8	27	7	26	347.3230	-32	8	67	7	66	357.6329	26
7	49	6	48	357.0904	16	8	28	7	27	347.6492	-3	8	68	7	67	357.8179	7
7	50	6	49	357.3395	-9	8	29	7	28	347.9719	24	8	69	7	68	358.0011	6
7	51	6	50	357.5864	-20	8	30	7	29	348.2874	13	8	70	7	69	358.1777	-26
7	52	6	51	357.8342	11	8	31	7	30	348.5960	-34	8	71	7	70	358.3533	-32
7	53	6	52	358.0759	16	8	32	7	31	348.9051	-45	8	72	7	71	358.5272	-19
7	54	6	53	358.3102	-18	8	33	7	32	349.2124	-39	8	73	7	72	358.6993	11
7	55	6	54	358.5565	103	8	34	7	33	349.5142	-55	8	74	7	73	358.8618	-19
7	56	6	55	358.7786	16	8	35	7	34	349.8173	-26	8	75	7	74	359.0275	19
7	57	6	56	359.0087	45												
									Na^{37}Cl								
0	2	0	1	0.8503850a	-182	1	21	0	20	365.4860	-57	1	45	0	44	373.0992	86
1	2	1	1	0.8441673a	104	1	22	0	21	365.8411	-54	1	46	0	45	373.3626	-24
2	2	2	1	0.8379230a	-276	1	23	0	22	366.2040	59	1	47	0	46	373.6466	106
0	9	0	8	3.8260245b	280	1	25	0	24	366.8955	40	1	48	0	47	373.9046	12
0	15	0	14	6.3741303b	182	1	26	0	25	367.2423	90	1	49	0	48	374.1718	43
0	17	0	16	7.2227114b	15	1	27	0	26	367.5701	-15	1	50	0	49	374.4307	27
1	9	1	8	3.7978951b	56	1	28	0	27	367.9014	-54	1	52	0	51	374.9480	91
1	12	1	11	5.0629549b	-68	1	29	0	28	368.2354	-31	1	53	0	52	375.1907	17
1	15	1	14	6.3272482b	-222	1	30	0	29	368.5675	4	1	54	0	53	375.4335	-21
1	6	0	5	359.7674	-126	1	31	0	30	368.8951	29	1	55	0	54	375.6793	4
1	7	0	6	360.1705	-127	1	32	0	31	369.2150	10	1	57	0	56	376.1631	84
1	8	0	7	360.5741	-92	1	33	0	32	369.5373	49	1	58	0	57	376.3954	80
1	9	0	8	360.9721	-80	1	34	0	33	369.8507	31	1	60	0	59	376.8435	14
1	12	0	11	362.1447	-68	1	35	0	34	370.1651	57	1	61	0	60	377.0580	-63
1	13	0	12	362.5300	-55	1	37	0	36	370.7777	50	1	62	0	61	377.2859	31
1	14	0	13	362.9146	-18	1	38	0	37	371.0715	-28	1	63	0	62	377.5002	24
1	16	0	15	363.6696	13	1	39	0	38	371.3762	36	1	64	0	63	377.7046	-47
1	17	0	16	364.0344	-51	1	40	0	39	371.6675	0	1	65	0	64	377.9161	-11
1	18	0	17	364.4049	-26	1	41	0	40	371.9627	38	1	66	0	65	378.1231	15
1	19	0	18	364.7664	-57	1	42	0	41	372.2574	104	1	67	0	66	378.3272	48
1	20	0	19	365.1332	-3	1	44	0	43	372.8143	14	1	69	0	68	378.7128	-4

TABLE 2—*Continued*

v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C
1	70	0	69	378.9146	113	2	21	1	20	362.0074	7	2	7	1	8	350.4037	-39
1	71	0	70	379.0936	39	2	22	1	21	362.3576	-13	2	8	1	9	349.9642	32
1	72	0	71	379.2711	-14	2	23	1	22	362.7022	-56	2	9	1	10	349.5142	30
1	73	0	72	379.4594	77	2	24	1	23	363.0561	27	2	10	1	11	349.0571	-14
1	74	0	73	379.6397	123	2	25	1	24	363.3938	-21	2	11	1	12	348.6060	32
1	75	0	74	379.8042	48	2	26	1	25	363.7320	-30	2	12	1	13	348.1434	-6
1	77	0	76	380.1446	121	2	27	1	26	364.0720	11	2	13	1	14	347.6806	-17
1	78	0	77	380.3014	78	2	28	1	27	364.4049	15	2	14	1	15	347.2123	-52
1	80	0	79	380.6115	66	2	30	1	29	365.0585	-1	2	15	1	16	346.7440	-57
1	81	0	80	380.7538	-12	2	31	1	30	365.3866	54	2	17	1	18	345.7993	-59
1	82	0	81	380.9022	6	2	32	1	31	365.7002	-4	2	18	1	19	345.3295	10
1	83	0	82	381.0519	75	2	33	1	32	366.0202	36	2	19	1	20	344.8474	-14
1	84	0	83	381.1828	-7	2	34	1	33	366.3298	6	2	20	1	21	344.3613	-48
1	85	0	84	381.3192	3	2	35	1	34	366.6385	-1	2	21	1	22	343.8727	-78
1	86	0	85	381.4465	-42	2	36	1	35	366.9453	7	3	20	2	19	358.1900	-120
1	87	0	86	381.5857	69	2	37	1	36	367.2423	-49	3	21	2	20	358.5437	-111
1	88	0	87	381.7140	109	2	38	1	37	367.5543	78	3	24	2	23	359.5976	40
1	90	0	89	381.9436	29	2	39	1	38	367.8423	-1	3	25	2	24	359.9379	44
1	91	0	90	382.0549	10	2	40	1	39	368.1358	8	3	26	2	25	360.2679	-21
1	92	0	91	382.1595	-39	2	41	1	40	368.4283	42	3	27	2	26	360.6025	-8
1	93	0	92	382.2661	-31	2	43	1	42	368.9918	-5	3	28	2	27	360.9323	-10
1	94	0	93	382.3673	-39	2	44	1	43	369.2670	-43	3	29	2	28	361.2675	75
1	95	0	94	382.4693	-2	2	45	1	44	369.5373	-96	3	30	2	29	361.5844	9
1	96	0	95	382.5670	30	2	48	1	47	370.3587	55	3	31	2	30	361.9022	-14
1	7	0	8	353.8030	-31	2	49	1	48	370.6190	40	3	32	2	31	362.2265	60
1	8	0	9	353.3468	-94	2	50	1	49	370.8734	-1	3	34	2	33	362.8527	83
1	9	0	10	352.8988	-44	2	51	1	50	371.1296	11	3	35	2	34	363.1527	14
1	10	0	11	352.4380	-92	2	52	1	51	371.3762	-39	3	36	2	35	363.4520	-29
1	12	0	13	351.5199	-60	2	53	1	52	371.6356	74	3	37	2	36	363.7555	3
1	13	0	14	351.0611	3	2	54	1	53	371.8731	2	3	38	2	37	364.0515	-7
1	14	0	15	350.5926	0	2	55	1	54	372.1150	10	3	39	2	38	364.3478	21
1	15	0	16	350.1175	-39	2	56	1	55	372.3513	-4	3	40	2	39	364.6349	-11
1	16	0	17	349.6504	32	2	57	1	56	372.5854	-5	3	41	2	40	364.9176	-52
1	18	0	19	348.6901	3	2	58	1	57	372.8143	-24	3	43	2	42	365.4860	-5
1	19	0	20	348.2034	-32	2	59	1	58	373.0475	36	3	44	2	43	365.7609	-24
1	20	0	21	347.7188	-16	2	60	1	59	373.2642	-34	3	45	2	44	366.0358	-9
1	22	0	23	346.7440	48	2	61	1	60	373.4825	-53	3	46	2	45	366.3032	-35
1	24	0	25	345.7523	62	2	62	1	61	373.7025	-20	3	49	2	48	367.0924	-39
1	25	0	26	345.2505	54	2	63	1	62	373.9193	16	3	52	2	51	367.8535	-16
1	32	0	33	341.6557	-10	2	64	1	63	374.1268	-6	3	53	2	52	368.0971	-41
1	33	0	34	341.1328	4	2	65	1	64	374.3303	-31	3	54	2	53	368.3504	66
1	34	0	35	340.5981	-72	2	66	1	65	374.5338	-23	3	55	2	54	368.5856	26
1	35	0	36	340.0749	-4	2	67	1	66	374.7325	-25	3	56	2	55	368.8226	39
1	36	0	37	339.5469	44	2	68	1	67	374.9325	20	3	57	2	56	369.0616	106
1	37	0	38	339.0157	89	2	69	1	68	375.1197	-27	3	58	2	57	369.2839	41
1	38	0	39	338.4737	55	2	71	1	70	375.5006	51	3	59	2	58	369.5026	-25
1	39	0	40	337.9280	12	2	72	1	71	375.6793	26	3	60	2	59	369.7237	-33
1	40	0	41	337.3760	-66	2	73	1	72	375.8570	27	3	62	2	61	370.1556	-46
1	41	0	42	336.8319	-36	2	74	1	73	376.0215	-67	3	63	2	62	370.3587	-128
1	42	0	43	336.2920	63	2	77	1	76	376.5292	5	3	64	2	63	370.5769	-24
1	43	0	44	335.7313	-18	2	78	1	77	376.6846	-36	3	65	2	64	370.7777	-60
1	44	0	45	335.1800	24	2	79	1	78	376.8435	-6	3	66	2	65	370.9872	27
2	5	1	4	355.9366	23	2	81	1	80	377.1468	17	3	67	2	66	371.1802	-15
2	6	1	5	356.3363	-14	2	82	1	81	377.2859	-43	3	68	2	67	371.3762	7
2	7	1	6	356.7392	14	2	83	1	82	377.4298	-18	3	69	2	68	371.5678	21
2	8	1	7	357.1356	6	2	85	1	84	377.7046	13	3	70	2	69	371.7503	-20
2	9	1	8	357.5350	62	2	86	1	85	377.8400	62	3	72	2	71	372.1150	-0
2	11	1	10	358.3102	30	2	88	1	87	378.0836	1	3	73	2	72	372.2902	-7
2	12	1	11	358.6993	78	2	89	1	88	378.1998	-30	3	75	2	74	372.6365	43
2	13	1	12	359.0756	29	2	90	1	89	378.3167	-17	3	76	2	75	372.7976	1
2	14	1	13	359.4565	59	2	91	1	90	378.4327	23	3	78	2	77	373.1188	17
2	15	1	14	359.8273	18	2	1	1	2	353.0216	-17	3	79	2	78	373.2771	55
2	16	1	15	360.2035	64	2	2	1	3	352.5904	-46	3	80	2	79	373.4237	13
2	17	1	16	360.5741	86	2	3	1	4	352.1558	-79	3	81	2	80	373.5679	-18
2	18	1	17	360.9323	17	2	4	1	5	351.7212	-81	3	82	2	81	373.7209	77
2	19	1	18	361.2972	47	2	5	1	6	351.2896	-21	3	83	2	82	373.8546	14
2	20	1	19	361.6560	48	2	6	1	7	350.8512	-0	3	84	2	83	373.9894	-1

Note: a and b mark pure rotational transitions from References 5 and 9, respectively.

TABLE 3

Observed Rotational Lines (in cm^{-1}) in the Vibration–Rotation Bands of $K^{35}Cl$

v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C	v′	J′	v″	J″	Obs	O-C
										$K^{35}Cl$							
0	13	0	12	3.3332907a	5	1	96	0	95	294.4183	60	1	39	0	40	266.0351	-42
0	20	0	19	5.1261290a	6	1	97	0	96	294.5067	27	1	40	0	41	265.7189	-30
0	25	0	24	6.4052142a	9	1	98	0	97	294.5921	-19	1	41	0	42	265.4039	6
0	30	0	29	7.6826669a	-5	1	99	0	98	294.6857	36	1	42	0	43	265.0822	-9
0	35	0	34	8.9581633a	-20	1	100	0	99	294.7685	2	1	43	0	44	264.7542	-73
1	13	1	12	3.3128398a	-1	1	101	0	100	294.8574	46	1	44	0	45	264.4368	-15
1	25	1	24	6.3658870a	-9	1	102	0	101	294.9326	-28	1	45	0	46	264.1067	-71
1	30	1	29	7.6354806a	25	1	103	0	102	295.0166	4	1	46	0	47	263.7822	-55
2	25	2	24	6.3267275a	-6	1	104	0	103	295.0955	5	1	47	0	48	263.4576	-27
1	19	0	18	282.0766	78	1	105	0	104	295.1744	24	1	48	0	49	263.1324	10
1	21	0	20	282.5203	40	1	106	0	105	295.2499	27	1	49	0	50	262.8031	21
1	22	0	21	282.7357	-18	1	107	0	106	295.3209	3	1	50	0	51	262.4718	26
1	23	0	22	282.9509	-63	1	108	0	107	295.3904	-18	1	51	0	52	262.1349	-11
1	24	0	23	283.1690	-62	1	109	0	108	295.4567	-50	1	52	0	53	261.7988	-25
1	25	0	24	283.3835	-81	1	110	0	109	295.5320	25	1	53	0	54	261.4626	-26
1	26	0	25	283.5976	-87	1	111	0	110	295.5996	42	1	54	0	55	261.1249	-27
1	27	0	26	283.8127	-67	1	112	0	111	295.6639	45	1	55	0	56	260.7838	-49
1	28	0	27	284.0252	-56	1	113	0	112	295.7189	-27	1	56	0	57	260.4470	-13
1	29	0	28	284.2392	-15	1	114	0	113	295.7825	7	1	57	0	58	260.1039	-26
1	39	0	38	286.2456	-20	1	115	0	114	295.8360	-43	1	58	0	59	259.7553	-80
1	40	0	39	286.4419	28	1	116	0	115	295.9007	40	1	59	0	60	259.4077	-109
1	41	0	40	286.6339	50	1	117	0	116	295.9536	22	1	61	0	62	258.7250	-0
1	42	0	41	286.8216	45	1	118	0	117	296.0034	-7	1	62	0	63	258.3719	-42
1	43	0	42	287.0106	70	1	119	0	118	296.0573	23	1	63	0	64	258.0159	-98
1	44	0	43	287.1997	113	1	120	0	119	296.1062	23	1	64	0	65	257.6615	-126
1	45	0	44	287.3796	81	1	121	0	120	296.1480	-30	1	65	0	66	257.3097	-113
1	46	0	45	287.5561	32	1	122	0	121	296.1925	-37	1	66	0	67	256.9500	-164
1	47	0	46	287.7357	30	1	123	0	122	296.2381	-13	1	67	0	68	256.5911	-194
1	48	0	47	287.9137	30	1	124	0	123	296.2727	-81	2	63	1	62	287.7972	43
1	49	0	48	288.0824	-47	1	125	0	124	296.3182	-20	2	64	1	63	287.9453	24
1	50	0	49	288.2589	-29	1	126	0	125	296.3524	-53	2	65	1	64	288.0919	7
1	51	0	50	288.4366	20	1	127	0	126	296.3902	-31	2	66	1	65	288.2399	22
1	52	0	51	288.6004	-55	1	128	0	127	296.4247	-24	2	67	1	66	288.3803	-23
1	53	0	52	288.7692	-62	1	129	0	128	296.4557	-32	2	68	1	67	288.5187	-71
1	54	0	53	288.9332	-100	1	130	0	129	296.4861	-26	2	69	1	68	288.6600	-73
1	55	0	54	289.1086	-7	1	131	0	130	296.5181	15	2	70	1	69	288.7976	-94
1	56	0	55	289.2688	-50	1	132	0	131	296.5471	45	2	71	1	70	288.9332	-118
1	58	0	57	289.5959	-14	1	133	0	132	296.5714	48	2	72	1	71	289.0749	-65
1	59	0	58	289.7549	-18	1	134	0	133	296.5913	26	2	74	1	73	289.3425	-63
1	60	0	59	289.9125	-17	1	135	0	134	296.6074	-15	2	75	1	74	289.4791	-8
1	62	0	61	290.2276	37	1	136	0	135	296.6295	24	2	76	1	75	289.6087	-5
1	63	0	62	290.3752	-10	1	137	0	136	296.6462	29	2	77	1	76	289.7362	-7
1	64	0	63	290.5265	-3	1	11	0	12	274.3250	83	2	78	1	77	289.8557	-72
1	65	0	64	290.6757	0	1	12	0	13	274.0472	56	2	79	1	78	289.9862	-8
1	66	0	65	290.8249	22	1	13	0	14	273.7711	62	2	80	1	79	290.1042	-53
1	68	0	67	291.1194	77	1	14	0	15	273.4951	85	2	81	1	80	290.2276	-26
1	69	0	68	291.2609	73	1	15	0	16	273.2081	13	2	82	1	81	290.3474	-18
1	70	0	69	291.4021	85	1	16	0	17	272.9327	71	2	83	1	82	290.4711	47
1	73	0	72	291.8083	49	1	17	0	18	272.6481	53	2	84	1	83	290.5859	40
1	74	0	73	291.9414	50	1	18	0	19	272.3635	51	2	85	1	84	290.7039	83
1	76	0	75	292.2027	54	1	20	0	21	271.7834	-18	2	86	1	85	290.8107	31
1	77	0	76	292.3280	30	1	21	0	22	271.5001	38	2	87	1	86	290.9193	15
1	78	0	77	292.4595	85	1	22	0	23	271.2027	-31	2	88	1	87	291.0251	-12
1	79	0	78	292.5771	19	1	23	0	24	270.9234	95	2	89	1	88	291.1372	43
1	80	0	79	292.6949	-27	1	24	0	25	270.6244	40	2	90	1	89	291.2435	56
1	81	0	80	292.8200	18	1	25	0	26	270.3276	21	2	91	1	90	291.3406	-4
1	82	0	81	292.9451	80	1	26	0	27	270.0289	-1	2	92	1	91	291.4485	61
1	83	0	82	293.0555	13	1	27	0	28	269.7395	85	2	93	1	92	291.5488	68
1	84	0	83	293.1693	-2	1	28	0	29	269.4353	38	2	95	1	94	291.7410	51
1	85	0	84	293.2839	10	1	29	0	30	269.1309	3	2	96	1	95	291.8380	78
1	86	0	85	293.3956	9	1	30	0	31	268.8242	-39	2	97	1	96	291.9271	44
1	87	0	86	293.5013	-32	1	31	0	32	268.5159	-83	2	98	1	97	292.0134	0
1	88	0	87	293.6054	-73	1	32	0	33	268.2211	23	2	99	1	98	292.0990	-33
1	89	0	88	293.7153	-36	1	33	0	34	267.9096	-22	2	100	1	99	292.1884	-10
1	90	0	89	293.8201	-34	1	34	0	35	267.6002	-33	2	102	1	101	292.3463	-120
1	91	0	90	293.9227	-34	1	35	0	36	267.2995	60	2	103	1	102	292.4356	-44
1	92	0	91	294.0224	-45	1	36	0	37	266.9814	-8	2	104	1	103	292.5193	-6
1	94	0	93	294.2197	-36	1	37	0	38	266.6688	-5	2	105	1	104	292.5986	7
1	95	0	94	294.3213	26	1	38	0	39	266.3500	-50	2	106	1	105	292.6674	-68

TABLE 3—*Continued*

v'	J'	v''	J''	Obs	O-C	v'	J'	v''	J''	Obs	O-C	v'	J'	v''	J''	Obs	O-C
2	107	1	106	292.7414	-73	3	61	2	60	285.0258	-108	3	118	2	117	290.9625	-4
2	108	1	107	292.8200	-12	3	62	2	61	285.1782	-116	3	119	2	118	291.0115	-28
2	109	1	108	292.8915	-5	3	63	2	62	285.3394	-18	3	120	2	119	291.0650	13
2	110	1	109	292.9628	18	3	64	2	63	285.4825	-86	3	121	2	120	291.1060	-52
2	111	1	110	293.0291	10	3	65	2	64	285.6311	-80	3	122	2	121	291.1547	-22
2	112	1	111	293.0932	-2	3	66	2	65	285.7850	-5	3	123	2	122	291.1986	-21
2	113	1	112	293.1600	31	3	67	2	66	285.9224	-78	3	124	2	123	291.2435	10
2	114	1	113	293.2180	-4	3	68	2	67	286.0679	-52	3	125	2	124	291.2887	62
2	115	1	114	293.2839	58	3	69	2	68	286.2177	34	3	126	2	125	291.3247	41
2	116	1	115	293.3388	28	3	70	2	69	286.3466	-72	3	127	2	126	291.3564	-4
2	117	1	116	293.3956	35	3	71	2	70	286.4887	-28	3	128	2	127	291.3891	-19
2	118	1	117	293.4462	0	3	72	2	71	286.6245	-31	4	91	3	90	286.5019	-162
2	119	1	118	293.5013	29	3	74	2	73	286.8910	-34	4	92	3	91	286.6105	-78
2	120	1	119	293.5497	8	3	75	2	74	287.0234	-19	4	93	3	92	286.7036	-130
2	121	1	120	293.5938	-36	3	76	2	75	287.1577	34	4	94	3	93	286.8074	-57
2	122	1	121	293.6460	20	3	78	2	77	287.4118	46	4	95	3	94	286.9062	-15
2	123	1	122	293.6876	-11	3	79	2	78	287.5393	82	4	96	3	95	287.0003	-2
2	124	1	123	293.7298	-17	3	80	2	79	287.6611	79	4	97	3	96	287.0907	-6
2	125	1	124	293.7768	43	3	81	2	80	287.7830	95	4	98	3	97	287.1854	50
2	126	1	125	293.8069	-46	3	82	2	81	287.8972	51	4	100	3	99	287.3609	83
2	127	1	126	293.8495	9	3	83	2	82	288.0138	49	4	101	3	100	287.4401	42
2	128	1	127	293.8802	-35	3	84	2	83	288.1248	8	4	102	3	101	287.5220	47
2	129	1	128	293.9130	-40	3	85	2	84	288.2399	27	4	103	3	102	287.6039	72
2	130	1	129	293.9389	-94	3	86	2	85	288.3474	-14	4	104	3	103	287.6751	8
2	131	1	130	293.9750	-27	3	87	2	86	288.4509	-75	4	105	3	104	287.7533	34
2	147	1	146	294.1844	62	3	88	2	87	288.5693	29	4	106	3	105	287.8302	66
3	33	2	32	280.0533	-137	3	89	2	88	288.6766	40	4	107	3	106	287.8972	18
3	34	2	33	280.2544	-124	3	90	2	89	288.7840	70	4	108	3	107	287.9626	-26
3	35	2	34	280.4579	-69	3	91	2	90	288.8815	19	4	109	3	108	288.0262	-68
3	36	2	35	280.6585	-29	3	92	2	91	288.9880	77	4	110	3	109	288.0919	-71
3	37	2	36	280.8600	38	3	93	2	92	289.0890	96	4	111	3	110	288.1537	-92
3	38	2	37	281.0541	47	3	95	2	94	289.2828	108	4	112	3	111	288.2108	-141
3	40	2	39	281.4394	85	3	96	2	95	289.3681	25	4	113	3	112	288.2783	-66
3	41	2	40	281.6297	105	3	97	2	96	289.4684	110	4	114	3	113	288.3355	-75
3	42	2	41	281.8075	16	3	98	2	97	289.5467	-8	4	115	3	114	288.3959	-31
3	43	2	42	281.9980	71	3	99	2	98	289.6381	25	4	116	3	115	288.4509	-21
3	44	2	43	282.1877	133	3	100	2	99	289.7224	4	4	117	3	116	288.5071	20
3	45	2	44	282.3615	54	3	101	2	100	289.8066	-0	4	118	3	117	288.5547	-5
3	46	2	45	282.5342	-19	3	102	2	101	289.8899	6	4	119	3	118	288.6004	-29
3	47	2	46	282.7192	47	3	103	2	102	289.9727	24	4	120	3	119	288.6469	-24
3	48	2	47	282.8936	23	3	104	2	103	290.0513	20	4	121	3	120	288.6928	-5
3	49	2	48	283.0639	-24	3	105	2	104	290.1262	-4	4	122	3	121	288.7366	13
3	50	2	49	283.2410	12	3	106	2	105	290.2033	13	4	123	3	122	288.7840	88
3	51	2	50	283.4113	-2	3	107	2	106	290.2767	12	4	124	3	123	288.8239	107
3	52	2	51	283.5816	1	3	108	2	107	290.3474	1	4	125	3	124	288.8639	149
3	53	2	52	283.7484	-16	3	109	2	108	290.4214	42	4	126	3	125	288.8947	119
3	54	2	53	283.9123	-45	3	110	2	109	290.4844	-9	4	127	3	126	288.9220	75
3	55	2	54	284.0708	-109	3	111	2	110	290.5524	9	4	128	3	127	288.9476	34
3	56	2	55	284.2392	-60	3	112	2	111	290.6145	-14	4	129	3	128	288.9738	20
3	57	2	56	284.4067	-1	3	113	2	112	290.6757	-27	4	130	3	129	288.9880	-93
3	58	2	57	284.5637	-31	3	115	2	114	290.7961	-17	4	131	3	130	289.0032	-176
3	59	2	58	284.7192	-59	3	116	2	115	290.8501	-46						
3	60	2	59	284.8689	-127	3	117	2	116	290.9060	-38						

Note: a marks pure rotational transitions from Ref. 9.

and KCl involved coaddition of 100 and 400 scans, respectively.

The spectra were measured using the PC-DECOMP, a program developed by J. Brault at the National Solar Observatory. This program determines the position of individual lines by fitting a Voigt lineshape function to each line. The spectra were calibrated using the measurements of H_2O lines (*37*) which were also present in our spectra as an impurity. The measurements of strong and unblended $Na^{35}Cl$ lines are expected to have a precision of about ±0.003 cm^{-1}. The uncertainty in the measurements of $Na^{37}Cl$ lines is expected to be somewhat worse because of the weaker intensity and overlapping from the major isotopomer. The lines of KCl are much weaker in intensity than NaCl, and $K^{37}Cl$ lines could not be identified in our spectra. The $K^{35}Cl$ lines are expected to be accurate to, at best, ±0.005 cm^{-1}.

TABLE 4

Rotational Constants (in cm^{-1}) of the $X^1\Sigma^+$ State of NaCl

v	T_v	B_v	$10^7 \times D_v$
		Na^{35}Cl	
0	0.0	0.217251914(65)[a]	3.11524(78)[b]
1	361.15111(18)	0.215637451(70)	3.10850(73)
2	718.80343(26)	0.214033094(92)	3.10109(70)
3	1072.99164(35)	0.21243904(16)	3.09352(69)
4	1423.75018(43)	0.21085530(20)	3.08580(69)
5	1771.11401(51)	0.20928199(26)	3.07808(69)
6	2115.11780(75)	0.20771859(35)	3.06983(70)
7	2455.7949(11)	0.20616567(75)	3.0620(12)
8	2793.1760(18)	0.2046246(13)	3.0560(21)
		Na^{37}Cl	
0	0.0	0.21260274(44)	2.9429(78)
1	357.29437(49)	0.21104144(22)	2.9396(72)
2	711.16501(70)	0.20948973(52)	2.9357(70)
3	1061.6469(15)	0.2079458(11)	2.9288(69)

[a] Numbers in parentheses are one standard deviation in last digits.

[b] $H_0 = -3.3(15) \times 10^{-15}$ cm^{-1}.

RESULTS AND DISCUSSION

The vibration–rotation bands of NaCl and KCl are located in the 340–390 and 240–300 cm^{-1} regions, respectively. The bands form R heads and the rotational structure of bands with high v values is heavily overlapped. Our Loomis–Wood program was very helpful in identifying the connecting R and P lines in each band, particularly in the severely overlapped regions. For KCl essentially all of the lines are blended.

The observed spectrum of NaCl consists of eight vibration–rotation bands, 1–0 to 8–7, of Na^{35}Cl spread from 350 to 387 cm^{-1}. The intensity of the higher vibrational bands decreases slowly with increasing vibration and it becomes difficult to identify the bands with $v > 8$ because of overlapping and the decline in intensity. In contrast to the previous infrared observations of Horiai *et al.* (*6*) and Uehara *et al.* (*7*), we have identified a number of P lines. The intensity of the Na^{37}Cl isotopomer is about 33% of the intensify of Na^{35}Cl as expected. The rotational lines only in the 1–0, 2–1, and 3–2 bands of Na^{37}Cl were identified and incorporated in the fit. A part of the high-resolution spectrum of the 1–0 band of NaCl near the R head is provided in Fig. 1 where some R lines of Na^{35}Cl have been marked.

The rotational lines belonging to the 1–0, 2–1, 3–2, and 4–3 bands of K^{35}Cl were identified in our high-resolution spectra although band heads up to 12–11 can be clearly seen. A part of the compressed spectrum of KCl showing the band heads is presented in Fig. 2 and a list of observed band heads is provided in Table 1. For technical reasons (the use of a bolometer) the KCl data are relatively poor compared to NaCl and a much less extensive analysis was carried out.

As expected for a $^1\Sigma^+ - {}^1\Sigma^+$ transition, each band consists of one R and one P branch. The wavenumbers of the observed transitions of NaCl and KCl are provided in Tables 2 and 3 respectively. The wavenumbers of NaCl and KCl were fit to the customary energy level expression:

$$F_v(J) = T_v + B_v J(J+1) - D_v[J(J+1)]^2 + H_v[J(J+1)]^3. \qquad [1]$$

In the final least-squares fit, approximate weights for the individual rotational lines were chosen on the basis of signal-to-noise ratio as well as freedom from blending. We have also included the previous microwave measurements of Honig *et al.* (*5*) and Clouser and Gordy (*7*), with appropriate weights in our final fit. The spectroscopic constants for the $X\,^1\Sigma^+$ state of NaCl and KCl obtained from the fit of the combined infrared and microwave data are provided

TABLE 5

Rotational Constants (in cm^{-1}) of the $X\,^1\Sigma^+$ State of KCl

v	T_v	B_v	$10^7 \times D_v$	$10^{14} \times H_v$
0	0.0	0.12824024(11)[a]	1.08807(60)	2.79(22)
1	277.49756(47)	0.12745368(11)	1.08762(57)	2.41(17)
2	552.4899(14)	0.12666947(13)	1.07926(61)	--
3	825.0724(22)	0.12590304(50)	1.08140(66)	--
4	1095.313(21)	0.1251600(34)	1.0943(15)	--

[a] Numbers in parentheses are one standard deviation in last digits.

in Tables 4 and 5, respectively. The molecular constants obtained in this study are in excellent agreement with values reported earlier from infrared studies (*5, 7*) but are more precise by an order of magnitude because of the inclusion of extensive data with high J and v values along with pure rotational lines. The rotational lines of $Na^{35}Cl$, $Na^{37}Cl$, and $K^{35}Cl$ were fit to the Dunham energy level expression (*38*)

$$E(v,\ J) = \sum Y_{ij}(v + 1/2)^i[J(J + 1)]^j. \tag{2}$$

The Dunham constants (Y_{ij}) for the $X\,^1\Sigma^+$ state of NaCl and KCl obtained from these fits are provided in Tables 6 and 7, respectively.

In another fit the combined $Na^{35}Cl$ and $Na^{37}Cl$ data sets were fit to the following expression to determine a set of mass-reduced Dunham U_{ij} coefficients and Born–Oppenheimer breakdown constants Δ_{ij} (*39, 40*):

$$E(v,\ J) = \sum U_{ij}\mu^{-(i+2j)/2}(v + 1/2)^i[J(J + 1)]^j \times \left(1 + \frac{m_e}{M_A}\Delta_{ij}^{A} + \frac{m_e}{M_B}\Delta_{ij}^{B}\right). \tag{3}$$

m_e is electron mass, M_A and M_B are masses of two atomic centers A and B, respectively, and Δ_{ij}^{A} and Δ_{ij}^{B} are Born–Oppenheimer breakdown constants for atoms A and B. It turns out that no Δ parameters were necessary in our fits.

Two fits of the combined NaCl data were obtained. In the first fit all U_{ij} parameters were allowed to vary. The constants obtained from this fit are reported in Table 8 under the column heading ‘‘unconstrained.’’ These unconstrained U_{ij} and Y_{ij} values of Tables 6 and 7 are thus empirical coefficients of polynomial fits. According to the Dunham model all of the parameters for a power series potential are uniquely determined by the U_{i0} and U_{i1} constants (*41, 42*). This means that U_{ij}’s with $j \geqslant 2$ can be expressed in terms of U_{i0}’s and U_{i1}’s. In the second fit, therefore, U_{i0}’s and U_{i1}’s were treated as adjustable parameters with the remaining U_{ij}’s fixed to the values satisfying these constraints. The constants obtained from this fit are also reported in Table 8 under the column heading ‘‘constrained.’’

TABLE 6

Dunham Constants (in cm^{-1}) of the $X\,^1\Sigma^+$ State of NaCl

Const.	$Na^{35}Cl$	$Na^{37}Cl$
Y_{10}	364.684163(391)	360.75003(145)
Y_{20}	-1.776085(189)	-1.736564(796)
$10^3\times Y_{30}$	5.9369(346)	5.452(135)
$10^5\times Y_{40}$	-1.231(207)	—
Y_{01}	0.2180630200(760)	0.213387680(446)
$10^3\times Y_{11}$	-1.6247876(562)	-1.571552(262)
$10^6\times Y_{21}$	5.1543(138)	4.9912(539)
$10^7\times Y_{02}$	-3.119044(755)	-2.95200(633)
$10^{10}\times Y_{12}$	6.397(206)	4.019(459)
$10^{12}\times Y_{22}$	8.37(110)	—
$10^{14}\times Y_{03}$	8.96(288)	—

[a] Numbers in parentheses are one standard deviation in last digits.

TABLE 7

Dunham Constants (in cm^{-1}) of the $X\,^1\Sigma^+$ State of KCl

Const.	$K^{35}Cl$
Y_{10}	280.07639(490)
Y_{20}	-1.31330(338)
$10^2\times Y_{30}$	1.4490(607)
Y_{01}	0.128632129(325)
$10^4\times Y_{11}$	-7.80915(746)
$10^6\times Y_{21}$	-5.545(473)
$10^6\times Y_{31}$	1.5963(906)
$10^7\times Y_{02}$	-1.08779(230)
$10^{10}\times Y_{12}$	-9.708(660)
$10^{10}\times Y_{22}$	7.514(216)
$10^{10}\times Y_{32}$	-1.2400(391)
$10^{13}\times Y_{03}$	1.47(107)
$10^{14}\times Y_{13}$	-1.274(301)

[a] Numbers in parentheses are one standard deviation in last digits.

There is no doubt that the Dunham constants reproduce the transition wavenumbers over the range of v and J values observed. It is well known, however, that this model is inadequate for extrapolating beyond the range of experimental measurements. The full advantage of high-quality, high-resolution spectra is achieved when the extracted spectroscopic information can also be applied in predicting the spectra well beyond the range of experimental measurements. The inherent failure of the Dunham model has led to the development of a more sophisticated approach of fitting observed measurements directly to the eigenvalues of the Schrödinger equation containing a parameterized potential energy function (*43–46*). The Born–Oppenheimer potential U^{BO} is represented by

$$U^{BO} = D_e\{1 - \exp[-\beta(R)]\}^2/\{1 - \exp[-\beta(\infty)]\}^2, \tag{4}$$

where

$$\beta(R) = z \sum \beta_i z^i, \tag{5}$$

$$\beta(\infty) = \sum \beta_i, \qquad [6]$$

and

$$z = (R - R_e)/(R + R_e). \qquad [7]$$

We call this approach to data reduction the parameterized potential model and the method is described in more detail in several previous publications (*45, 46*). This fit provides a set of β_i parameters which describe (Eq. [4]) the internuclear potential function (*45, 46*). These parameters for NaCl are provided in Table 9. Only statistically determined parameters are listed in this table along with 1σ uncertainties.

Our measurements of NaCl rotational lines are in good agreement with the measurements of Horiai *et al.* (*6*) and Uehara *et al.* (*7*) where they overlap. The present set of Dunham constants for Na^{35}Cl and Na^{37}Cl (Table 6) are also in excellent agreement with the previous values (*6, 7*). Because of our more extensive data set including bands up to 8–7, however, the present constants for Na^{35}Cl are more precise than the previous values (*5, 7*). A comparison of present band head positions of KCl with those reported by Uehara *et al.* (*13*) indicates that on average their values are about 0.07 cm^{-1} higher than the present measurements. At this point it is worth mentioning that Uehara *et al.*'s spectra were recorded at a resolution of 0.1 cm^{-1} whereas the present spectra were recorded at 0.01 cm^{-1} resolution. Thus the present molecular constants of KCl in Tables 5 and 7 are much more precise than previous values of Uehara *et al.* (*13*). For example, the present values of Y_{10}, Y_{20}, and Y_{01} constants are 280.0764(49), −1.3133(34), and 0.12863213(33) cm^{-1}, respectively, compared to the corresponding values of 279.963(22), −1.2306(83), and 0.128631(52) cm^{-1}, respectively, obtained by Uehara *et al.* (*13*).

TABLE 9

Internuclear Potential Energy Parameters (in cm^{-1}) for the $X\,^1\Sigma^+$ State of NaCl

Parameter	Value	Uncertainty
D_e/cm^{-1}	34120.0[a]	—
R_e/Å	2.360796042	2.15×10^{-7}
β_0	4.224459	1.71×10^{-3}
β_1	0.150329	3.86×10^{-3}
β_2	0.399367	4.87×10^{-3}
β_3	7.922000	5.91×10^{-2}
β_4	-5.573758	5.42×10^{-1}
M(Na)/u	22.989768	
M(^{35}Cl)/u	34.968853	
M(^{37}Cl)/u	36.965903	

[a] Fixed to value in Ref. 47.

TABLE 8

Mass Reduced Dunham Constants (in cm^{-1}) for the $X\,^1\Sigma^+$ State of NaCl

Const.	Unconstrained	Constrained
U_{10}	1358.20379(145)	1358.20342(153)
U_{20}	-24.63286(265)	-24.63228(283)
U_{30}	0.305575(183)	0.305157(192)
$10^{3}\times U_{40}$	-2.162(411)	-2.054(420)
U_{01}	3.02468394(106)	3.024682410(486)
$10^{2}\times U_{11}$	-8.393156(300)	-8.392648(169)
$10^{4}\times U_{21}$	9.8831(280)	9.8594(107)
$10^{5}\times U_{02}$	-6.00196(146)	-6.0003
$10^{7}\times U_{12}$	4.801(152)	4.8324
$10^{8}\times U_{22}$	2.344(312)	2.5841
$10^{10}\times U_{32}$		-2.7211
$10^{11}\times U_{03}$	11.61(791)	-9.1179
$10^{11}\times U_{13}$		2.5565
$10^{13}\times U_{23}$		-1.5197
$10^{15}\times U_{04}$		-4.8462
$10^{16}\times U_{14}$		5.4755
$10^{17}\times U_{24}$		3.4469
$10^{20}\times U_{05}$		8.7537
$10^{20}\times U_{15}$		1.6829
$10^{24}\times U_{06}$		4.0752
$10^{24}\times U_{16}$		1.3648
$10^{28}\times U_{07}$		2.1918
$10^{32}\times U_{08}$		1.1062

[a] Numbers in parentheses are one standard deviation in last digits.

CONCLUSION

The infrared emission spectra of NaCl and KCl have been observed using a Fourier transform spectrometer. The vibration–rotation spectra of a number of bands of Na^{35}Cl, Na^{37}Cl, and K^{35}Cl have been measured and the line positions fitted to extract molecular constants for individual vibrational levels and Dunham coefficients. The lines of Na^{35}Cl and Na^{37}Cl were combined in another fit to determine the mass-reduced Dunham parameters U_{ij}. A second set of mass-reduced constants was also obtained using the same data set but with only the U_{i0}'s and U_{i1}'s treated as variables and the rest of the U_{ij}'s were fixed by constraints imposed by the Dunham model. The lines of NaCl have also been fit with a parameterized potential model to extract a potential energy function.

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