

NOTE

FTIR Emission Spectra and Molecular Constants for DCI

HCl is an important gas which is used as an absolute wavenumber standard and has been used in studies of the breakdown of the Born–Oppenheimer approximation (1–3). Recently, HCl was observed in the infrared region in the upper atmosphere (4) and in the IR absorption spectra of the atmospheres of Venus (5) and an S-type star (6).

The HCl fundamental has previously been measured in absorption by Rank *et al.* (7) and Guelachvili *et al.* (8), as well as by Rinsland *et al.* (9) during a recent experiment on room temperature HCl. Measurements on hot HCl have been reported by Webb and Rao from absorption spectra (10) and by Le Blanc *et al.* and Clayton *et al.* from emission spectra (11, 12). The pure rotational lines were measured by tunable far-infrared spectrometry (13, 14) and submillimeter-wave techniques (15, 16). A set of Einstein A coefficients were also calculated for HCl (17).

While spectra of both the fundamental and hot bands of HCl are known, there are no measurements available for the hot bands of DCI. Absorption spectra of the fundamental were recently measured by Klee and Ogilvie (18). Other previous studies of DCI include measurements of the fundamental by Guelachvili *et al.* (8) and of the fundamental and overtone bands by Webb and Rao (10). Pure rotational spectra of DCI were observed by Fusina *et al.* (19) with a tunable far-infrared spectrometer, and by Klaus *et al.* (16) by submillimeter-wave techniques.

We report here new high-resolution infrared emission spectra of DCI. This spectrum was accidentally observed while we were trying to measure the infrared spectrum of DBO (20). It was recorded with a Bruker IFS 120 HR Fourier transform spectrometer. Solid boron and calcium chloride in a tantalum boat were heated to 1000°C in a tube furnace, while D₂ gas was passed through the tube at a pressure of 50 Torr. The emission spectrum was recorded at a resolution of 0.01 cm⁻¹ over the 1600–2900 cm⁻¹ range, using a KBr beamsplitter and an HgCdTe detector. The reaction between D₂ and calcium chloride gave DCI as a product.

Vibration–rotation line positions of the $\nu = 1 \rightarrow 0$, $2 \rightarrow 1$, $3 \rightarrow 2$, and $4 \rightarrow 3$ bands of D³⁵Cl, and of the $\nu = 1 \rightarrow 0$, $2 \rightarrow 1$, and $3 \rightarrow 2$ bands of D³⁷Cl were measured. For the more intense bands, strong unblended lines were measured to an estimated precision of ± 0.0002 cm⁻¹, while for the weaker $\nu = 3 \rightarrow 2$ and $\nu = 4 \rightarrow 3$ bands, the typical uncertainties for unblended lines were ± 0.0004 and ± 0.002 cm⁻¹, respectively.

Our measured line positions are reported in Table 1A for D³⁵Cl and Table 1B for D³⁷Cl.¹ The signal-to-noise ratio for the strongest lines was better than 25. The spectral analysis to determine the line positions was carried out using PC Decomp, a program developed by J. W. Brault. The rovibrational lines were calibrated with CO lines, which were present as an impurity in the spectrum. The CO line positions were taken from the book by Maki and Wells (21). For completeness, Tables 1A and 1B also list the literature data used in the present fits.

As the next stage of our analysis, separate sets of band constants were determined for D³⁵Cl and D³⁷Cl. The input to these fits consisted of the new

results reported here plus pure rotational (16, 19) and rovibrational (18) measurements from the literature, with all line positions being weighted by the inverse square of their estimated uncertainties. These data sets for D³⁵Cl and D³⁷Cl were fitted to the familiar band constant expression (22)

$$E(\nu, J) = T_\nu + B_\nu[J(J+1)] - D_\nu[J(J+1)]^2 + H_\nu[J(J+1)]^3 + \dots, \quad [1]$$

where T_ν is the vibrational energy, and B_ν , D_ν , H_ν , ... etc. are the usual inertial rotation and centrifugal distortion constants. The constants obtained from these fits are reported in Table 2.

A combined isotopomer analysis was then performed using the DCI data sets described above, together with analogous high-quality literature data for H³⁵Cl and H³⁷Cl. This was done both in order to determine Born–Oppenheimer breakdown correction terms for this system and because this combined analysis allows us to obtain more extensive and reliable DCI constants than can be determined from the data for each isotopomer considered alone. In particular, the FTIR HCl measurements (9, 11) include data for levels up to $\nu(\text{HCl}) = 3$, while the usual first-order semiclassical scaling relationship (22–24) shows that the present DCI results only span the energy range up to $\nu(\text{HCl}) \approx 2.72$ for D³⁵Cl and to $\nu(\text{HCl}) \approx 2.01$ for D³⁷Cl. Similarly, the highest observed J level in the HCl data used is $J(\text{HCl}) = 31$, while semiclassical scaling shows that the highest DCI rotational level observed here ($J(\text{DCI}) = 35$) corresponds to $J(\text{HCl}) \approx 24.95$. Thus, DCI constants yielded by this combined isotopomer analysis will be valid for a wider range of energy than is spanned by the DCI data itself.

Following Ref. (25), transitions of isotopomer α of species A–B formed from atoms of mass M_A^α and M_B^α are expressed as differences between level energies written as

$$E^\alpha(\nu, J) = \sum_{(l,m) \neq (0,0)} Y_{lm}^\alpha \left(\frac{\mu_1}{\mu_\alpha} \right)^{m+1/2} (\nu + 1/2)^l [J(J+1)]^m + \sum_{(l,m) \geq (0,0)} \left\{ \frac{\Delta M_A^\alpha}{M_A^\alpha} \delta_{l,m}^A + \frac{\Delta M_B^\alpha}{M_B^\alpha} \delta_{l,m}^B \right\} \left(\frac{\mu_1}{\mu_\alpha} \right)^{m+1/2} \times (\nu + 1/2)^l [J(J+1)]^m, \quad [2]$$

where μ_α is the usual atomic reduced mass of isotopomer α , $\Delta M_A^\alpha = M_A^\alpha - M_A^1$, and $\alpha = 1$ identifies a selected reference species, in this case the most abundant isotopomer, ¹H³⁵Cl. The semiclassical and Born–Oppenheimer breakdown correction coefficients $\delta_{l,m}^A$ determined here are simply related to the older Watson Δ correction parameters $\Delta_{l,m}^A = -\delta_{l,m}^A M_A^1 (\mu_1)^{m+1/2} / U_{l,m} m_e$ (25). The conventional Dunham constants for minority ($\alpha \neq 1$) isotopomers are readily generated from the expression

$$Y_{lm}^\alpha = \left\{ Y_{lm}^1 + \frac{\Delta M_A^\alpha}{M_A^\alpha} \delta_{l,m}^A + \frac{\Delta M_B^\alpha}{M_B^\alpha} \delta_{l,m}^B \right\} \left(\frac{\mu_1}{\mu_\alpha} \right)^{m+1/2}. \quad [3]$$

¹ The data used in the present analysis may also be obtained electronically from authors RJL (leroy@UWaterloo.ca) or PFB (bernath@UWaterloo.ca).

TABLE 1A
 $D^{35}Cl$ Line Positions (in cm^{-1}), Uncertainties,^a and the Differences^a
 from Predictions Yielded by the Constants of Table 3

v'	j'	v''	j''	observed	u_{obs}^a	$(c-o)^a$	v'	j'	v''	j''	observed	u_{obs}^a	$(c-o)^a$
0	1	0	0	10.7839843 ^b	17	-5	1	11	0	12	1947.79009 ^d	4	0
0	2	0	1	21.5646150 ^c	63	-58	1	12	0	13	1934.57710 ^d	4	-9
0	3	0	2	32.3385169 ^c	33	24	1	13	0	14	1921.18455 ^d	4	-1
0	4	0	3	43.1023717 ^c	130	-111	1	14	0	15	1907.61607 ^d	6	19
0	5	0	4	53.8527876 ^c	23	-31	1	15	0	16	1893.87576 ^d	6	4
0	6	0	5	64.5864487 ^c	33	2	1	19	0	20	1837.26388	20	37
0	7	0	6	75.3000141 ^c	130	58	1	20	0	21	1822.71659	20	41
0	9	0	8	96.6535964 ^c	13	-3	1	21	0	22	1808.01889	20	31
0	12	0	11	128.4505566 ^c	17	5	1	22	0	23	1793.17435	20	12
0	15	0	14	159.8890997 ^c	13	0	1	23	0	24	1778.18638	20	-1
0	17	0	16	180.6061274 ^c	86	-66	1	24	0	25	1763.05843	20	4
1	1	1	0	10.5591371 ^b	330	-36	1	25	0	26	1747.79430	20	4
1	2	1	1	21.1145855 ^b	6700	3541	1	26	0	27	1732.39738	20	13
1	1	0	0	2101.61784 ^d	4	2	1	27	0	28	1716.87161	20	-11
1	2	0	1	2111.94883 ^d	4	-1	1	28	0	29	1701.22019	20	-37
1	3	0	2	2122.04829 ^d	4	1	1	29	0	30	1685.44595	20	0
1	4	0	3	2131.91308 ^d	4	-3	1	30	0	31	1669.55335	20	-2
1	5	0	4	2141.53984 ^d	4	0	1	31	0	32	1653.54537	20	4
1	6	0	5	2150.92553 ^d	4	-5	1	32	0	33	1637.42688	200	-131
1	7	0	6	2160.06680 ^d	4	3	2	27	1	28	1669.84492	600	1152
1	8	0	7	2168.96079 ^d	4	-1	2	26	1	27	1685.12955	600	770
1	9	0	8	2177.60423 ^d	4	2	2	25	1	26	1700.28239	600	645
1	10	0	9	2185.99423 ^d	4	-1	2	24	1	25	1715.30714	20	61
1	11	0	10	2194.12767 ^d	4	4	2	23	1	24	1730.19065	20	-14
1	12	0	11	2202.00178 ^d	4	0	2	22	1	23	1744.93391	20	-27
1	13	0	12	2209.61355 ^d	4	0	2	21	1	22	1759.53403	20	-39
1	14	0	13	2216.96019 ^d	4	-3	2	20	1	21	1773.98728	20	-29
1	15	0	14	2224.03891 ^d	4	-8	2	19	1	20	1788.29041	20	-23
1	16	0	15	2230.84680 ^d	4	0	2	18	1	19	1802.43969	20	-3
1	17	0	16	2237.38189 ^d	40	-50	2	17	1	18	1816.43104	20	86
1	18	0	17	2243.63678	200	316	2	16	1	17	1830.26354	20	-20
1	19	0	18	2249.62081	200	-96	2	15	1	16	1843.93054	20	-9
1	20	0	19	2255.32044	200	-184	2	14	1	15	1870.75752	20	-10
1	21	0	20	2260.73485	20	-117	2	13	1	14	1883.91050	20	-32
1	22	0	21	2265.86238	20	28	2	12	1	13	1896.88445	20	-5
1	23	0	22	2270.70293	20	22	2	11	1	12	1909.67683	20	-29
1	24	0	23	2275.25257	20	25	2	10	1	11	1922.28316	20	-10
1	25	0	24	2279.50943	20	-4	2	9	1	10	1934.70049	20	-4
1	26	0	25	2283.47080	20	-16	2	8	1	9	1946.92516	20	2
1	27	0	26	2287.13467	20	-28	2	7	1	8	1958.95365	20	13
1	28	0	27	2290.49871	20	-18	2	6	1	7	1970.78263	20	11
1	29	0	28	2293.56119	20	-21	2	5	1	6	1993.82781	20	13
1	30	0	29	2296.31929	20	44	2	4	1	5	2005.03731	20	-1
1	31	0	30	2298.77332	20	-51	2	3	1	4	2026.81283	20	-30
1	32	0	31	2300.91824	20	8	2	2	1	3	2047.70722	20	14
1	33	0	32	2302.75424	20	14	2	1	0	2	2067.69521	20	9
1	34	0	33	2304.28004	100	-87	2	0	1	1	2095.92024	20	-24
1	0	0	1	2080.27471 ^d	4	3	2	6	1	5	2104.84652	20	43
1	1	0	2	2069.26924 ^d	4	3	2	7	1	6	2113.52784	20	21
1	2	0	3	2058.04573 ^d	4	-4	2	8	1	7	2130.14037	20	21
1	3	0	4	2046.60741 ^d	4	1	2	9	1	8	2138.06581	20	21
1	4	0	5	2034.95791 ^d	4	-1	2	10	1	9	2145.73332	20	32
1	5	0	6	2023.10058 ^d	4	3	2	11	1	10	2153.14034	20	22
1	6	0	7	2011.03902 ^d	4	0	2	12	1	11	2160.28368	20	26
1	7	0	8	1998.77661 ^d	4	3	2	13	1	12	2167.16092	20	7
1	8	0	9	1986.31708 ^d	4	-7	2	14	1	13	2173.76886	20	7
1	9	0	10	1973.66364 ^d	4	2	2	15	1	14	2178.10516	20	-8
1	10	0	11	1960.82020 ^d	4	-4	2	16	1	15	2186.16691	20	-13
							2	17	1	16	2186.16691	20	-13
							2	18	1	17	2191.95141	20	0
							2	19	1	18	2191.95141	20	0

TABLE 1A—Continued

v'	j'	v''	j''	observed	u_{obs}^a	(c-o) ^a	v'	j'	v''	j''	observed	u_{obs}^a	(c-o) ^a
2	20	1	19	2197.45542	20	100	3	13	2	12	2096.99832	40	-27
2	21	1	20	2202.67837	200	93	3	14	2	13	2103.93614	40	2
2	22	1	21	2207.61783	200	-25	3	15	2	14	2110.60906	40	20
2	23	1	22	2212.26724	200	162	3	16	2	15	2117.01437	40	24
2	24	1	23	2216.63116	200	-39	3	17	2	16	2123.15050	200	-101
2	26	1	25	2224.47798	200	-67	3	18	2	17	2129.01150	40	-27
2	27	1	26	2227.95833	200	-87	3	19	2	18	2134.59860	200	-141
2	28	1	27	2231.13780	200	150	3	20	2	19	2139.90415	40	66
3	20	2	21	1725.51552	40	17	3	21	2	20	2144.93098	40	58
3	19	2	20	1739.58058	40	-15	4	16	3	17	1731.62537	200	-153
3	18	2	19	1753.49162	40	9	4	15	3	16	1744.82106	200	79
3	17	2	18	1767.24616	40	-10	4	14	3	15	1757.85522	200	-252
3	16	2	17	1780.83999	40	-1	4	13	3	14	1770.71356	200	-59
3	15	2	16	1794.27038	40	-39	4	12	3	13	1783.39853	200	67
3	14	2	15	1807.53351	40	-92	4	11	3	12	1795.90879	200	-82
3	13	2	14	1820.62466	40	-37	4	10	3	11	1808.23575	200	8
3	12	2	13	1833.54174	40	-15	4	9	3	10	1820.37919	200	15
3	11	2	12	1846.28116	40	-16	4	8	3	9	1832.33509	200	0
3	10	2	11	1858.83922	40	-19	4	7	3	8	1844.09772	200	193
3	9	2	10	1871.21231	40	-10	4	6	3	7	1855.66796	200	165
3	8	2	9	1883.39718	40	-13	4	5	3	6	1867.03055	1000	1101
3	7	2	8	1895.38976	40	34	4	4	3	5	1878.21151	200	63
3	6	2	7	1907.18806	40	-17	4	3	3	4	1889.17578	200	218
3	5	2	6	1918.78705	40	-5	4	2	3	3	1899.92086	1000	1481
3	4	2	5	1930.18386	40	13	4	0	3	1	1920.81366	200	-21
3	3	2	4	1941.37599	40	-53	4	2	3	1	1950.48586	200	71
3	2	2	3	1952.35804	40	-2	4	3	3	2	1959.93141	1000	-509
3	1	2	0	1994.13315	200	-105	4	5	3	4	1978.11086	200	-119
3	2	2	1	2004.01971	40	31	4	6	3	5	1986.84500	200	198
3	3	2	2	2013.67874	40	45	4	7	3	6	1995.34201	200	188
3	5	2	4	2032.29861	40	-22	4	8	3	7	2003.59707	200	27
3	6	2	5	2041.25213	40	-3	4	9	3	8	2011.60498	200	-70
3	7	2	6	2049.96414	40	23	4	10	3	9	2019.36324	200	-152
3	8	2	7	2058.43184	40	30	4	11	3	10	2026.86507	200	162
3	9	2	8	2066.65217	40	18	4	12	3	11	2034.11929	200	-304
3	10	2	9	2074.62245	40	-46	4	13	3	12	2041.10623	200	130
3	11	2	10	2082.33810	40	0	4	14	3	13	2047.84191	200	-423
3	12	2	11	2089.79784	40	-9	4	16	3	15	2060.50394	200	-59

^a Relative to last digit of the observation.^b From Ref. 16.^c Ref. 19.^d Ref. 18.

The results obtained on performing a simultaneous fit to the present D³⁵Cl and D³⁷Cl data sets and to analogous high-quality literature infrared (9, 11) and microwave (16) data for HCl using Eq. [2] are presented in Table 3. These fits were performed with atomic masses taken from the 1993 mass table (26), using program DSParFit (25), which uses a sequential rounding and refitting procedure to minimize the numbers of significant digits required to accurately represent the data (27). The “All-Isotopomer Fit” H³⁵Cl column in Table 3 presents the results of this simultaneous fit to all 292 HCl and 360 DCl data; for the user’s convenience, parameter sets for the minority isotopomers generated from the former using Eq. [3] are presented in the last three columns of this table. Note that our definition of the reference isotopomer means that $\Delta M_A^* = 0$ for both atoms of H³⁵Cl, so the level energies of all four isotopomers may be generated from the $Y_{l,m}^a$ parameters alone. The dimensionless standard error (27) for this combined isotopomer fit is $\bar{\sigma}_f = 0.985$, which means that on average, predictions yielded by the fitted constants agree with the experimental data to within 0.985 times the estimated experimental uncertainties. The $\bar{\sigma}_f$ values shown for the minority isotopomers were obtained by comparing the

experimental data with predictions generated using the listed (derived) $\{Y_{l,m}\}$ constants for these species. For D³⁵Cl and D³⁷Cl, these $\bar{\sigma}_f$ values are especially equivalent to those (1.171 and 0.855, respectively) associated with the independent band constant fits summarized in Table 2.

While not shown, the correlated uncertainties in the DCl parameters in Table 3 are all roughly $[\mu(\text{H}^{35}\text{Cl})/\mu(\text{DCl})]^{l+m/2}$ times those shown for the corresponding H³⁵Cl parameters. Because of the improved statistics associated with the fit to the larger data set, these are substantially smaller than the analogous uncertainties obtained in Dunham expansion fits to the data for one isotopomer at a time, while the quality of fit is essentially the same. Moreover, because of the greater range of v and J associated with the HCl data, the DCl parameters obtained from the combined isotopomer analysis include higher order vibrational and rotational expansion constants than could be reliably obtained from independent analyses of the D³⁵Cl and D³⁷Cl data. Thus, the DCl band constants recommended here are those calculated from the expansion coefficients in Table 3, rather than the independent-fit results shown in Table 2.

TABLE 1B
D³⁷Cl Line Positions (in cm⁻¹), Uncertainties,^a and the Differences^a
from Predictions Yielded by the Constants of Table 3

<i>v'</i>	<i>j'</i>	<i>v''</i>	<i>j''</i>	observed	<i>u</i> _{obs} ^a	(<i>c-o</i>) ^a	<i>v'</i>	<i>j'</i>	<i>v''</i>	<i>j''</i>	observed	<i>u</i> _{obs} ^a	(<i>c-o</i>) ^a
0	1	0	0	10.7524250 ^b	20	-9	1	13	0	12	2206.30060 ^d	4	4
0	2	0	1	21.5015095 ^c	10	1	1	14	0	13	2213.63128 ^d	12	-5
0	3	0	2	32.2439210 ^c	20	-19	1	15	0	14	2220.69508 ^d	25	2
0	4	0	3	42.9763201 ^c	20	-12	1	18	0	17	2240.25897	60	40
0	5	0	4	53.6953828 ^c	20	-28	1	19	0	18	2246.22920	60	38
0	6	0	5	64.3977826 ^c	20	-28	1	20	0	19	2251.91973	20	20
0	7	0	6	75.0801954 ^c	20	86	1	21	0	20	2257.32793	20	0
0	9	0	8	96.3719133 ^c	70	41	1	22	0	21	2262.45100	20	16
0	12	0	11	128.0774508 ^c	30	-17	1	23	0	22	2267.28715	20	10
0	15	0	14	159.4266496 ^c	30	35	1	24	0	23	2271.83386	20	2
0	17	0	16	180.0855293 ^c	60	-62	1	25	0	24	2276.08897	20	-19
1	1	1	0	10.5285668 ^b	50	-36	1	26	0	25	2280.04976	20	-2
1	2	1	1	21.0534668 ^b	5000	3517	1	27	0	26	2283.71463	20	-4
1	34	0	35	1603.40990	60	42	1	28	0	27	2287.08096	20	27
1	33	0	34	1619.69108	60	-12	1	29	0	28	2290.14753	20	6
1	32	0	33	1635.86748	60	-79	1	30	0	29	2292.91224	60	-56
1	31	0	32	1651.93420	20	0	1	32	0	31	2297.52591	200	-66
1	30	0	31	1667.89011	20	3	2	29	1	30	1637.33205	80	-48
1	29	0	30	1683.73101	20	11	2	28	1	29	1652.81179	80	-141
1	28	0	29	1699.45388	20	-15	2	27	1	28	1668.16832	80	-113
1	27	0	28	1715.05460	20	-6	2	26	1	27	1683.39865	20	-5
1	26	0	27	1730.53046	60	-37	2	25	1	26	1698.50112	20	11
1	25	0	26	1745.87681	20	8	2	24	1	25	1713.47152	20	10
1	24	0	25	1761.09190	60	-46	2	23	1	24	1728.30756	80	-121
1	23	0	24	1776.17032	20	-9	2	21	1	22	1757.55505	20	-15
1	22	0	23	1791.10954	20	17	2	20	1	21	1771.96188	20	-12
1	21	0	22	1805.90626	20	8	2	19	1	20	1786.21928	20	-28
1	20	0	21	1820.55640	20	16	2	18	1	19	1800.32318	20	-7
1	19	0	20	1835.05670	20	9	2	17	1	18	1814.27068	20	-11
1	18	0	19	1849.40327	20	18	2	16	1	17	1828.05794	20	-9
1	17	0	18	1863.59274	20	23	2	15	1	16	1841.68142	20	0
1	14	0	15	1905.18257 ^d	25	14	2	13	1	14	1868.42344	20	-13
1	13	0	14	1918.70764 ^d	25	7	2	12	1	13	1881.53465	20	-8
1	12	0	13	1932.05746 ^d	12	16	2	11	1	12	1894.46794	20	7
1	11	0	12	1945.22878 ^d	4	7	2	10	1	11	1907.22011	20	-1
1	10	0	11	1958.21786 ^d	4	-4	2	9	1	10	1919.78735	20	-1
1	9	0	10	1971.02090 ^d	12	8	2	8	1	9	1932.16621	20	0
1	8	0	9	1983.63483 ^d	4	-6	2	7	1	8	1944.35322	20	2
1	7	0	8	1996.05565 ^d	4	0	2	6	1	7	1956.34497	20	-2
1	6	0	7	2008.28014 ^d	4	-4	2	5	1	6	1968.13809	20	-22
1	5	0	6	2020.30461 ^d	4	1	2	4	1	5	1979.72933	60	-77
1	4	0	5	2032.12574 ^d	4	-3	2	3	1	4	1991.11421	60	-62
1	3	0	4	2043.73990 ^d	4	1	2	2	1	3	2002.28969	20	-14
1	2	0	3	2055.14379 ^d	4	-2	2	1	1	2	2013.25273	60	34
1	1	0	2	2066.33385 ^d	4	2	2	0	1	1	2024.00061	20	16
1	0	0	1	2077.30682 ^d	4	0	2	1	1	0	2044.83557	20	-12
1	1	0	0	2098.58780 ^d	4	0	2	2	1	1	2054.91607	20	-24
1	2	0	1	2108.88919 ^d	4	1	2	3	1	2	2064.76715	20	8
1	3	0	2	2118.96013 ^d	4	2	2	4	1	3	2074.38640	20	3
1	4	0	3	2128.79745 ^d	4	-4	2	5	1	4	2083.77010	20	15
1	5	0	4	2138.39776 ^d	4	2	2	6	1	5	2092.91598	60	-45
1	6	0	5	2147.75812 ^d	4	-2	2	7	1	6	2101.81934	20	-17
1	7	0	6	2156.87520 ^d	4	0	2	8	1	7	2110.47803	20	6
1	8	0	7	2165.74602 ^d	4	2	2	10	1	9	2127.04945	20	19
1	9	0	8	2174.36752 ^d	4	1	2	11	1	10	2134.95592	60	40
1	10	0	9	2182.73672 ^d	4	-4	2	12	1	11	2142.60626	20	11
1	11	0	10	2190.85054 ^d	4	-2	2	13	1	12	2149.99691	20	1
1	12	0	11	2198.70615 ^d	4	-1	2	14	1	13	2157.12514	20	-1
							2	15	1	14	2163.98844	20	-21

TABLE 1B—Continued

v'	j'	v''	j''	observed	u_{obs}^a	$(c-o)^a$	v'	j'	v''	j''	observed	u_{obs}^a	$(c-o)^a$
2	16	1	15	2170.58335	20	13	3	11	2	12	1844.00818	40	22
2	17	1	16	2176.90825	20	-6	3	10	2	11	1856.52748	40	-6
2	18	1	17	2182.95973	20	-1	3	9	2	10	1868.86266	40	-32
2	19	1	18	2188.73561	20	-14	3	8	2	9	1881.00953	40	17
2	20	1	19	2194.23395	80	-105	3	7	2	8	1892.96578	40	27
2	21	1	20	2199.44952	20	-1	3	6	2	7	1904.72821	40	-23
2	22	1	21	2204.38288	20	-3	3	5	2	6	1916.29113	40	92
2	23	1	22	2209.03104	60	-52	3	4	2	5	1927.65500	40	-13
2	24	1	23	2213.39006	20	12	3	5	2	4	2029.47854	40	49
2	25	1	24	2217.45965	20	-12	3	6	2	5	2038.40934	40	-6
2	26	1	25	2221.23561	80	70	3	7	2	6	2047.09917	40	2
2	28	1	27	2227.90577	200	-234	3	8	2	7	2055.54578	40	-8
2	29	1	28	2230.79228	200	-276	3	9	2	8	2063.74529	40	47
3	25	2	26	1651.35179	200	108	3	10	2	9	2071.69606	40	35
3	23	2	24	1680.68022	200	236	3	11	2	10	2079.39474	40	-7
3	22	2	23	1695.13870	200	170	3	12	2	11	2086.83705	40	60
3	21	2	22	1709.45197	200	369	3	13	2	12	2094.02273	40	-26
3	20	2	21	1723.62344	200	148	3	14	2	13	2100.94585	40	44
3	19	2	20	1737.64626	200	-151	3	15	2	14	2107.60771	200	-137
3	18	2	19	1751.51359	200	-190	3	16	2	15	2113.99706	200	281
3	17	2	18	1765.22239	40	-9	3	17	2	16	2120.12381	40	36
3	15	2	16	1792.16039	40	22	3	18	2	17	2125.98264	600	-604
3	14	2	15	1805.38166	40	-29	3	20	2	19	2136.85343	200	200
3	13	2	14	1818.43368	200	-177	3	21	2	20	2141.87749	40	-74
3	12	2	13	1831.30873	40	1	3	22	2	21	2146.61618	40	-16

^a Relative to last digit of the observation.^b From Ref. 16.^c Ref. 19.^d Ref. 18.

TABLE 2
 Band Constants from Independent Fits to Data for $X^1\Sigma^+$ State $D^{35}\text{Cl}$
 (Upper Entries) and $D^{37}\text{Cl}$ (Lower Entries)

constant	$v = 0$	$v = 1$	$v = 2$	$v = 3$	$v = 4$
G_v	—	2091.05872 (3)	4128.43035 (21)	6112.4489 (5)	8043.376 (2)
	—	2088.059239 (24)	4122.58868 (13)	6103.9208 (5)	—
B_v	5.39227196 (40)	5.2798447 (9)	5.1681257 (51)	5.056998 (10)	4.94626 (4)
	5.3764904 (2)	5.2645578 (7)	5.1533269 (31)	5.042685 (8)	—
$10^4 D_v$	1.39955 (3)	1.386673 (53)	1.37474 (35)	1.36335 (57)	1.345 (2)
	1.391341 (21)	1.378568 (48)	1.36647 (18)	1.35522 (40)	—
$10^9 H_v$	2.282 (8)	2.238 (11)	2.22 (8)	2.06 (8)	—
	2.2646 (65)	2.224 (11)	2.134 (38)	2.03 (5)	—
$10^{14} L_v$	-5.8 (5)	-6.3 (6)	-10 (7)	—	—
	-6.0 (5)	-6.7 (8)	-4 (2)	—	—

Note. The numbers in parentheses are the 95% confidence limit uncertainties in the last significant digits shown.

TABLE 3
Parameters for $X^1\Sigma^+$ State HCl and DCl Obtained from a Simultaneous Fit of 652 High-Resolution Infrared and Microwave Data for All Four Isotopomers to Eq. [2]

constant	Generated from the H ^{35}Cl constants and Eq.(3)			
	All-isotopomer Fit H ^{35}Cl	H ^{37}Cl	D ^{35}Cl	D ^{37}Cl
$Y_{1,0}$	2990.92476 (300)	2988.6603355	2145.132622	2141.974380
$Y_{2,0}$	-52.79996 (290)	-52.7200529	-27.1592560	-27.0793489
$Y_{3,0}$	0.21803 (110)	0.2175352	0.07993137	0.07957888
$Y_{4,0}$	-0.01146 (14)	-0.01142534	-0.003032167	-0.003014351
$Y_{0,1}$	10.5933002 (25)	10.577269724	5.448783774	5.432753231
$Y_{1,1}$	-0.3069985 (81)	-0.30630185	-0.113234481	-0.112735116
$10^4 Y_{2,1}$	16.28 (8)	16.23076	4.28500	4.25983
$10^4 Y_{3,1}$	-0.765 (31)	-0.762109	-0.145168	-0.144103
$10^4 Y_{4,1}$	-0.045 (4)	-0.044796	-0.0061244	-0.0060705
$10^4 Y_{0,2}$	-5.31668 (4)	-5.3005997	-1.40632931	-1.39806617
$10^4 Y_{1,2}$	0.07377 (6)	0.07349121	0.01381107	0.01370971
$10^4 Y_{2,2}$	-0.00365 (2)	-0.00363345	-0.00045188	-0.00044790
$10^8 Y_{0,3}$	1.6954 (10)	1.687714	0.230333	0.228306
$10^8 Y_{1,3}$	-0.0547 (14)	-0.054411	-0.0049491	-0.0048984
$10^{12} Y_{0,4}$	-0.787 (7)	-0.78225	-0.055095	-0.054449
$10^{12} Y_{1,4}$	-0.042 (10)	-0.04171	-0.0021088	-0.0020810
$10^2 \delta_{1,0}^{\text{H}}$	8.99 (36)	—	—	—
$10^2 \delta_{2,0}^{\text{H}}$	0.0 (3)	—	—	—
$10^2 \delta_{3,0}^{\text{H}}$	-0.273 (56)	—	—	—
$10^4 \delta_{0,1}^{\text{H}}$	-7.802 (25)	—	—	—
$10^4 \delta_{1,1}^{\text{H}}$	1.188 (57)	—	—	—
$10^4 \delta_{2,1}^{\text{H}}$	-0.17 (3)	—	—	—
$10^7 \delta_{0,2}^{\text{H}}$	2.99 (10)	—	—	—
$10^7 \delta_{1,2}^{\text{H}}$	-1.98 (19)	—	—	—
$10^7 \delta_{2,2}^{\text{H}}$	0.66 (8)	—	—	—
$10^{11} \delta_{0,3}^{\text{H}}$	-6 (2)	—	—	—
$10^{11} \delta_{1,3}^{\text{H}}$	8 (2)	—	—	—
$10^3 \delta_{1,0}^{\text{Cl}}$	-6.4 (5)	—	—	—
$10^5 \delta_{0,1}^{\text{Cl}}$	2.5 (4)	—	—	—
No. of data	652	135	193	167
No. parameters	29	0	0	0
$\bar{\sigma}_f$	0.985	0.938	1.148	0.862

Note. The numbers in parentheses are the 95% confidence limit uncertainties in the last significant digits shown.

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