

Table 1: Observed ro-vibrational transitions of X²Π CCl

J'	J''	$2\times\Omega'$	parity ^b	isotope ^c	Wavenumber cm ^{-1d}	Uncertainty ×100 ^e	Observed - Calculated ×10 ^{4f}
<i>(a) v = 1 - 0</i>							
47.5	48.5	1	0	0	784.9844	0.2	-23
47.5	48.5	1	1	0	784.9935	0.2	-29
46.5	47.5	3	1	0	785.0078	0.25	-41
46.5	47.5	3	0	0	785.0078	0.25	-49
43.5	44.5	1	0	0	792.8109	0.2	9
43.5	44.5	1	1	0	792.8211	0.2	8
42.5	43.5	3	1	0	792.8502	0.25	11
42.5	43.5	3	0	0	792.8502	0.25	5
39.5	40.5	1	0	0	800.4484	0.1	2
39.5	40.5	1	1	0	800.4598	0.1	6
38.5	39.5	3	1	0	800.5023	0.1	8
38.5	39.5	1	0	0	802.3266	0.1	-20
38.5	39.5	1	1	0	802.3383	0.1	-14
37.5	38.5	3	1	0	802.3820	0.1	-34
37.5	38.5	3	0	0	802.3855	0.1	-3
36.5	37.5	1	0	0	806.0530	0.1	-7
36.5	37.5	1	1	0	806.0649	0.1	-2
35.5	36.5	3	1	0	806.1182	0.1	6
35.5	36.5	3	0	0	806.1211	0.1	31
34.5	35.5	1	0	0	809.7300	0.1	-13
34.5	35.5	1	1	0	809.7417	0.1	-12
33.5	34.5	3	1	0	809.8000	0.1	-23
33.5	34.5	3	0	0	809.8028	0.1	2
31.5	32.5	3	1	0	813.4354	0.1	-36
31.5	32.5	3	0	0	813.4374	0.1	-19
30.5	31.5	1	0	0	816.9443	0.1	21
30.5	31.5	1	1	0	816.9565	0.1	22
29.5	30.5	3	1	0	817.0291	0.15	18
29.5	30.5	3	0	0	817.0291	0.15	16
39.5	40.5	1	0	1	795.4962	0.1	10
39.5	40.5	1	1	1	795.5075	0.1	14
38.5	39.5	3	1	1	795.5427	0.1	-13
38.5	39.5	3	0	1	795.5458	0.1	13

J'	J''	$2 \times \Omega'$	parity ^b	isotope ^c	Wavenumber cm^{-1d}	Uncertainty $\times 100^e$	Observed - Calculated $\times 10^{4f}$
37.5	38.5	1	0	1	799.1888	0.1	25
37.5	38.5	1	1	1	799.1979	0.1	4
36.5	37.5	3	1	1	799.2463	0.15	43
36.5	37.5	3	0	1	799.2463	0.15	39
35.5	36.5	1	0	1	802.8318	0.1	8
35.5	36.5	1	1	1	802.8437	0.1	13
34.5	35.5	3	1	1	802.8920	0.1	-14
34.5	35.5	3	0	1	802.8955	0.1	17
33.5	34.5	1	0	1	806.4312	0.1	24
33.5	34.5	1	1	1	806.4442	0.1	37
32.5	33.5	3	1	1	806.4969	0.1	-11
32.5	33.5	3	0	1	806.4996	0.1	13
31.5	32.5	1	0	1	809.9804	0.1	10
31.5	32.5	1	1	1	809.9922	0.1	9
30.5	31.5	3	1	1	810.0545	0.1	-9
30.5	31.5	3	0	1	810.0567	0.1	11
29.5	30.5	1	0	1	813.4823	0.1	-2
29.5	30.5	1	1	1	813.4948	0.1	1
28.5	29.5	3	1	1	813.5646	0.1	-5
28.5	29.5	3	0	1	813.5658	0.1	5
27.5	28.5	1	0	1	816.9409	0.1	31
27.5	28.5	1	1	1	816.9529	0.1	28
26.5	27.5	3	1	1	817.0285	0.15	17
26.5	27.5	3	0	1	817.0285	0.15	16
<i>(b) v = 2 - 1</i>							
42.5	43.5	1	0	0	784.7684	0.2	-6
42.5	43.5	1	1	0	784.7796	0.2	1
41.5	42.5	3	1	0	784.8144	0.25	18
41.5	42.5	3	0	0	784.8144	0.25	12
40.5	41.5	1	1	0	788.5562	0.2	-49
39.5	40.5	3	1	0	788.5993	0.25	-17
39.5	40.5	3	0	0	788.5993	0.25	-22
36.5	37.5	1	0	0	795.9713	0.2	-24
36.5	37.5	1	1	0	795.9859	0.1	9
35.5	36.5	3	1	0	796.0377	0.2	-7
34.5	35.5	1	0	0	799.6151	0.1	2

J'	J''	$2 \times \Omega'$	parity ^b	isotope ^c	Wavenumber cm^{-1d}	Uncertainty $\times 100^e$	Observed - Calculated $\times 10^{4f}$
34.5	35.5	1	1	0	799.6272	0.1	7
33.5	34.5	3	1	0	799.6880	0.15	14
33.5	34.5	3	0	0	799.6880	0.15	11
32.5	33.5	1	0	0	803.2068	0.1	-19
32.5	33.5	1	1	0	803.2197	0.1	-9
31.5	32.5	3	1	0	803.2872	0.1	-2
31.5	32.5	3	0	0	803.2894	0.1	17
32.5	33.5	1	0	0	803.2089	0.1	2
32.5	33.5	1	1	0	803.2211	0.1	5
29.5	30.5	3	1	0	806.8400	0.1	-3
29.5	30.5	3	0	0	806.8413	0.1	8
30.5	31.5	1	0	0	806.7554	0.1	7
30.5	31.5	1	1	0	806.7672	0.1	4
27.5	28.5	3	1	0	810.3432	0.1	-17
27.5	28.5	3	0	0	810.3450	0.1	-1
28.5	29.5	1	0	0	810.2526	0.1	1
28.5	29.5	1	1	0	810.2651	0.1	2
25.5	26.5	3	1	0	813.7999	0.1	-10
25.5	26.5	3	0	0	813.8005	0.1	-6
26.5	27.5	1	0	0	813.7014	0.1	-4
26.5	27.5	1	1	0	813.7145	0.1	2
23.5	24.5	3	0	0	817.2112	0.15	32
23.5	24.5	3	1	0	817.2112	0.15	34
24.5	25.5	1	0	0	817.1031	0.1	9
24.5	25.5	1	1	0	817.1155	0.1	6
15.5	16.5	1	0	0	831.7889	0.1	-9
15.5	16.5	1	1	0	831.8027	0.1	-5
14.5	15.5	3	0	0	831.9207	0.15	-9
14.5	15.5	3	1	0	831.9207	0.15	-9
12.5	13.5	1	1	0	836.4657	0.5	-65
11.5	12.5	3	0	0	836.5974	0.15	-2
11.5	12.5	3	1	0	836.5974	0.15	-2
10.5	11.5	1	0	0	839.5058	0.1	-16
10.5	11.5	1	1	0	839.5197	0.1	-12
9.5	10.5	3	0	0	839.6470	0.15	-33
9.5	10.5	3	1	0	839.6470	0.15	-33

J'	J''	$2 \times \Omega'$	parity ^b	isotope ^c	Wavenumber cm^{-1d}	Uncertainty $\times 100^e$	Observed - Calculated $\times 10^{4f}$
8.5	9.5	1	0	0	842.5046	0.1	2
8.5	9.5	1	1	0	842.5181	0.1	2
7.5	8.5	3	0	0	842.6505	0.15	-5
7.5	8.5	3	1	0	842.6505	0.15	-5
6.5	7.5	1	0	0	845.4500	0.1	6
6.5	7.5	1	1	0	845.4641	0.1	11
3.5	4.5	1	0	0	849.7697	0.1	7
3.5	4.5	1	1	0	849.7824	0.1	-1
2.5	3.5	3	0	0	849.9221	0.15	1
2.5	3.5	3	1	0	849.9221	0.15	1
6.5	5.5	1	0	0	864.5972	0.1	0
7.5	6.5	3	0	0	864.7343	0.15	-6
7.5	6.5	3	1	0	864.7343	0.15	-6
7.5	6.5	1	1	0	865.8502	0.1	2
7.5	6.5	1	0	0	865.8624	0.1	-6
8.5	7.5	1	1	0	867.1019	0.1	-4
8.5	7.5	1	0	0	867.1146	0.1	-6
9.5	8.5	3	0	0	867.2499	0.15	1
9.5	8.5	3	1	0	867.2499	0.15	1
9.5	8.5	1	1	0	868.3398	0.1	-11
9.5	8.5	1	0	0	868.3530	0.1	-7
10.5	9.5	3	0	0	868.4847	0.15	-17
10.5	9.5	3	1	0	868.4847	0.15	-17
12.5	11.5	1	1	0	871.9724	0.1	-17
12.5	11.5	1	0	0	871.9849	0.1	-17
18.5	17.5	1	1	0	878.8615	0.1	-41
18.5	17.5	1	0	0	878.8767	0.1	-7
39.5	40.5	1	0	1	785.5975	0.2	-49
39.5	40.5	1	1	1	785.6087	0.2	-46
38.5	39.5	3	1	1	785.6498	0.25	-23
38.5	39.5	3	0	1	785.6498	0.25	-28
31.5	32.5	1	0	1	799.9459	0.1	13
31.5	32.5	1	1	1	799.9575	0.1	10
30.5	31.5	3	1	1	800.0247	0.15	36
30.5	31.5	3	0	1	800.0247	0.15	34
29.5	30.5	1	0	1	803.4143	0.1	9

J'	J''	$2 \times \Omega'$	parity ^b	isotope ^c	Wavenumber cm^{-1d}	Uncertainty $\times 100^e$	Observed - Calculated $\times 10^{4f}$
29.5	30.5	1	1	1	803.4266	0.1	11
28.5	29.5	3	1	1	803.4960	0.1	-5
28.5	29.5	3	0	1	803.4986	0.1	19
27.5	28.5	1	0	1	806.8331	0.1	-18
27.5	28.5	1	1	1	806.8500	0.1	28
26.5	27.5	3	1	1	806.9267	0.15	24
26.5	27.5	3	0	1	806.9267	0.15	22
25.5	26.5	1	0	1	810.2093	0.1	7
25.5	26.5	1	1	1	810.2221	0.1	11
24.5	25.5	3	1	1	810.3048	0.15	5
24.5	25.5	3	0	1	810.3048	0.15	4
23.5	24.5	1	0	1	813.5354	0.1	12
23.5	24.5	1	1	1	813.5492	0.1	24
22.5	23.5	3	1	1	813.6368	0.15	8
22.5	23.5	3	0	1	813.6368	0.15	7
21.5	22.5	1	0	1	816.8122	0.1	8
21.5	22.5	1	1	1	816.8251	0.1	9
20.5	21.5	3	1	1	816.9224	0.15	34
20.5	21.5	3	0	1	816.9224	0.15	33
(c) $\nu = 3 - 2$							
31.5	32.5	1	0	0	794.9527	0.1	-15
31.5	32.5	1	1	0	794.9647	0.1	-15
30.5	31.5	3	1	0	795.0349	0.15	-21
30.5	31.5	3	0	0	795.0349	0.15	-23
28.5	29.5	1	0	0	800.1665	0.1	-5
28.5	29.5	1	1	0	800.1789	0.1	-4
27.5	28.5	3	1	0	800.2595	0.15	-5
27.5	28.5	3	0	0	800.2595	0.15	-7
26.5	27.5	1	0	0	803.5826	0.1	3
26.5	27.5	1	1	0	803.5953	0.1	5
25.5	26.5	3	1	0	803.6819	0.15	1
25.5	26.5	3	0	0	803.6819	0.15	-1
25.5	26.5	1	0	0	805.2716	0.1	-2
25.5	26.5	1	1	0	805.2844	0.1	0
24.5	25.5	3	1	0	805.3738	0.15	-8
24.5	25.5	3	0	0	805.3738	0.15	-9

J'	J''	$2 \times \Omega'$	parity ^b	isotope ^c	Wavenumber cm^{-1d}	Uncertainty $\times 100^e$	Observed - Calculated $\times 10^{4f}$
24.5	25.5	1	0	0	806.9502	0.1	10
24.5	25.5	1	1	0	806.9624	0.1	5
23.5	24.5	3	1	0	807.0539	0.15	-13
23.5	24.5	3	0	0	807.0539	0.15	-14
22.5	23.5	1	0	0	810.2668	0.1	-6
22.5	23.5	1	1	0	810.2799	0.1	-4
21.5	22.5	3	1	0	810.3792	0.15	-4
21.5	22.5	3	0	0	810.3792	0.15	-5
20.5	21.5	1	0	0	813.5367	0.15	2
20.5	21.5	1	1	0	813.5500	0.15	5
19.5	20.5	3	1	0	813.6551	0.15	4
19.5	20.5	3	0	0	813.6551	0.15	3
18.5	19.5	1	0	0	816.7565	0.1	3
18.5	19.5	1	1	0	816.7696	0.1	2
17.5	18.5	3	1	0	816.8819	0.15	18
17.5	18.5	3	0	0	816.8819	0.15	17
34.5	35.5	1	0	1	784.8047	0.2	6
34.5	35.5	1	1	1	784.8169	0.2	13
33.5	34.5	3	1	1	784.8765	0.25	51
33.5	34.5	3	0	1	784.8765	0.25	48
32.5	33.5	1	0	1	788.3041	0.2	-45
31.5	32.5	3	1	1	788.3827	0.25	2
31.5	32.5	3	0	1	788.3827	0.25	-1
28.5	29.5	1	0	1	795.1786	0.1	5
28.5	29.5	1	1	1	795.1860	0.1	-43
27.5	28.5	3	1	1	795.2646	0.15	-4
27.5	28.5	3	0	1	795.2646	0.15	-5
25.5	26.5	1	0	1	800.2078	0.1	9
25.5	26.5	1	1	1	800.2209	0.1	16
24.5	25.5	3	1	1	800.3046	0.15	16
24.5	25.5	3	0	1	800.3046	0.15	14
23.5	24.5	1	0	1	803.5012	0.1	12
23.5	24.5	1	1	1	803.5125	0.1	-1
22.5	23.5	3	1	1	803.6038	0.15	17
22.5	23.5	3	0	1	803.6038	0.15	16
21.5	22.5	3	1	1	805.2322	0.15	-14

J'	J''	$2 \times \Omega'$	parity ^b	isotope ^c	Wavenumber cm^{-1d}	Uncertainty $\times 100^e$	Observed - Calculated $\times 10^{4f}$
21.5	22.5	3	0	1	805.2322	0.15	-15
21.5	22.5	1	0	1	806.7469	0.15	18
21.5	22.5	1	1	1	806.7558	0.15	-21
20.5	21.5	3	1	1	806.8552	0.15	21
20.5	21.5	3	0	1	806.8552	0.15	21
16.5	17.5	1	0	1	814.6466	0.1	4
16.5	17.5	1	1	1	814.6614	0.1	21
14.5	15.5	1	0	1	817.7211	0.1	0
14.5	15.5	1	1	1	817.7335	0.1	-7
13.5	14.5	3	1	1	817.8469	0.15	1
13.5	14.5	3	0	1	817.8469	0.15	1
<i>(d) v = 4 - 3</i>							
25.5	26.5	1	0	0	795.2647	0.1	-1
25.5	26.5	1	1	0	795.2763	0.1	-11
24.5	25.5	3	1	0	795.3671	0.15	-10
24.5	25.5	3	0	0	795.3671	0.15	-11
22.5	23.5	1	0	0	800.2104	0.1	-7
22.5	23.5	1	1	0	800.2235	0.1	-4
20.5	21.5	1	0	0	803.4477	0.1	-3
20.5	21.5	1	1	0	803.4609	0.1	-1
19.5	20.5	3	1	0	803.5664	0.15	-1
19.5	20.5	3	0	0	803.5664	0.15	-2
18.5	19.5	1	0	0	806.6362	0.15	1
18.5	19.5	1	1	0	806.6487	0.15	-5
17.5	18.5	3	1	0	806.7602	0.15	1
17.5	18.5	3	0	0	806.7602	0.15	0
16.5	17.5	1	0	0	809.7735	0.1	-14
16.5	17.5	1	1	0	809.7867	0.1	-14
15.5	16.5	3	1	0	809.9046	0.15	4
15.5	16.5	3	0	0	809.9046	0.15	3
13.5	14.5	1	0	0	814.3896	0.1	-4
13.5	14.5	1	1	0	814.4032	0.2	-2
12.5	13.5	3	1	0	814.5278	0.15	12
12.5	13.5	3	0	0	814.5278	0.15	12
11.5	12.5	1	0	0	817.4057	0.1	14
11.5	12.5	1	1	0	817.4190	0.1	13

J'	J''	$2 \times \Omega'$	parity ^b	isotope ^c	Wavenumber cm^{-1d}	Uncertainty $\times 100^e$	Observed - Calculated $\times 10^{4f}$
10.5	11.5	3	1	0	817.5453	0.1	2
10.5	11.5	3	0	0	817.5453	0.1	2
28.5	29.5	1	0	1	785.3515	0.2	-11
28.5	29.5	1	1	1	785.3632	0.2	-15
27.5	28.5	3	1	1	785.4450	0.25	49
27.5	28.5	3	0	1	785.4450	0.25	47
21.5	22.5	3	1	1	795.3101	0.15	-9
21.5	22.5	3	0	1	795.3101	0.15	-10
19.5	20.5	1	0	1	799.9729	0.1	10
19.5	20.5	1	1	1	799.9856	0.1	8
18.5	19.5	3	1	1	800.0858	0.15	1
18.5	19.5	3	0	1	800.0858	0.15	1
<i>(e) v = 5 - 4</i>							
25.5	26.5	1	0	0	785.3853	0.2	61
25.5	26.5	1	1	0	785.3976	0.2	59
24.5	25.5	3	1	0	785.4884	0.25	53
24.5	25.5	3	0	0	785.4884	0.25	52
21.5	22.5	1	0	0	791.8843	0.1	-9
21.5	22.5	1	1	0	791.8977	0.1	-3
20.5	21.5	3	1	0	791.9987	0.15	-25
20.5	21.5	3	0	0	791.9987	0.15	-26
19.5	20.5	1	0	0	795.0642	0.1	-18
19.5	20.5	1	1	0	795.0773	0.1	-17
18.5	19.5	3	1	0	795.1864	0.15	-13
18.5	19.5	3	0	0	795.1864	0.15	-14
16.5	17.5	1	0	0	799.7472	0.1	11
16.5	17.5	1	1	0	799.7602	0.1	9
15.5	16.5	3	1	0	799.8745	0.15	-13
15.5	16.5	3	0	0	799.8745	0.15	-13
14.5	15.5	1	0	0	802.8052	0.1	2
14.5	15.5	1	1	0	802.8188	0.1	5
13.5	14.5	3	1	0	802.9393	0.15	-1
13.5	14.5	3	0	0	802.9393	0.15	-2
12.5	13.5	1	0	0	805.8150	0.1	5
12.5	13.5	1	1	0	805.8297	0.1	19
11.5	12.5	3	1	0	805.9533	0.15	0

J'	J''	$2 \times \Omega^a$	parity ^b	isotope ^c	Wavenumber cm ⁻¹ ^d	Uncertainty ×100 ^e	Observed - Calculated ×10 ⁴ ^f
11.5	12.5	3	0	0	805.9533	0.15	-1

^a Twice the projection of \mathbf{J} on the molecular axis for the states involved in the transition.

^b For e levels, we have defined parity = 1, for f levels, parity = 0. The listed transitions all obey the selection rules $e \leftrightarrow e$ and $f \leftrightarrow f$.

^c Isotope number 0 is C³⁵Cl, 1 is C³⁷Cl.

^d Observed wavenumber for the transition in cm⁻¹.

^e Estimated measurement uncertainty, in cm⁻¹, accorded this point in the fitting.

^f Observed - calculated residual computed using the parameters in table 3.