

**Observed Transition Frequencies for CH<sup>35</sup>ClF<sub>2</sub>-H<sup>12</sup>C<sup>12</sup>CH**

<u>J'</u>	<u>K<sub>a</sub>'</u>	<u>K<sub>c</sub>'</u>	<u>F' + 1/2</u>	<u>J''</u>	<u>K<sub>a</sub>''</u>	<u>K<sub>c</sub>''</u>	<u>F'' + 1/2</u>	<u>Frequency (MHz)</u>	<u>Obs. - Calc. (MHz)</u>
2	0	2	3	1	0	1	2	4997.9879	0.0015
2	0	2	4	1	0	1	3	4999.2977	0.0019
2	1	1	4	1	1	0	3	5210.5939	0.0026
2	1	1	3	1	1	0	2	5219.2850	0.0011
3	1	3	4	2	1	2	4	7205.4268	-0.0007
3	1	3	2	2	1	2	1	7209.3602	-0.0029
3	1	3	3	2	1	2	2	7211.1401	0.0007
3	1	3	5	2	1	2	4	7212.3808	-0.0004
3	1	3	4	2	1	2	3	7214.1538	0.0014
3	1	3	3	2	1	2	3	7217.4130	0.0012
3	1	3	2	2	1	2	2	7218.1322	-0.0002
3	0	3	3	2	0	2	3	7459.2182	0.0005
3	0	3	4	2	0	2	3	7461.7282	0.0007
3	0	3	5	2	0	2	4	7463.6775	-0.0009
3	0	3	3	2	0	2	2	7464.4535	-0.0035
3	0	3	2	2	0	2	1	7466.3212	-0.0048
3	2	2	3	2	2	1	2	7519.9682	0.0026
3	2	2	4	2	2	1	3	7526.2641	-0.0024
3	2	1	2	2	2	0	1	7568.0472	-0.0044
3	2	1	5	2	2	0	4	7574.8125	-0.0022
3	2	1	3	2	2	0	2	7578.6275	0.0007
3	2	1	3	2	2	0	3	7583.8725	-0.0086
3	2	1	4	2	2	0	3	7585.3959	-0.0025
3	1	2	5	2	1	1	4	7809.6820	0.0023
3	1	2	4	2	1	1	3	7811.4185	0.0033
3	1	2	2	2	1	1	1	7813.1812	0.0016
3	1	2	3	2	1	1	2	7814.9246	-0.0028
3	1	2	4	2	1	1	4	7828.8471	-0.0030
4	1	4	3	3	1	3	2	9600.1493	0.0004
4	1	4	4	3	1	3	3	9600.4699	0.0002
4	1	4	6	3	1	3	5	9601.0831	0.0001
4	1	4	5	3	1	3	4	9601.3918	0.0013
4	1	4	4	3	1	3	4	9603.7254	-0.0037
4	1	4	3	3	1	3	3	9607.1415	-0.0004
4	0	4	3	3	0	3	3	9883.3952	0.0004
4	0	4	4	3	0	3	4	9883.9154	-0.0010
4	0	4	5	3	0	3	4	9885.0028	0.0024
4	0	4	4	3	0	3	3	9886.4276	0.0015
4	0	4	6	3	0	3	5	9887.3220	0.0058
4	0	4	3	3	0	3	2	9888.9256	0.0052
4	0	4	5	3	0	3	5	9890.4154	0.0046
4	2	3	3	3	2	2	2	10012.8784	-0.0037
4	2	3	6	3	2	2	5	10014.0231	0.0008
4	2	3	4	3	2	2	3	10016.0911	0.0070
4	2	3	5	3	2	2	4	10017.1634	-0.0033
4	3	2	3	3	3	1	2	10045.1096	0.0068
4	3	1	4	3	3	0	3	10057.4331	0.0002
4	2	2	3	3	2	1	3	10149.7273	-0.0036
4	2	2	3	3	2	1	2	10152.9073	-0.0023

4	2	2	6	3	2	1	5	10154.5648	-0.0031
4	2	2	4	3	2	1	4	10156.9961	0.0066
4	2	2	4	3	2	1	3	10158.5140	0.0073
4	2	2	5	3	2	1	4	10160.0495	0.0006
4	2	2	5	3	2	1	5	10163.2849	-0.0013
4	1	3	3	3	1	2	3	10378.2139	-0.0045
4	1	3	6	3	1	2	5	10395.1987	-0.0021
4	1	3	5	3	1	2	4	10395.3731	0.0046
4	1	3	5	3	1	2	5	10414.5313	-0.0076
5	1	5	5	4	1	4	4	11977.3716	0.0022
5	1	5	4	4	1	4	3	11977.5796	-0.0052
5	1	5	6	4	1	4	5	11977.7677	0.0045
5	1	5	7	4	1	4	6	11977.9829	-0.0050
5	0	5	6	4	0	4	5	12261.9975	-0.0078
5	0	5	5	4	0	4	4	12262.9628	-0.0031
5	0	5	7	4	0	4	6	12264.6572	0.0017
5	0	5	4	4	0	4	3	12265.5893	0.0039
5	2	4	4	4	2	3	3	12499.6051	0.0001
5	2	4	7	4	2	3	6	12499.7451	-0.0010
5	2	4	6	4	2	3	5	12501.0033	0.0042
5	3	3	7	4	3	2	6	12572.2556	-0.0021
5	3	3	6	4	3	2	5	12576.6255	-0.0006
5	3	2	4	4	3	1	3	12584.6891	-0.0027
5	3	2	7	4	3	1	6	12586.1365	0.0033
5	3	2	5	4	3	1	4	12589.3207	0.0026
5	3	2	6	4	3	1	5	12590.7437	-0.0035
5	2	3	6	4	2	2	6	12782.2364	0.0068
5	1	4	4	4	1	3	4	12944.2576	0.0015
5	1	4	7	4	1	3	6	12962.1102	0.0016
5	1	4	5	4	1	3	4	12963.0573	0.0032
5	1	4	4	4	1	3	3	12963.5712	-0.0029
6	1	6	6	5	1	5	6	14343.6347	0.0029
6	0	6	7	5	0	5	6	14596.9046	0.0016
6	0	6	6	5	0	5	5	14597.5348	-0.0001
6	0	6	8	5	0	5	7	14599.4915	-0.0010
6	0	6	5	5	0	5	4	14600.1151	-0.0021
6	3	3	5	5	3	2	4	15133.4923	0.0006
6	3	3	8	5	3	2	7	15134.1055	0.0002
6	3	3	6	5	3	2	5	15136.5892	-0.0034
6	1	5	7	5	1	4	6	15502.5877	-0.0056
6	1	5	5	5	1	4	4	15504.7396	-0.0026
6	1	5	7	5	1	4	7	15521.3974	0.0039
7	1	6	8	6	1	5	7	18009.7802	-0.0008
7	1	6	7	6	1	5	6	18010.7052	0.0006
7	1	6	9	6	1	5	8	18011.2789	0.0008
7	1	6	6	6	1	5	5	18012.0770	0.0006

**Observed Transition Frequencies for CH<sup>37</sup>ClF<sub>2</sub>-H<sup>12</sup>C<sup>12</sup>CH**

<u>J'</u>	<u>K<sub>a</sub>'</u>	<u>K<sub>c</sub>'</u>	<u>F' + 1/2</u>	<u>J''</u>	<u>K<sub>a</sub>''</u>	<u>K<sub>c</sub>''</u>	<u>F'' + 1/2</u>	<u>Frequency (MHz)</u>	<u>Obs. - Calc. (MHz)</u>
3	1	3	2	2	1	2	1	7150.9879	0.0050
3	1	3	5	2	1	2	4	7153.3386	-0.0019
3	1	3	4	2	1	2	3	7154.7081	-0.0034
3	0	3	4	2	0	2	3	7408.8689	0.0042
3	0	3	5	2	0	2	4	7410.5003	0.0000
3	0	3	3	2	0	2	2	7411.0397	0.0021
3	0	3	2	2	0	2	1	7412.6017	-0.0002
3	2	1	2	2	2	0	1	7529.5209	-0.0013
3	2	1	5	2	2	0	4	7534.8511	-0.0081
3	2	1	3	2	2	0	2	7537.9184	-0.0061
3	2	1	4	2	2	0	3	7543.2577	-0.0080
3	1	2	5	2	1	1	4	7773.2831	-0.0050
3	1	2	4	2	1	1	3	7774.6250	0.0008
3	1	2	2	2	1	1	1	7776.0538	0.0030
3	1	2	3	2	1	1	2	7777.3948	0.0009
4	1	4	3	3	1	3	2	9519.9775	-0.0040
4	1	4	4	3	1	3	3	9520.2038	-0.0012
4	1	4	6	3	1	3	5	9520.7083	0.0016
4	1	4	5	3	1	3	4	9520.9225	0.0011
4	0	4	4	3	0	3	3	9809.0750	-0.0017
4	0	4	6	3	0	3	5	9809.8696	0.0016
4	0	4	3	3	0	3	2	9811.1444	0.0067
4	2	3	3	3	2	2	2	9949.7947	-0.0054
4	2	3	6	3	2	2	5	9950.5656	0.0029
4	2	3	4	3	2	2	3	9952.1822	0.0019
4	2	3	5	3	2	2	4	9953.1048	0.0072
4	2	2	3	3	2	1	2	10104.8327	0.0053
4	2	2	6	3	2	1	5	10106.0819	0.0043
4	2	2	4	3	2	1	3	10109.2831	0.0035
4	2	2	5	3	2	1	4	10110.5288	0.0019
4	1	3	6	3	1	2	5	10344.2537	-0.0016
4	1	3	5	3	1	2	4	10344.3409	-0.0023
4	1	3	3	3	1	2	2	10345.9717	0.0093
4	1	3	4	3	1	2	3	10346.0542	-0.0032
5	1	5	5	4	1	4	4	11874.7677	-0.0003
5	1	5	4	4	1	4	3	11874.9628	-0.0040
5	1	5	6	4	1	4	5	11875.0730	-0.0001
5	1	5	7	4	1	4	6	11875.2790	0.0012
5	0	5	6	4	0	4	5	12157.4230	0.0008
5	0	5	5	4	0	4	4	12158.1792	0.0003
5	0	5	7	4	0	4	6	12159.5835	-0.0026
5	0	5	4	4	0	4	3	12160.3251	-0.0022
5	2	3	4	4	2	2	3	12714.5780	-0.0015
5	2	3	7	4	2	2	6	12714.9757	-0.0014
5	2	3	5	4	2	2	4	12717.6954	-0.0023
5	2	3	6	4	2	2	5	12718.0842	0.0049
5	1	4	6	4	1	3	5	12893.9629	0.0036
5	1	4	7	4	1	3	6	12894.4397	-0.0056
5	1	4	5	4	1	3	4	12895.1337	-0.0032

5	1	4	4	4	1	3	3	12895.6079	-0.0015
6	0	6	7	5	0	5	6	14463.4458	0.0050
6	0	6	6	5	0	5	5	14463.9269	-0.0018
6	0	6	8	5	0	5	7	14465.5113	-0.0011

**Observed Transition Frequencies for CH<sup>35</sup>ClF<sub>2</sub>-H<sup>13</sup>C<sup>13</sup>CH**

<u>J'</u>	<u>K<sub>a</sub>'</u>	<u>K<sub>c</sub>'</u>	<u>F' + 1/2</u>	<u>J''</u>	<u>K<sub>a</sub>''</u>	<u>K<sub>c</sub>''</u>	<u>F'' + 1/2</u>	<u>Frequency (MHz)</u>	<u>Obs. - Calc. (MHz)</u>
3	1	3	2	2	1	2	1	6896.9781	0.0009
3	1	3	3	2	1	2	2	6898.7863	0.0042
3	1	3	5	2	1	2	4	6900.0058	-0.0007
3	1	3	4	2	1	2	3	6901.8108	0.0000
3	0	3	4	2	0	2	3	7134.2694	0.0014
3	0	3	5	2	0	2	4	7136.0228	0.0018
3	0	3	3	2	0	2	2	7136.9338	0.0020
3	0	3	2	2	0	2	1	7138.6412	-0.0004
3	2	2	2	2	2	1	1	7174.4067	0.0000
3	2	2	5	2	2	1	4	7180.5034	-0.0055
3	2	2	3	2	2	1	2	7182.9252	0.0007
3	2	2	4	2	2	1	3	7189.2096	-0.0004
3	2	1	2	2	2	0	1	7221.5979	0.0043
3	2	1	5	2	2	0	4	7228.2862	-0.0026
3	2	1	3	2	2	0	2	7231.9658	-0.0013
3	2	1	4	2	2	0	3	7238.6730	0.0018
3	1	2	5	2	1	1	4	7450.8394	-0.0072
3	1	2	4	2	1	1	3	7452.6210	-0.0014
3	1	2	2	2	1	1	1	7454.3224	-0.0001
3	1	2	3	2	1	1	2	7456.1082	-0.0020
4	1	4	3	3	1	3	2	9186.1165	-0.0019
4	1	4	4	3	1	3	3	9186.4867	-0.0016
4	1	4	6	3	1	3	5	9187.0667	-0.0017
4	1	4	5	3	1	3	4	9187.4195	-0.0014
4	0	4	5	3	0	3	4	9458.5087	0.0017
4	0	4	4	3	0	3	3	9459.8886	-0.0020
4	0	4	6	3	0	3	5	9460.6194	-0.0011
4	0	4	3	3	0	3	2	9462.1826	-0.0012
4	2	3	6	3	2	2	5	9566.5506	0.0013
4	2	3	4	3	2	2	3	9568.6365	0.0010
4	2	3	5	3	2	2	4	9569.7098	0.0014
4	2	2	3	3	2	1	2	9682.7194	-0.0003
4	2	2	6	3	2	1	5	9684.2822	0.0001
4	2	2	4	3	2	1	3	9688.1059	0.0012
4	2	2	5	3	2	1	4	9689.6452	-0.0012
4	1	3	6	3	1	2	5	9920.0134	0.0024
4	1	3	5	3	1	2	4	9920.2553	0.0030
4	1	3	3	3	1	2	2	9922.1477	0.0034
4	1	3	4	3	1	2	3	9922.3997	0.0035
5	1	5	5	4	1	4	4	11463.4495	-0.0009
5	1	5	4	4	1	4	3	11463.6128	-0.0013
5	1	5	6	4	1	4	5	11463.8528	-0.0005
5	1	5	7	4	1	4	6	11464.0273	0.0010
5	0	5	6	4	0	4	5	11742.4571	0.0027
5	0	5	5	4	0	4	4	11743.4058	-0.0044
5	0	5	7	4	0	4	6	11744.9467	0.0004
5	0	5	4	4	0	4	3	11745.8429	0.0051
5	1	4	6	4	1	3	5	12373.4362	-0.0020
5	1	4	7	4	1	3	6	12373.8654	0.0001

5	1	4	5	4	1	3	4	12374.8971	0.0017
5	1	4	4	4	1	3	3	12375.3044	-0.0049
6	1	6	6	5	1	5	5	13729.4553	-0.0024
6	1	6	7	5	1	5	6	13729.6681	0.0014
6	1	6	5	5	1	5	4	13729.8663	-0.0016
6	1	6	8	5	1	5	7	13730.0893	0.0047
6	0	6	7	5	0	5	6	13987.8285	-0.0040
6	0	6	6	5	0	5	5	13988.4757	0.0021
6	0	6	8	5	0	5	7	13990.3284	0.0000

**Observed Transition Frequencies for CH<sup>37</sup>ClF<sub>2</sub>-H<sup>13</sup>C<sup>13</sup>CH**

<u>J'</u>	<u>K<sub>a</sub>'</u>	<u>K<sub>c</sub>'</u>	<u>F' + 1/2</u>	<u>J''</u>	<u>K<sub>a</sub>''</u>	<u>K<sub>c</sub>''</u>	<u>F'' + 1/2</u>	<u>Frequency (MHz)</u>	<u>Obs. - Calc. (MHz)</u>
3	1	3	2	2	1	2	1	6840.8213	-0.0025
3	1	3	3	2	1	2	2	6842.2286	0.0046
3	1	3	5	2	1	2	4	6843.2047	0.0031
3	1	3	4	2	1	2	3	6844.6010	0.0046
3	0	3	4	2	0	2	3	7083.4834	0.0019
3	0	3	5	2	0	2	4	7084.9517	0.0017
3	0	3	3	2	0	2	2	7085.5972	-0.0018
3	0	3	2	2	0	2	1	7087.0350	0.0013
3	1	2	5	2	1	1	4	7414.4874	-0.0044
3	1	2	4	2	1	1	3	7415.8560	-0.0041
4	1	4	3	3	1	3	2	9109.2080	-0.0075
4	1	4	4	3	1	3	3	9109.4818	0.0054
4	1	4	6	3	1	3	5	9109.9554	0.0029
4	1	4	5	3	1	3	4	9110.2079	0.0017
4	0	4	5	3	0	3	4	9385.2842	0.0005
4	0	4	4	3	0	3	3	9386.3979	0.0007
4	0	4	6	3	0	3	5	9387.0650	0.0035
4	0	4	3	3	0	3	2	9388.2800	-0.0045
4	1	3	5	3	1	2	4	9869.6891	-0.0023
4	1	3	4	3	1	2	3	9871.3813	-0.0064
5	1	5	5	4	1	4	4	11365.2835	0.0033
5	1	5	4	4	1	4	3	11365.4344	-0.0032
5	1	5	6	4	1	4	5	11365.5871	-0.0072
5	1	5	7	4	1	4	6	11365.7566	-0.0006
5	0	5	6	4	0	4	5	11643.7855	-0.0013
5	0	5	5	4	0	4	4	11644.5392	0.0002
5	0	5	7	4	0	4	6	11645.8281	0.0011
5	0	5	4	4	0	4	3	11646.5459	-0.0021
5	1	4	6	4	1	3	5	12307.1913	0.0024
5	1	4	7	4	1	3	6	12307.5850	0.0050
5	1	4	5	4	1	3	4	12308.3439	-0.0015
5	1	4	4	4	1	3	3	12308.7335	0.0060

**Principal axis coordinates (Å) from an Inertial Fit of  $I_a$  and  $I_b$  from all four isotopologues**

	a	b	c
Cl	0.730	1.293	0.000
C	0.635	-0.446	0.000
H	-0.413	-0.780	0.000
F	1.234	-0.950	-1.095
F	1.234	-0.950	1.095
C	-2.796	0.427	0.000
H	-2.330	1.380	0.000
H	-3.790	-1.607	0.000
C	-3.324	-0.654	0.000

**Principal axis coordinates (Å) from ab initio structure C**

	a	b	c
Cl	0.790	1.303	0.000
C	0.585	-0.461	0.000
H	-0.470	-0.694	0.000
F	1.178	-0.982	1.088
F	1.178	-0.982	-1.088
C	-2.819	0.490	0.000
H	-2.433	1.479	0.000
H	-3.642	-1.629	0.000
C	-3.248	-0.644	0.000