Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

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Rovibrational states of $ClHCl^-$ isotopologues up to high J: a joint theoretical and spectroscopic investigation

5 tables

1 figure

Table S1: Parameters of the empirically corrected potential energy function (PEF) for $ClHCl^-$.[a]

i	j	k	C_{ijk}	i	j	k	C_{ijk}	i	j	k	C_{ijk}
2	0	0	0.0773450	4	10	0	-0.0003822	0	2	2	-0.0374900
3	0	0	-0.0498158	4	12	0	-0.0008301	0	2	4	-0.0242871
4	0	0	0.0217425	5	2	0	0.0043572	0	2	6	-0.0036517
5	0	0	-0.0073538	5	4	0	0.0029379	0	2	8	-0.0002589
6	0	0	0.0016019	5	6	0	-0.0039644	0	2	10	-0.0000155
7	0	0	-0.0002199	5	10	0	0.0011371	0	4	2	0.0346458
8	0	0	0.0000373	5	14	0	-0.0000888	0	4	4	0.0211774
0	2	0	0.0279182	6	2	0	0.0004641	0	4	6	0.0040776
0	4	0	0.0094792	6	4	0	0.0014947	0	4	8	0.0002984
0	6	0	-0.0052787	6	6	0	-0.0027613	0	4	10	0.0000106
0	8	0	0.0007825	6	10	0	0.0004136	0	6	2	-0.0219698
0	10	0	0.0010154	6	14	0	-0.0000118	0	6	4	-0.0116997
0	12	0	-0.0007509	7	2	0	-0.0000241	0	6	6	-0.0023983
0	14	0	0.0001502	7	4	0	-0.0002386	0	6	8	-0.0001638
0	0	2	0.0014935	7	6	0	-0.0001067	0	6	10	-0.0000015
0	0	4	0.0163532	7	10	0	0.0000193	0	8	2	0.0129756
0	0	6	0.0014307	8	2	0	-0.0000941	0	8	4	0.0028007
0	0	8	0.0000561	8	6	0	-0.0000194	0	8	6	0.0008171
0	0	10	0.0000079	9	2	0	-0.0000126	0	8	8	0.0000521
1	2	0	0.0422749	9	4	0	0.0000284	0	8	10	-0.0000014
1	4	0	-0.0326682	1	0	2	-0.0593934	0	10	2	-0.0064233
1	6	0	0.0106962	1	0	4	-0.0294132	0	10	4	0.0006585
1	8	0	0.0045854	1	0	6	-0.0022362	0	10	6	-0.0002259
1	10	0	-0.0060801	1	0	8	-0.0001489	0	10	8	-0.0000053
1	12	0	0.0016207	1	0	10	-0.0000094	0	12	2	0.0019839
1	14	0	-0.0000463	2	0	2	0.0633335	0	12	4	-0.0005229
2	2	0	-0.0620863	2	0	4	0.0257936	0	12	6	0.0000615
2	4	0	0.0434672	2	0	6	0.0017940	0	12	8	-0.0000021
2	6	0	-0.0219992	2	0	8	0.0001110	0	14	2	-0.0002593
2	8	0	0.0025206	2	0	10	0.0000028	0	14	4	0.0000819
2	10	0	0.0084360	3	0	2	-0.0392638	0	14	6	-0.0000084
2	12	0	-0.0060076	3	0	4	-0.0140165	1	2	2	0.1036151
2	14	0	0.0011217	3	0	6	-0.0007201	1	2	4	0.0530646
3	2	0	0.0445309	3	0	8	-0.0000269	1	2	6	0.0069237
3	4	0	-0.0284852	4	0	2	0.0165319	1	2	8	0.0004039
3	6	0	-0.0004861	4	0	4	0.0044420	1	2	10	0.0000129
3	8	0	0.0005326	4	0	6	0.0000995	1	4	2	-0.0884463
3	10	0	0.0127926	4	0	8	0.0000026	1	4	4	-0.0502295
3	12	0	-0.0079993	5	0	2	-0.0039371	1	4	6	-0.0071554
3	14	0	0.0011842	5	0	4	-0.0006891	1	4	8	-0.0003176
4	2	0	-0.0225733	6	0	2	0.0003383	1	4	10	-0.0000052
4	4	0	0.0171729	6	0	4	0.0000522	1	6	2	0.0425572
4	6	0	-0.0159340	6	0	6	-0.0000013	1	6	4	0.0283437
4	8	0	0.0107322	8	0	2	-0.0000045	1	6	6	0.0035653

i	j	k	C_{ijk}	i	j	k	C_{ijk}	i	j	k	C_{ijk}
1	6	8	0.0000767	2	6	6	-0.0009960	3	10	6	-0.0000019
1	8	2	-0.0026121	2	6	8	-0.0000101	3	12	2	0.0001912
1	8	4	-0.0104877	2	8	2	0.0259203	3	14	2	0.0000564
1	8	6	-0.0009429	2	8	4	0.0046366	3	14	4	-0.0000053
1	8	8	0.0000139	2	8	6	-0.0000514	4	2	2	-0.0284133
1	10	2	-0.0092066	2	10	2	-0.0144457	4	2	4	-0.0046260
1	10	4	0.0031668	2	10	4	-0.0002950	4	2	6	-0.0000068
1	10	6	0.0000908	2	10	6	0.0000495	4	4	2	0.0102814
1	10	8	-0.0000074	2	12	2	0.0049889	4	4	4	0.0010613
1	12	2	0.0044067	2	12	4	-0.0000910	4	6	2	0.0014769
1	12	4	-0.0007329	2	14	2	-0.0005842	4	8	4	-0.0000024
1	12	6	0.0000130	2	14	4	0.0000062	4	10	2	-0.0006812
1	14	2	-0.0006235	3	2	2	0.0828252	4	14	2	0.0000439
1	14	4	0.0000745	3	2	4	0.0251071	5	2	2	0.0021479
1	14	6	-0.0000019	3	2	6	0.0012225	5	2	6	-0.0000045
2	2	2	-0.1207533	3	2	8	0.0000076	5	4	2	0.0009016
2	2	4	-0.0521229	3	4	2	-0.0640956	5	4	4	0.0000905
2	2	6	-0.0049219	3	4	4	-0.0150123	5	6	4	-0.0000175
2	2	8	-0.0001652	3	4	6	-0.0005451	5	10	2	-0.0000458
2	2	10	-0.0000013	3	6	2	0.0230008	6	2	2	0.0005882
2	4	2	0.1089015	3	6	4	0.0030830	7	2	2	0.0000338
2	4	4	0.0448765	3	6	6	0.0000797	7	4	2	-0.0000679
2	4	6	0.0037785	3	8	2	-0.0036975	7	10	2	0.0000020
2	4	8	0.0000714	3	8	4	0.0001078	8	6	2	0.0000011
2	6	2	-0.0569755	3	10	2	-0.0006633				
2	6	4	-0.0198517	3	10	4	-0.0000455				

[a] The PEF is expanded around the empirically corrected equilibrium structure (r_e = 1.55766 Å). All PEF terms are given in atomic units. The effect of coordinate scaling is included in the coefficients C_{ijk}.

Table S2. Parameters of the electric dipole moment function (EDMF) for $^{35}ClH^{35}Cl^{-}$.[a]

i	j	k	D''_{ijk}	i	j	k	$D^{\perp}_{ijk}$
0	1	0	1.8662590	0	0	1	-0.0958950
0	3	0	-0.3191300	0	0	3	-0.0082370
0	5	0	0.0467460	0	0	5	0.0066070
0	7	0	-0.0022550	1	0	1	-0.0761800
0	9	0	0.0001670	1	0	3	-0.009900
1	1	0	0.0299220	2	0	1	-0.002680
2	1	0	0.0615390	2	0	3	0.0205600
3	1	0	-0.0287760	3	0	1	-0.0056020
4	1	0	-0.0171080	0	2	1	-0.0117640
5	1	0	0.0222630	0	4	1	0.0128130
6	1	0	0.0119550	0	6	1	-0.0029680
1	3	0	0.1530650	0	8	1	0.0004010
2	3	0	-0.0668060	0	2	3	-0.0038770
3	3	0	0.0497760	0	4	3	0.0066880
4	3	0	-0.0418190	0	6	3	-0.0019780
1	5	0	-0.0438490	1	2	1	-0.0278100
2	5	0	0.0222500	2	2	1	0.0109380
0	1	2	-0.0163420				
0	1	4	-0.0046820				
0	3	2	-0.0768290				
0	5	2	0.0172560				
1	1	2	0.0332150				
2	1	2	-0.0381390				
1	3	2	0.0033180				

[a] All EDMF terms are given in atomic units; for definition of coordinates see Eqs. (3) and (4).

Table S3. Calculated rovibrational energies (in cm^{-1}) for states with $l = 0$.

	$^{35}ClH^{35}Cl^-$			$^{37}ClH^{35}Cl^-$			$^{37}ClH^{37}Cl^-$		
J	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$
0	0.0000	722.8965	983.1216	0.0000	722.9568	979.7641	0.0000	723.0197	976.3593
1	0.1947	723.0811	983.3052	0.1895	723.1364	979.9428	0.1842	723.1943	976.5330
2	0.5842	723.4502	983.6724	0.5684	723.4956	980.3002	0.5527	723.5436	976.8806
3	1.1684	724.0039	984.2232	1.1369	724.0344	980.8362	1.1054	724.0676	977.4018
4	1.9473	724.7421	984.9577	1.8948	724.7528	981.5510	1.8422	724.7661	978.0969
5	2.9210	725.6649	985.8757	2.8422	725.6508	982.4444	2.7634	725.6393	978.9657
6	4.0894	726.7723	986.9773	3.9790	726.7284	983.5164	3.8687	726.6872	980.0082
7	5.4524	728.0642	988.2625	5.3053	727.9856	984.7672	5.1582	727.9097	981.2245
8	7.0102	729.5406	989.7313	6.8210	729.4224	986.1966	6.6320	729.3068	982.6145
9	8.7627	731.2016	991.3836	8.5262	731.0387	987.8046	8.2899	730.8785	984.1783
10	10.7099	733.0471	993.2196	10.4209	732.8347	989.5913	10.1321	732.6248	985.9157
11	12.8518	735.0772	995.2390	12.5050	734.8101	991.5566	12.1584	734.5458	987.8269
12	15.1883	737.2918	997.4420	14.7784	736.9652	993.7005	14.3689	736.6414	989.9118
13	17.7196	739.6909	999.8285	17.2414	739.2998	996.0230	16.7635	738.9116	992.1703
14	20.4454	742.2745	1002.3986	19.8937	741.8140	998.5242	19.3423	741.3563	994.6025
15	23.3659	745.0426	1005.1521	22.7353	744.5077	1001.2039	22.1052	743.9757	997.2084
16	26.4810	747.9952	1008.0891	25.7664	747.3809	1004.0621	25.0523	746.7696	999.9880
17	29.7907	751.1322	1011.2096	28.9868	750.4337	1007.0989	28.1834	749.7381	1002.9411
18	33.2950	754.4538	1014.5135	32.3965	753.6660	1010.3143	31.4987	752.8811	1006.0679
19	36.9939	757.9598	1018.0009	35.9956	757.0777	1013.7081	34.9980	756.1987	1009.3683
20	40.8873	761.6502	1021.6716	39.7840	760.6690	1017.2804	38.6814	759.6908	1012.8423
21	44.9753	765.5251	1025.5257	43.7617	764.4397	1021.0312	42.5489	763.3575	1016.4898
22	49.2577	769.5844	1029.5632	47.9286	768.3899	1024.9605	46.6004	767.1987	1020.3108
23	53.7347	773.8281	1033.7840	52.2848	772.5196	1029.0682	50.8359	771.2143	1024.3054
24	58.4061	778.2562	1038.1881	56.8302	776.8287	1033.3542	55.2554	775.4044	1028.4734
25	63.2720	782.8686	1042.7756	61.5648	781.3172	1037.8187	59.8588	779.7690	1032.8150
26	68.3323	787.6654	1047.5462	66.4886	785.9851	1042.4615	64.6462	784.3081	1037.3300
27	73.5871	792.6466	1052.5001	71.6016	790.8323	1047.2826	69.6176	789.0216	1042.0184

	$^{35}ClH^{35}Cl^-$			$^{37}ClH^{35}Cl^-$			$^{37}ClH^{37}Cl^-$		
J	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$
28	79.0361	797.8120	1057.6372	76.9037	795.8590	1052.2820	74.7728	793.9095	1046.8801
29	84.6796	803.1618	1062.9575	82.3949	801.0650	1057.4597	80.1119	798.9718	1051.9153
30	90.5173	808.6958	1068.4609	88.0753	806.4503	1062.8156	85.6349	804.2085	1057.1238
31	96.5494	814.4141	1074.1474	93.9446	812.0149	1068.3498	91.3417	809.6195	1062.5056
32	102.7757	820.3166	1080.0169	100.0030	817.7588	1074.0621	97.2323	815.2049	1068.0607
33	109.1962	826.4033	1086.0695	106.2504	823.6820	1079.9525	103.3067	820.9646	1073.7891
34	115.8109	832.6742	1092.3052	112.6868	829.7844	1086.0211	109.5648	826.8986	1079.6906
35	122.6198	839.1293	1098.7237	119.3121	836.0660	1092.2677	116.0067	833.0068	1085.7653
36	129.6229	845.7685	1105.3252	126.1263	842.5268	1098.6924	122.6322	839.2893	1092.0132
37	136.8200	852.5917	1112.1096	133.1294	849.1667	1105.2950	129.4414	845.7460	1098.4342
38	144.2112	859.5991	1119.0768	140.3214	855.9858	1112.0757	136.4342	852.3769	1105.0283
39	151.7964	866.7905	1126.2268	147.7021	862.9840	1119.0342	143.6107	859.1820	1111.7954
40	159.5756	874.1659	1133.5596	155.2717	870.1612	1126.1706	150.9706	866.1612	1118.7356
41	167.5488	881.7252	1141.0751	163.0299	877.5175	1133.4849	158.5142	873.3145	1125.8486
42	175.7158	889.4685	1148.7733	170.9769	885.0528	1140.9769	166.2412	880.6418	1133.1346
43	184.0768	897.3957	1156.6541	179.1125	892.7671	1148.6468	174.1516	888.1432	1140.5935
44	192.6316	905.5068	1164.7174	187.4368	900.6603	1156.4943	182.2455	895.8187	1148.2253
45	201.3801	913.8017	1172.9633	195.9496	908.7324	1164.5195	190.5227	903.6681	1156.0298
46	210.3225	922.2804	1181.3917	204.6510	916.9833	1172.7223	198.9833	911.6914	1164.0071
47	219.4585	930.9429	1190.0025	213.5409	925.4131	1181.1026	207.6272	919.8886	1172.1570
48	228.7881	939.7890	1198.7957	222.6192	934.0217	1189.6605	216.4544	928.2598	1180.4797
49	238.3114	948.8188	1207.7712	231.8860	942.8090	1198.3959	225.4648	936.8047	1188.9749
50	248.0283	958.0323	1216.9290	241.3411	951.7751	1207.3086	234.6583	945.5234	1197.6428
51	257.9386	967.4293	1226.2690	250.9845	960.9197	1216.3988	244.0350	954.4159	1206.4831
52	268.0424	977.0099	1235.7911	260.8163	970.2431	1225.6662	253.5948	963.4821	1215.4959
53	278.3397	986.7739	1245.4954	270.8362	979.7449	1235.1109	263.3377	972.7219	1224.6811
54	288.8303	996.7213	1255.3817	281.0444	989.4253	1244.7328	273.2635	982.1354	1234.0387
55	299.5142	1006.8522	1265.4500	291.4406	999.2842	1254.5319	283.3723	991.7224	1243.5686
56	310.3914	1017.1664	1275.7002	302.0250	1009.3215	1264.5080	293.6640	1001.4829	1253.2708
57	321.4618	1027.6638	1286.1322	312.7974	1019.5372	1274.6612	304.1386	1011.4170	1263.1451

	$^{35}ClH^{35}Cl^-$			$^{37}ClH^{35}Cl^-$			$^{37}ClH^{37}Cl^-$		
J	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$
58	332.7253	1038.3445	1296.7461	323.7578	1029.9312	1284.9914	314.7960	1021.5245	1273.1916
59	344.1819	1049.2083	1307.5417	334.9061	1040.5035	1295.4985	325.6361	1031.8053	1283.4102
60	355.8316	1060.2553	1318.5190	346.2423	1051.2540	1306.1824	336.6590	1042.2595	1293.8008
61	367.6743	1071.4853	1329.6779	357.7663	1062.1826	1317.0431	347.8645	1052.8869	1304.3634
62	379.7099	1082.8982	1341.0183	369.4780	1073.2894	1328.0805	359.2526	1063.6876	1315.0979
63	391.9383	1094.4942	1352.5402	381.3775	1084.5742	1339.2946	370.8233	1074.6614	1326.0042
64	404.3596	1106.2729	1364.2434	393.4647	1096.0370	1350.6853	382.5765	1085.8084	1337.0824
65	416.9736	1118.2345	1376.1281	405.7394	1107.6778	1362.2525	394.5121	1097.1284	1348.3322
66	429.7803	1130.3788	1388.1939	418.2016	1119.4963	1373.9962	406.6301	1108.6214	1359.7538
67	442.7795	1142.7058	1400.4410	430.8514	1131.4927	1385.9163	418.9305	1120.2874	1371.3469
68	455.9714	1155.2154	1412.8691	443.6885	1143.6669	1398.0127	431.4131	1132.1262	1383.1116
69	469.3557	1167.9075	1425.4784	456.7130	1156.0187	1410.2853	444.0779	1144.1378	1395.0477
70	482.9325	1180.7821	1438.2685	469.9248	1168.5481	1422.7342	456.9250	1156.3222	1407.1552
71	496.7016	1193.8391	1451.2396	483.3238	1181.2551	1435.3591	469.9540	1168.6793	1419.4341
72	510.6630	1207.0784	1464.3914	496.9100	1194.1395	1448.1601	483.1652	1181.2090	1431.8842
73	524.8166	1220.4999	1477.7240	510.6832	1207.2013	1461.1370	496.5583	1193.9112	1444.5055
74	539.1623	1234.1035	1491.2373	524.6435	1220.4405	1474.2899	510.1333	1206.7859	1457.2979
75	553.7001	1247.8893	1504.9311	538.7908	1233.8568	1487.6185	523.8902	1219.8331	1470.2614
76	568.4299	1261.8571	1518.8054	553.1249	1247.4504	1501.1229	537.8288	1233.0526	1483.3959
77	583.3517	1276.0068	1532.8601	567.6459	1261.2211	1514.8029	551.9492	1246.4443	1496.7013
78	598.4653	1290.3383	1547.0951	582.3536	1275.1688	1528.6585	566.2512	1260.0083	1510.1774
79	613.7707	1304.8516	1561.5104	597.2480	1289.2934	1542.6896	580.7348	1273.7444	1523.8244
80	629.2677	1319.5465	1576.1058	612.3290	1303.5949	1556.8962	595.3999	1287.6525	1537.6420
81	644.9564	1334.4231	1590.8812	627.5965	1318.0732	1571.2780	610.2464	1301.7326	1551.6302
82	660.8367	1349.4811	1605.8367	643.0506	1332.7281	1585.8351	625.2744	1315.9846	1565.7890
83	676.9084	1364.7206	1620.9721	658.6909	1347.5597	1600.5674	640.4836	1330.4084	1580.1182
84	693.1715	1380.1414	1636.2872	674.5176	1362.5678	1615.4748	655.8741	1345.0040	1594.6177
85	709.6259	1395.7434	1651.7821	690.5306	1377.7524	1630.5572	671.4457	1359.7712	1609.2876
86	726.2715	1411.5265	1667.4566	706.7296	1393.1133	1645.8144	687.1984	1374.7100	1624.1277
87	743.1082	1427.4907	1683.3106	723.1148	1408.6505	1661.2466	703.1322	1389.8203	1639.1378

	$^{35}ClH^{35}Cl^-$			$^{37}ClH^{35}Cl^-$			$^{37}ClH^{37}Cl^-$		
J	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$	$(0,0^0,0)$	$(0,0^0,1)$	$(1,0^0,1)$
88	760.1361	1443.6358	1699.3441	739.6860	1424.3638	1676.8534	719.2468	1405.1019	1654.3181
89	777.3548	1459.9618	1715.5569	756.4430	1440.2533	1692.6350	735.5424	1420.5549	1669.6683
90	794.7645	1476.4685	1731.9489	773.3859	1456.3187	1708.5911	752.0187	1436.1791	1685.1883
91	812.3650	1493.1558	1748.5202	790.5146	1472.5600	1724.7216	768.6757	1451.9745	1700.8782
92	830.1561	1510.0238	1765.2705	807.8289	1488.9771	1741.0266	785.5133	1467.9409	1716.7378
93	848.1379	1527.0721	1782.1997	825.3288	1505.5699	1757.5059	802.5315	1484.0782	1732.7670
94	866.3102	1544.3008	1799.3079	843.0142	1522.3383	1774.1594	819.7301	1500.3864	1748.9658
95	884.6729	1561.7097	1816.5948	860.8850	1539.2822	1790.9870	837.1092	1516.8654	1765.3340
96	903.2260	1579.2987	1834.0605	878.9412	1556.4015	1807.9887	854.6685	1533.5150	1781.8716
97	921.9693	1597.0678	1851.7047	897.1825	1573.6962	1825.1643	872.4081	1550.3353	1798.5784
98	940.9028	1615.0168	1869.5274	915.6091	1591.1660	1842.5138	890.3278	1567.3260	1815.4545
99	960.0264	1633.1455	1887.5286	934.2206	1608.8109	1860.0370	908.4275	1584.4870	1832.4997
100	979.3399	1651.4540	1905.7080	953.0172	1626.6307	1877.7339	926.7072	1601.8184	1849.7140
101	998.8432	1669.9419	1924.0657	971.9986	1644.6255	1895.6044	945.1667	1619.3199	1867.0972
102	1018.5364	1688.6094	1942.6015	991.1648	1662.7950	1913.6484	963.8061	1636.9915	1884.6492
103	1038.4192	1707.4562	1961.3153	1010.5156	1681.1392	1931.8658	982.6252	1654.8331	1902.3701
104	1058.4915	1726.4822	1980.2070	1030.0511	1699.6579	1950.2565	1001.6238	1672.8446	1920.2596
105	1078.7534	1745.6873	1999.2765	1049.7710	1718.3511	1968.8204	1020.8020	1691.0258	1938.3177
106	1099.2045	1765.0714	2018.5239	1069.6754	1737.2185	1987.5575	1040.1596	1709.3766	1956.5444
107	1119.8450	1784.6343	2037.9488	1089.7640	1756.2602	2006.4676	1059.6965	1727.8970	1974.9395
108	1140.6746	1804.3760	2057.5513	1110.0369	1775.4760	2025.5507	1079.4127	1746.5869	1993.5030
109	1161.6932	1824.2963	2077.3313	1130.4938	1794.8657	2044.8067	1099.3080	1765.4460	2012.2347
110	1182.9008	1844.3950	2097.2887	1151.1347	1814.4292	2064.2354	1119.3824	1784.4744	2031.1347

Table S4: Calculated rovibrational energies (in cm^{-1}) for states with $l = 1$ of $^{35}ClH^{35}Cl^{-}$.

J	$(0,1^1,0)e$	$(0,1^1,0)f$	$(1,1^1,0)e$	$(1,1^1,0)f$
1	795.8488	795.8484	1090.4322	1090.4323
2	796.2417	796.2406	1090.8217	1090.8219
3	796.8310	796.8288	1091.4058	1091.4063
4	797.6168	797.6131	1092.1847	1092.1855
5	798.5990	798.5935	1093.1583	1093.1595
6	799.7777	799.7700	1094.3266	1094.3283
7	801.1528	801.1425	1095.6896	1095.6918
8	802.7242	802.7111	1097.2472	1097.2501
9	804.4921	804.4757	1098.9996	1099.0032
10	806.4563	806.4363	1100.9466	1100.9510
11	808.6170	808.5930	1103.0882	1103.0936
12	810.9739	810.9457	1105.4245	1105.4309
13	813.5272	813.4944	1107.9555	1107.9629
14	816.2768	816.2391	1110.6810	1110.6896
15	819.2227	819.1797	1113.6011	1113.6110
16	822.3648	822.3164	1116.7158	1116.7271
17	825.7032	825.6489	1120.0250	1120.0378
18	829.2378	829.1774	1123.5288	1123.5431
19	832.9686	832.9018	1127.2271	1127.2431
20	836.8955	836.8221	1131.1199	1131.1376
21	841.0186	840.9382	1135.2071	1135.2267
22	845.3377	845.2502	1139.4887	1139.5104
23	849.8529	849.7580	1143.9648	1143.9886
24	854.5642	854.4616	1148.6352	1148.6612
25	859.4714	859.3610	1153.5000	1153.5283
26	864.5746	864.4561	1158.5591	1158.5899
27	869.8737	869.7470	1163.8125	1163.8459
28	875.3686	875.2335	1169.2601	1169.2962
29	881.0594	880.9158	1174.9020	1174.9409
30	886.9460	886.7936	1180.7380	1180.7799
31	893.0284	892.8671	1186.7681	1186.8132
32	899.3064	899.1361	1192.9924	1193.0407
33	905.7801	905.6006	1199.4107	1199.4624
34	912.4494	912.2607	1206.0230	1206.0783
35	919.3143	919.1163	1212.8293	1212.8883
36	926.3747	926.1672	1219.8295	1219.8925
37	933.6305	933.4136	1227.0236	1227.0907
38	941.0818	940.8553	1234.4116	1234.4828
39	948.7284	948.4924	1241.9933	1242.0690
40	956.5703	956.3247	1249.7688	1249.8491
41	964.6075	964.3523	1257.7380	1257.8230
42	972.8398	972.5751	1265.9008	1265.9908
43	981.2673	980.9930	1274.2572	1274.3524
44	989.8899	989.6060	1282.8071	1282.9077

45	998.7075	998.4141	1291.5505	1291.6567
46	1007.7201	1007.4172	1300.4873	1300.5993
47	1016.9275	1016.6153	1309.6174	1309.7355
48	1026.3298	1026.0083	1318.9409	1319.0652
49	1035.9269	1035.5962	1328.4575	1328.5884
50	1045.7186	1045.3789	1338.1674	1338.3050
51	1055.7050	1055.3563	1348.0703	1348.2150
52	1065.8860	1065.5285	1358.1663	1358.3183
53	1076.2615	1075.8954	1368.4553	1368.6148
54	1086.8315	1086.4568	1378.9372	1379.1045
55	1097.5958	1097.2128	1389.6119	1389.7874
56	1108.5544	1108.1633	1400.4793	1400.6633
57	1119.7072	1119.3083	1411.5395	1411.7322
58	1131.0542	1130.6476	1422.7922	1422.9940
59	1142.5952	1142.1812	1434.2375	1434.4486
60	1154.3303	1153.9091	1445.8753	1446.0961
61	1166.2593	1165.8312	1457.7054	1457.9363
62	1178.3822	1177.9474	1469.7278	1469.9692
63	1190.6988	1190.2577	1481.9425	1482.1946
64	1203.2091	1202.7620	1494.3492	1494.6125
65	1215.9131	1215.4602	1506.9480	1507.2229
66	1228.8106	1228.3523	1519.7388	1520.0257
67	1241.9015	1241.4382	1532.7214	1533.0207
68	1255.1858	1254.7178	1545.8958	1546.2080
69	1268.6634	1268.1911	1559.2619	1559.5873
70	1282.3342	1281.8580	1572.8196	1573.1588
71	1296.1981	1295.7184	1586.5687	1586.9222
72	1310.2550	1309.7722	1600.5092	1600.8775
73	1324.5049	1324.0194	1614.6411	1615.0246
74	1338.9476	1338.4599	1628.9641	1629.3634
75	1353.5830	1353.0936	1643.4781	1643.8938
76	1368.4112	1367.9204	1658.1832	1658.6158
77	1383.4318	1382.9403	1673.0791	1673.5293
78	1398.6450	1398.1532	1688.1658	1688.6341
79	1414.0505	1413.5589	1703.4431	1703.9302
80	1429.6483	1429.1575	1718.9109	1719.4175
81	1445.4383	1444.9488	1734.5691	1735.0958
82	1461.4203	1460.9327	1750.4176	1750.9652
83	1477.5943	1477.1092	1766.4562	1767.0255
84	1493.9602	1493.4782	1782.6849	1783.2765
85	1510.5178	1510.0395	1799.1034	1799.7183
86	1527.2671	1526.7932	1815.7117	1816.3507
87	1544.2079	1543.7390	1832.5096	1833.1736
88	1561.3402	1560.8770	1849.4970	1850.1868
89	1578.6637	1578.2069	1866.6738	1867.3904
90	1596.1785	1595.7288	1884.0397	1884.7842
91	1613.8844	1613.4426	1901.5947	1902.3680
92	1631.7812	1631.3480	1919.3385	1920.1418

93	1649.8689	1649.4451	1937.2710	1938.1055
94	1668.1472	1667.7338	1955.3921	1956.2589
95	1686.6162	1686.2139	1973.7016	1974.6020
96	1705.2757	1704.8853	1992.1993	1993.1346
97	1724.1255	1723.7480	2010.8850	2011.8566
98	1743.1655	1742.8018	2029.7586	2030.7679
99	1762.3956	1762.0466	2048.8198	2049.8684
100	1781.8157	1781.4824	2068.0684	2069.1579
101	1801.4255	1801.1090	2087.5043	2088.6364
102	1821.2250	1820.9263	2107.1271	2108.3037
103	1841.2140	1840.9342	2126.9368	2128.1597
104	1861.3924	1861.1326	2146.9330	2148.2042
105	1881.7600	1881.5214	2167.1155	2168.4372
106	1902.3167	1902.1005	2187.4840	2188.8585
107	1923.0622	1922.8697	2208.0384	2209.4680
108	1943.9965	1943.8290	2228.7782	2230.2656
109	1965.1194	1964.9782	2249.7032	2251.2510
110	1986.4307	1986.3173	2270.8131	2272.4243
111	2007.9301	2007.8460	2292.1075	2293.7851
112	2029.6177	2029.5643	2313.5861	2315.3336
113	2051.4931	2051.4721	2335.2485	2337.0693
114	2073.5562	2073.5693	2357.0942	2358.9923
115	2095.8067	2095.8556	2379.1230	2381.1025
116	2118.2445	2118.3310	2401.3343	2403.3995
117	2140.8694	2140.9955	2423.7276	2425.8834
118	2163.6812	2163.8487	2446.3024	2448.5539
119	2186.6795	2186.8907	2469.0580	2471.4109
120	2209.8643	2210.1213	2491.9939	2494.4543

Table S5: Calculated effective spectroscopic constants (in cm^{-1}) for the $(0,1^1,0)$ and $(1,1^1,0)$ states of $^{37}ClH^{35}Cl^-$ and $^{37}ClH^{37}Cl^-$.[a]

Isotopomer	State	J_{max}	G_v	B_v	D_v (x 10^7)	q_v (x 10^3)	q_D (x 10^7)
$^{37}ClH^{35}Cl^-$	$(0,1^1,0)$	10	795.64	0.095481	0.5210	-0.172	0.22
		30	795.64	0.095481	0.5044	-0.171	0.20
		50	795.64	0.095479	0.4925	-0.168	0.17
		70	795.64	0.095476	0.4802	-0.162	0.15
		90	795.64	0.095472	0.4702	-0.152	0.13
		110	795.65	0.095468	0.4645	-0.143	0.11
	$(1,1^1,0)$	10	1086.34	0.094763	0.4664	0.040	-0.05
		30	1086.34	0.094763	0.4671	0.040	-0.05
		50	1086.34	0.094763	0.4688	0.040	-0.05
		70	1086.34	0.094764	0.4721	0.039	-0.05
		90	1086.34	0.094767	0.4784	0.036	-0.06
		110	1086.33	0.094775	0.4907	0.023	-0.08
$^{37}ClH^{37}Cl^-$	$(0,1^1,0)$	10	795.53	0.092831	0.4809	-0.159	0.20
		30	795.53	0.092830	0.4742	-0.159	0.18
		50	795.53	0.092829	0.4636	-0.156	0.16
		70	795.53	0.092826	0.4526	-0.150	0.14
		90	795.54	0.092822	0.4435	-0.141	0.12
		110	795.54	0.092819	0.4383	-0.133	0.11
	$(1,1^1,0)$	10	1082.29	0.092146	0.4394	0.040	-0.05
		30	1082.29	0.092146	0.4401	0.040	-0.05
		50	1082.29	0.092146	0.4418	0.040	-0.05
		70	1082.29	0.092147	0.4449	0.039	-0.05
		90	1082.29	0.092149	0.4506	0.036	-0.06
		110	1082.28	0.092157	0.4619	0.024	-0.07

[a] See Eqs. (7) and (8) for definition.