

Supplemental Material

Insights of the Peroxychloroformyl Radical ClC(O)OO via Microwave Spectrum

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Table S1. Observed transition frequencies of the *trans*-³⁵ClC(O)OO radical. (in MHz)

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
3	0	3	2.5	1.0	2	0	2	1.5	0.0	15080.783	15080.783	0.000
3	0	3	2.5	2.0	2	0	2	1.5	1.0	15078.766	15078.763	0.003
3	0	3	2.5	3.0	2	0	2	1.5	2.0	15083.502	15083.500	0.002
3	0	3	2.5	4.0	2	0	2	1.5	3.0	15085.120	15085.119	0.001
3	0	3	3.5	2.0	2	0	2	2.5	1.0	15065.671	15065.672	-0.001
3	0	3	3.5	2.0	2	0	2	2.5	2.0	15078.194	15078.192	0.002
3	0	3	3.5	3.0	2	0	2	2.5	2.0	15064.970	15064.972	-0.002
3	0	3	3.5	4.0	2	0	2	2.5	3.0	15067.137	15067.137	0.000
3	0	3	3.5	5.0	2	0	2	2.5	4.0	15067.515	15067.515	0.000
3	1	3	2.5	1.0	2	1	2	1.5	0.0	14175.600	14175.600	0.000
3	1	3	2.5	2.0	2	1	2	1.5	1.0	14171.830	14171.833	-0.003
3	1	3	2.5	3.0	2	1	2	1.5	2.0	14172.626	14172.627	-0.001
3	1	3	2.5	4.0	2	1	2	1.5	3.0	14176.329	14176.330	-0.001
3	1	3	3.5	2.0	2	1	2	2.5	1.0	14288.603	14288.603	0.000
3	1	3	3.5	3.0	2	1	2	2.5	2.0	14285.002	14285.002	0.000
3	1	3	3.5	3.0	2	1	2	2.5	3.0	14288.372	14288.371	0.001
3	1	3	3.5	4.0	2	1	2	2.5	3.0	14284.715	14284.715	0.000
3	1	3	3.5	5.0	2	1	2	2.5	4.0	14288.834	14288.833	0.001
3	1	2	2.5	2.0	2	1	1	1.5	1.0	16116.459	16116.459	0.000
3	1	2	2.5	3.0	2	1	1	1.5	2.0	16116.979	16116.980	-0.001
3	1	2	2.5	4.0	2	1	1	1.5	3.0	16120.065	16120.066	-0.001
3	1	2	3.5	2.0	2	1	1	2.5	1.0	16217.684	16217.680	0.004
3	1	2	3.5	3.0	2	1	1	2.5	2.0	16213.880	16213.880	0.000
3	1	2	3.5	4.0	2	1	1	2.5	3.0	16213.477	16213.477	0.000
3	1	2	3.5	5.0	2	1	1	2.5	4.0	16217.608	16217.608	0.000
4	0	4	3.5	2.0	3	0	3	2.5	1.0	19917.096	19917.101	-0.005
4	0	4	3.5	3.0	3	0	3	2.5	2.0	19916.501	19916.499	0.002
4	0	4	3.5	4.0	3	0	3	2.5	3.0	19918.583	19918.583	0.000
4	0	4	3.5	5.0	3	0	3	2.5	4.0	19918.931	19918.930	0.001
4	0	4	4.5	3.0	3	0	3	3.5	2.0	19899.903	19899.904	-0.001
4	0	4	4.5	4.0	3	0	3	3.5	3.0	19899.729	19899.730	-0.001
4	0	4	4.5	5.0	3	0	3	3.5	4.0	19901.087	19901.087	0.000
4	0	4	4.5	6.0	3	0	3	3.5	5.0	19901.273	19901.274	-0.001
4	1	4	3.5	2.0	3	1	3	2.5	1.0	18917.558	18917.555	0.003
4	1	4	3.5	3.0	3	1	3	2.5	2.0	18915.907	18915.904	0.003
4	1	4	3.5	4.0	3	1	3	2.5	3.0	18916.916	18916.915	0.001
4	1	4	3.5	5.0	3	1	3	2.5	4.0	18918.582	18918.582	0.000
4	1	4	4.5	3.0	3	1	3	3.5	2.0	18974.900	18974.897	0.003
4	1	4	4.5	4.0	3	1	3	3.5	3.0	18973.427	18973.426	0.001
4	1	4	4.5	5.0	3	1	3	3.5	4.0	18973.935	18973.935	0.000
4	1	4	4.5	6.0	3	1	3	3.5	5.0	18975.700	18975.700	0.000

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
4	1	3	3.5	3.0	3	1	2	2.5	2.0	21500.318	21500.319	-0.001
4	1	3	3.5	4.0	3	1	2	2.5	3.0	21501.137	21501.138	-0.001
4	1	3	3.5	5.0	3	1	2	2.5	4.0	21502.741	21502.743	-0.002
4	1	3	4.5	3.0	3	1	2	3.5	2.0	21541.276	21541.275	0.001
4	1	3	4.5	4.0	3	1	2	3.5	3.0	21539.653	21539.653	0.000
4	1	3	4.5	5.0	3	1	2	3.5	4.0	21540.125	21540.126	-0.001
4	1	3	4.5	6.0	3	1	2	3.5	5.0	21541.859	21541.860	-0.001
4	2	3	3.5	5.0	3	2	2	2.5	4.0	20150.636	20150.643	-0.007
4	2	3	4.5	5.0	3	2	2	3.5	4.0	20386.048	20386.047	0.001
4	2	3	4.5	6.0	3	2	2	3.5	5.0	20392.340	20392.340	0.000
4	2	2	3.5	5.0	3	2	1	2.5	4.0	20566.086	20566.085	0.001
4	2	2	4.5	6.0	3	2	1	3.5	5.0	20802.814	20802.814	0.000
5	0	5	4.5	3.0	4	0	4	3.5	2.0	24608.830	24608.827	0.003
5	0	5	4.5	4.0	4	0	4	3.5	3.0	24608.637	24608.635	0.002
5	0	5	4.5	5.0	4	0	4	3.5	4.0	24609.784	24609.790	-0.006
5	0	5	4.5	6.0	4	0	4	3.5	5.0	24609.816	24609.811	0.005
5	0	5	5.5	4.0	4	0	4	4.5	3.0	24593.944	24593.936	0.008
5	0	5	5.5	5.0	4	0	4	4.5	4.0	24593.969	24593.973	-0.004
5	0	5	5.5	6.0	4	0	4	4.5	5.0	24594.893	24594.891	0.002
5	0	5	5.5	7.0	4	0	4	4.5	6.0	24595.005	24595.006	-0.001
5	1	5	4.5	3.0	4	1	4	3.5	2.0	23600.263	23600.269	-0.006
5	1	5	4.5	4.0	4	1	4	3.5	3.0	23599.649	23599.647	0.002
5	1	5	4.5	5.0	4	1	4	3.5	4.0	23600.479	23600.478	0.001
5	1	5	4.5	6.0	4	1	4	3.5	5.0	23601.153	23601.151	0.002
5	1	5	5.5	4.0	4	1	4	4.5	3.0	23635.821	23635.822	-0.001
5	1	5	5.5	5.0	4	1	4	4.5	4.0	23635.128	23635.130	-0.002
5	1	4	4.5	4.0	4	1	3	3.5	3.0	26804.285	26804.282	0.003
5	1	4	4.5	5.0	4	1	3	3.5	4.0	26805.013	26805.015	-0.002
5	1	4	4.5	6.0	4	1	3	3.5	5.0	26805.650	26805.650	0.000
5	1	4	5.5	4.0	4	1	3	4.5	3.0	26821.674	26821.676	-0.002
5	1	4	5.5	6.0	4	1	3	4.5	5.0	26821.421	26821.421	0.000
5	1	4	5.5	7.0	4	1	3	4.5	6.0	26822.344	26822.345	-0.001
6	0	6	5.5	4.0	5	0	5	4.5	3.0	29126.209	29126.210	-0.001
6	0	6	5.5	5.0	5	0	5	4.5	4.0	29126.791	29126.792	-0.001
6	0	6	5.5	6.0	5	0	5	4.5	5.0	29127.785	29127.785	0.000
6	0	6	5.5	7.0	5	0	5	4.5	6.0	29127.500	29127.502	-0.002
6	0	6	6.5	5.0	5	0	5	5.5	4.0	29153.103	29153.106	-0.003
6	0	6	6.5	6.0	5	0	5	5.5	5.0	29153.238	29153.238	0.000
6	0	6	6.5	7.0	5	0	5	5.5	6.0	29153.844	29153.844	0.000
6	0	6	6.5	8.0	5	0	5	5.5	7.0	29153.995	29153.994	0.001
6	1	6	5.5	4.0	5	1	5	4.5	3.0	28252.093	28252.095	-0.002
6	1	6	5.5	5.0	5	1	5	4.5	4.0	28251.073	28251.073	0.000

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
6	1	6	5.5	6.0	5	1	5	4.5	5.0	28251.553	28251.552	0.001
6	1	6	5.5	7.0	5	1	5	4.5	6.0	28252.413	28252.414	-0.001
6	1	6	6.5	5.0	5	1	5	5.5	4.0	28263.237	28263.235	0.002
6	1	6	6.5	6.0	5	1	5	5.5	5.0	28262.792	28262.791	0.001
6	1	6	6.5	7.0	5	1	5	5.5	6.0	28263.303	28263.304	-0.001
6	1	6	6.5	8.0	5	1	5	5.5	7.0	28263.774	28263.774	0.000

6	1	5	5.5	4.0	5	1	4	4.5	3.0	32032.216	32032.212	0.004
6	1	5	5.5	5.0	5	1	4	4.5	4.0	32031.732	32031.734	-0.002
6	1	5	5.5	6.0	5	1	4	4.5	5.0	32032.262	32032.261	0.001
6	1	5	5.5	7.0	5	1	4	4.5	6.0	32032.601	32032.601	0.000
6	1	5	6.5	5.0	5	1	4	5.5	4.0	32034.055	32034.057	-0.002
6	1	5	6.5	6.0	5	1	4	5.5	5.0	32033.658	32033.658	0.000
6	1	5	6.5	7.0	5	1	4	5.5	6.0	32034.109	32034.109	0.000
6	1	5	6.5	8.0	5	1	4	5.5	7.0	32034.635	32034.635	0.000

1	1	1	0.5	2.0	0	0	0	0.5	1.0	12534.153	12534.150	0.003
1	1	1	1.5	2.0	0	0	0	0.5	2.0	11818.841	11818.840	0.001
1	1	1	1.5	3.0	0	0	0	0.5	2.0	11811.736	11811.741	-0.005

2	2	0	1.5	3.0	1	1	1	0.5	2.0	32920.705	32920.705	0.000
2	2	0	2.5	3.0	1	1	1	1.5	2.0	32034.841	32034.837	0.004
2	2	0	2.5	4.0	1	1	1	1.5	3.0	32027.068	32027.063	0.005

2	2	1	1.5	3.0	1	1	0	0.5	2.0	32214.391	32214.396	-0.005
2	2	1	2.5	2.0	1	1	0	1.5	1.0	31355.589	31355.589	0.000
2	2	1	2.5	3.0	1	1	0	1.5	2.0	31356.586	31356.591	-0.005
2	2	1	2.5	4.0	1	1	0	1.5	3.0	31349.741	31349.741	0.000

2	1	2	1.5	3.0	1	0	1	0.5	2.0	16743.853	16743.851	0.002
2	1	2	2.5	2.0	1	0	1	1.5	1.0	16334.205	16334.209	-0.004
2	1	2	2.5	3.0	1	0	1	1.5	2.0	16338.847	16338.848	-0.001
2	1	2	2.5	4.0	1	0	1	1.5	3.0	16332.456	16332.459	-0.003
3	2	2	3.5	4.0	2	1	1	2.5	3.0	35871.960	35871.956	0.004
3	2	2	3.5	5.0	2	1	1	2.5	4.0	35865.596	35865.594	0.002

3	1	3	2.5	4.0	2	0	2	1.5	3.0	20788.205	20788.207	-0.002
3	1	3	3.5	4.0	2	0	2	2.5	3.0	20510.471	20510.471	0.000
3	1	3	3.5	5.0	2	0	2	2.5	4.0	20507.351	20507.351	0.000

4	0	4	4.5	4.0	3	1	3	3.5	3.0	14458.212	14458.212	0.000
4	0	4	4.5	5.0	3	1	3	3.5	4.0	14457.751	14457.753	-0.002
4	0	4	4.5	6.0	3	1	3	3.5	5.0	14461.438	14461.438	0.000

4	1	4	3.5	5.0	3	0	3	2.5	4.0	24621.668	24621.670	-0.002
4	1	4	4.5	4.0	3	0	3	3.5	3.0	24414.949	24414.945	0.004
4	1	4	4.5	5.0	3	0	3	3.5	4.0	24417.270	24417.269	0.001
4	1	4	4.5	6.0	3	0	3	3.5	5.0	24415.534	24415.536	-0.002

Table S2. Observed transition frequencies of the *trans*-³⁷ClC(O)OO radical. (in MHz)

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
3	0	3	2.5	3.0	2	0	2	1.5	2.0	14727.289	14727.289	0.000
3	0	3	2.5	4.0	2	0	2	1.5	3.0	14728.577	14728.577	0.000
3	0	3	3.5	2.0	2	0	2	2.5	1.0	14710.210	14710.211	-0.001
3	0	3	3.5	3.0	2	0	2	2.5	2.0	14709.705	14709.706	-0.001
3	0	3	3.5	4.0	2	0	2	2.5	3.0	14711.438	14711.436	0.002
3	0	3	3.5	5.0	2	0	2	2.5	4.0	14711.763	14711.762	0.001
3	1	3	3.5	2.0	2	1	2	2.5	1.0	13962.681	13962.681	0.000
3	1	3	3.5	3.0	2	1	2	2.5	2.0	13959.821	13959.821	0.000
3	1	3	3.5	3.0	2	1	2	2.5	3.0	13962.465	13962.462	0.003
3	1	3	3.5	4.0	2	1	2	2.5	3.0	13959.597	13959.596	0.001
3	1	3	3.5	5.0	2	1	2	2.5	4.0	13962.879	13962.878	0.001
3	1	2	2.5	2.0	2	1	1	1.5	1.0	15704.415	15704.413	0.002
3	1	2	2.5	3.0	2	1	1	1.5	2.0	15704.832	15704.833	-0.001
3	1	2	2.5	4.0	2	1	1	1.5	3.0	15707.274	15707.273	0.001
3	1	2	3.5	3.0	2	1	1	2.5	2.0	15802.671	15802.671	0.000
3	1	2	3.5	4.0	2	1	1	2.5	3.0	15802.364	15802.362	0.002
3	1	2	3.5	5.0	2	1	1	2.5	4.0	15805.658	15805.657	0.001
4	0	4	3.5	2.0	3	0	3	2.5	1.0	19459.063	19459.064	-0.001
4	0	4	3.5	3.0	3	0	3	2.5	2.0	19458.611	19458.607	0.004
4	0	4	3.5	4.0	3	0	3	2.5	3.0	19460.246	19460.245	0.001
4	0	4	3.5	5.0	3	0	3	2.5	4.0	19460.534	19460.534	0.000
4	0	4	4.5	3.0	3	0	3	3.5	2.0	19442.482	19442.480	0.002
4	0	4	4.5	4.0	3	0	3	3.5	3.0	19442.367	19442.365	0.002
4	0	4	4.5	5.0	3	0	3	3.5	4.0	19443.441	19443.439	0.002
4	0	4	4.5	6.0	3	0	3	3.5	5.0	19443.597	19443.597	0.000
4	1	4	3.5	2.0	3	1	3	2.5	1.0	18487.143	18487.141	0.002
4	1	4	3.5	3.0	3	1	3	2.5	2.0	18485.824	18485.824	0.000
4	1	4	3.5	4.0	3	1	3	2.5	3.0	18486.624	18486.623	0.001
4	1	4	3.5	5.0	3	1	3	2.5	4.0	18487.954	18487.953	0.001
4	1	4	4.5	3.0	3	1	3	3.5	2.0	18544.712	18544.713	-0.001
4	1	4	4.5	4.0	3	1	3	3.5	3.0	18543.546	18543.547	-0.001
4	1	4	4.5	5.0	3	1	3	3.5	4.0	18543.955	18543.953	0.002
4	1	4	4.5	6.0	3	1	3	3.5	5.0	18545.358	18545.359	-0.001
1	1	1	1.5	3.0	0	0	0	0.5	2.0	11735.620	11735.621	-0.001
2	1	2	1.5	2.0	1	0	1	0.5	2.0	16569.140	16569.139	0.001
2	1	2	1.5	3.0	1	0	1	0.5	2.0	16572.861	16572.862	-0.001
2	1	2	2.5	2.0	1	0	1	1.5	1.0	16161.872	16161.870	0.002
2	1	2	2.5	3.0	1	0	1	1.5	2.0	16166.038	16166.038	0.000
2	1	2	2.5	4.0	1	0	1	1.5	3.0	16161.050	16161.051	-0.001
4	0	4	3.5	5.0	3	1	3	2.5	4.0	13653.691	13653.690	0.001
4	0	4	4.5	4.0	3	1	3	3.5	3.0	13899.165	13899.163	0.002

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
4	0	4	4.5	5.0	3	1	3	3.5	4.0	13898.782	13898.781	0.001
4	0	4	4.5	6.0	3	1	3	3.5	5.0	13901.738	13901.739	-0.001

Table S3. Observed transition frequencies of the *cis*-³⁵ClC(O)OO radical. (in MHz)

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
2	0	2	1.5	1.0	1	0	1	0.5	1.0	12569.292	12569.288	0.004
2	0	2	1.5	2.0	1	0	1	0.5	1.0	12566.912	12566.912	0.000
2	0	2	1.5	3.0	1	0	1	0.5	2.0	12569.419	12569.418	0.001
2	0	2	2.5	2.0	1	0	1	1.5	2.0	12551.503	12551.504	-0.001
2	0	2	2.5	3.0	1	0	1	1.5	2.0	12547.919	12547.918	0.001
2	0	2	2.5	4.0	1	0	1	1.5	3.0	12551.974	12551.974	0.000
2	1	2	1.5	3.0	1	1	1	0.5	2.0	11817.506	11817.504	0.002
2	1	2	2.5	3.0	1	1	1	1.5	2.0	11724.078	11724.080	-0.002
2	1	2	2.5	4.0	1	1	1	1.5	3.0	11725.431	11725.433	-0.002
2	1	1	1.5	3.0	1	1	0	0.5	2.0	15736.957	15736.955	0.002
2	1	1	2.5	3.0	1	1	0	1.5	2.0	15487.948	15487.948	0.000
2	1	1	2.5	4.0	1	1	0	1.5	3.0	15487.606	15487.606	0.000
3	0	3	2.5	2.0	2	0	2	1.5	1.0	17391.378	17391.377	0.001
3	0	3	2.5	2.0	2	0	2	1.5	2.0	17393.752	17393.753	-0.001
3	0	3	2.5	3.0	2	0	2	1.5	2.0	17390.950	17390.952	-0.002
3	0	3	2.5	4.0	2	0	2	1.5	3.0	17394.260	17394.260	0.000
3	0	3	3.5	2.0	2	0	2	2.5	1.0	17407.650	17407.650	0.000
3	0	3	3.5	3.0	2	0	2	2.5	2.0	17404.773	17404.773	0.000
3	0	3	3.5	3.0	2	0	2	2.5	3.0	17408.358	17408.360	-0.002
3	0	3	3.5	4.0	2	0	2	2.5	3.0	17404.391	17404.391	0.000
3	0	3	3.5	5.0	2	0	2	2.5	4.0	17407.249	17407.249	0.000
3	1	3	2.5	1.0	2	1	2	1.5	0.0	17090.312	17090.312	0.000
3	1	3	2.5	2.0	2	1	2	1.5	1.0	17088.855	17088.855	0.000
3	1	3	2.5	3.0	2	1	2	1.5	2.0	17090.422	17090.421	0.001
3	1	3	2.5	4.0	2	1	2	1.5	3.0	17091.994	17091.993	0.001
3	1	3	3.5	2.0	2	1	2	2.5	1.0	17054.660	17054.658	0.002
3	1	3	3.5	3.0	2	1	2	2.5	2.0	17053.125	17053.124	0.001
3	1	3	3.5	3.0	2	1	2	2.5	3.0	17057.688	17057.688	0.000
3	1	3	3.5	4.0	2	1	2	2.5	3.0	17053.562	17053.562	0.000
3	1	3	3.5	5.0	2	1	2	2.5	4.0	17055.012	17055.012	0.000
3	1	2	2.5	1.0	2	1	1	1.5	1.0	22393.880	22393.882	-0.002
3	1	2	2.5	2.0	2	1	1	1.5	1.0	22398.369	22398.371	-0.002
3	1	2	2.5	3.0	2	1	1	1.5	2.0	22394.682	22394.685	-0.003
3	1	2	2.5	4.0	2	1	1	1.5	3.0	22396.815	22396.817	-0.002
3	1	2	3.5	3.0	2	1	1	2.5	2.0	22274.618	22274.614	0.004
3	1	2	3.5	5.0	2	1	1	2.5	4.0	22275.074	22275.071	0.003
3	2	2	3.5	4.0	2	2	1	2.5	3.0	20447.126	20447.125	0.001
3	2	2	3.5	5.0	2	2	1	2.5	4.0	20447.454	20447.455	-0.001
3	2	1	2.5	2.0	2	2	0	1.5	1.0	23850.186	23850.188	-0.002
3	2	1	2.5	3.0	2	2	0	1.5	2.0	23851.037	23851.038	-0.001
3	2	1	2.5	4.0	2	2	0	1.5	3.0	23847.796	23847.798	-0.002

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
3	2	1	3.5	2.0	2	2	0	2.5	1.0	23497.246	23497.242	0.004
3	2	1	3.5	3.0	2	2	0	2.5	2.0	23499.629	23499.628	0.001
3	2	1	3.5	4.0	2	2	0	2.5	3.0	23499.802	23499.802	0.000
3	2	1	3.5	5.0	2	2	0	2.5	4.0	23497.308	23497.308	0.000
4	0	4	3.5	2.0	3	0	3	2.5	1.0	22202.923	22202.924	-0.001
4	0	4	3.5	3.0	3	0	3	2.5	2.0	22201.352	22201.350	0.002
4	0	4	3.5	4.0	3	0	3	2.5	3.0	22201.815	22201.815	0.000
4	0	4	3.5	5.0	3	0	3	2.5	4.0	22203.442	22203.443	-0.001
4	0	4	4.5	3.0	3	0	3	3.5	2.0	22204.964	22204.967	-0.003
4	0	4	4.5	5.0	3	0	3	3.5	4.0	22203.611	22203.611	0.000
4	0	4	4.5	6.0	3	0	3	3.5	5.0	22205.110	22205.109	0.001
4	1	4	3.5	2.0	3	1	3	2.5	1.0	22128.760	22128.759	0.001
4	1	4	3.5	3.0	3	1	3	2.5	2.0	22127.555	22127.555	0.000
4	1	4	3.5	4.0	3	1	3	2.5	3.0	22128.236	22128.234	0.002
4	1	4	3.5	5.0	3	1	3	2.5	4.0	22129.494	22129.494	0.000
4	1	4	4.5	3.0	3	1	3	3.5	2.0	22115.511	22115.513	-0.002
4	1	4	4.5	4.0	3	1	3	3.5	3.0	22114.304	22114.304	0.000
4	1	4	4.5	5.0	3	1	3	3.5	4.0	22114.609	22114.609	0.000
4	1	4	4.5	6.0	3	1	3	3.5	5.0	22115.776	22115.775	0.001
2	2	0	1.5	1.0	1	1	1	0.5	1.0	22585.423	22585.426	-0.003
2	2	0	1.5	2.0	1	1	1	0.5	1.0	22589.257	22589.258	-0.001
2	2	0	1.5	2.0	1	1	1	0.5	2.0	22588.597	22588.595	0.002
2	2	0	1.5	3.0	1	1	1	0.5	2.0	22585.207	22585.208	-0.001
2	2	0	2.5	1.0	1	1	1	1.5	0.0	22191.911	22191.911	0.000
2	2	0	2.5	1.0	1	1	1	1.5	1.0	22197.594	22197.592	0.002
2	2	0	2.5	2.0	1	1	1	1.5	1.0	22201.429	22201.427	0.002
2	2	0	2.5	2.0	1	1	1	1.5	2.0	22207.202	22207.204	-0.002
2	2	0	2.5	3.0	1	1	1	1.5	2.0	22208.972	22208.972	0.000
2	2	0	2.5	3.0	1	1	1	1.5	3.0	22205.456	22205.458	-0.002
2	2	0	2.5	4.0	1	1	1	1.5	3.0	22200.171	22200.171	0.000
2	2	1	1.5	1.0	1	1	0	0.5	1.0	19308.276	19308.280	-0.004
2	2	1	1.5	2.0	1	1	0	0.5	1.0	19307.863	19307.867	-0.004
2	2	1	1.5	2.0	1	1	0	0.5	2.0	19308.199	19308.197	0.002
2	2	1	1.5	3.0	1	1	0	0.5	2.0	19309.159	19309.163	-0.004
2	2	1	1.5	3.0	1	1	0	1.5	3.0	19639.123	19639.115	0.008
2	2	1	2.5	1.0	1	1	0	1.5	0.0	19306.645	19306.643	0.002
2	2	1	2.5	2.0	1	1	0	1.5	1.0	19301.816	19301.813	0.003
2	2	1	2.5	2.0	1	1	0	1.5	2.0	19297.311	19297.311	0.000
2	2	1	2.5	3.0	1	1	0	1.5	2.0	19296.792	19296.791	0.001
2	2	1	2.5	3.0	1	1	0	1.5	3.0	19303.262	19303.261	0.001
2	2	1	2.5	4.0	1	1	0	1.5	3.0	19301.972	19301.971	0.001
2	1	2	1.5	2.0	1	0	1	0.5	1.0	12959.142	12959.145	-0.003

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
2	1	2	1.5	2.0	1	0	1	0.5	2.0	12956.809	12956.808	0.001
2	1	2	1.5	3.0	1	0	1	0.5	2.0	12963.746	12963.745	0.001
2	1	2	2.5	2.0	1	0	1	1.5	1.0	13012.352	13012.352	0.000
2	1	2	2.5	3.0	1	0	1	1.5	2.0	13009.391	13009.391	0.000
2	1	2	2.5	4.0	1	0	1	1.5	3.0	13015.253	13015.253	0.000
3	2	2	2.5	1.0	2	1	1	1.5	0.0	24204.325	24204.325	0.000
3	2	2	2.5	2.0	2	1	1	1.5	1.0	24198.246	24198.248	-0.002
3	2	2	2.5	2.0	2	1	1	1.5	2.0	24191.581	24191.580	0.001
3	2	2	2.5	3.0	2	1	1	1.5	2.0	24192.188	24192.190	-0.002
3	2	2	2.5	4.0	2	1	1	1.5	3.0	24198.246	24198.248	-0.002
3	2	2	3.5	2.0	2	1	1	2.5	1.0	24264.952	24264.951	0.001
3	2	2	3.5	3.0	2	1	1	2.5	2.0	24259.132	24259.130	0.002
3	2	2	3.5	3.0	2	1	1	2.5	3.0	24256.823	24256.824	-0.001
3	2	2	3.5	4.0	2	1	1	2.5	3.0	24255.969	24255.968	0.001
3	2	2	3.5	5.0	2	1	1	2.5	4.0	24261.821	24261.819	0.002
3	1	3	2.5	2.0	2	0	2	1.5	1.0	17483.292	17483.293	-0.001
3	1	3	2.5	2.0	2	0	2	1.5	2.0	17485.671	17485.669	0.002
3	1	3	2.5	3.0	2	0	2	1.5	2.0	17482.653	17482.654	-0.001
3	1	3	2.5	4.0	2	0	2	1.5	3.0	17486.320	17486.320	0.000
3	1	3	3.5	2.0	2	0	2	2.5	1.0	17518.835	17518.835	0.000
3	1	3	3.5	3.0	2	0	2	2.5	2.0	17515.573	17515.574	-0.001
3	1	3	3.5	4.0	2	0	2	2.5	3.0	17515.033	17515.035	-0.002
3	1	3	3.5	5.0	2	0	2	2.5	4.0	17518.290	17518.292	-0.002
4	1	4	3.5	2.0	3	0	3	2.5	1.0	22221.041	22221.042	-0.001
4	1	4	3.5	3.0	3	0	3	2.5	2.0	22219.472	22219.471	0.001
4	1	4	3.5	3.0	3	0	3	2.5	3.0	22222.274	22222.273	0.001
4	1	4	3.5	4.0	3	0	3	2.5	3.0	22219.936	22219.936	0.000
4	1	4	3.5	5.0	3	0	3	2.5	4.0	22221.554	22221.554	0.000
4	1	4	4.5	3.0	3	0	3	3.5	2.0	22226.697	22226.698	-0.001
4	1	4	4.5	4.0	3	0	3	3.5	3.0	22225.103	22225.105	-0.002
4	1	4	4.5	5.0	3	0	3	3.5	4.0	22225.253	22225.253	0.000
4	1	4	4.5	5.0	3	0	3	3.5	5.0	22219.340	22219.335	0.005
4	1	4	4.5	6.0	3	0	3	3.5	5.0	22226.818	22226.818	0.000

Table S4. Observed transition frequencies of the *cis*-³⁷ClC(O)OO radical. (in MHz)

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
3	0	3	3.5	2.0	2	0	2	2.5	1.0	17124.384	17124.379	0.005
3	0	3	3.5	3.0	2	0	2	2.5	2.0	17122.411	17122.413	-0.002
3	0	3	3.5	4.0	2	0	2	2.5	3.0	17122.321	17122.321	0.000
3	0	3	3.5	5.0	2	0	2	2.5	4.0	17124.270	17124.271	-0.001
3	1	3	3.5	2.0	2	1	2	2.5	1.0	16756.103	16756.104	-0.001
3	1	3	3.5	3.0	2	1	2	2.5	2.0	16754.747	16754.745	0.002
3	1	3	3.5	4.0	2	1	2	2.5	3.0	16755.027	16755.029	-0.002
3	1	3	3.5	5.0	2	1	2	2.5	4.0	16756.326	16756.329	-0.003
3	1	2	2.5	3.0	2	1	1	1.5	2.0	21987.593	21987.596	-0.003
3	1	2	2.5	4.0	2	1	1	1.5	3.0	21989.208	21989.208	0.000
3	1	2	3.5	3.0	2	1	1	2.5	2.0	21861.713	21861.713	0.000
3	1	2	3.5	4.0	2	1	1	2.5	3.0	21860.541	21860.540	0.001
3	1	2	3.5	5.0	2	1	1	2.5	4.0	21862.220	21862.217	0.003
4	0	4	3.5	3.0	3	0	3	2.5	2.0	21831.852	21831.856	-0.004
4	0	4	3.5	4.0	3	0	3	2.5	3.0	21832.298	21832.296	0.002
4	0	4	3.5	5.0	3	0	3	2.5	4.0	21833.493	21833.496	-0.003
4	0	4	4.5	3.0	3	0	3	3.5	2.0	21836.378	21836.378	0.000
4	0	4	4.5	4.0	3	0	3	3.5	3.0	21835.264	21835.264	0.000
4	0	4	4.5	5.0	3	0	3	3.5	4.0	21835.446	21835.446	0.000
4	0	4	4.5	6.0	3	0	3	3.5	5.0	21836.539	21836.538	0.001
4	1	4	3.5	2.0	3	1	3	2.5	1.0	21753.046	21753.042	0.004
4	1	4	3.5	3.0	3	1	3	2.5	2.0	21752.103	21752.102	0.001
4	1	4	3.5	4.0	3	1	3	2.5	3.0	21752.661	21752.662	-0.001
4	1	4	3.5	5.0	3	1	3	2.5	4.0	21753.650	21753.651	-0.001
4	1	4	4.5	3.0	3	1	3	3.5	2.0	21739.115	21739.114	0.001
4	1	4	4.5	4.0	3	1	3	3.5	3.0	21738.165	21738.166	-0.001
4	1	4	4.5	5.0	3	1	3	3.5	4.0	21738.420	21738.421	-0.001
4	1	4	4.5	6.0	3	1	3	3.5	5.0	21739.335	21739.336	-0.001
2	2	0	1.5	3.0	1	1	1	0.5	2.0	22240.892	22240.891	0.001
2	2	0	2.5	1.0	1	1	1	1.5	0.0	21860.232	21860.231	0.001
2	2	0	2.5	2.0	1	1	1	1.5	1.0	21867.047	21867.048	-0.001
2	2	0	2.5	3.0	1	1	1	1.5	2.0	21872.310	21872.310	0.000
2	2	0	2.5	4.0	1	1	1	1.5	3.0	21865.977	21865.978	-0.001
2	2	1	1.5	3.0	1	1	0	0.5	2.0	19058.733	19058.733	0.000
2	2	1	2.5	2.0	1	1	0	1.5	1.0	19070.678	19070.680	-0.002
2	2	1	2.5	3.0	1	1	0	1.5	2.0	19067.460	19067.458	0.002
2	2	1	2.5	4.0	1	1	0	1.5	3.0	19070.281	19070.280	0.001
3	2	2	2.5	2.0	2	1	1	1.5	2.0	23861.869	23861.870	-0.001
3	2	2	2.5	3.0	2	1	1	1.5	2.0	23862.384	23862.384	0.000
3	2	2	2.5	4.0	2	1	1	1.5	3.0	23865.937	23865.936	0.001
3	2	2	3.5	2.0	2	1	1	2.5	1.0	23947.889	23947.890	-0.001

N'	K_a'	K_c'	J'	F'	N	K_a	K_c	J	F	Observed	Calculated	O.-C.
3	2	2	3.5	3.0	2	1	1	2.5	2.0	23944.576	23944.576	0.000
3	2	2	3.5	4.0	2	1	1	2.5	3.0	23942.796	23942.796	0.000
3	2	2	3.5	5.0	2	1	1	2.5	4.0	23946.138	23946.137	0.001
3	1	3	2.5	2.0	2	0	2	1.5	1.0	17205.764	17205.766	-0.002
3	1	3	2.5	3.0	2	0	2	1.5	2.0	17205.702	17205.700	0.002
3	1	3	2.5	4.0	2	0	2	1.5	3.0	17208.225	17208.224	0.001
3	1	3	3.5	2.0	2	0	2	2.5	1.0	17246.401	17246.400	0.001
3	1	3	3.5	3.0	2	0	2	2.5	2.0	17244.227	17244.227	0.000
3	1	3	3.5	4.0	2	0	2	2.5	3.0	17244.050	17244.050	0.000
3	1	3	3.5	5.0	2	0	2	2.5	4.0	17246.215	17246.216	-0.001
4	1	4	3.5	3.0	3	0	3	2.5	2.0	21851.733	21851.731	0.002
4	1	4	3.5	4.0	3	0	3	2.5	3.0	21852.175	21852.174	0.001
4	1	4	3.5	5.0	3	0	3	2.5	4.0	21853.357	21853.356	0.001
4	1	4	4.5	4.0	3	0	3	3.5	3.0	21859.980	21859.980	0.000
4	1	4	4.5	5.0	3	0	3	3.5	4.0	21860.149	21860.150	-0.001
4	1	4	4.5	6.0	3	0	3	3.5	5.0	21861.280	21861.281	-0.001