2,2,3,3,3-pentafluoro-1-propanol and its dimers: structural diversity, conformational conversion, and tunneling motion

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Point S1. Gaussian keywords used in the calculations.

Calculations	Employed keywords
Geometry optimization	Freq, fopt=(verytight,MaxCycles=200), int=SuperFine; empiricaldispersion=gd3bj
Harmonic calculation	Freq=(VCD,VibRot), or Freq=(savenormalmodes,VibRot)
	B3LYP, Def2-QZVP, empiricaldispersion=gd3bj; PBE1PBE, Def2-TZVPD, empiricaldispersion=gd3bj; MP2, cc-pVTZ
Anharmonic calculations	Freq=Anharmonic, fopt=tight, int=SuperFine (for TZVP); and fopt=verytight, (for QZVP)
Transition calculation	opt=(calcall,ts,noeigentest), scf=verytight, int=grid=SuperFine
Rigid PES scan	scan
BSSE correction	density=current, counterpoise=2
Common keywords	output=picket

The G16 optimized geometry files for the five PFP monomeric conformers and ten binary PFP conformers are provided as a zip file.

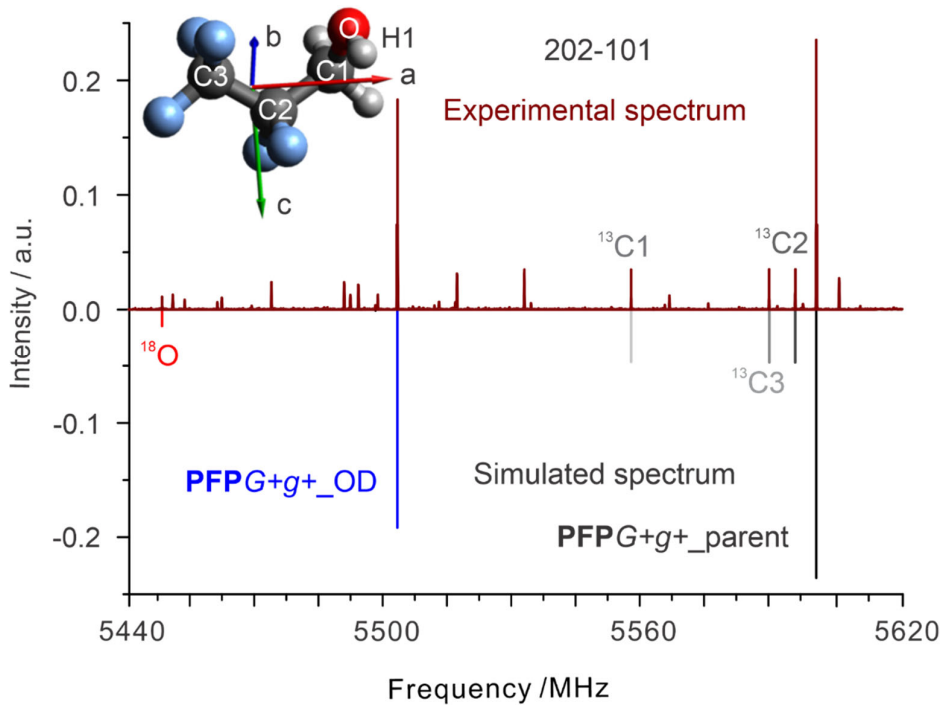

Figure S1. Experimental spectra of the **PFP***G+g+*/**PFP***G-g-* monomer and isotopologues species of its 2,0,2-1,0,1 transition of the PFP+D_2O mixture in the Ne atmosphere. The experimental spectroscopic constants, the calculated electric dipole moment components and a rotational temperature of 0.5 K were used for the spectral simulations. The experimental spectra were recorded by averaging about 900 k free induction decays.

Table S1. Rotational transition frequencies of the parent **PFP***G+g+* monomer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
4	1	3	4	1	4	2118.1766	2118.1757	0.0009
4	1	3	4	0	4	2234.4507	2234.4470	0.0037
2	2	1	2	1	2	2343.7751	2343.7759	-0.0008
5	3	2	5	2	3	2669.1246	2669.1171	0.0075
3	2	2	3	1	3	2698.7252	2698.7308	-0.0056
2	2	1	2	0	2	2742.2867	2742.2813	0.0054
1	0	1	0	0	0	2827.3625	2827.3649	-0.0024
4	3	2	4	2	2	2875.5745	2875.5743	0.0002
4	3	1	4	2	2	2929.1759	2929.1783	-0.0024
3	2	2	3	0	3	2932.0002	2931.9996	0.0006
3	2	1	3	1	3	2940.0504	2940.0449	0.0055
5	1	4	5	1	5	3057.9251	3057.9234	0.0017
5	1	4	5	0	5	3109.7134	3109.7116	0.0018
3	3	1	3	2	1	3151.2002	3151.1982	0.0020
3	3	0	3	2	1	3159.1253	3159.1271	-0.0018
4	2	3	4	1	4	3176.1133	3176.1103	0.0030
4	2	3	4	0	4	3292.3845	3292.3816	0.0029
7	2	5	7	1	6	3323.4127	3323.4166	-0.0039
1	1	1	0	0	0	3391.4452	3391.4460	-0.0008
3	3	1	3	2	2	3392.5119	3392.5124	-0.0005
3	3	0	3	2	2	3400.4417	3400.4413	0.0004
8	4	4	8	3	5	3504.7134	3504.7115	0.0019
4	3	2	4	2	3	3516.9767	3516.9731	0.0036
4	3	1	4	2	3	3570.5764	3570.5771	-0.0007
1	1	0	0	0	0	3608.6252	3608.6251	0.0001
5	3	3	5	2	4	3741.7379	3741.7370	0.0009
5	2	4	5	1	5	3765.1378	3765.1347	0.0031
7	4	3	7	3	4	3852.1488	3852.1447	0.0041
6	1	5	6	1	6	4031.1306	4031.1310	-0.0004
6	1	5	6	0	6	4052.5756	4052.5796	-0.0040
6	4	2	6	3	3	4199.5003	4199.4997	0.0006
5	4	2	5	3	2	4440.3648	4440.3667	-0.0019
6	2	5	6	1	6	4445.0748	4445.0748	0.0000
5	4	1	5	3	2	4449.2129	4449.2107	0.0022
6	2	5	6	0	6	4466.5241	4466.5234	0.0007
4	3	2	4	1	3	4574.9098	4574.9077	0.0021
4	4	1	4	3	1	4582.8165	4582.8174	-0.0009

4	4	0	4	3	1	4583.8245	4583.8225	0.0020
4	4	1	4	3	2	4636.4252	4636.4213	0.0039
4	4	0	4	3	2	4637.4252	4637.4265	-0.0013
5	4	2	5	3	3	4639.9873	4639.9885	-0.0012
5	4	1	5	3	3	4648.8374	4648.8325	0.0049
6	4	3	6	3	4	4685.3709	4685.3729	-0.0020
3	3	1	3	1	2	4796.0998	4796.1013	-0.0015
2	0	2	1	1	0	4821.8646	4821.8626	0.0020
7	1	6	7	0	7	4984.0842	4984.0838	0.0004
2	0	2	1	1	1	5039.0416	5039.0417	-0.0001
7	2	6	7	1	7	5190.2748	5190.2741	0.0007
7	2	6	7	0	7	5198.7375	5198.7372	0.0003
9	2	7	9	1	8	5298.6371	5298.6385	-0.0014
2	1	2	1	1	1	5437.5501	5437.5471	0.0030
3	0	3	2	2	0	5498.4876	5498.4794	0.0082
2	0	2	1	0	1	5603.1252	5603.1228	0.0024
16	7	10	16	6	10	5607.0499	5607.0505	-0.0006
3	1	3	2	2	0	5731.7499	5731.7482	0.0017
7	5	2	7	4	3	5744.0115	5744.0109	0.0006
3	1	3	2	2	1	5783.3512	5783.3501	0.0011
2	1	1	1	1	0	5871.9007	5871.9045	-0.0038
6	5	2	6	4	2	5872.9503	5872.9495	0.0008
6	5	1	6	4	2	5874.1992	5874.1928	0.0064
7	5	3	7	4	4	5882.1009	5882.1059	-0.0050
6	5	2	6	4	3	5915.4113	5915.4108	0.0005
6	5	1	6	4	3	5916.6501	5916.6541	-0.0040
5	5	1	5	4	2	5948.6377	5948.6388	-0.0011
5	5	0	5	4	2	5948.7518	5948.7538	-0.0020
2	1	2	1	0	1	6001.6258	6001.6282	-0.0024
3	3	0	3	1	3	6099.1759	6099.1720	0.0039
2	1	1	1	0	1	6653.1624	6653.1647	-0.0023
3	1	2	2	2	1	7078.5005	7078.4920	0.0085
2	2	1	1	1	0	7564.1377	7564.1439	-0.0062
2	2	1	1	1	1	7781.3249	7781.3230	0.0019
2	2	0	1	1	1	7832.9249	7832.9250	-0.0001
3	0	3	2	1	2	7893.8624	7893.8572	0.0052
3	1	3	2	1	2	8127.1255	8127.1261	-0.0006
3	0	3	2	0	2	8292.3626	8292.3627	-0.0001
3	1	3	2	0	2	8525.6366	8525.6315	0.0051
3	2	1	2	2	0	8671.7874	8671.7931	-0.0057

3	1	2	2	1	1	8770.7373	8770.7314	0.0059
3	2	2	2	1	1	10174.3128	10174.3204	-0.0076
4	1	3	3	2	2	10210.7759	10210.7678	0.0081
4	1	4	3	1	3	10791.3235	10791.3229	0.0006
4	0	4	3	0	3	10908.3154	10908.3204	-0.0050
4	1	4	3	0	3	11024.5874	11024.5917	-0.0043
3	2	1	2	1	2	11067.1631	11067.1710	-0.0079
4	2	3	3	2	2	11268.7021	11268.7024	-0.0003
4	3	2	3	3	1	11393.1709	11393.1632	0.0077
4	3	1	3	3	0	11438.8359	11438.8382	-0.0023
3	2	1	2	0	2	11465.6751	11465.6764	-0.0013
4	1	3	3	1	2	11614.3506	11614.3567	-0.0061
4	2	2	3	2	1	11668.7858	11668.7870	-0.0012
3	3	1	2	2	0	11822.9882	11822.9913	-0.0031
3	3	0	2	2	1	11882.5215	11882.5222	-0.0007

Table S2. Rotational transition frequencies of the ^{13}C1 **PFP***G+g+* monomer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
1	0	1	0	0	0	2821.5499	2821.5462	0.0037
2	0	2	1	1	1	5025.3692	5025.3719	-0.0027
2	0	2	1	0	1	5591.8859	5591.8897	-0.0038
2	1	2	1	1	1	5426.4317	5426.4331	-0.0014
2	1	1	1	1	0	5859.7439	5859.7426	0.0013
3	1	3	2	1	2	8110.6692	8110.6716	-0.0024
3	0	3	2	0	2	8276.2352	8276.2370	-0.0018
3	2	2	2	2	1	8464.6249	8464.6220	0.0029
3	2	1	2	2	0	8653.0074	8653.0022	0.0052
3	1	2	2	1	1	8752.8158	8752.8132	0.0026
2	1	2	1	0	1	5992.9497	5992.9509	-0.0012
1	1	1	0	0	0	3388.0637	3388.0640	-0.0003
4	1	4	3	1	3	10769.6749	10769.6654	0.0095
4	0	4	3	0	3	10887.3503	10887.3543	-0.0040
4	2	3	3	2	2	11245.7507	11245.7536	-0.0029
4	1	3	3	1	2	11591.2039	11591.2043	-0.0004
4	2	2	3	2	1	11643.5418	11643.5450	-0.0032
4	3	2	3	3	1	11369.3098	11369.3063	0.0035
4	3	1	3	3	0	11414.3763	11414.3807	-0.0044

Table S3. Rotational transition frequencies of the ^{13}C2 **PFP***G+g+* monomer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
1	0	1	0	0	0	2821.5499	2821.5462	0.0037
1	1	1	0	0	0	3388.0637	3388.0646	-0.0009
2	0	2	1	1	1	5025.3692	5025.3712	-0.0020
2	1	2	1	1	1	5426.4317	5426.4332	-0.0015
2	0	2	1	0	1	5591.8859	5591.8897	-0.0038
2	1	1	1	1	0	5859.7439	5859.7424	0.0015
2	1	2	1	0	1	5992.9497	5992.9517	-0.0020
3	1	3	2	1	2	8110.6692	8110.6720	-0.0028
3	0	3	2	0	2	8276.2352	8276.2373	-0.0021
3	2	2	2	2	1	8464.6249	8464.6199	0.0050
3	2	1	2	2	0	8653.0074	8653.0040	0.0034
3	1	2	2	1	1	8752.8158	8752.8125	0.0033
4	1	4	3	1	3	10769.6749	10769.6672	0.0077
4	0	4	3	0	3	10887.3503	10887.3560	-0.0057
4	2	3	3	2	2	11245.7507	11245.7481	0.0026
4	3	2	3	3	1	11369.3098	11369.3053	0.0045
4	3	1	3	3	0	11414.3763	11414.3834	-0.0071
4	1	3	3	1	2	11591.2039	11591.2014	0.0025
4	2	2	3	2	1	11643.5418	11643.5482	-0.0064

Table S4. Rotational transition frequencies of the ^{13}C3 **PFP***G+g+* monomer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
1	0	1	0	0	0	2803.8751	2803.8736	0.0015
4	2	3	4	0	4	3294.7262	3294.7250	0.0012
2	0	2	1	1	1	4984.5821	4984.5749	0.0072
2	1	2	1	1	1	5395.8754	5395.8762	-0.0008
2	0	2	1	0	1	5559.1334	5559.1362	-0.0028
2	1	1	1	1	0	5819.6126	5819.6100	0.0026
3	1	3	2	1	2	8066.2327	8066.2370	-0.0043
3	0	3	2	0	2	8231.9672	8231.9752	-0.0080
3	2	2	2	2	1	8411.6093	8411.6038	0.0055
3	2	1	2	2	0	8591.2359	8591.2341	0.0018
3	1	2	2	1	1	8694.6374	8694.6407	-0.0033
4	1	4	3	1	3	10712.3142	10712.3188	-0.0046

4	0	4	3	0	3	10832.6252	10832.6183	0.0069
4	2	3	3	2	2	11177.1461	11177.1363	0.0098
4	3	2	3	3	1	11294.8546	11294.8569	-0.0023
4	3	1	3	3	0	11336.4269	11336.4306	-0.0037
4	1	3	3	1	2	11518.2085	11518.2068	0.0017
4	2	2	3	2	1	11559.0900	11559.0952	-0.0052

Table S5. Rotational transition frequencies of the ^{18}O **PFP***G+g+* monomer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
1	0	1	0	0	0	2748.4296	2748.4297	-0.0001
2	1	2	1	1	1	5282.6485	5282.6530	-0.0045
2	0	2	1	0	1	5447.9456	5447.9479	-0.0023
2	1	1	1	1	0	5711.0621	5711.0589	0.0032
2	1	2	1	0	1	5866.9892	5866.9912	-0.0020
3	1	3	2	1	2	7896.2145	7896.2196	-0.0051
3	0	3	2	0	2	8064.4076	8064.4088	-0.0012
3	2	2	2	2	1	8245.2788	8245.2747	0.0041
3	2	1	2	2	0	8426.1497	8426.1421	0.0076
3	1	2	2	1	1	8531.6242	8531.6232	0.0010
4	1	4	3	1	3	10485.3052	10485.3058	-0.0006
4	0	4	3	0	3	10607.8009	10607.7935	0.0074
4	2	3	3	2	2	10955.1228	10955.1252	-0.0024
4	2	2	3	2	1	11340.1359	11340.1423	-0.0064

Table S6. Rotational transition frequencies of **PFP***G+g+* (OD) monomer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
1	0	1	0	0	0	2775.4753	2775.4718	0.0035
2	2	1	2	0	2	2792.4624	2792.4586	0.0038
3	2	2	3	0	3	2967.4377	2967.4336	0.0041
5	1	4	5	1	5	2970.0485	2970.0515	-0.0030
4	3	1	4	2	2	3023.6855	3023.6874	-0.0019
4	2	3	4	1	4	3174.2238	3174.2185	0.0053
3	3	0	3	2	1	3243.0107	3243.0098	0.0009
4	2	3	4	0	4	3304.6794	3304.6782	0.0012

1	1	1	0	0	0	3356.9505	3356.9566	-0.0061
3	3	1	3	2	2	3458.3393	3458.3375	0.0018
1	1	0	0	0	0	3566.6067	3566.6074	-0.0007
4	3	2	4	2	3	3572.9503	3572.9555	-0.0052
5	2	4	5	1	5	3742.9258	3742.9273	-0.0015
5	3	3	5	2	4	3781.2447	3781.2479	-0.0032
5	2	4	5	0	5	3803.1582	3803.1566	0.0016
6	1	5	6	1	6	3933.5895	3933.5924	-0.0029
5	3	3	5	1	4	4554.1207	4554.1236	-0.0029
4	4	0	4	3	1	4691.3615	4691.3578	0.0037
4	3	2	4	1	3	4697.1863	4697.1925	-0.0062
2	0	2	1	1	0	4712.5872	4712.5826	0.0046
4	4	1	4	3	2	4737.0556	4737.0518	0.0038
5	4	2	5	3	3	4737.8015	4737.7989	0.0026
2	0	2	1	1	1	4922.2332	4922.2334	-0.0002
2	1	2	1	1	1	5341.2953	5341.2910	0.0043
2	0	2	1	0	1	5503.7124	5503.7182	-0.0058
2	1	1	1	1	0	5760.5932	5760.5918	0.0014
2	1	2	1	0	1	5922.7751	5922.7757	-0.0006
2	2	1	1	1	0	7505.0417	7505.0412	0.0005
3	1	3	2	1	2	7985.1005	7985.1069	-0.0064
3	0	3	2	0	2	8151.4335	8151.4363	-0.0028
3	2	2	2	2	1	8326.4173	8326.4113	0.0060
3	2	1	2	2	0	8501.3749	8501.3722	0.0027
3	1	2	2	1	1	8607.2001	8607.2022	-0.0021
4	1	4	3	1	3	10605.1499	10605.1507	-0.0008
4	0	4	3	0	3	10727.4135	10727.4192	-0.0057
4	2	3	3	2	2	11064.6656	11064.6638	0.0018
4	3	2	3	3	1	11179.2853	11179.2818	0.0035
4	1	3	3	1	2	11404.0869	11404.0852	0.0017

Table S7. Rotational transition frequencies of the **PFP***Tg+* monomer. The ground state is noted as “0” and “1” for the excited states.

J’	K_a’	K_c’	stat	*J”*	K_a”	K_c”	stat	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
1	0	1	0	0	0	0	0	2436.3895	2436.4022	-0.0127
5	0	5	0	4	1	3	1	2962.0498	2962.0471	0.0027
4	2	3	0	3	3	0	0	3077.6048	3077.6022	0.0026
4	2	2	0	3	3	1	0	3091.8937	3091.8950	-0.0013
6	1	6	1	6	2	4	0	3167.1012	3167.1018	-0.0006
3	1	3	0	2	2	0	0	3184.6473	3184.6494	-0.0021
3	1	3	1	2	2	0	1	3185.6693	3185.6715	-0.0022
6	1	5	0	5	2	3	1	3318.5042	3318.5020	0.0023
5	1	5	1	5	2	3	0	3319.1439	3319.1410	0.0029
3	1	2	0	2	2	1	0	3428.0946	3428.0945	0.0001
3	1	3	1	3	2	1	0	3526.1166	3526.1152	0.0014
2	0	2	0	1	1	1	0	3558.1396	3558.1380	0.0016
2	0	2	1	1	1	1	1	3558.3332	3558.3305	0.0027
2	1	2	1	2	2	0	0	3589.3117	3589.3089	0.0028
3	2	1	0	2	1	1	1	3601.2569	3601.2576	-0.0007
4	1	3	0	3	0	3	1	3630.8305	3630.8301	0.0004
1	1	1	0	0	0	0	0	3750.1398	3750.1432	-0.0034
1	1	1	1	0	0	0	1	3750.1398	3750.1357	0.0041
4	2	2	0	4	1	3	0	3813.3126	3813.3087	0.0039
4	2	2	1	4	1	3	1	3828.0002	3828.0003	-0.0001
3	2	1	0	3	1	2	0	3884.7715	3884.7721	-0.0006
3	2	1	1	3	1	2	1	3891.0456	3891.0462	-0.0006
2	2	0	1	2	1	1	1	3941.7009	3941.7013	-0.0004
2	2	0	0	2	1	1	0	3941.9003	3941.9019	-0.0016
5	1	4	1	5	2	4	0	3958.0753	3958.0807	-0.0054
2	2	1	0	2	1	2	0	4062.2089	4062.2098	-0.0009
6	1	5	1	6	2	5	0	4080.1371	4080.1357	0.0014
3	2	2	0	3	1	3	0	4122.5122	4122.5106	0.0016
3	2	2	1	3	1	3	1	4129.1326	4129.1313	0.0013
1	1	0	1	2	0	2	0	4134.2127	4134.2086	0.0041
4	2	3	0	4	1	4	0	4203.1221	4203.1189	0.0032
4	2	3	1	4	1	4	1	4218.7051	4218.7041	0.0010
2	2	0	1	3	1	2	0	4225.2147	4225.2158	-0.0011
5	2	4	0	5	1	5	0	4304.1645	4304.1626	0.0019
5	2	4	1	5	1	5	1	4331.0607	4331.0597	0.0010
5	5	0	0	5	4	2	1	4364.9799	4364.9798	0.0001
5	5	1	0	5	4	1	1	4364.9799	4364.9784	0.0015

8	1	7	1	8	2	7	0	4381.2747	4381.2740	0.0007
6	2	5	0	6	1	6	0	4425.7402	4425.7385	0.0017
7	2	6	0	7	1	7	0	4567.8628	4567.8671	-0.0043
2	1	2	0	1	1	1	0	4832.2625	4832.2619	0.0006
2	1	2	1	1	1	1	1	4832.8413	4832.8409	0.0004
2	0	2	0	1	0	1	0	4871.8797	4871.8790	0.0007
2	0	2	1	1	0	1	1	4872.0127	4872.0094	0.0033
2	1	1	0	1	1	0	0	4913.0999	4913.1003	-0.0004
2	1	1	1	1	1	0	1	4913.7369	4913.7341	0.0028
6	0	6	0	5	1	4	1	5268.5113	5268.5143	-0.0030
5	2	4	0	4	3	1	0	5516.7739	5516.7716	0.0024
4	1	4	1	3	2	1	1	5530.3004	5530.3031	-0.0027
4	1	4	0	3	2	1	0	5535.4219	5535.4139	0.0080
5	2	3	0	4	3	2	0	5550.2375	5550.2418	-0.0043
4	1	3	0	3	2	2	0	5944.2252	5944.2251	0.0001
4	2	2	0	3	1	2	1	5984.0328	5984.0340	-0.0012
3	0	3	1	2	1	2	1	6031.2382	6031.2462	-0.0080
3	0	3	0	2	1	2	0	6031.3855	6031.3837	0.0018
2	1	2	0	1	0	1	0	6146.0007	6146.0029	-0.0022
2	1	2	1	1	0	1	1	6146.5181	6146.5198	-0.0017
5	1	4	0	4	0	4	1	6172.4253	6172.4255	-0.0002
4	2	3	0	3	1	3	1	6212.4183	6212.4175	0.0008
3	3	0	0	2	2	0	1	6320.4875	6320.4868	0.0007
3	3	1	0	2	2	1	1	6321.3562	6321.3563	-0.0001
1	0	1	1	1	1	1	0	6338.2127	6338.2123	0.0004
2	0	2	1	2	1	2	0	6377.9626	6377.9598	0.0028
3	0	3	1	3	1	3	0	6435.9016	6435.9057	-0.0041
4	0	4	1	4	1	4	0	6510.0377	6510.0383	-0.0006
6	3	3	0	6	2	4	0	6592.3502	6592.3471	0.0031
5	0	5	1	5	1	5	0	6597.7049	6597.7033	0.0016
5	3	2	1	5	2	3	1	6601.6811	6601.6790	0.0021
5	3	2	0	5	2	3	0	6624.6394	6624.6415	-0.0021
4	3	1	1	4	2	2	1	6635.6835	6635.6827	0.0008
4	3	1	0	4	2	2	0	6646.7004	6646.6990	0.0014
4	3	2	1	4	2	3	1	6649.0732	6649.0734	-0.0002
5	3	3	0	5	2	4	0	6656.5402	6656.5463	-0.0061
3	3	0	1	3	2	1	1	6659.5035	6659.5069	-0.0034
4	3	2	0	4	2	3	0	6660.6243	6660.6242	0.0001
3	3	0	0	3	2	1	0	6660.9304	6660.9305	-0.0001
3	3	1	1	3	2	2	1	6664.0365	6664.0384	-0.0019

3	3	1	0	3	2	2	0	6665.6372	6665.6388	-0.0016
6	0	6	1	6	1	6	0	6695.6826	6695.6826	0.0000
7	0	7	1	7	1	7	0	6800.3514	6800.3507	0.0007
3	1	3	0	2	1	2	0	7247.8108	7247.8107	0.0001
3	1	3	1	2	1	2	1	7248.7242	7248.7215	0.0027
3	0	3	0	2	0	2	0	7305.5082	7305.5076	0.0006
3	0	3	1	2	0	2	1	7305.7547	7305.7565	-0.0018
3	2	2	0	2	2	1	0	7308.1116	7308.1115	0.0001
3	2	1	0	2	2	0	0	7311.9151	7311.9151	0.0000
4	0	4	0	3	1	3	0	8519.9516	8519.9538	-0.0022
3	1	3	0	2	0	2	0	8521.9333	8521.9346	-0.0013
2	2	1	0	1	1	0	0	8854.0524	8854.0506	0.0018
2	2	1	1	1	1	0	1	8854.5206	8854.5190	0.0016
3	1	3	1	3	0	3	0	8869.8096	8869.8080	0.0016
2	2	0	0	1	1	1	0	8895.4214	8895.4232	-0.0018
2	2	0	1	1	1	1	1	8895.8941	8895.8908	0.0033
2	1	2	1	2	0	2	0	8926.5913	8926.5941	-0.0028
1	1	1	1	1	0	1	0	8965.6325	8965.6322	0.0003
4	1	4	0	3	1	3	0	9662.6775	9662.6796	-0.0021
4	1	4	0	3	0	3	0	10879.103	10879.1066	-0.0028
5	0	5	0	4	1	4	0	11020.911	11020.9116	-0.0002
2	0	2	1	1	1	0	0	11169.800	11169.8007	-0.0006
3	2	2	0	2	1	1	0	11249.063	11249.0618	0.0017
3	2	2	1	2	1	1	1	11256.503	11256.5041	-0.0007
3	2	1	0	2	1	2	0	11375.082	11375.0764	0.0064
1	1	0	1	0	0	0	0	11442.486	11442.4898	-0.0030

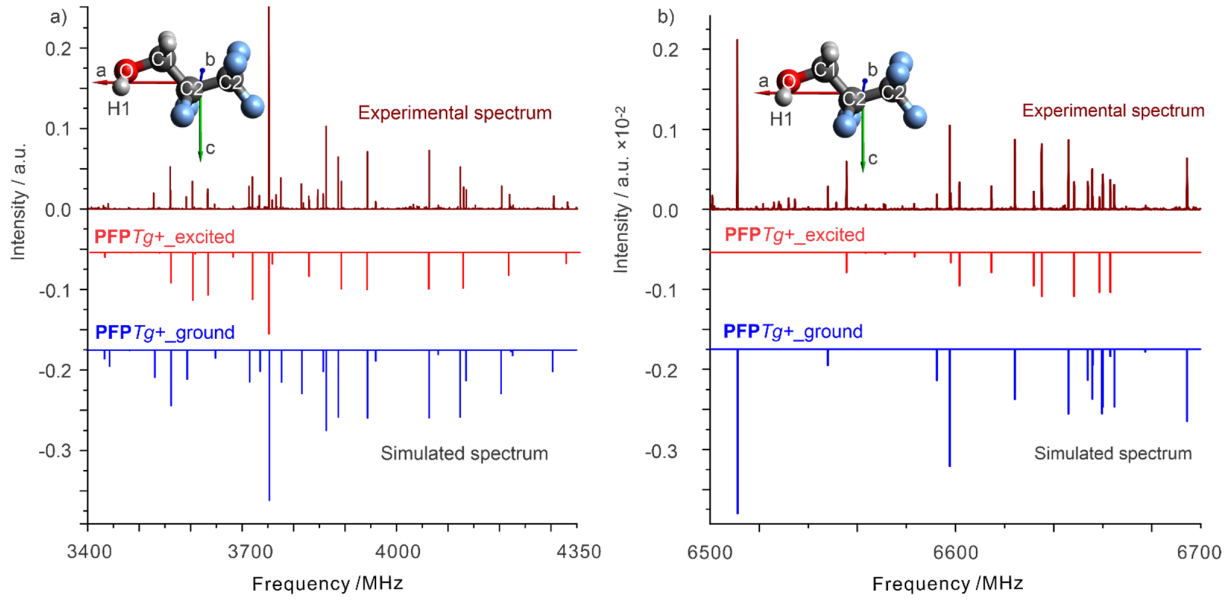

Figure S2. Experimental spectra of **PFP***Tg*+/**PFP***Tg*- monomer transitions measured using neon as a carrier gas. The ground state transitions are presented in blue and those of excited state in red. The known transitions of the **PFP***G*+*g*+/**PFP***G*-*g*- monomer and the PFP monohydrate species are removed for clarity. The experimental spectroscopic constants, the calculated electric dipole moment components, and a rotational temperature of 0.6 K were used for the spectral simulations. Please note that the b) 6.5-6.7 GHz is outside the usual operational range of the TWT and the power is lower at the higher frequency end. The experimental spectra were recorded by averaging about 900 k free induction decays.

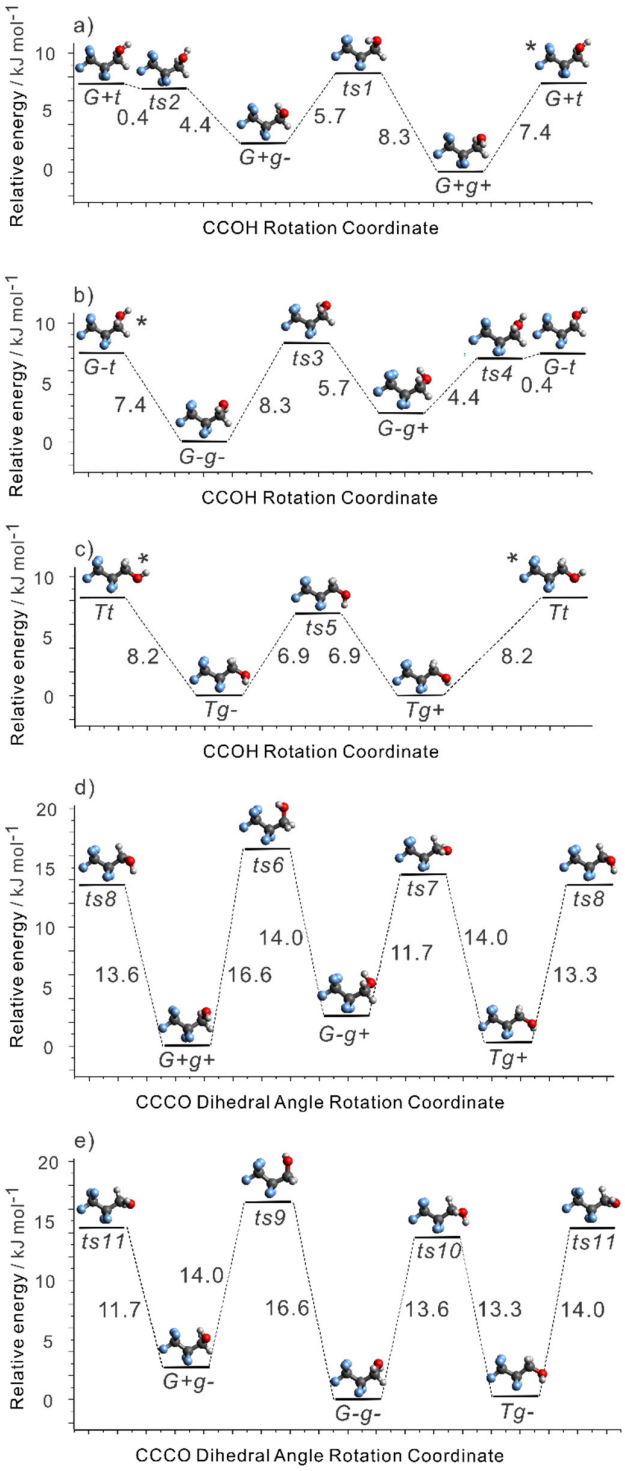

Figure S3. The interconversion barriers after *ZPE* corrections in kJ mol^{-1} of the **PFP** conformers at the B3LYP-D3(BJ)/def2-QZVP level. * indicates that the *t*-conformers are unstable, i.e., above the nearby transition states (see also Figure 4 in the main text).

Table S8. Experimental Kraitchman's coordinates (in Å) in the principal inertia axis of **PFP***G+g+*/*G-g-*.

Atom	*a*	*b*	*c*
^{13}C1	1.64862(91)[i]	-0.025(60)	0.6826(22)
^{13}C2	0.3892(39)	-0.5664(27)	0.0 [ii]
^{13}C3	-0.8365(18)	0.3012(50)	0.0
^{18}O1	2.12666(71)	1.1634113)	0.0
^{2}H1	2.42133(62)	0.8965(17)	-0.8446(18)

[i] Costain errors in units of the least significant digits are given in brackets.

[ii] Non-physical value and set to 0.0.

Table S9. The r_o structural parameters obtained from the STRFIT fit for **PFP***G+g+*/*G-g-*.[a]

parameter	exp. [b]	theo. [c]	Parameter	exp. [b]	theo. [c]
C1-C2 /Å	1.5448(34)	1.5247	H1-O1-C1 /°	105.1(25)	109.42
C2-C3 /Å	1.483(11)	1.5504	O1-C1-C2 /°	119.1(21)	113.32
C1-O1 /Å	1.334(35)	1.4038	H1-O1-C1-C2 /°	69.0(23)	62.92
H1-O1 /Å	0.892(39)	0.9615	O1-C1-C2-C3 /°	59.2(25)	63.34

[a] Bond lengths and angles are listed with four and two digits after the decimal points, respectively for consistency. These do not necessarily reflect their uncertainties. The atom numberings are provided in Figure 1.

[b] Structural parameters without error bars are directly read from the STRFIT output geometry.

[c] The equilibrium geometry at the B3LYP-D3(BJ)/def2-QZVP level of theory.

Table S10. Experimental r_0 coordinates (in Å) of **PFP***G-g-* monomer in the principal inertia axis based on the STRFIT geometry.[a]

Atom	*a*	*b*	*c*
C1	-1.648(17)	-0.057(16)	0.584(42)
H2	-1.431(37)	-0.393(44)	1.596(48)
H3	-2.393(15)	0.742(18)	0.637(35)
C2	-0.4262(52)	0.5645(22)	0.0181(19)
F1	-0.137(15)	1.679(21)	0.738(36)
F2	-0.662(30)	0.949(38)	-1.2693(45)
C3	0.8444(26)	-0.3141(32)	0.0075(11)
F3	0.708(15)	-1.352(22)	-0.819(33)
F4	1.083(28)	-0.779(37)	1.2427(93)
F5	1.9029(86)	0.401(11)	-0.385(41)
O1	-2.1231(74)	-1.1752(91)	0.0338(83)
H1	-2.430(14)	-0.928(35)	-0.766(35)

[a] The experimental rotational constants were used and some structural parameters were fixed at the values obtained at the B3LYP-D3BJ/def2-QZVP level.

Table S11. The r_e^{SE} geometry parameters obtained from the STRFIT fit for **PFP***G+g+/G-g-*.[a]

parameter	semi-exp.[b]	theo.[c]	Parameter	semi-exp.[b]	theo.[c]
C1-C2 /Å	1.5192(21)	1.5148	H1-O1-C1 /°	107.16(50)	107.82
C2-C3 /Å	1.54609(73)	1.5378	O1-C1-C2 /°	113.61(40)	112.99
C1-O1 /Å	1.3985(77)	1.4041	H1-O1-C1-C2 /°	65.43(45)	61.03
H1-O1 /Å	0.9560(87)	0.9624	O1-C1-C2-C3 /°	62.66(43)	62.63

[a] Bond lengths and angles are listed with four and two digits after the decimal points, respectively for consistency. These do not necessarily reflect their uncertainties. The atom numberings are in Figure 1.

[b] Structural parameters without error bars are directly read from the STRFIT output geometry.

[c] The equilibrium structural parameters at the MP2/cc-pVTZ level of theory.

Table S12. The r_e^{SE} coordinates (in Å) of **PFP***G+g+/G-g-* in its principal inertia axis.[a]

Atom	*a*	*b*	*c*
C1	-1.6511(37)	-0.0164(36)	0.6726(83)
H2	-2.3892(34)	0.7890(38)	0.6961(68)
H3	-1.4070(81)	-0.2922(93)	1.6941(89)
C2	-0.4150(11)	0.57638(44)	0.01799(35)
F1	-0.6916(62)	0.8885(77)	-1.27503(40)
F2	-0.0897(27)	1.7175(37)	0.6670(75)
C3	0.84404(58)	-0.32092(69)	0.01168(23)
F3	0.6698(28)	-1.3890(41)	-0.7583(70)
F4	1.8916(20)	0.3619(24)	-0.4443(80)
F5	1.1114(58)	-0.7260(76)	1.2555(14)
O1	-2.1258(16)	-1.1668(19)	0.0345(17)
H1	-2.4234(31)	-0.9044(79)	-0.8354(76)

[a] The semi-experimental equilibrium rotational constants were used. Some structural parameters were fixed at the values obtained at the MP2/cc-pVTZ level. See the main text for details.

Table S13. Comparison of the experimental bond lengths (in Å), angles (˚) and dihedral angle (˚) with the theoretical predictions at the indicated level of theory.

Atom	r_0	r_s	r_e^{SE}	MP2[a]	PBE[b]	B3LYP[c]
C1-C2 /Å	1.5448(34)	1.531(21)	1.5192(21)	1.51480	1.51906	1.52472
C2-C3 /Å	1.483(11)	1.5017(48)	1.54609(73)	1.53779	1.54484	1.55044
C1-O1 /Å	1.334(35)	1.452(49)	1.3985(77)	1.40409	1.39434	1.40379
H1-O1 /Å	0.892(39)	0.9337(18)	0.9560(87)	0.96240	0.96191	0.96149
H1-O1-C1 /°	105.1(25)	107.1(13)	107.16(50)	107.815	109.119	109.417
O1-C1-C2 /°	119.1(21)	110.5(15)	113.61(40)	112.994	113.407	113.320
H1-O1-C1-C2 /°	69.0(23)	67.1(20)	65.43(45)	61.027	62.111	62.919
O1-C1-C2-C3 /°	59.2(25)	63.6(15)	62.66(43)	62.634	64.144	63.337

[a] At the MP2/cc-pVTZ level of theory.

[b] At the PBE1PBE-D3BJ/def2-TZVPD level of theory.

[c] At the B3LYP-D3BJ/def2-QZVP level of theory.

Table S14. Full list of the properties of the for 2,2,3,3,3-pentafluoro-1-propanol homodimer conformations predicted at the B3LYP- D3(BJ)/def2-QZVP level of theory.

#	Homodimers	ΔE_{raw} [a]	ΔE_0 [b]	ΔE_b [c]	A [d]	B [d]	C [d]	$\lvert\mu_a\rvert$ [e]	$\lvert\mu_b\rvert$ [e]	$\lvert\mu_c\rvert$ [e]
I	**PFP***G+g+***PFP***Tg+*	0.0	0.0	23.4	990.7	156.9	154.3	2.7	0.6	1.0
2	**PFP***G+g+***PFP***G+g+*	0.7	0.4	22.8	848.5	171.1	167.2	2.0	1.1	0.3
3	**PFP***Tg+***PFP***Tg+*	0.3	0.4	23.3	767.4	185.9	172.1	2.7	0.1	0.9
4	**PFP***G+g+***PFP***G-g-*	1.1	0.5	22.6	793.7	191.5	184.0	2.4	1.6	0.1
5	**PFP***G+g+***PFP***Tg-*	0.9	0.5	22.9	793.9	179.3	169.0	2.8	-1.5	-0.7
6	**PFP***Tg+***PFP***G-g-*	1.0	0.6	22.8	679.3	229.4	202.9	2.6	1.2	0.3
7	**PFP***Tg+***PFP***Tg-*	1.0	0.7	23.0	650.4	218.2	189.7	3.0	1.2	0.1
8	**PFP***G+g+***PFP***Tg+*	0.8	0.9	22.5	764.3	169.4	160.7	0.7	0.8	0.5
9	**PFP***Tg+***PFP***G+g+*	1.3	0.9	22.5	724.2	187.1	180.5	2.1	0.6	0.6
10	**PFP***G+g+***PFP***G+g+*_2	0.9	1.0	22.2	834.6	161.4	155.5	0.6	1.0	0.3
11	**PFP***G+g+***PFP***G-g-*_2	1.4	1.0	22.1	715.3	194.3	189.6	0.9	2.2	0.7
12	**PFP***G+g+***PFP***G+g+*_3	1.7	1.4	21.7	714.1	215.9	200.5	1.4	3.5	0.3
13	**PFP***G+g+***PFP***Tg-*_2	1.7	1.5	22.0	715.4	176.3	164.6	0.6	1.8	1.0
14	**PFP***G+g+***PFP***Tg+*_2	2.0	1.7	21.7	709.7	202.1	185.6	1.1	2.6	1.9
15	**PFP***G+g+***PFP***G-g-*_3	2.2	1.8	21.3	738.4	197.5	188.5	1.2	3.3	0.4
16	**PFP***G+g+***PFP***Tg-*_3	2.3	2.1	-21.3	830.5	175.7	167.8	1.4	2.9	1.2
17	**PFP***G+g+***PFP***G-g+*	2.3	2.1	-23.6	830.0	187.1	177.3	2.8	0.3	1.2
18	**PFP***Tg+***PFP***G-g+*	2.3	2.3	-23.8	680.3	225.6	200.3	2.8	0.0	0.8
19	**PFP***Tg+***PFP***G+g+*_2	2.8	2.5	-20.9	806.0	141.8	138.0	0.9	0.6	0.5
20	**PFP***G+g-***PFP***Tg-*	3.0	2.6	-23.4	825.5	182.1	178.1	3.3	0.1	1.4
21	**PFP***Tg+***PFP***G+g+*_3	3.0	2.6	-20.8	810.8	173.5	171.3	0.7	3.4	1.0
22	**PFP***Tg+***PFP***Tg+*_2	3.0	2.8	-21.0	963.1	122.7	120.1	0.5	0.7	0.4
23	**PFP***Tg+***PFP***G-g-*_2	3.3	2.9	-20.5	877.9	156.9	151.5	0.5	2.3	2.5
24	**PFP***Tg+* **PFP***Tg+*_2	3.3	2.9	-20.8	813.6	153.6	146.6	1.0	1.1	3.3
25	**PFP***G+g+***PFP***G+g-*	3.4	3.0	-22.8	925.5	164.9	160.6	3.1	1.0	0.8
26	**PFP***G+g-***PFP***G-g-*	3.6	3.0	-22.7	736.8	200.5	196.5	2.7	1.0	1.0
27	**PFP***Tg+***PFP***Tg-*_2	3.2	3.0	-20.7	835.0	146.3	142.3	1.0	0.8	0.3
28	**PFP***G+g+***PFP***G-g-*_4	2.9	3.1	-22.7	718.6	196.3	185.4	0.7	0.9	0.2
29	**PFP***Tg+***PFP***Tg-*_3	3.3	3.1	-20.7	1031.9	133.6	132.0	1.0	1.1	3.1
30	**PFP***Tg+***PFP***G+g-*_2	3.6	3.3	-22.7	762.4	190.6	176.4	3.3	0.7	0.2
31	**PFP***G+g+***PFP***G+g-*_2	3.6	3.5	-22.3	715.1	215.3	200.0	1.4	2.3	2.1
32	**PFP***G+g-***PFP***Tg+*	4.1	3.6	-22.5	721.2	207.8	192.8	3.2	1.0	1.1
33	**PFP***G+g+* **PFP***Tg-*_2	4.1	3.8	-19.7	790.9	157.7	155.9	0.0	0.3	1.8
34	**PFP***G+g+***PFP***G+g-*_3	4.3	4.0	-21.7	839.0	157.7	153.8	1.3	1.8	0.7
35	**PFP***G+g-***PFP***G+g+*	4.9	4.1	-21.6	715.5	209.1	208.4	2.7	1.4	0.2
36	**PFP***G+g-***PFP***G+g+*_2	4.7	4.2	-21.5	745.1	207.1	190.6	2.1	2.1	0.6
37	**PFP***G+g+***PFP***G-g+*_2	4.6	4.3	-21.5	833.4	178.8	170.7	1.7	2.7	1.5
38	**PFP***G+g-***PFP***G+g-*	5.1	4.7	-23.7	725.6	216.4	200.5	3.4	0.4	1.1

39	**PFP***G+g-***PFP***Tg-_2*	4.7	4.7	-21.3	852.1	157.3	152.1	0.3	0.4	0.7
40	**PFP***G+g-***PFP***G-g-_2*	4.7	4.7	-21.3	870.9	158.8	151.8	0.4	0.3	0.6
41	**PFP***G+g-***PFP***G-g-_3*	5.3	4.8	-21.0	754.1	198.6	196.4	1.3	0.4	3.7
42	**PFP***Tg+***PFP***G+g-*	5.0	4.8	-21.3	834.4	167.3	160.6	0.8	0.9	3.1
43	**PFP***Tg+***PFP***G-g+_2*	5.1	4.8	-21.2	786.8	149.0	140.0	0.6	0.7	0.2
44	**PFP***Tg+***PFP***G-g-_3*	5.3	4.9	-18.5	859.0	146.2	138.9	0.0	0.8	1.5
45	**PFP***Tg+***PFP***Tg-_4*	5.2	4.9	-18.8	718.8	161.4	148.4	0.3	1.0	1.3
46	**PFP***G+g-***PFP***G+g+_3*	5.6	5.0	-20.7	799.6	176.2	166.5	1.3	2.0	2.8
47	**PFP***G+g-***PFP***Tg-_2*	5.6	5.1	-21.0	788.4	183.7	170.6	1.8	1.3	3.5
48	**PFP***G+g-***PFP***G+g+_4*	5.7	5.1	-20.6	776.0	193.7	188.7	1.4	1.4	3.3
49	**PFP***Tg+***PFP***G-g+_3*	5.3	5.2	-20.9	770.9	171.0	158.0	0.9	0.6	0.7
50	**PFP***G+g-***PFP***Tg+_2*	5.7	5.3	-20.7	903.9	169.7	163.4	1.8	0.7	3.4
51	**PFP***Tg+***PFP***G-g+_4*	5.7	5.4	-20.7	963.4	143.7	141.5	1.4	0.7	3.3
52	**PFP***G+g-***PFP***Tg+_3*	6.0	5.7	-20.4	816.7	158.5	153.7	1.2	0.5	1.7
53	**PFP***G+g-***PFP***G-g+*	6.6	6.1	-22.3	809.6	190.3	182.9	3.4	0.1	1.2
54	**PFP***G+g+***PFP***G+t*	7.3	6.2	-26.1	883.3	180.0	177.1	0.2	0.5	2.0
55	**PFP***G+g-***PFP***G+g-_2*	6.7	6.8	-21.5	790.8	185.4	170.4	0.4	0.2	0.7
56	**PFP***Tg+***PFP***G+t*	8.2	7.1	-25.5	846.9	174.6	167.2	0.4	1.0	2.0
57	**PFP***G+g+***PFP***G-t*	7.8	7.2	-25.2	876.2	161.4	156.9	1.1	0.6	1.6
58	**PFP***G+g-***PFP***G-g+_2*	7.7	7.2	-21.2	790.4	178.8	168.3	1.7	0.0	3.3
59	**PFP***Tg+***PFP***G-t*	9.0	7.3	-25.4	793.6	169.2	161.3	1.2	0.3	2.7
60	**PFP***G+g-***PFP***G+g-_3*	8.0	7.5	-20.9	866.3	173.7	165.1	2.2	0.6	3.5
61	**PFP***G+g+***PFP***G+t_2*	8.5	7.6	-24.7	800.7	177.8	174.8	1.4	0.9	1.1
62	**PFP***Tg+***PFP***Tt*	9.0	7.8	-26.0	706.2	193.8	175.7	0.9	0.7	2.0
63	**PFP***G+g+***PFP***Tt*	8.5	7.8	-25.6	818.4	165.6	158.0	1.1	0.2	1.6
64	**PFP***G+g-***PFP***G-g+_3*	8.0	7.8	-20.6	778.0	182.7	169.0	0.9	0.2	1.9
65	**PFP***G+g-***PFP***G-t*	9.2	8.3	-26.7	817.2	191.1	183.9	1.0	2.8	0.5
66	**PFP***Tg+***PFP***G-t_2*	9.7	8.4	-24.3	722.6	209.4	198.6	-0.6	0.7	1.7
67	**PFP***Tg+***PFP***G-t_3*	9.9	8.6	-24.1	896.7	145.5	141.0	0.1	1.9	0.6
68	**PFP***G+t***PFP***G+g+*	10.4	9.0	-16.7	739.7	210.3	192.0	3.9	2.8	0.8
69	**PFP***G+g-***PFP***Tt*	10.2	9.1	-33.6	779.4	187.2	182.5	1.6	2.1	1.5
70	**PFP***Tg+***PFP***Tt_2*	10.4	9.2	-24.5	1080.5	123.0	121.9	0.2	2.0	0.8
71	**PFP***G+g-***PFP***G+t*	10.9	9.3	-25.7	764.8	188.7	187.8	2.0	1.2	2.6
72	**PFP***G+g-***PFP***G+t_2*	10.8	9.8	-25.2	743.9	213.0	202.6	0.8	2.1	0.8
73	**PFP***G+g-***PFP***Tt_2*	13.2	12.3	-30.4	863.8	163.5	158.3	0.0	2.0	2.3
74	**PFP***G+g+***PFP***G-t_2*	16.7	14.1	-18.3	707.2	214.7	202.1	3.3	4.2	1.6
75	**PFP***G+g+***PFP***Tt_2*	17.1	15.0	-18.5	737.4	193.6	180.3	3.0	4.5	0.9
76	**PFP***G+t* **PFP***G-t*	18.8	16.4	-25.2	767.7	164.2	161.0	5.4	2.4	2.2
77	**PFP***G+t***PFP***G+t*	18.9	16.6	-25.0	806.6	156.6	153.6	5.1	3.1	1.3
78	**PFP***G+t* **PFP***G-t_2*	21.1	18.8	-22.8	865.7	154.2	145.6	2.9	2.3	0.6

Table S15. Rotational transition frequencies of the **PFP***G+g+***PFP***Tg+* homodimer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
5	1	5	4	1	4	1547.7504	1547.7511	-0.0007
5	0	5	4	0	4	1554.0237	1554.0248	-0.0011
5	3	3	4	3	2	1554.1742	1554.1747	-0.0005
5	3	2	4	3	1	1554.1742	1554.1749	-0.0007
5	4	2	4	4	1	1554.1783	1554.1792	-0.0009
5	4	1	4	4	0	1554.1783	1554.1792	-0.0009
5	2	3	4	2	2	1554.2502	1554.2495	0.0007
5	1	4	4	1	3	1560.4817	1560.4821	-0.0004
6	1	6	5	1	5	1857.2792	1857.2794	-0.0002
6	0	6	5	0	5	1864.7596	1864.7598	-0.0002
6	2	5	5	2	4	1864.9428	1864.9433	-0.0005
6	3	3	5	3	2	1865.0113	1865.0113	0.0000
6	3	4	5	3	3	1865.0113	1865.0109	0.0004
6	4	3	5	4	2	1865.0130	1865.0128	0.0002
6	4	2	5	4	1	1865.0130	1865.0128	0.0002
6	5	2	5	5	1	1865.0251	1865.0253	-0.0002
6	5	1	5	5	0	1865.0251	1865.0253	-0.0002
6	2	4	5	2	3	1865.1463	1865.1459	0.0004
6	1	5	5	1	4	1872.5552	1872.5557	-0.0005
4	1	3	3	0	3	2096.4035	2096.4031	0.0004
7	1	7	6	1	6	2166.7959	2166.7957	0.0002
7	0	7	6	0	6	2175.4569	2175.4567	0.0002
7	2	6	6	2	5	2175.7438	2175.7435	0.0003
7	3	5	6	3	4	2175.8486	2175.8477	0.0009
7	3	4	6	3	3	2175.8486	2175.8487	-0.0001
7	2	5	6	2	4	2176.0674	2176.0675	-0.0001
7	1	6	6	1	5	2184.6170	2184.6169	0.0001
5	1	4	4	0	4	2413.6276	2413.6271	0.0005
8	1	8	7	1	7	2476.2999	2476.2981	0.0018
8	0	8	7	0	7	2486.1093	2486.1091	0.0002
8	2	7	7	2	6	2486.5326	2486.5327	-0.0001
8	4	5	7	4	4	2486.6753	2486.6757	-0.0004
8	4	4	7	4	3	2486.6753	2486.6757	-0.0004
8	3	5	7	3	4	2486.6863	2486.6872	-0.0009
8	3	6	7	3	5	2486.6863	2486.6852	0.0011
8	5	4	7	5	3	2486.6863	2486.6870	-0.0007
8	5	3	7	5	2	2486.6863	2486.6870	-0.0007
8	6	3	7	6	2	2486.7095	2486.7096	-0.0001

8	6	2	7	6	1	2486.7095	2486.7096	-0.0001
8	2	6	7	2	5	2487.0187	2487.0187	0.0000
8	1	7	7	1	6	2496.6631	2496.6634	-0.0003
6	1	5	5	0	5	2732.1585	2732.1581	0.0004
9	1	9	8	1	8	2785.7853	2785.7848	0.0005
9	0	9	8	0	8	2796.7118	2796.7109	0.0009
9	2	8	8	2	7	2797.3096	2797.3094	0.0002
9	4	6	8	4	5	2797.5041	2797.5047	-0.0006
9	4	5	8	4	4	2797.5041	2797.5047	-0.0006
9	5	4	8	5	3	2797.5131	2797.5137	-0.0006
9	5	5	8	5	4	2797.5131	2797.5137	-0.0006
9	3	7	8	3	6	2797.5237	2797.5233	0.0004
9	3	6	8	3	5	2797.5265	2797.5270	-0.0005
9	6	3	8	6	2	2797.5378	2797.5371	0.0007
9	6	4	8	6	3	2797.5378	2797.5371	0.0007
9	2	7	8	2	6	2798.0028	2798.0034	-0.0006
9	1	8	8	1	7	2808.6939	2808.6932	0.0007
12	0	12	11	1	11	2968.6564	2968.6566	-0.0002
7	1	7	6	0	6	2980.7249	2980.7232	0.0017
7	1	6	6	0	6	3052.0161	3052.0152	0.0009
13	0	13	12	1	11	3094.4809	3094.4799	0.0010
10	1	10	9	1	9	3095.2543	3095.2539	0.0004
10	0	10	9	0	9	3107.2561	3107.2557	0.0004
10	2	9	9	2	8	3108.0723	3108.0720	0.0003
10	4	6	9	4	5	3108.3319	3108.3318	0.0001
10	4	7	9	4	6	3108.3319	3108.3318	0.0001
10	5	6	9	5	5	3108.3373	3108.3371	0.0002
10	5	5	9	5	4	3108.3373	3108.3371	0.0002
10	3	8	9	3	7	3108.3612	3108.3620	-0.0008
10	6	5	9	6	4	3108.3612	3108.3606	0.0006
10	6	4	9	6	3	3108.3612	3108.3606	0.0006
10	3	7	9	3	6	3108.3683	3108.3685	-0.0002
10	2	8	9	2	7	3109.0253	3109.0258	-0.0005
10	1	9	9	1	8	3120.7035	3120.7039	-0.0004
8	1	8	7	0	7	3281.5645	3281.5646	-0.0001
8	1	7	7	0	7	3373.2244	3373.2219	0.0025
14	0	14	13	1	12	3386.6249	3386.6255	-0.0006
11	1	11	10	1	10	3404.7049	3404.7036	0.0013
11	0	11	10	0	10	3417.7375	3417.7375	0.0000
11	2	10	10	2	9	3418.8197	3418.8190	0.0007

11	4	7	10	4	6	3419.1566	3419.1568	-0.0002
11	5	7	10	5	6	3419.1566	3419.1569	-0.0003
11	4	8	10	4	7	3419.1566	3419.1567	-0.0001
11	5	6	10	5	5	3419.1566	3419.1569	-0.0003
11	3	8	10	3	7	3419.2118	3419.2118	0.0000
11	2	9	10	2	8	3420.0885	3420.0898	-0.0013
11	1	10	10	1	9	3432.6942	3432.6934	0.0008
3	2	2	2	1	1	3475.6751	3475.6742	0.0009
3	2	1	2	1	1	3475.7031	3475.7032	-0.0001
15	0	15	14	1	13	3677.0296	3677.0302	-0.0006
9	1	8	8	0	8	3695.8044	3695.8059	-0.0015
12	1	12	11	1	11	3714.1342	3714.1321	0.0021
12	0	12	11	0	11	3728.1501	3728.1503	-0.0002
12	2	11	11	2	10	3729.5478	3729.5488	-0.0010
12	5	7	11	5	6	3729.9723	3729.9728	-0.0005
12	5	8	11	5	7	3729.9723	3729.9728	-0.0005
12	4	8	11	4	7	3729.9785	3729.9794	-0.0009
12	4	9	11	4	8	3729.9785	3729.9793	-0.0008
12	6	6	11	6	5	3729.9924	3729.9940	-0.0016
12	6	7	11	6	6	3729.9924	3729.9940	-0.0016
12	3	10	11	3	9	3730.0406	3730.0412	-0.0006
12	3	9	11	3	8	3730.0582	3730.0575	0.0007
12	2	10	11	2	9	3731.1995	3731.1994	0.0001
12	1	11	11	1	10	3744.6613	3744.6594	0.0019
10	1	10	9	0	9	3879.7854	3879.7834	0.0020
10	1	9	9	0	9	4019.7999	4019.7990	0.0009
13	1	13	12	1	12	4023.5364	4023.5375	-0.0011
13	0	13	12	0	12	4038.4883	4038.4881	0.0002
13	2	12	12	2	11	4040.2611	4040.2599	0.0012
13	5	9	12	5	8	4040.7841	4040.7843	-0.0002
13	5	8	12	5	7	4040.7841	4040.7843	-0.0002
13	4	9	12	4	8	4040.8005	4040.7994	0.0011
13	4	10	12	4	9	4040.8005	4040.7993	0.0012
13	3	11	12	3	10	4040.8806	4040.8814	-0.0008
13	2	11	12	2	10	4042.3603	4042.3583	0.0020
13	1	12	12	1	11	4056.5999	4056.5995	0.0004
18	3	16	18	2	16	4311.9884	4311.9898	-0.0014
17	3	15	17	2	15	4315.9212	4315.9200	0.0012
16	3	14	16	2	14	4319.2337	4319.2341	-0.0004
14	1	14	13	1	13	4332.9164	4332.9184	-0.0020

11	3	8	11	2	10	4332.9164	4332.9158	0.0006
20	3	17	20	2	19	4344.6631	4344.6636	-0.0005
11	1	10	10	0	10	4345.2372	4345.2366	0.0006
14	0	14	13	0	13	4348.7445	4348.7452	-0.0007
14	2	13	13	2	12	4350.9506	4350.9507	-0.0001
14	2	12	13	2	11	4353.5711	4353.5702	0.0009
14	1	13	13	1	12	4368.5121	4368.5114	0.0007
6	2	5	5	1	5	4431.0751	4431.0760	-0.0009
17	0	17	16	1	16	4598.3176	4598.3197	-0.0021
15	1	15	14	1	14	4642.2746	4642.2729	0.0017
15	0	15	14	0	14	4658.9158	4658.9161	-0.0003
15	2	14	14	2	13	4661.6199	4661.6196	0.0003
15	4	11	14	4	10	4662.4316	4662.4310	0.0006
15	4	12	14	4	11	4662.4316	4662.4307	0.0009
15	7	8	14	7	7	4662.4422	4662.4419	0.0003
15	7	9	14	7	8	4662.4422	4662.4419	0.0003
15	2	13	14	2	12	4664.8384	4664.8382	0.0002
12	1	11	11	0	11	4672.1581	4672.1584	-0.0003
15	1	14	14	1	13	4680.3907	4680.3928	-0.0021
7	2	6	6	1	6	4749.5386	4749.5401	-0.0015
18	0	18	17	1	17	4926.2831	4926.2839	-0.0008
16	1	16	15	1	15	4951.5993	4951.5996	-0.0003
16	0	16	15	0	15	4968.9937	4968.9956	-0.0019
16	2	15	15	2	14	4972.2645	4972.2652	-0.0007
16	5	12	15	5	11	4973.1893	4973.1892	0.0001
16	5	11	15	5	10	4973.1893	4973.1892	0.0001
16	6	10	15	6	9	4973.1941	4973.1941	0.0000
16	6	11	15	6	10	4973.1941	4973.1941	0.0000
16	7	10	15	7	9	4973.2314	4973.2311	0.0003
16	7	9	15	7	8	4973.2314	4973.2311	0.0003
16	4	13	15	4	12	4973.2425	4973.2417	0.0008
16	4	12	15	4	11	4973.2425	4973.2421	0.0004
16	3	14	15	3	13	4973.3995	4973.4019	-0.0024
16	3	13	15	3	12	4973.4708	4973.4713	-0.0005
16	2	14	15	2	13	4976.1649	4976.1657	-0.0008
16	1	15	15	1	14	4992.2416	4992.2410	0.0006
13	1	12	12	0	12	5000.6072	5000.6077	-0.0005
14	1	14	13	0	13	5063.4414	5063.4434	-0.0020
9	5	4	10	4	6	5234.2559	5234.2564	-0.0005
9	5	4	10	4	7	5234.2559	5234.2565	-0.0006

9	5	5	10	4	7	5234.2559	5234.2565	-0.0006
9	5	5	10	4	6	5234.2559	5234.2564	-0.0005
17	1	17	16	1	16	5260.8945	5260.8968	-0.0023
17	0	17	16	0	16	5278.9783	5278.9788	-0.0005
17	2	16	16	2	15	5282.8854	5282.8858	-0.0004
17	5	12	16	5	11	5283.9791	5283.9798	-0.0007
17	6	11	16	6	10	5283.9791	5283.9777	0.0014
17	6	12	16	6	11	5283.9791	5283.9777	0.0014
17	5	13	16	5	12	5283.9791	5283.9798	-0.0007
17	7	10	16	7	9	5284.0119	5284.0125	-0.0006
17	7	11	16	7	10	5284.0119	5284.0125	-0.0006
17	4	13	16	4	12	5284.0514	5284.0499	0.0015
17	4	13	16	4	12	5284.0514	5284.0499	0.0015
17	4	14	16	4	13	5284.0514	5284.0491	0.0023
17	3	15	16	3	14	5284.2405	5284.2411	-0.0006
17	3	14	16	3	13	5284.3351	5284.3352	-0.0001
17	2	15	16	2	14	5287.5563	5287.5553	0.0010
9	2	7	8	1	7	5300.5392	5300.5404	-0.0012
17	1	16	16	1	15	5304.0525	5304.0535	-0.001
14	1	13	13	0	13	5330.6316	5330.6311	0.0005
15	1	15	14	0	14	5356.9734	5356.9711	0.0023
9	2	8	8	1	8	5390.2871	5390.2883	-0.0012
8	5	3	9	4	5	5545.0754	5545.0746	0.0008
8	5	4	9	4	5	5545.0754	5545.0746	0.0008
8	5	4	9	4	6	5545.0754	5545.0746	0.0008
8	5	3	9	4	6	5545.0754	5545.0746	0.0008
18	1	18	17	1	17	5570.1609	5570.1632	-0.0023
18	0	18	17	0	17	5588.8602	5588.8610	-0.0008
18	2	17	17	2	16	5593.4813	5593.4799	0.0014
18	5	14	17	5	13	5594.7624	5594.7642	-0.0018
18	5	13	17	5	12	5594.7624	5594.7642	-0.0018
18	3	16	17	3	15	5595.0783	5595.0792	-0.0009
18	3	15	17	3	14	5595.2067	5595.2045	0.0022
18	2	16	17	2	15	5599.0096	5599.0094	0.0002
18	1	17	17	1	16	5615.8274	5615.8278	-0.0004
16	1	16	15	0	15	5649.6539	5649.6546	-0.0007
7	5	3	8	4	5	5855.8921	5855.8923	-0.0002
7	5	3	8	4	4	5855.8921	5855.8923	-0.0002
7	5	2	8	4	4	5855.8921	5855.8923	-0.0002
7	5	2	8	4	5	5855.8921	5855.8923	-0.0002

19	1	19	18	1	18	5879.4001	5879.3973	0.0028
19	0	19	18	0	18	5898.6361	5898.6383	-0.0022
19	2	18	18	2	17	5904.0467	5904.046	0.0007
19	6	13	18	6	12	5905.5219	5905.5219	0.0000
19	6	14	18	6	13	5905.5219	5905.5219	0.0000
19	4	16	18	4	15	5905.6555	5905.6527	0.0028
19	4	15	18	4	14	5905.6555	5905.6543	0.0012
19	3	17	18	3	16	5905.9143	5905.9157	-0.0014
19	3	16	18	3	15	5906.0802	5906.0800	0.0002
19	2	17	18	2	16	5910.5295	5910.5300	-0.0005
19	1	18	18	1	17	5927.5621	5927.5612	0.0009
16	1	15	15	0	15	5995.6054	5995.6036	0.0018
20	1	20	19	1	19	6188.5998	6188.5977	0.0021
20	0	20	19	0	19	6208.3048	6208.3070	-0.0022
20	2	19	19	2	18	6214.5827	6214.5825	0.0002
20	5	15	19	5	14	6216.3127	6216.3131	-0.0004
20	5	16	19	5	15	6216.3127	6216.3131	-0.0004
20	4	16	19	4	15	6216.4497	6216.4506	-0.0009
20	4	17	19	4	16	6216.4497	6216.4484	0.0013
20	3	18	19	3	17	6216.7507	6216.7500	0.0007
20	3	17	19	3	16	6216.9629	6216.9626	0.0003
20	2	18	19	2	17	6222.1192	6222.1187	0.0005
20	1	19	19	1	18	6239.2499	6239.2510	-0.0011

Table S16. Rotational transition frequencies of the **PFP***G*+*g*+**PFP***G*+*g*+ homodimer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
5	1	4	4	1	3	1692.1842	1692.1846	-0.0004
14	2	12	14	1	13	1892.3407	1892.3395	0.0012
6	1	6	5	1	5	2007.2750	2007.2730	0.0020
6	0	6	5	0	5	2018.4760	2018.4738	0.0022
6	2	5	5	2	4	2018.9797	2018.9800	-0.0003
6	4	3	5	4	2	2019.1249	2019.1259	-0.0010
6	5	1	5	5	0	2019.1249	2019.1232	0.0017
6	5	2	5	5	1	2019.1249	2019.1232	0.0017
6	4	2	5	4	1	2019.1249	2019.1260	-0.0011
6	3	4	5	3	3	2019.1513	2019.1499	0.0014
6	3	3	5	3	2	2019.1513	2019.1523	-0.0010
6	2	4	5	2	3	2019.5544	2019.5551	-0.0007

6	2	4	6	1	5	2024.0249	2024.0263	-0.0014
6	1	5	5	1	4	2030.5623	2030.5641	-0.0018
4	2	3	4	1	4	2082.9547	2082.9521	0.0026
5	2	4	5	1	5	2092.6932	2092.6963	-0.0031
5	1	5	4	0	4	2341.4008	2341.4013	-0.0005
7	1	7	6	1	6	2341.7434	2341.7425	0.0009
7	0	7	6	0	6	2354.6222	2354.6220	0.0002
7	2	6	6	2	5	2355.4160	2355.4196	-0.0036
7	2	5	6	2	4	2356.3410	2356.3392	0.0018
7	1	6	6	1	5	2368.9140	2368.9118	0.0022
9	0	9	8	1	8	2405.9095	2405.9095	0.0000
6	1	6	5	0	5	2666.4509	2666.4530	-0.0020
8	1	8	7	1	7	2676.1745	2676.1777	-0.0032
8	0	8	7	0	7	2690.6492	2690.6489	0.0003
8	2	7	7	2	6	2691.8322	2691.8329	-0.0007
8	6	2	7	6	1	2692.1523	2692.1530	-0.0007
8	5	3	7	5	2	2692.1523	2692.1517	0.0006
8	5	4	7	5	3	2692.1523	2692.1517	0.0006
8	6	3	7	6	2	2692.1523	2692.1530	-0.0007
8	4	4	7	4	3	2692.1708	2692.1707	0.0001
8	4	5	7	4	4	2692.1708	2692.1707	0.0001
8	3	6	7	3	5	2692.2345	2692.2346	-0.0001
8	3	5	7	3	4	2692.2455	2692.2455	0.0000
8	2	6	7	2	5	2693.2106	2693.2112	-0.0006
8	1	7	7	1	6	2707.2218	2707.2221	-0.0003
2	2	1	1	1	0	2734.5922	2734.5907	0.0015
2	2	1	1	1	1	2738.4768	2738.4734	0.0034
2	2	0	1	1	1	2738.492	2738.4898	0.0022
10	0	10	9	1	9	2757.6115	2757.6088	0.0027
7	1	7	6	0	6	2989.7209	2989.7218	-0.0009
9	1	9	8	1	8	3010.5744	3010.5739	0.0005
9	0	9	8	0	8	3026.5362	3026.5380	-0.0018
9	6	4	8	6	3	3028.6583	3028.6580	0.0003
9	6	3	8	6	2	3028.6583	3028.658	0.0003
9	5	5	8	5	4	3028.6627	3028.6621	0.0006
9	5	4	8	5	3	3028.6627	3028.6621	0.0006
9	7	3	8	7	2	3028.6687	3028.6687	0.0000
9	7	2	8	7	1	3028.6687	3028.6687	0.0000
9	4	5	8	4	4	3028.6951	3028.6940	0.0011
9	4	6	8	4	5	3028.6951	3028.6939	0.0012

9	3	7	8	3	6	3028.7859	3028.7864	-0.0005
9	3	6	8	3	5	3028.8058	3028.8065	-0.0007
9	2	7	8	2	6	3030.1843	3030.1828	0.0015
9	1	8	8	1	7	3045.4892	3045.4893	-0.0001
3	2	2	2	1	1	3067.2245	3067.2213	0.0032
3	2	1	2	1	2	3078.9504	3078.9514	-0.0010
7	1	6	6	0	6	3098.4206	3098.4184	0.0022
11	0	11	10	1	10	3110.5206	3110.5208	-0.0002
8	1	8	7	0	7	3311.2767	3311.2775	-0.0008
10	1	10	9	1	9	3344.9260	3344.9269	-0.0009
10	0	10	9	0	9	3362.2766	3362.2732	0.0034
10	2	9	9	2	8	3364.5643	3364.5655	-0.0012
10	6	5	9	6	4	3365.1576	3365.1581	-0.0005
10	6	4	9	6	3	3365.1576	3365.1581	-0.0005
10	7	4	9	7	3	3365.1659	3365.1659	0.0000
10	7	3	9	7	2	3365.1659	3365.1659	0.0000
10	5	6	9	5	5	3365.1699	3365.1695	0.0004
10	5	5	9	5	4	3365.1699	3365.1695	0.0004
10	8	2	9	8	1	3365.1859	3365.1858	0.0001
10	8	3	9	8	2	3365.1859	3365.1858	0.0001
10	4	7	9	4	6	3365.2186	3365.2178	0.0008
10	4	6	9	4	5	3365.2186	3365.2180	0.0006
10	3	8	9	3	7	3365.3440	3365.3449	-0.0009
10	3	7	9	3	6	3365.3794	3365.3793	0.0001
10	2	8	9	2	7	3367.2630	3367.2654	-0.0024
10	1	9	9	1	8	3383.7040	3383.7074	-0.0034
4	2	3	3	1	2	3397.9084	3397.9057	0.0027
15	3	12	15	2	13	3412.4134	3412.4138	-0.0004
14	3	11	14	2	12	3418.5862	3418.5859	0.0003
4	2	2	3	1	3	3421.4479	3421.4480	-0.0001
13	3	10	13	2	11	3423.6509	3423.6529	-0.0020
12	3	9	12	2	10	3427.7417	3427.7417	0.0000
11	3	8	11	2	9	3430.9761	3430.9774	-0.0013
10	3	7	10	2	8	3433.4798	3433.4807	-0.0009
9	3	6	9	2	7	3435.3668	3435.3668	0.0000
8	3	6	8	2	6	3436.7238	3436.7230	0.0008
8	3	5	8	2	6	3436.7419	3436.7431	-0.0012
7	3	5	7	2	5	3437.6996	3437.6995	0.0001
7	3	4	7	2	5	3437.7082	3437.7087	-0.0005
6	3	4	6	2	4	3438.3493	3438.3495	-0.0002

6	3	3	6	2	4	3438.3535	3438.3532	0.0003
5	3	3	5	2	3	3438.7551	3438.7547	0.0004
5	3	2	5	2	3	3438.7551	3438.7559	-0.0008
4	3	2	4	2	2	3438.9878	3438.9852	0.0026
4	3	1	4	2	2	3438.9878	3438.9855	0.0023
5	3	2	5	2	4	3439.3311	3439.3313	-0.0002
5	3	3	5	2	4	3439.3311	3439.3301	0.0010
6	3	4	6	2	5	3439.5018	3439.5000	0.0018
6	3	3	6	2	5	3439.5018	3439.5036	-0.0018
7	3	5	7	2	6	3439.7694	3439.7696	-0.0002
7	3	4	7	2	6	3439.7789	3439.7788	0.0001
8	3	6	8	2	7	3440.1709	3440.1713	-0.0004
9	3	7	9	2	8	3440.7418	3440.7417	0.0001
10	3	8	10	2	9	3441.5211	3441.5211	0.0000
11	3	9	11	2	10	3442.5535	3442.5540	-0.0005
12	3	10	12	2	11	3443.8894	3443.8883	0.0011
13	3	11	13	2	12	3445.5748	3445.5753	-0.0005
14	3	12	14	2	13	3447.6695	3447.6694	0.0001
15	3	13	15	2	14	3450.2276	3450.2280	-0.0004
8	1	7	7	0	7	3451.0163	3451.0186	-0.0023
16	3	14	16	2	15	3453.3107	3453.3108	-0.0001
17	3	15	17	2	16	3456.9792	3456.9800	-0.0008
18	3	16	18	2	17	3461.2982	3461.2997	-0.0015
12	0	12	11	1	11	3464.5096	3464.5093	0.0003
19	3	17	19	2	18	3466.3355	3466.3357	-0.0002
20	3	18	20	2	19	3472.1557	3472.1550	0.0007
9	1	9	8	0	8	3631.1998	3631.2024	-0.0026
11	1	11	10	1	10	3679.2328	3679.2325	0.0003
11	0	11	10	0	10	3697.8386	3697.839	-0.0004
11	2	10	10	2	9	3700.8746	3700.8773	-0.0027
11	6	5	10	6	4	3701.6523	3701.6527	-0.0004
11	6	6	10	6	5	3701.6523	3701.6527	-0.0004
11	7	4	10	7	3	3701.6567	3701.6564	0.0003
11	7	5	10	7	4	3701.6567	3701.6564	0.0003
11	5	6	10	5	5	3701.6753	3701.6735	0.0018
11	5	7	10	5	6	3701.6753	3701.6735	0.0018
11	4	8	10	4	7	3701.7426	3701.7424	0.0002
11	4	7	10	4	6	3701.7426	3701.7427	-0.0001
11	3	9	10	3	8	3701.9066	3701.9102	-0.0036
11	3	8	10	3	7	3701.9651	3701.9662	-0.0011

11	2	9	10	2	8	3704.4686	3704.4695	-0.0009
11	1	10	10	1	9	3721.8702	3721.8703	-0.0001
5	2	4	4	1	3	3726.6449	3726.6446	0.0003
5	2	4	4	1	4	3765.4691	3765.4699	-0.0008
5	2	3	4	1	4	3766.0442	3766.0453	-0.0011
13	0	13	12	1	12	3819.4314	3819.4285	0.0029
6	5	2	7	4	4	3834.8055	3834.8051	0.0004
6	5	1	7	4	4	3834.8055	3834.8051	0.0004
6	5	2	7	4	3	3834.8055	3834.8051	0.0004
6	5	1	7	4	3	3834.8055	3834.8051	0.0004
19	1	19	18	2	16	3872.7705	3872.7702	0.0003
14	7	8	15	6	10	3894.1702	3894.1703	-0.0001
14	7	7	15	6	10	3894.1702	3894.1703	-0.0001
14	7	8	15	6	9	3894.1702	3894.1703	-0.0001
14	7	7	15	6	9	3894.1702	3894.1703	-0.0001
17	1	16	16	2	14	3895.1622	3895.1629	-0.0007
10	1	10	9	0	9	3949.5886	3949.5913	-0.0027
12	1	12	11	1	11	4013.4868	4013.4869	-0.0001
12	0	12	11	0	11	4033.2204	4033.2210	-0.0006
12	2	11	11	2	10	4037.1467	4037.1479	-0.0012
12	7	6	11	7	5	4038.1406	4038.1394	0.0012
12	7	5	11	7	4	4038.1406	4038.1394	0.0012
12	6	6	11	6	5	4038.1406	4038.1412	-0.0006
12	6	7	11	6	6	4038.1406	4038.1412	-0.0006
12	8	5	11	8	4	4038.1557	4038.1561	-0.0004
12	8	4	11	8	3	4038.1557	4038.1561	-0.0004
12	5	8	11	5	7	4038.1737	4038.1738	-0.0001
12	5	7	11	5	6	4038.1737	4038.1738	-0.0001
12	4	9	11	4	8	4038.2688	4038.2677	0.0011
12	4	8	11	4	7	4038.2688	4038.2683	0.0005
12	3	10	11	3	9	4038.4821	4038.4821	0.0000
12	3	9	11	3	8	4038.5691	4038.5691	0.0000
12	2	10	11	2	9	4041.8046	4041.8048	-0.0002
6	2	5	5	1	4	4053.4424	4053.4399	0.0025
12	1	11	11	1	10	4059.9713	4059.9716	-0.0003
6	2	4	5	1	5	4112.8253	4112.8267	-0.0014
10	1	9	9	0	9	4163.0263	4163.0284	-0.0021
14	0	14	13	1	13	4175.1237	4175.1249	-0.0012
11	1	11	10	0	10	4266.5482	4266.5507	-0.0025
13	1	13	12	1	12	4347.689	4347.6863	0.0027

13	2	12	12	2	11	4373.3757	4373.3734	0.0023
13	7	7	12	7	6	4374.6143	4374.6143	0.0000
13	7	6	12	7	5	4374.6143	4374.6143	0.0000
13	6	7	12	6	6	4374.6232	4374.6231	0.0001
13	6	8	12	6	7	4374.6232	4374.6231	0.0001
13	8	5	12	8	4	4374.6279	4374.6279	0.0000
13	8	6	12	8	5	4374.6279	4374.6279	0.0000
13	5	9	12	5	8	4374.6718	4374.6700	0.0018
13	5	8	12	5	7	4374.6718	4374.6700	0.0018
13	4	10	12	4	9	4374.7962	4374.7938	0.0024
13	4	9	12	4	8	4374.7962	4374.7949	0.0013
13	3	11	12	3	10	4375.063	4375.0604	0.0026
13	3	10	12	3	9	4375.1922	4375.1908	0.0014
7	2	6	6	1	5	4378.2959	4378.2954	0.0005
13	2	11	12	2	10	4379.2793	4379.2797	-0.0004
13	1	12	12	1	11	4398.0046	4398.0048	-0.0002
3	3	1	2	2	0	4448.7061	4448.7062	-0.0001
3	3	0	2	2	0	4448.7061	4448.7062	-0.0001
3	3	0	2	2	1	4448.7227	4448.7227	0.0000
3	3	1	2	2	1	4448.7227	4448.7226	0.0001
7	2	5	6	1	6	4461.8928	4461.8929	-0.0001
15	0	15	14	1	14	4531.4382	4531.4385	-0.0003
12	1	12	11	0	11	4582.1961	4582.1986	-0.0025
14	1	14	13	1	13	4681.8250	4681.8272	-0.0022
8	2	7	7	1	6	4701.2166	4701.2165	0.0001
14	0	14	13	0	13	4703.3831	4703.3827	0.0004
14	2	13	13	2	12	4709.5478	4709.5503	-0.0025
14	7	7	13	7	6	4711.0798	4711.0803	-0.0005
14	7	8	13	7	7	4711.0798	4711.0803	-0.0005
14	8	7	13	8	6	4711.0901	4711.0898	0.0003
14	8	6	13	8	5	4711.0901	4711.0898	0.0003
14	6	8	13	6	7	4711.0974	4711.0978	-0.0004
14	6	9	13	6	8	4711.0974	4711.0978	-0.0004
14	9	6	13	9	5	4711.1177	4711.1176	0.0001
14	9	5	13	9	4	4711.1177	4711.1176	0.0001
14	5	9	13	5	8	4711.1631	4711.1619	0.0012
14	5	10	13	5	9	4711.1631	4711.1619	0.0012
14	4	11	13	4	10	4711.3222	4711.3207	0.0015
14	4	10	13	4	9	4711.3222	4711.3226	-0.0004
14	3	12	13	3	11	4711.6438	4711.6444	-0.0006

14	3	11	13	3	10	4711.8346	4711.8339	0.0007
14	2	12	13	2	11	4716.9007	4716.9009	-0.0002
14	1	13	13	1	12	4735.9606	4735.9628	-0.0022
4	3	2	3	2	1	4785.1868	4785.1865	0.0003
4	3	1	3	2	1	4785.1868	4785.1868	0.0000
4	3	2	3	2	2	4785.2697	4785.2687	0.0010
4	3	1	3	2	2	4785.2697	4785.2690	0.0007
20	4	16	20	3	17	4805.9052	4805.9056	-0.0004
18	4	14	18	3	15	4809.2241	4809.2242	-0.0001
20	4	17	20	3	18	4810.1935	4810.1931	0.0004
17	4	13	17	3	14	4810.4631	4810.4628	0.0003
19	4	16	19	3	17	4810.8983	4810.8979	0.0004
16	4	12	16	3	13	4811.4733	4811.4728	0.0005
18	4	15	18	3	16	4811.5435	4811.5425	0.0010
17	4	14	17	3	15	4812.1215	4812.1229	-0.0014
15	4	11	15	3	12	4812.2891	4812.2878	0.0013
16	4	13	16	3	14	4812.6366	4812.6375	-0.0009
14	4	11	14	3	11	4812.9328	4812.9336	-0.0008
14	4	10	14	3	11	4812.9376	4812.9377	-0.0001
15	4	12	15	3	13	4813.0863	4813.0864	-0.0001
8	2	6	7	1	7	4813.3591	4813.3616	-0.0025
13	4	9	13	3	10	4813.4488	4813.4491	-0.0003
14	4	11	14	3	12	4813.4711	4813.4711	0.0000
11	4	8	11	3	9	4814.2761	4814.2758	0.0003
11	4	7	11	3	9	4814.2761	4814.2765	-0.0004
10	4	7	10	3	7	4814.3691	4814.369	0.0001
10	4	6	10	3	7	4814.3691	4814.3693	-0.0002
10	4	6	10	3	8	4814.4438	4814.444	-0.0002
10	4	7	10	3	8	4814.4438	4814.4437	0.0001
9	4	6	9	3	7	4814.5705	4814.5708	-0.0003
9	4	5	9	3	7	4814.5705	4814.5709	-0.0004
8	4	5	8	3	5	4814.6431	4814.6431	0.0000
8	4	4	8	3	5	4814.6431	4814.6432	-0.0001
6	4	2	6	3	3	4814.7646	4814.7646	0.0000
6	4	3	6	3	3	4814.7646	4814.7646	0.0000
6	4	2	6	3	4	4814.7682	4814.7682	0.0000
6	4	3	6	3	4	4814.7682	4814.7682	0.0000
4	4	0	4	3	2	4814.8039	4814.8039	0.0000
4	4	1	4	3	1	4814.8039	4814.8036	0.0003
4	4	0	4	3	1	4814.8039	4814.8036	0.0003

4	4	1	4	3	2	4814.8039	4814.8039	0.0000
16	0	16	15	1	15	4888.2054	4888.2048	0.0006
13	1	13	12	0	12	4896.6652	4896.6639	0.0013
15	1	15	14	1	14	5015.9073	5015.9065	0.0008
9	2	8	8	1	7	5022.2124	5022.2104	0.0020
15	0	15	14	0	14	5038.1379	5038.1408	-0.0029
15	2	14	14	2	13	5045.6757	5045.6747	0.0010
15	7	9	14	7	8	5047.5372	5047.5368	0.0004
15	7	8	14	7	7	5047.5372	5047.5368	0.0004
15	8	8	14	8	7	5047.5411	5047.5411	0.0000
15	8	7	14	8	6	5047.5411	5047.5411	0.0000
15	6	9	14	6	8	5047.5661	5047.5648	0.0013
15	6	10	14	6	9	5047.5661	5047.5648	0.0013
15	5	11	14	5	10	5047.6499	5047.6490	0.0009
15	5	10	14	5	9	5047.6499	5047.6490	0.0009
15	4	12	14	4	11	5047.8499	5047.8485	0.0014
15	4	11	14	4	10	5047.8499	5047.8515	-0.0016
15	3	13	14	3	12	5048.2322	5048.2333	-0.0011
15	3	12	14	3	11	5048.5003	5048.5015	-0.0012
15	2	13	14	2	12	5054.6759	5054.6736	0.0023
15	1	14	14	1	13	5073.8375	5073.8386	-0.0011
5	3	3	4	2	2	5121.5979	5121.6012	-0.0033
5	3	2	4	2	2	5121.5994	5121.6024	-0.0030
5	3	3	4	2	3	5121.8492	5121.8478	0.0014
5	3	2	4	2	3	5121.8492	5121.8491	0.0001
9	2	7	8	1	8	5167.3662	5167.3667	-0.0005
14	1	14	13	0	13	5210.0839	5210.0850	-0.0011
17	0	17	16	1	16	5245.2597	5245.2572	0.0025
10	2	9	9	1	8	5341.2901	5341.2866	0.0035
16	1	16	15	1	15	5349.9222	5349.9212	0.0010
16	0	16	15	0	15	5372.6760	5372.6729	0.0031
16	2	15	15	2	14	5381.7415	5381.7431	-0.0016
16	8	8	15	8	7	5383.9809	5383.9810	-0.0001
16	8	9	15	8	8	5383.9809	5383.9810	-0.0001
16	7	9	15	7	8	5383.9824	5383.9831	-0.0007
16	7	10	15	7	9	5383.9832	5383.9831	0.0000
16	5	12	15	5	11	5384.1314	5384.1311	0.0003
16	5	11	15	5	10	5384.1314	5384.1311	0.0003
16	4	12	15	4	11	5384.3798	5384.3819	-0.0021
16	4	13	15	4	12	5384.3798	5384.3771	0.0027

16	3	14	15	3	13	5384.8258	5384.8259	-0.0001
16	3	13	15	3	12	5385.1975	5385.1969	0.0006
16	2	14	15	2	13	5392.6003	5392.6005	-0.0002
16	1	15	15	1	14	5411.6256	5411.6247	0.0009
6	3	4	5	2	3	5457.9042	5457.9046	-0.0004
6	3	3	5	2	3	5457.9084	5457.9082	0.0002
6	3	4	5	2	4	5458.4803	5458.4799	0.0004
6	3	3	5	2	4	5458.4837	5458.4836	0.0001
15	1	15	14	0	14	5522.6101	5522.6089	0.0012
10	2	8	9	1	9	5524.0571	5524.0581	-0.0010
10	2	8	9	1	9	5524.0571	5524.0581	-0.0010
18	0	18	17	1	17	5602.4274	5602.4290	-0.0016
11	2	10	10	1	9	5658.4556	5658.4564	-0.0008
17	1	17	16	1	16	5683.8688	5683.8686	0.0002
17	0	17	16	0	16	5706.9760	5706.9736	0.0024
17	2	16	16	2	15	5717.7500	5717.7518	-0.0018
17	7	11	16	7	10	5720.4167	5720.4186	-0.0019
17	7	10	16	7	9	5720.4167	5720.4186	-0.0019
17	6	12	16	6	11	5720.4749	5720.4734	0.0015
17	6	11	16	6	10	5720.4749	5720.4734	0.0015
17	5	12	16	5	11	5720.6081	5720.6078	0.0003
17	5	13	16	5	12	5720.6081	5720.6077	0.0004
17	4	14	16	4	13	5720.9072	5720.9064	0.0008
17	4	13	16	4	12	5720.9135	5720.9138	-0.0003
17	3	15	16	3	14	5721.4209	5721.4210	-0.0001
17	3	14	16	3	13	5721.9239	5721.9238	0.0001
17	2	15	16	2	14	5730.6822	5730.6820	0.0002
17	1	16	16	1	15	5749.3120	5749.3133	-0.0013
7	3	5	6	2	4	5794.0375	5794.0388	-0.0013
7	3	5	6	2	5	5795.1899	5795.1892	0.0007
7	3	4	6	2	5	5795.1983	5795.1983	0.0000
16	1	16	15	0	15	5834.3876	5834.3893	-0.0017
11	2	9	10	1	10	5883.6022	5883.6007	0.0015
19	0	19	18	1	18	5959.5543	5959.5563	-0.0020
12	2	11	11	1	10	5973.7346	5973.7340	0.0006
18	1	18	17	1	17	6017.7464	6017.7464	0.0000
18	0	18	17	0	17	6041.0380	6041.0404	-0.0024
18	2	17	17	2	16	6053.6964	6053.6973	-0.0009
18	8	10	17	8	9	6056.8241	6056.8236	0.0005
18	8	11	17	8	10	6056.8241	6056.8236	0.0005

18	9	9	17	9	8	6056.8388	6056.8380	0.0008
18	9	10	17	9	9	6056.8388	6056.8380	0.0008
18	7	12	17	7	11	6056.8438	6056.8425	0.0013
18	7	11	17	7	10	6056.8438	6056.8425	0.0013
18	6	12	17	6	11	6056.9143	6056.9138	0.0005
18	6	13	17	6	12	6056.9143	6056.9138	0.0005
18	5	13	17	5	12	6057.0773	6057.0787	-0.0014
18	5	14	17	5	13	6057.0773	6057.0787	-0.0014
18	4	15	17	4	14	6057.4365	6057.4365	0.0000
18	4	14	17	4	13	6057.4475	6057.4476	-0.0001
18	3	16	17	3	15	6058.0187	6058.0170	0.0017
18	3	15	17	3	14	6058.6877	6058.6862	0.0015
18	2	16	17	2	15	6068.915	6068.9157	-0.0007
18	1	17	17	1	16	6086.8968	6086.8963	0.0005
8	3	6	7	2	5	6129.9341	6129.9341	0.0000
8	3	5	7	2	5	6129.9541	6129.9542	-0.0001
8	3	6	7	2	6	6132.0048	6132.0042	0.0006
8	3	5	7	2	6	6132.0254	6132.0243	0.0011
17	1	17	16	0	16	6145.5826	6145.5850	-0.0024
4	4	1	3	3	1	6160.8909	6160.8907	0.0002
4	4	1	3	3	0	6160.8909	6160.8907	0.0002
4	4	0	3	3	0	6160.8909	6160.8907	0.0002
4	4	0	3	3	1	6160.8909	6160.8907	0.0002
12	2	10	11	1	11	6246.1709	6246.1730	-0.0021
13	2	12	12	1	11	6287.1365	6287.1357	0.0008
19	1	19	18	1	18	6351.5501	6351.5523	-0.0022
19	0	19	18	0	18	6374.8755	6374.8737	0.0018
19	2	18	18	2	17	6389.5747	6389.5758	-0.0011
19	8	11	18	8	10	6393.2239	6393.2246	-0.0007
19	8	12	18	8	11	6393.2239	6393.2246	-0.0007
19	7	12	18	7	11	6393.2533	6393.2542	-0.0009
19	7	13	18	7	12	6393.2533	6393.2542	-0.0009
19	6	14	18	6	13	6393.3447	6393.3443	0.0004
19	6	13	18	6	12	6393.3447	6393.3443	0.0004
19	5	14	18	5	13	6393.5437	6393.5436	0.0001
19	5	15	18	5	14	6393.5437	6393.5435	0.0002
19	4	16	18	4	15	6393.9669	6393.9673	-0.0004
19	4	15	18	4	14	6393.9829	6393.9835	-0.0006
19	3	17	18	3	16	6394.6137	6394.6118	0.0019
19	3	16	18	3	15	6395.4892	6395.4885	0.0007

19	2	17	18	2	16	6407.2973	6407.2964	0.0009
19	1	18	18	1	17	6424.3645	6424.3652	-0.0007
9	3	7	8	2	6	6465.5073	6465.5093	-0.0020
5	4	2	4	3	2	6497.4081	6497.4082	-0.0001
5	4	1	4	3	1	6497.4081	6497.4079	0.0002
5	4	2	4	3	1	6497.4081	6497.4079	0.0002
5	4	1	4	3	2	6497.4081	6497.4082	-0.0001
20	1	20	19	1	19	6685.2871	6685.2845	0.0026
20	0	20	19	0	19	6708.4752	6708.4764	-0.0012
20	2	19	19	2	18	6725.3861	6725.3840	0.0021
20	6	14	19	6	13	6729.7624	6729.7643	-0.0019
20	6	15	19	6	14	6729.7624	6729.7643	-0.0019
20	5	15	19	5	14	6729.9989	6730.0021	-0.0032
20	5	16	19	5	15	6729.9989	6730.0018	-0.0029
20	4	17	19	4	16	6730.499	6730.4985	0.0005
20	4	16	19	4	15	6730.5228	6730.5218	0.0010
20	3	17	19	3	16	6732.3375	6732.3354	0.0021
20	1	19	19	1	18	6761.7128	6761.7112	0.0016
6	4	2	5	3	3	6833.9174	6833.9181	-0.0007
6	4	3	5	3	2	6833.9174	6833.9169	0.0005
6	4	3	5	3	3	6833.9174	6833.9181	-0.0007
6	4	2	5	3	2	6833.9174	6833.9169	0.0005
6	4	3	5	3	2	6833.9176	6833.9169	0.0007
6	4	3	5	3	3	6833.9176	6833.9181	-0.0005
6	4	2	5	3	2	6833.9176	6833.9169	0.0007
6	4	2	5	3	3	6833.9176	6833.9181	-0.0005
7	4	3	6	3	4	7170.4168	7170.4163	0.0005

Table S17. Rotational transition frequencies of the **PFP***G+g+***PFP***G-g-* homodimer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
5	0	5	4	0	4	1890.5178	1890.5179	-0.0001
5	4	2	4	4	1	1892.2365	1892.2362	0.0003
5	4	1	4	4	0	1892.2365	1892.2362	0.0003
5	3	3	4	3	2	1892.3315	1892.3318	-0.0003
5	3	2	4	3	1	1892.3434	1892.3419	0.0015
5	2	3	4	2	2	1893.4575	1893.4579	-0.0004
5	1	4	4	1	3	1911.5501	1911.5483	0.0018
4	1	4	3	0	3	2078.3412	2078.3405	0.0007
11	2	10	11	1	11	2078.4078	2078.4121	-0.0043
7	0	7	6	1	6	2119.3551	2119.3574	-0.0023
6	1	6	5	1	5	2246.0844	2246.0883	-0.0039
6	0	6	5	0	5	2267.7601	2267.7608	-0.0007
6	2	5	5	2	4	2270.1257	2270.1275	-0.0018
6	5	1	5	5	0	2270.6529	2270.6534	-0.0005
6	5	2	5	5	1	2270.6529	2270.6534	-0.0005
6	4	2	5	4	1	2270.7331	2270.7326	0.0005
6	4	3	5	4	2	2270.7331	2270.7326	0.0005
6	3	4	5	3	3	2270.8907	2270.8900	0.0007
6	3	3	5	3	2	2270.9168	2270.917	-0.0002
6	2	4	5	2	3	2272.8505	2272.8513	-0.0008
6	1	5	5	1	4	2293.6303	2293.6277	0.0026
17	2	16	17	1	17	2436.4199	2436.4216	-0.0017
5	1	5	4	0	4	2437.3762	2437.3745	0.0017
8	0	8	7	1	7	2520.0031	2520.0060	-0.0029
7	1	7	6	1	6	2620.1428	2620.1441	-0.0013
7	0	7	6	0	6	2644.5389	2644.5415	-0.0026
7	2	6	6	2	5	2648.2736	2648.2735	0.0001
7	6	2	6	6	1	2649.0619	2649.0627	-0.0008
7	6	1	6	6	0	2649.0619	2649.0627	-0.0008
7	5	2	6	5	1	2649.1354	2649.1339	0.0015
7	5	3	6	5	2	2649.1354	2649.1339	0.0015
7	4	3	6	4	2	2649.2586	2649.25600	0.0026
7	4	4	6	4	3	2649.2586	2649.2557	0.0029
7	3	5	6	3	4	2649.4925	2649.4941	-0.0016
7	3	4	6	3	3	2649.5573	2649.5547	0.0026
7	2	5	6	2	4	2652.6197	2652.6201	-0.0004
7	1	6	6	1	5	2675.5756	2675.5770	-0.0014
6	1	6	5	0	5	2792.9486	2792.9449	0.0037

9	0	9	8	1	8	2922.3877	2922.3896	-0.0019
14	3	11	14	2	12	2929.5863	2929.5900	-0.0037
13	3	10	13	2	11	2950.8703	2950.8722	-0.0019
12	3	9	12	2	10	2968.5528	2968.5553	-0.0025
11	3	8	11	2	9	2982.8936	2982.8937	-0.0001
8	1	8	7	1	7	2994.0697	2994.0716	-0.0019
10	3	7	10	2	8	2994.2135	2994.2119	0.0016
9	3	6	9	2	7	3002.8836	3002.8797	0.0039
8	3	5	8	2	6	3009.2908	3009.2901	0.0007
7	3	4	7	2	5	3013.8369	3013.8381	-0.0012
6	3	3	6	2	4	3016.9041	3016.9035	0.0006
5	3	2	5	2	3	3018.8409	3018.8378	0.0031
4	3	1	4	2	2	3019.9561	3019.9539	0.0022
3	3	0	3	2	1	3020.5179	3020.5190	-0.0011
8	0	8	7	0	7	3020.7911	3020.7927	-0.0016
4	3	2	4	2	3	3021.1211	3021.1210	0.0001
5	3	3	5	2	4	3021.5548	3021.5538	0.0010
6	3	4	6	2	5	3022.3148	3022.3164	-0.0016
7	3	5	7	2	6	3023.5394	3023.5370	0.0024
8	3	6	8	2	7	3025.3613	3025.3618	-0.0005
8	2	7	7	2	6	3026.3217	3026.3234	-0.0017
8	5	4	7	5	3	3027.6302	3027.6320	-0.0018
8	5	3	7	5	2	3027.6302	3027.6320	-0.0018
8	4	5	7	4	4	3027.8095	3027.8100	-0.0005
8	4	4	7	4	3	3027.8095	3027.8108	-0.0013
9	3	7	9	2	8	3027.9525	3027.9530	-0.0005
8	3	6	7	3	5	3028.1475	3028.1482	-0.0007
8	3	5	7	3	4	3028.2715	3028.2692	0.0023
10	3	8	10	2	9	3031.4852	3031.4874	-0.0022
11	3	9	11	2	10	3036.1538	3036.1540	-0.0002
12	3	10	12	2	11	3042.1522	3042.1523	-0.0001
13	3	11	13	2	12	3049.6886	3049.6897	-0.0011
8	1	7	7	1	6	3057.3735	3057.3709	0.0026
15	3	13	15	2	14	3070.2346	3070.2382	-0.0036
16	3	14	16	2	15	3083.6859	3083.6835	0.0024
17	3	15	17	2	16	3099.5312	3099.5318	-0.0006
18	3	16	18	2	17	3117.9951	3117.9955	-0.0004
19	3	17	19	2	18	3139.2816	3139.2816	0.0000
7	1	7	6	0	6	3145.3276	3145.3282	-0.0006
10	0	10	9	1	9	3326.0163	3326.0142	0.0021

9	1	9	8	1	8	3367.8551	3367.8571	-0.0020
9	0	9	8	0	8	3396.4566	3396.4553	0.0013
9	2	8	8	2	7	3404.2627	3404.2635	-0.0008
9	7	3	8	7	2	3405.9171	3405.9169	0.0002
9	7	2	8	7	1	3405.9171	3405.9169	0.0002
9	6	4	8	6	3	3406.0111	3406.0097	0.0014
9	6	3	8	6	2	3406.0111	3406.0097	0.0014
9	5	4	8	5	3	3406.1503	3406.1503	0.0000
9	5	5	8	5	4	3406.1503	3406.1503	0.0000
9	4	6	8	4	5	3406.4001	3406.3999	0.0002
9	4	5	8	4	4	3406.4001	3406.4018	-0.0017
9	3	7	8	3	6	3406.8542	3406.8548	-0.0006
9	3	6	8	3	5	3407.0758	3407.0765	-0.0007
9	2	7	8	2	6	3413.4864	3413.4869	-0.0005
9	1	8	8	1	7	3438.9856	3438.9823	0.0033
8	1	8	7	0	7	3494.8584	3494.8584	0.0000
11	0	11	10	1	10	3730.3613	3730.3649	-0.0036
10	1	10	9	1	9	3741.4875	3741.4884	-0.0009
10	0	10	9	0	9	3771.4777	3771.4817	-0.0040
10	2	9	9	2	8	3782.0799	3782.0804	-0.0005
10	8	3	9	8	2	3784.2907	3784.2911	-0.0004
10	8	2	9	8	1	3784.2907	3784.2911	-0.0004
10	7	4	9	7	3	3784.3801	3784.3805	-0.0004
10	7	3	9	7	2	3784.3801	3784.3805	-0.0004
10	6	4	9	6	3	3784.5043	3784.5027	0.0016
10	6	5	9	6	4	3784.5043	3784.5027	0.0016
10	5	5	9	5	4	3784.6898	3784.6913	-0.0015
10	5	6	9	5	5	3784.6898	3784.6913	-0.0015
10	4	7	9	4	6	3785.0314	3785.0294	0.0020
10	4	6	9	4	5	3785.0314	3785.0337	-0.0023
10	3	8	9	3	7	3785.6159	3785.6148	0.0011
10	3	7	9	3	6	3785.9962	3785.9943	0.0019
10	2	8	9	2	7	3794.6652	3794.6622	0.0030
10	1	9	9	1	8	3820.3831	3820.3819	0.0012
9	1	9	8	0	8	3841.9186	3841.9228	-0.0042
14	1	13	13	2	12	3880.0187	3880.0185	0.0002
6	2	5	5	1	4	4023.4117	4023.4112	0.0005
11	1	11	10	1	10	4114.9544	4114.9554	-0.0010
12	0	12	11	1	11	4134.9232	4134.9219	0.0013
11	0	11	10	0	10	4145.8371	4145.8391	-0.0020

3	3	1	2	2	0	4156.0804	4156.0801	0.0003
3	3	0	2	2	1	4156.1603	4156.1587	0.0016
11	2	10	10	2	9	4159.7629	4159.7606	0.0023
11	9	2	10	9	1	4162.6499	4162.6503	-0.0004
11	9	3	10	9	2	4162.6499	4162.6503	-0.0004
11	8	4	10	8	3	4162.7388	4162.7397	-0.0009
11	8	3	10	8	2	4162.7388	4162.7397	-0.0009
11	7	4	10	7	3	4162.8527	4162.8530	-0.0003
11	7	5	10	7	4	4162.8527	4162.8530	-0.0003
11	6	5	10	6	4	4163.0115	4163.0107	0.0008
11	6	6	10	6	5	4163.0115	4163.0107	0.0008
11	5	6	10	5	5	4163.2574	4163.2575	-0.0001
11	5	7	10	5	6	4163.2574	4163.2575	-0.0001
11	4	8	10	4	7	4163.7021	4163.7029	-0.0008
11	4	7	10	4	6	4163.7111	4163.7113	-0.0002
11	3	9	10	3	8	4164.4283	4164.4272	0.0011
11	3	8	10	3	7	4165.0434	4165.0429	0.0005
11	2	9	10	2	8	4176.3618	4176.3610	0.0008
18	4	14	18	3	15	4194.3123	4194.3120	0.0003
11	1	10	10	1	9	4201.5383	4201.5385	-0.0002
15	1	14	14	2	13	4311.1868	4311.1881	-0.0013
12	1	12	11	1	11	4488.2483	4488.2498	-0.0015
12	0	12	11	0	11	4519.5128	4519.5125	0.0003
11	1	11	10	0	10	4530.4296	4530.4296	0.0000
4	3	2	3	2	1	4534.3327	4534.3324	0.0003
4	3	1	3	2	2	4534.7255	4534.7260	-0.0005
12	2	11	11	2	10	4537.2909	4537.2908	0.0001
13	0	13	12	1	12	4539.1791	4539.1792	-0.0001
12	10	2	11	10	1	4540.9921	4540.9926	-0.0005
12	10	3	11	10	2	4540.9921	4540.9926	-0.0005
12	9	3	11	9	2	4541.0852	4541.0843	0.0009
12	9	4	11	9	3	4541.0852	4541.0843	0.0009
12	8	5	11	8	4	4541.1939	4541.1940	-0.0001
12	8	4	11	8	3	4541.1939	4541.1940	-0.0001
12	7	6	11	7	5	4541.3371	4541.3353	0.0018
12	7	5	11	7	4	4541.3371	4541.3353	0.0018
12	6	7	11	6	6	4541.5368	4541.5351	0.0017
12	6	6	11	6	5	4541.5368	4541.5351	0.0017
12	5	7	11	5	6	4541.8516	4541.8515	0.0001
12	5	8	11	5	7	4541.8516	4541.8514	0.0002

12	4	9	11	4	8	4542.4223	4542.4242	-0.0019
12	4	8	11	4	7	4542.4395	4542.4400	-0.0005
12	3	10	11	3	9	4543.2899	4543.2891	0.0008
12	3	9	11	3	8	4544.2433	4544.2448	-0.0015
12	2	10	11	2	9	4558.5833	4558.5832	0.0001
12	1	11	11	1	10	4582.4175	4582.4182	-0.0007
13	1	13	12	1	12	4861.3646	4861.3653	-0.0007
13	0	13	12	0	12	4892.5082	4892.5071	0.0011
5	3	3	4	2	2	4912.2823	4912.2823	0.0000
5	3	2	4	2	3	4913.4651	4913.4662	-0.0011
13	2	12	12	2	11	4914.6583	4914.6581	0.0002
13	10	4	12	10	3	4919.4122	4919.4118	0.0004
13	10	3	12	10	2	4919.4122	4919.4118	0.0004
13	9	4	12	9	3	4919.5218	4919.5213	0.0005
13	9	5	12	9	4	4919.5218	4919.5213	0.0005
13	8	5	12	8	4	4919.6516	4919.6544	-0.0028
13	8	6	12	8	5	4919.6516	4919.6544	-0.0028
13	7	6	12	7	5	4919.8269	4919.8285	-0.0016
13	7	7	12	7	6	4919.8269	4919.8285	-0.0016
13	6	7	12	6	6	4920.0768	4920.0776	-0.0008
13	6	8	12	6	7	4920.0768	4920.0776	-0.0008
13	5	9	12	5	8	4920.4757	4920.4756	0.0001
13	5	8	12	5	7	4920.4757	4920.4759	-0.0002
13	4	10	12	4	9	4921.1942	4921.1970	-0.0028
13	4	9	12	4	8	4921.2258	4921.2251	0.0007
13	3	11	12	3	10	4922.1952	4922.1955	-0.0003
13	3	10	12	3	9	4923.6254	4923.6250	0.0004
13	2	11	12	2	10	4941.3067	4941.3080	-0.0013
14	0	14	13	1	13	4942.6639	4942.6630	0.0009
13	1	12	12	1	11	4962.9843	4962.9846	-0.0003
8	2	6	7	1	7	4966.9739	4966.9738	0.0001
9	2	8	8	1	7	5075.6966	5075.6960	0.0006
17	1	16	16	2	15	5180.3792	5180.3797	-0.0005
14	1	14	13	1	13	5234.2968	5234.2978	-0.0010
14	0	14	13	0	13	5264.8491	5264.8491	0.0000
6	3	4	5	2	3	5289.7146	5289.7144	0.0002
14	2	13	13	2	12	5291.8502	5291.8497	0.0005
6	3	3	5	2	4	5292.4852	5292.4842	0.0010
14	11	4	13	11	3	5297.7189	5297.7198	-0.0009
14	11	3	13	11	2	5297.7189	5297.7198	-0.0009

14	10	4	13	10	3	5297.8326	5297.8317	0.0009
14	10	5	13	10	4	5297.8326	5297.8317	0.0009
14	9	6	13	9	5	5297.9612	5297.9615	-0.0003
14	9	5	13	9	4	5297.9612	5297.9615	-0.0003
14	8	7	13	8	6	5298.1213	5298.1213	0.0000
14	8	6	13	8	5	5298.1217	5298.1213	0.0004
14	7	8	13	7	7	5298.3358	5298.3332	0.0026
14	7	7	13	7	6	5298.3358	5298.3332	0.0026
14	6	9	13	6	8	5298.6406	5298.6396	0.0010
14	6	8	13	6	7	5298.6406	5298.6396	0.0010
14	5	10	13	5	9	5299.1329	5299.1326	0.0003
14	5	9	13	5	8	5299.1329	5299.1332	-0.0003
14	3	12	13	3	11	5301.1396	5301.1395	0.0001
14	3	11	13	3	10	5303.2111	5303.2113	-0.0002
14	2	12	13	2	11	5324.4948	5324.4935	0.0013
14	1	13	13	1	12	5343.2002	5343.1989	0.0013
15	0	15	14	1	14	5344.9507	5344.9497	0.0010
10	2	9	9	1	8	5418.7947	5418.7941	0.0006
15	1	15	14	1	14	5607.0427	5607.0449	-0.0022
18	1	17	17	2	16	5617.7958	5617.7977	-0.0019
15	0	15	14	0	14	5636.5851	5636.5844	0.0007
7	3	5	6	2	4	5666.3574	5666.3572	0.0002
15	2	14	14	2	13	5668.8542	5668.8533	0.0009
7	3	4	6	2	5	5671.9118	5671.9115	0.0003
15	11	4	14	11	3	5676.1212	5676.1226	-0.0014
15	11	5	14	11	4	5676.1212	5676.1226	-0.0014
15	10	5	14	10	4	5676.2537	5676.2524	0.0013
15	10	6	14	10	5	5676.2537	5676.2524	0.0013
15	9	7	14	9	6	5676.4055	5676.4050	0.0005
15	9	6	14	9	5	5676.4055	5676.4050	0.0005
15	8	8	14	8	7	5676.5964	5676.5954	0.0010
15	8	7	14	8	6	5676.5964	5676.5954	0.0010
15	7	9	14	7	8	5676.8518	5676.8505	0.0013
15	7	8	14	7	7	5676.8518	5676.8505	0.0013
15	6	9	14	6	8	5677.2238	5677.2226	0.0012
15	6	10	14	6	9	5677.2238	5677.2226	0.0012
15	5	11	14	5	10	5677.8266	5677.8250	0.0016
15	5	10	14	5	9	5677.8266	5677.8260	0.0006
15	4	12	14	4	11	5678.9114	5678.9107	0.0007
15	4	11	14	4	10	5678.9889	5678.9886	0.0003

15	3	13	14	3	12	5680.1116	5680.1120	-0.0004
15	3	12	14	3	11	5683.0342	5683.0340	0.0002
15	2	13	14	2	12	5708.0765	5708.0774	-0.0009
15	1	14	14	1	13	5723.0186	5723.0192	-0.0006
16	0	16	15	1	15	5745.6823	5745.6804	0.0019
11	2	10	10	1	9	5758.1735	5758.1728	0.0007
16	1	16	15	1	15	5979.6066	5979.6065	0.0001
16	0	16	15	0	15	6007.7756	6007.7756	0.0000
8	3	6	7	2	5	6041.8851	6041.8853	-0.0002
16	2	15	15	2	14	6045.6595	6045.6569	0.0026
8	3	5	7	2	6	6051.9077	6051.9072	0.0005
16	12	4	15	12	3	6054.3914	6054.3917	-0.0003
16	12	5	15	12	4	6054.3914	6054.3917	-0.0003
16	11	6	15	11	5	6054.5249	6054.5241	0.0008
16	11	5	15	11	4	6054.5249	6054.5241	0.0008
16	10	7	15	10	6	6054.6761	6054.6741	0.0020
16	10	6	15	10	5	6054.6761	6054.6741	0.0020
16	9	7	15	9	6	6054.8503	6054.8523	-0.0020
16	9	8	15	9	7	6054.8503	6054.8523	-0.0020
16	8	8	15	8	7	6055.0752	6055.0771	-0.0019
16	8	9	15	8	8	6055.0752	6055.0771	-0.0019
16	7	9	15	7	8	6055.3808	6055.3812	-0.0004
16	7	10	15	7	9	6055.3808	6055.3812	-0.0004
16	6	11	15	6	10	6055.8284	6055.8282	0.0002
16	6	10	15	6	9	6055.8284	6055.8282	0.0002
16	5	12	15	5	11	6056.5559	6056.5551	0.0008
16	5	11	15	5	10	6056.5559	6056.5571	-0.0012
16	4	13	15	4	12	6057.8575	6057.8573	0.0002
16	4	12	15	4	11	6057.9804	6057.9805	-0.0001
16	3	14	15	3	13	6059.1005	6059.1023	-0.0018
16	3	13	15	3	12	6063.1254	6063.1257	-0.0003
16	2	14	15	2	13	6091.9803	6091.9801	0.0002
12	2	11	11	1	10	6093.9251	6093.9251	0.0000
16	1	15	15	1	14	6102.4043	6102.4017	0.0026
17	0	17	16	1	16	6144.5714	6144.5716	-0.0002
17	1	17	16	1	16	6351.9853	6351.9841	0.0012
17	0	17	16	0	16	6378.4964	6378.4977	-0.0013
9	3	7	8	2	6	6415.9225	6415.9230	-0.0005
17	2	16	16	2	15	6422.2503	6422.2492	0.0011
13	2	12	12	1	11	6426.1645	6426.1650	-0.0005

9	3	6	8	2	7	6432.6605	6432.6602	0.0003
17	11	6	16	11	5	6432.9254	6432.9244	0.0010
17	11	7	16	11	6	6432.9254	6432.9244	0.0010
17	10	7	16	10	6	6433.0945	6433.0966	-0.0021
17	10	8	16	10	7	6433.0945	6433.0966	-0.0021
17	9	8	16	9	7	6433.3052	6433.3035	0.0017
17	9	9	16	9	8	6433.3052	6433.3035	0.0017
17	8	10	16	8	9	6433.5652	6433.5669	-0.0017
17	8	9	16	8	8	6433.5652	6433.5669	-0.0017
17	7	11	16	7	10	6433.9266	6433.9263	0.0003
17	7	10	16	7	9	6433.9266	6433.9263	0.0003
17	6	11	16	6	10	6434.4578	6434.4578	0.0000
17	6	12	16	6	11	6434.4578	6434.4577	0.0001
17	5	13	16	5	12	6435.3255	6435.3257	-0.0002
17	5	12	16	5	11	6435.3287	6435.3290	-0.0003
17	4	14	16	4	13	6436.8678	6436.8667	0.0011
17	4	13	16	4	12	6437.0558	6437.0558	0.0000
17	3	15	16	3	14	6438.0972	6438.0975	-0.0003
17	3	14	16	3	13	6443.5203	6443.5212	-0.0009
17	2	15	16	2	14	6476.1114	6476.1089	0.0025
17	1	16	16	1	15	6481.3009	6481.3001	0.0008
18	0	18	17	1	17	6541.4205	6541.4196	0.0009
17	1	17	16	0	16	6585.9079	6585.9103	-0.0024
18	1	18	17	1	17	6724.1827	6724.1809	0.0018
18	0	18	17	0	17	6748.8327	6748.8321	0.0006
14	2	13	13	1	12	6755.0291	6755.0301	-0.0010
18	2	17	17	2	16	6798.6196	6798.6195	0.0001
18	7	12	17	7	11	6812.4884	6812.4866	0.0018
18	7	11	17	7	10	6812.4884	6812.4866	0.0018
18	6	12	17	6	11	6813.1108	6813.1130	-0.0022
18	6	13	17	6	12	6813.1108	6813.1129	-0.0021
18	5	14	17	5	13	6814.1376	6814.1390	-0.0014
18	5	13	17	5	12	6814.1438	6814.1446	-0.0008
18	4	15	17	4	14	6815.9400	6815.9404	-0.0004
18	4	14	17	4	13	6816.2223	6816.2233	-0.0010
18	3	16	17	3	15	6817.0824	6817.0832	-0.0008
18	3	15	17	3	14	6824.2548	6824.2563	-0.0015
18	1	17	17	1	16	6859.6707	6859.6673	0.0034
18	2	16	17	2	15	6860.3624	6860.3637	-0.0013
19	1	19	18	1	18	7096.1995	7096.2017	-0.0022

19	0	19	18	0	18	7118.8596	7118.8610	-0.0014
13	2	11	12	1	12	7144.7546	7144.7527	0.0019
11	3	9	10	2	8	7157.8158	7157.8158	0.0000
19	2	18	18	2	17	7174.7579	7174.7576	0.0003
19	6	13	18	6	12	7191.7986	7191.7953	0.0033
19	6	14	18	6	13	7191.7986	7191.7952	0.0034
19	5	15	18	5	14	7192.9950	7192.9976	-0.0026
19	5	14	18	5	13	7193.0046	7193.0069	-0.0023
19	3	16	18	3	15	7205.3662	7205.3671	-0.0009
19	1	18	18	1	17	7237.4539	7237.4553	-0.0014
19	1	19	18	0	18	7278.9622	7278.9631	-0.0009
20	1	20	19	1	19	7468.0533	7468.0525	0.0008
20	0	20	19	0	19	7488.6635	7488.6624	0.0011

Table S18. Rotational transition frequencies of the **PFP***G*+*g*+**PFP***Tg*- homodimer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
6	1	6	5	1	5	2078.0416	2078.0412	0.0004
6	0	6	5	0	5	2106.8438	2106.8487	-0.0049
6	2	5	5	2	4	2111.2251	2111.2323	-0.0072
6	3	4	5	3	3	2112.6405	2112.6450	-0.0045
6	3	3	5	3	2	2112.7068	2112.7124	-0.0056
6	2	4	5	2	3	2116.2631	2116.2727	-0.0096
6	1	5	5	1	4	2143.4046	2143.4149	-0.0103
11	2	10	11	1	11	2216.6591	2216.6524	0.0067
5	1	5	4	0	4	2295.6553	2295.6597	-0.0044
7	1	7	6	1	6	2423.8601	2423.8576	0.0025
7	0	7	6	0	6	2455.8326	2455.8328	-0.0002
7	2	6	6	2	5	2462.7261	2462.7259	0.0002
7	3	5	6	3	4	2464.9905	2464.9787	0.0118
7	3	4	6	3	3	2465.1392	2465.1301	0.0091
7	2	5	6	2	4	2470.7578	2470.7519	0.0059
7	1	6	6	1	5	2500.0613	2500.0513	0.0100
6	1	6	5	0	5	2616.6717	2616.6751	-0.0034
8	1	8	7	1	7	2769.4501	2769.4485	0.0016
8	0	8	7	0	7	2803.8747	2803.8702	0.0045
8	2	7	7	2	6	2814.0500	2814.0452	0.0048

8	3	6	7	3	5	2817.4054	2817.4006	0.0048
8	3	5	7	3	4	2817.7092	2817.7030	0.0062
8	2	6	7	2	5	2826.0043	2825.9973	0.0070
8	1	7	7	1	6	2856.3896	2856.3940	-0.0044
9	1	9	8	1	8	3114.7879	3114.7929	-0.0050
9	0	9	8	0	8	3150.8764	3150.8788	-0.0024
9	2	8	8	2	7	3165.1749	3165.1658	0.0091
9	5	4	8	5	3	3168.7001	3168.7064	-0.0063
9	5	5	8	5	4	3168.7065	3168.7064	0.0001
9	3	7	8	3	6	3169.9139	3169.9122	0.0017
9	3	6	8	3	5	3170.4667	3170.4657	0.0010
9	2	7	8	2	6	3182.0628	3182.0649	-0.0021
9	1	8	8	1	7	3212.3890	3212.3886	0.0004
4	2	3	3	1	2	3224.2138	3224.2211	-0.0073
8	1	8	7	0	7	3247.2969	3247.2998	-0.0029
18	3	16	18	2	17	3254.1338	3254.1332	0.0006
17	3	14	17	2	16	3266.8303	3266.8314	-0.0011
4	2	3	3	1	3	3289.6618	3289.6664	-0.0046
4	2	2	3	1	3	3291.8323	3291.8373	-0.0050
14	1	13	13	2	11	3424.2687	3424.2714	-0.0027
20	3	17	20	2	19	3445.5515	3445.5509	0.0006
10	1	10	9	1	9	3459.8742	3459.8737	0.0005
10	0	10	9	0	9	3496.8001	3496.8103	-0.0102
10	2	9	9	2	8	3516.0665	3516.0635	0.0030
10	3	8	9	3	7	3522.5166	3522.5108	0.0058
10	3	7	9	3	6	3523.4656	3523.4574	0.0082
10	2	8	9	2	7	3538.9756	3538.9762	-0.0006
5	2	4	4	1	3	3554.3613	3554.3534	0.0079
5	2	3	4	1	3	3559.4101	3559.4130	-0.0029
10	1	9	9	1	8	3567.9723	3567.9759	-0.0036
5	2	4	4	1	4	3663.4155	3663.4213	-0.0058
5	2	3	4	1	4	3668.4752	3668.4809	-0.0057
11	1	11	10	1	10	3804.6754	3804.6782	-0.0028
11	0	11	10	0	10	3841.6534	3841.6572	-0.0038
11	2	10	10	2	9	3866.7253	3866.7144	0.0109
10	1	10	9	0	9	3867.2088	3867.2173	-0.0085
11	3	9	10	3	8	3875.1927	3875.1896	0.0031
11	3	8	10	3	7	3876.7241	3876.7231	0.0010
6	2	5	5	1	4	3879.0626	3879.0511	0.0115
11	2	9	10	2	8	3896.7065	3896.7114	-0.0049

11	1	10	10	1	9	3923.0801	3923.0913	-0.0112
12	1	12	11	1	11	4149.1904	4149.1982	-0.0078
11	1	11	10	0	10	4175.0882	4175.0852	0.0030
12	0	12	11	0	11	4185.4546	4185.4569	-0.0023
12	2	11	11	2	10	4217.0984	4217.0955	0.0029
12	3	10	11	3	9	4227.9489	4227.9373	0.0116
12	3	9	11	3	8	4230.3227	4230.3129	0.0098
12	2	10	11	2	9	4255.2008	4255.2052	-0.0044
12	1	11	11	1	10	4277.6643	4277.6647	-0.0004
7	2	6	6	1	6	4427.3174	4427.3143	0.0031
7	2	5	6	1	6	4445.4369	4445.4404	-0.0035
12	1	12	11	0	11	4482.6303	4482.6262	0.0041
13	1	13	12	1	12	4493.4246	4493.4296	-0.0050
13	0	13	12	0	12	4528.2825	4528.2898	-0.0073
13	2	12	12	2	11	4567.1868	4567.1843	0.0025
13	3	11	12	3	10	4580.7409	4580.7384	0.0025
13	3	10	12	3	9	4584.2883	4584.2829	0.0054
13	2	11	12	2	10	4614.3418	4614.3484	-0.0066
13	1	12	12	1	11	4631.6214	4631.6202	0.0012
13	1	13	12	0	12	4790.6004	4790.5989	0.0015
8	2	7	7	1	7	4817.5038	4817.5019	0.0019
14	1	14	13	1	13	4837.3673	4837.3727	-0.0054
8	2	6	7	1	7	4847.5759	4847.5801	-0.0042
14	0	14	13	0	13	4870.2738	4870.2729	0.0009
14	2	13	13	2	12	4916.9612	4916.9594	0.0018
14	7	8	13	7	7	4929.0915	4929.0917	-0.0002
14	7	7	13	7	6	4929.0915	4929.0917	-0.0002
14	3	12	13	3	11	4933.5745	4933.5732	0.0013
14	3	11	13	3	10	4938.6952	4938.6940	0.0012
14	2	12	13	2	11	4973.9917	4973.9934	-0.0017
14	1	13	13	1	12	4984.8729	4984.8769	-0.0040
14	1	14	13	0	13	5099.6831	5099.6817	0.0014
15	1	15	14	1	14	5181.0278	5181.0315	-0.0037
9	2	8	8	1	8	5213.2255	5213.2192	0.0063
9	2	7	8	1	8	5260.1966	5260.1965	0.0001
15	2	14	14	2	13	5266.3924	5266.4004	-0.0080
15	3	13	14	3	12	5286.4192	5286.4179	0.0013
15	3	12	14	3	11	5293.6238	5293.6114	0.0124
15	1	14	14	1	13	5337.3434	5337.3495	-0.0061
15	1	15	14	0	14	5410.4503	5410.4403	0.0100

16	1	16	15	1	15	5524.4023	5524.4137	-0.0114
16	0	16	15	0	15	5552.2682	5552.2684	-0.0002
16	2	15	15	2	14	5615.4871	5615.4885	-0.0014
16	6	11	15	6	10	5634.3852	5634.3829	0.0023
16	6	10	15	6	9	5634.3852	5634.3830	0.0022
16	3	14	15	3	13	5639.2451	5639.2456	-0.0005
16	3	13	15	3	12	5649.1019	5649.1021	-0.0002
10	2	8	9	1	9	5684.3788	5684.3798	-0.0010
16	1	15	15	1	14	5688.9479	5688.9508	-0.0029
17	0	17	16	0	16	5892.5752	5892.5838	-0.0086
17	2	16	16	2	15	5964.2032	5964.2065	-0.0033
17	4	14	16	4	13	5991.1179	5991.1135	0.0044
17	4	13	16	4	12	5991.7468	5991.7460	0.0008
17	3	15	16	3	14	5992.0254	5992.0261	-0.0007
17	3	14	16	3	13	6005.2272	6005.2326	-0.0054
18	4	15	17	4	14	6344.3496	6344.3430	0.0066
18	3	16	17	3	15	6344.7349	6344.7270	0.0079
18	4	14	17	4	13	6345.2928	6345.2874	0.0054
18	1	18	17	0	17	6356.3859	6356.3776	0.0083
19	9	10	18	9	9	6689.1961	6689.2021	-0.0060
19	9	11	18	9	10	6689.1961	6689.2021	-0.0060
19	8	12	18	8	11	6689.7857	6689.7875	-0.0018
19	8	11	18	8	10	6689.7857	6689.7875	-0.0018
19	6	13	18	6	12	6691.9395	6691.9370	0.0025
19	6	14	18	6	13	6691.9395	6691.9363	0.0032
19	3	17	18	3	16	6697.3056	6697.3141	-0.0085
19	4	16	18	4	15	6697.6859	6697.6806	0.0053
19	4	15	18	4	14	6699.062	6699.0584	0.0036
6	1	6	5	1	5	2078.0416	2078.0412	0.0004
6	0	6	5	0	5	2106.8438	2106.8487	-0.0049
6	2	5	5	2	4	2111.2251	2111.2323	-0.0072
6	3	4	5	3	3	2112.6405	2112.6450	-0.0045
6	3	3	5	3	2	2112.7068	2112.7124	-0.0056
6	2	4	5	2	3	2116.2631	2116.2727	-0.0096
6	1	5	5	1	4	2143.4046	2143.4149	-0.0103
11	2	10	11	1	11	2216.6591	2216.6524	0.0067
5	1	5	4	0	4	2295.6553	2295.6597	-0.0044
7	1	7	6	1	6	2423.8601	2423.8576	0.0025
7	0	7	6	0	6	2455.8326	2455.8328	-0.0002
7	2	6	6	2	5	2462.7261	2462.7259	0.0002

7	3	5	6	3	4	2464.9905	2464.9787	0.0118
7	3	4	6	3	3	2465.1392	2465.1301	0.0091
7	2	5	6	2	4	2470.7578	2470.7519	0.0059
7	1	6	6	1	5	2500.0613	2500.0513	0.0100
6	1	6	5	0	5	2616.6717	2616.6751	-0.0034
8	1	8	7	1	7	2769.4501	2769.4485	0.0016
8	0	8	7	0	7	2803.8747	2803.8702	0.0045
8	2	7	7	2	6	2814.0500	2814.0452	0.0048
8	3	6	7	3	5	2817.4054	2817.4006	0.0048
8	3	5	7	3	4	2817.7092	2817.7030	0.0062
8	2	6	7	2	5	2826.0043	2825.9973	0.0070
8	1	7	7	1	6	2856.3896	2856.3940	-0.0044
9	1	9	8	1	8	3114.7879	3114.7929	-0.005
9	0	9	8	0	8	3150.8764	3150.8788	-0.0024
9	2	8	8	2	7	3165.1749	3165.1658	0.0091
9	5	4	8	5	3	3168.7001	3168.7064	-0.0063
9	5	5	8	5	4	3168.7065	3168.7064	0.0001
9	3	7	8	3	6	3169.9139	3169.9122	0.0017
9	3	6	8	3	5	3170.4667	3170.4657	0.0010
9	2	7	8	2	6	3182.0628	3182.0649	-0.0021
9	1	8	8	1	7	3212.3890	3212.3886	0.0004
4	2	3	3	1	2	3224.2138	3224.2211	-0.0073
8	1	8	7	0	7	3247.2969	3247.2998	-0.0029
18	3	16	18	2	17	3254.1338	3254.1332	0.0006
17	3	14	17	2	16	3266.8303	3266.8314	-0.0011
4	2	3	3	1	3	3289.6618	3289.6664	-0.0046
4	2	2	3	1	3	3291.8323	3291.8373	-0.0050
14	1	13	13	2	11	3424.2687	3424.2714	-0.0027
20	3	17	20	2	19	3445.5515	3445.5509	0.0006
10	1	10	9	1	9	3459.8742	3459.8737	0.0005
10	0	10	9	0	9	3496.8001	3496.8103	-0.0102
10	2	9	9	2	8	3516.0665	3516.0635	0.0030
10	3	8	9	3	7	3522.5166	3522.5108	0.0058
10	3	7	9	3	6	3523.4656	3523.4574	0.0082
10	2	8	9	2	7	3538.9756	3538.9762	-0.0006
5	2	4	4	1	3	3554.3613	3554.3534	0.0079
5	2	3	4	1	3	3559.4101	3559.4130	-0.0029
10	1	9	9	1	8	3567.9723	3567.9759	-0.0036
5	2	4	4	1	4	3663.4155	3663.4213	-0.0058
5	2	3	4	1	4	3668.4752	3668.4809	-0.0057

11	1	11	10	1	10	3804.6754	3804.6782	-0.0028
11	0	11	10	0	10	3841.6534	3841.6572	-0.0038
11	2	10	10	2	9	3866.7253	3866.7144	0.0109
10	1	10	9	0	9	3867.2088	3867.2173	-0.0085
11	3	9	10	3	8	3875.1927	3875.1896	0.0031
11	3	8	10	3	7	3876.7241	3876.7231	0.0010
6	2	5	5	1	4	3879.0626	3879.0511	0.0115
11	2	9	10	2	8	3896.7065	3896.7114	-0.0049
11	1	10	10	1	9	3923.0801	3923.0913	-0.0112
12	1	12	11	1	11	4149.1904	4149.1982	-0.0078
11	1	11	10	0	10	4175.0882	4175.0852	0.0030
12	0	12	11	0	11	4185.4546	4185.4569	-0.0023
12	2	11	11	2	10	4217.0984	4217.0955	0.0029
12	3	10	11	3	9	4227.9489	4227.9373	0.0116
12	3	9	11	3	8	4230.3227	4230.3129	0.0098
12	2	10	11	2	9	4255.2008	4255.2052	-0.0044
12	1	11	11	1	10	4277.6643	4277.6647	-0.0004
7	2	6	6	1	6	4427.3174	4427.3143	0.0031
7	2	5	6	1	6	4445.4369	4445.4404	-0.0035
12	1	12	11	0	11	4482.6303	4482.6262	0.0041
13	1	13	12	1	12	4493.4246	4493.4296	-0.0050
13	0	13	12	0	12	4528.2825	4528.2898	-0.0073
13	2	12	12	2	11	4567.1868	4567.1843	0.0025
13	3	11	12	3	10	4580.7409	4580.7384	0.0025
13	3	10	12	3	9	4584.2883	4584.2829	0.0054
13	2	11	12	2	10	4614.3418	4614.3484	-0.0066
13	1	12	12	1	11	4631.6214	4631.6202	0.0012
13	1	13	12	0	12	4790.6004	4790.5989	0.0015
8	2	7	7	1	7	4817.5038	4817.5019	0.0019
14	1	14	13	1	13	4837.3673	4837.3727	-0.0054
8	2	6	7	1	7	4847.5759	4847.5801	-0.0042
14	0	14	13	0	13	4870.2738	4870.2729	0.0009
14	2	13	13	2	12	4916.9612	4916.9594	0.0018
14	7	8	13	7	7	4929.0915	4929.0917	-0.0002
14	7	7	13	7	6	4929.0915	4929.0917	-0.0002
14	3	12	13	3	11	4933.5745	4933.5732	0.0013
14	3	11	13	3	10	4938.6952	4938.6940	0.0012
14	2	12	13	2	11	4973.9917	4973.9934	-0.0017
14	1	13	13	1	12	4984.8729	4984.8769	-0.0040
14	1	14	13	0	13	5099.6831	5099.6817	0.0014

15	1	15	14	1	14	5181.0278	5181.0315	-0.0037
9	2	8	8	1	8	5213.2255	5213.2192	0.0063
9	2	7	8	1	8	5260.1966	5260.1965	0.0001
15	2	14	14	2	13	5266.3924	5266.4004	-0.0080
15	3	13	14	3	12	5286.4192	5286.4179	0.0013
15	3	12	14	3	11	5293.6238	5293.6114	0.0124
15	1	14	14	1	13	5337.3434	5337.3495	-0.0061
15	1	15	14	0	14	5410.4503	5410.4403	0.0100
16	1	16	15	1	15	5524.4023	5524.4137	-0.0114
16	0	16	15	0	15	5552.2682	5552.2684	-0.0002
16	2	15	15	2	14	5615.4871	5615.4885	-0.0014
16	6	11	15	6	10	5634.3852	5634.3829	0.0023
16	6	10	15	6	9	5634.3852	5634.3830	0.0022
16	3	14	15	3	13	5639.2451	5639.2456	-0.0005
16	3	13	15	3	12	5649.1019	5649.1021	-0.0002
10	2	8	9	1	9	5684.3788	5684.3798	-0.0010
16	1	15	15	1	14	5688.9479	5688.9508	-0.0029
17	0	17	16	0	16	5892.5752	5892.5838	-0.0086
17	2	16	16	2	15	5964.2032	5964.2065	-0.0033
17	4	14	16	4	13	5991.1179	5991.1135	0.0044
17	4	13	16	4	12	5991.7468	5991.7460	0.0008
17	3	15	16	3	14	5992.0254	5992.0261	-0.0007
17	3	14	16	3	13	6005.2272	6005.2326	-0.0054
18	4	15	17	4	14	6344.3496	6344.3430	0.0066
18	3	16	17	3	15	6344.7349	6344.7270	0.0079
18	4	14	17	4	13	6345.2928	6345.2874	0.0054
18	1	18	17	0	17	6356.3859	6356.3776	0.0083
19	9	10	18	9	9	6689.1961	6689.2021	-0.0060
19	9	11	18	9	10	6689.1961	6689.2021	-0.0060
19	8	12	18	8	11	6689.7857	6689.7875	-0.0018
19	8	11	18	8	10	6689.7857	6689.7875	-0.0018
19	6	13	18	6	12	6691.9395	6691.9370	0.0025
19	6	14	18	6	13	6691.9395	6691.9363	0.0032
19	3	17	18	3	16	6697.3056	6697.3141	-0.0085
19	4	16	18	4	15	6697.6859	6697.6806	0.0053
19	4	15	18	4	14	6699.0620	6699.0584	0.0036

Table S19. Rotational transition frequencies of the **PFP***Tg*+**PFP***Tg*+ homodimer.

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz

5	2	4	4	2	3	1822.8436	1822.8441	-0.0005
5	4	1	4	4	0	1824.1194	1824.1191	0.0003
5	4	2	4	4	1	1824.1194	1824.1188	0.0006
5	3	3	4	3	2	1824.4157	1824.4158	-0.0001
5	3	2	4	3	1	1824.4879	1824.4866	0.0013
5	2	3	4	2	2	1828.4627	1828.4626	0.0001
6	1	6	5	1	5	2141.6195	2141.6198	-0.0003
6	0	6	5	0	5	2178.3675	2178.3682	-0.0007
6	2	5	5	2	4	2186.8803	2186.8807	-0.0004
6	5	2	5	5	1	2188.9004	2188.8983	0.0021
6	5	1	5	5	0	2188.9004	2188.8983	0.0021
6	4	3	5	4	2	2189.1351	2189.1346	0.0005
6	4	2	5	4	1	2189.1351	2189.1358	-0.0007
6	3	4	5	3	3	2189.6225	2189.6216	0.0009
6	3	3	5	3	2	2189.8112	2189.8101	0.0011
6	2	4	5	2	3	2196.6552	2196.6537	0.0015
6	1	5	5	1	4	2230.1466	2230.1482	-0.0016
7	1	7	6	1	6	2497.5667	2497.5675	-0.0008
7	0	7	6	0	6	2537.3250	2537.3231	0.0019
7	2	6	6	2	5	2550.6263	2550.6278	-0.0015
7	6	1	6	6	0	2553.6851	2553.6863	-0.0012
7	6	2	6	6	1	2553.6851	2553.6863	-0.0012
7	5	3	6	5	2	2553.8733	2553.8729	0.0004
7	5	2	6	5	1	2553.8733	2553.8729	0.0004
7	4	4	6	4	3	2554.255	2554.2545	0.0005
7	4	3	6	4	2	2554.2585	2554.2585	0.0000
7	3	5	6	3	4	2554.9762	2554.9738	0.0024
7	3	4	6	3	3	2555.3958	2555.3974	-0.0016
7	2	5	6	2	4	2566.1109	2566.1129	-0.0020
7	1	6	6	1	5	2600.6397	2600.6418	-0.0021
8	1	8	7	1	7	2853.1032	2853.1033	-0.0001
8	0	8	7	0	7	2894.5688	2894.5691	-0.0003
8	2	7	7	2	6	2914.0370	2914.0381	-0.0011
8	7	2	7	7	1	2918.4797	2918.4803	-0.0006
8	7	1	7	7	0	2918.4797	2918.4803	-0.0006
8	6	3	7	6	2	2918.6342	2918.6332	0.0010
8	6	2	7	6	1	2918.6342	2918.6332	0.0010
8	5	4	7	5	3	2918.9207	2918.9204	0.0003
8	5	3	7	5	2	2918.9207	2918.9205	0.0002
8	4	5	7	4	4	2919.4943	2919.4949	-0.0006

8	4	4	7	4	3	2919.5063	2919.5059	0.0004
8	3	6	7	3	5	2920.4719	2920.4735	-0.0016
8	3	5	7	3	4	2921.3175	2921.3186	-0.0011
15	2	13	14	3	11	2927.4618	2927.4623	-0.0005
9	3	6	9	2	8	2930.1817	2930.1821	-0.0004
8	2	6	7	2	5	2936.9284	2936.9303	-0.0019
8	1	7	7	1	6	2970.5357	2970.5344	0.0013
16	1	16	15	2	14	3021.1349	3021.1345	0.0004
13	3	10	13	2	12	3026.7665	3026.7665	0.0000
4	2	2	3	1	2	3159.8280	3159.8278	0.0002
9	1	9	8	1	8	3208.1987	3208.1982	0.0006
4	2	3	3	1	3	3244.3218	3244.3212	0.0006
9	0	9	8	0	8	3250.0499	3250.0510	-0.0011
9	2	8	8	2	7	3277.0653	3277.0649	0.0004
9	8	1	8	8	0	3283.2802	3283.2796	0.0006
9	8	2	8	8	1	3283.2802	3283.2796	0.0006
9	7	2	8	7	1	3283.4077	3283.4062	0.0015
9	7	3	8	7	2	3283.4077	3283.4062	0.0015
9	6	4	8	6	3	3283.6342	3283.6339	0.0003
9	6	3	8	6	2	3283.6342	3283.6339	0.0003
9	5	5	8	5	4	3284.0502	3284.0514	-0.0012
9	5	4	8	5	3	3284.0502	3284.0516	-0.0014
9	4	6	8	4	5	3284.8709	3284.8716	-0.0007
9	4	5	8	4	4	3284.8979	3284.8980	-0.0001
9	3	7	8	3	6	3286.1118	3286.1117	0.0001
9	3	6	8	3	5	3287.6562	3287.6558	0.0004
9	2	7	8	2	6	3309.1090	3309.1091	-0.0001
9	1	8	8	1	7	3339.7042	3339.7058	-0.0016
7	1	6	6	0	6	3351.5649	3351.5647	0.0002
5	2	3	4	1	3	3500.5076	3500.5096	-0.0020
10	1	10	9	1	9	3562.8352	3562.8333	0.0019
10	0	10	9	0	9	3603.8130	3603.8148	-0.0018
5	2	4	4	1	4	3638.5136	3638.5136	0.0000
10	2	9	9	2	8	3639.6630	3639.6631	-0.0001
10	8	2	9	8	1	3648.1890	3648.1879	0.0011
10	8	3	9	8	2	3648.1890	3648.1879	0.0011
10	7	4	9	7	3	3648.3757	3648.3729	0.0028
10	7	3	9	7	2	3648.3757	3648.3729	0.0028
10	6	5	9	6	4	3648.6980	3648.6951	0.0029
10	6	4	9	6	3	3648.6980	3648.6952	0.0028

10	5	5	9	5	4	3649.2760	3649.2768	-0.0008
10	5	6	9	5	5	3649.2760	3649.2762	-0.0002
10	4	7	9	4	6	3650.4003	3650.3990	0.0013
10	4	6	9	4	5	3650.4583	3650.4560	0.0023
10	3	8	9	3	7	3651.8706	3651.8696	0.0010
10	3	7	9	3	6	3654.5042	3654.5038	0.0004
10	2	8	9	2	7	3682.5520	3682.5497	0.0023
10	1	9	9	1	8	3708.0238	3708.0229	0.0009
6	2	4	5	1	4	3838.0031	3838.0014	0.0016
11	1	11	10	1	10	3917.0002	3917.0003	-0.0001
11	0	11	10	0	10	3956.0112	3956.0086	0.0026
3	3	0	2	2	0	3995.9802	3995.9789	0.0013
3	3	1	2	2	1	3996.2577	3996.2581	-0.0004
11	2	10	10	2	9	4001.7870	4001.7890	-0.0020
11	9	3	10	9	2	4012.9763	4012.9768	-0.0005
11	9	2	10	9	1	4012.9763	4012.9768	-0.0005
11	8	4	10	8	3	4013.1284	4013.1276	0.0008
11	8	3	10	8	2	4013.1284	4013.1276	0.0008
11	7	4	10	7	3	4013.3843	4013.3850	-0.0007
11	7	5	10	7	4	4013.3843	4013.3850	-0.0007
11	6	6	10	6	5	4013.8249	4013.8237	0.0012
11	6	5	10	6	4	4013.8249	4013.8237	0.0012
11	5	6	10	5	5	4014.6054	4014.6067	-0.0013
11	5	7	10	5	6	4014.6054	4014.6052	0.0002
11	4	8	10	4	7	4016.0887	4016.0898	-0.0011
11	4	7	10	4	6	4016.2014	4016.2037	-0.0023
11	3	9	10	3	8	4017.7180	4017.7179	0.0001
11	3	8	10	3	7	4021.9712	4021.9706	0.0006
11	2	9	10	2	8	4057.0478	4057.0483	-0.0005
11	1	10	10	1	9	4075.3389	4075.3396	-0.0007
7	2	5	6	1	5	4173.9641	4173.9661	-0.0020
18	0	18	17	1	16	4183.4154	4183.4165	-0.0011
9	1	8	8	0	8	4229.9121	4229.9126	-0.0005
12	1	12	11	1	11	4270.7003	4270.7002	0.0001
12	0	12	11	0	11	4306.8637	4306.865	-0.0013
4	3	1	3	2	1	4360.1226	4360.1229	-0.0003
4	3	2	3	2	2	4361.5127	4361.5112	0.0015
12	2	11	11	2	10	4363.3990	4363.4010	-0.0020
12	10	2	11	10	1	4377.7723	4377.7722	0.0001
12	10	3	11	10	2	4377.7723	4377.7722	0.0001

12	9	4	11	9	3	4377.8925	4377.8934	-0.0009
12	9	3	11	9	2	4377.8925	4377.8934	-0.0009
12	8	4	11	8	3	4378.1018	4378.1017	0.0001
12	8	5	11	8	4	4378.1018	4378.1017	0.0001
12	7	6	11	7	5	4378.4461	4378.4469	-0.0008
12	7	5	11	7	4	4378.4461	4378.4469	-0.0008
12	6	7	11	6	6	4379.0253	4379.0262	-0.0009
12	6	6	11	6	5	4379.0253	4379.0262	-0.0009
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12	5	7	11	5	6	4380.0519	4380.0522	-0.0003
12	4	9	11	4	8	4381.9559	4381.9549	0.0010
12	4	8	11	4	7	4382.1669	4382.1677	-0.0008
12	3	10	11	3	9	4383.6180	4383.6179	0.0001
12	3	9	11	3	8	4390.1780	4390.1759	0.0021
16	1	15	15	2	13	4391.4757	4391.4765	-0.0008
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8	2	6	7	1	6	4510.2555	4510.2545	0.0010
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5	3	3	4	2	3	4727.3605	4727.3614	-0.0009
13	9	4	12	9	3	4742.8375	4742.8363	0.0012
13	9	5	12	9	4	4742.8375	4742.8363	0.0012
13	8	5	12	8	4	4743.1125	4743.1135	-0.0010
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13	7	7	12	7	6	4743.5626	4743.5634	-0.0008
13	6	8	12	6	7	4744.3120	4744.3095	0.0025
13	6	7	12	6	6	4744.3120	4744.3095	0.0025
13	5	9	12	5	8	4745.6168	4745.6172	-0.0004
13	5	8	12	5	7	4745.6243	4745.6244	-0.0001
13	4	10	12	4	9	4748.0020	4748.0017	0.0003
13	4	9	12	4	8	4748.3782	4748.3789	-0.0007
13	3	11	12	3	10	4749.5225	4749.5217	0.0008
13	3	10	12	3	9	4759.2486	4759.2480	0.0006
13	1	12	12	1	11	4806.3295	4806.3295	0.0000
13	2	11	12	2	10	4807.9965	4807.9968	-0.0003

9	2	7	8	1	7	4848.8277	4848.8292	-0.0015
8	2	7	7	1	7	4865.5748	4865.5743	0.0005
14	1	14	13	1	13	4976.7475	4976.7480	-0.0005
14	0	14	13	0	13	5005.7163	5005.7171	-0.0008
6	3	3	5	2	3	5084.5730	5084.5726	0.0004
14	2	13	13	2	12	5084.9336	5084.9333	0.0003
6	3	4	5	2	4	5094.1386	5094.1389	-0.0003
14	11	4	13	11	3	5107.4497	5107.4508	-0.0011
14	11	3	13	11	2	5107.4497	5107.4508	-0.0011
14	10	5	13	10	4	5107.5854	5107.5838	0.0016
14	10	4	13	10	3	5107.5854	5107.5838	0.0016
14	9	5	13	9	4	5107.8094	5107.8074	0.0020
14	9	6	13	9	5	5107.8094	5107.8074	0.0020
14	8	7	13	8	6	5108.1642	5108.1660	-0.0018
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14	5	9	13	5	8	5111.3353	5111.3350	0.0003
14	4	11	13	4	10	5114.2349	5114.2347	0.0002
14	4	10	13	4	9	5114.8733	5114.8730	0.0003
14	3	12	13	3	11	5115.3742	5115.3739	0.0003
14	3	11	13	3	10	5129.3173	5129.3178	-0.0005
11	1	10	10	0	10	5159.4092	5159.4093	-0.0001
14	1	13	13	1	12	5169.6651	5169.6658	-0.0007
14	2	12	13	2	11	5183.7346	5183.7338	0.0008
10	2	8	9	1	8	5191.6753	5191.6731	0.0022
15	1	15	14	1	14	5329.1379	5329.1384	-0.0005
15	0	15	14	0	14	5354.2852	5354.2844	0.0008
7	3	4	6	2	4	5443.3158	5443.3163	-0.0005
15	2	14	14	2	13	5444.7865	5444.7880	-0.0015
7	3	5	6	2	5	5462.2312	5462.2320	-0.0008
15	12	4	14	12	3	5472.2411	5472.2408	0.0003
15	12	3	14	12	2	5472.2411	5472.2408	0.0003
15	11	5	14	11	4	5472.3403	5472.3418	-0.0015
15	11	4	14	11	3	5472.3403	5472.3418	-0.0015
15	10	5	14	10	4	5472.5189	5472.5205	-0.0016
15	10	6	14	10	5	5472.5204	5472.5205	0.0000

15	9	6	14	9	5	5472.8094	5472.8091	0.0003
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15	8	7	14	8	6	5473.2613	5473.2623	-0.0010
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15	7	8	14	7	7	5473.9778	5473.9777	0.0001
15	6	9	14	6	8	5475.1462	5475.1460	0.0002
15	6	10	14	6	9	5475.1462	5475.1455	0.0007
15	5	11	14	5	10	5477.1686	5477.1688	-0.0002
15	5	10	14	5	9	5477.1960	5477.1961	-0.0001
15	4	12	14	4	11	5480.6535	5480.6534	0.0001
15	3	13	14	3	12	5481.1119	5481.1130	-0.0011
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15	1	14	14	1	13	5531.3422	5531.3432	-0.0010
11	2	9	10	1	9	5540.7002	5540.6984	0.0018
15	2	13	14	2	12	5559.1741	5559.1752	-0.0011
16	1	16	15	1	15	5681.1423	5681.1440	-0.0017
16	0	16	15	0	15	5702.5997	5702.5983	0.0014
8	3	5	7	2	5	5798.5214	5798.5221	-0.0007
16	2	15	15	2	14	5803.9983	5803.9992	-0.0009
8	3	6	7	2	6	5832.0764	5832.0776	-0.0012
16	12	5	15	12	4	5837.1071	5837.1089	-0.0018
16	12	4	15	12	3	5837.1071	5837.1089	-0.0018
16	11	5	15	11	4	5837.2486	5837.2479	0.0007
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16	10	6	15	10	5	5837.4802	5837.4797	0.0005
16	10	7	15	10	6	5837.4802	5837.4797	0.0005
16	9	7	15	9	6	5837.8453	5837.8435	0.0018
16	9	8	15	9	7	5837.8453	5837.8435	0.0018
16	8	8	15	8	7	5838.4048	5838.4056	-0.0008
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16	7	10	15	7	9	5839.2870	5839.2848	0.0022
16	7	9	15	7	8	5839.2870	5839.2848	0.0022
16	6	11	15	6	10	5840.7130	5840.7120	0.0010
16	6	10	15	6	9	5840.7130	5840.7129	0.0001
16	3	14	15	3	13	5846.6750	5846.6730	0.0020
16	4	13	15	4	12	5847.2521	5847.2525	-0.0004

16	4	12	15	4	11	5848.8853	5848.8867	-0.0014
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16	1	15	15	1	14	5891.2177	5891.2184	-0.0007
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16	2	14	15	2	13	5934.0113	5934.0115	-0.0002
17	1	17	16	1	16	6032.7986	6032.7973	0.0013
17	0	17	16	0	16	6050.8291	6050.8296	-0.0005
9	3	6	8	2	6	6149.2492	6149.2476	0.0016
17	2	16	16	2	15	6162.5472	6162.5475	-0.0003
17	12	6	16	12	5	6201.9883	6201.9870	0.0013
17	12	5	16	12	4	6201.9883	6201.9870	0.0013
17	11	7	16	11	6	6202.1694	6202.1700	-0.0006
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17	10	7	16	10	6	6202.4629	6202.4629	0.0000
17	10	8	16	10	7	6202.4629	6202.4629	0.0000
17	9	9	16	9	8	6202.9127	6202.9127	0.0000
17	9	8	16	9	7	6202.9127	6202.9127	0.0000
17	8	10	16	8	9	6203.5985	6203.5991	-0.0006
17	8	9	16	8	8	6203.5985	6203.5991	-0.0006
9	3	7	8	2	7	6204.1501	6204.1512	-0.0011
17	7	11	16	7	10	6204.6644	6204.6645	-0.0001
17	7	10	16	7	9	6204.6644	6204.6645	-0.0001
17	6	11	16	6	10	6206.3871	6206.3883	-0.0012
17	6	12	16	6	11	6206.3871	6206.3866	0.0005
17	5	13	16	5	12	6209.3369	6209.3370	-0.0001
17	5	12	16	5	11	6209.4227	6209.4233	-0.0006
17	3	15	16	3	14	6211.9850	6211.9851	-0.0001
17	4	14	16	4	13	6214.0197	6214.0209	-0.0012
17	4	13	16	4	12	6216.5146	6216.5151	-0.0005
17	3	14	16	3	13	6246.6247	6246.6254	-0.0007
17	1	16	16	1	15	6249.1865	6249.1853	0.0012
13	2	11	12	1	11	6264.1702	6264.1714	-0.0012
17	2	15	16	2	14	6307.9791	6307.9804	-0.0013
18	1	18	17	1	17	6384.1334	6384.1323	0.0011
18	0	18	17	0	17	6399.0951	6399.0936	0.0015
10	3	7	9	2	7	6494.6413	6494.6423	-0.0010
18	2	17	17	2	16	6520.4192	6520.4197	-0.0005
18	12	7	17	12	6	6566.8751	6566.8757	-0.0006
18	12	6	17	12	5	6566.8751	6566.8757	-0.0006
18	11	8	17	11	7	6567.1085	6567.1091	-0.0006

18	11	7	17	11	6	6567.1085	6567.1091	-0.0006
18	10	9	17	10	8	6567.4715	6567.4716	-0.0001
18	10	8	17	10	7	6567.4715	6567.4716	-0.0001
18	9	10	17	9	9	6568.0189	6568.0190	-0.0001
18	9	9	17	9	8	6568.0189	6568.0190	-0.0001
18	8	10	17	8	9	6568.8446	6568.8458	-0.0012
18	8	11	17	8	10	6568.8446	6568.8458	-0.0012
18	7	12	17	7	11	6570.1215	6570.1215	0.0000
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18	6	13	17	6	12	6572.1759	6572.1762	-0.0003
18	6	12	17	6	11	6572.1802	6572.1796	0.0006
18	5	14	17	5	13	6575.6748	6575.6740	0.0008
18	5	13	17	5	12	6575.8195	6575.8194	0.0001
18	3	16	17	3	15	6576.9806	6576.9801	0.0005
10	3	8	9	2	8	6578.9563	6578.9558	0.0005
18	4	15	17	4	14	6580.9413	6580.9408	0.0005
18	4	14	17	4	13	6584.6463	6584.6463	0.0000
18	1	17	17	1	16	6605.1925	6605.1926	-0.0001
12	2	11	11	1	11	6606.3573	6606.3573	0.0000
18	3	15	17	3	14	6621.6229	6621.6238	-0.0009
18	2	16	17	2	15	6680.8646	6680.8651	-0.0005
19	1	19	18	1	18	6735.1836	6735.1835	0.0001
11	3	8	10	2	8	6834.0635	6834.0632	0.0003
19	2	18	18	2	17	6877.6103	6877.6098	0.0005
19	7	12	18	7	11	6935.6617	6935.6606	0.0011
19	7	13	18	7	12	6935.6617	6935.6605	0.0012
19	6	14	18	6	13	6938.0886	6938.0879	0.0007
19	6	13	18	6	12	6938.0938	6938.0940	-0.0002
19	4	16	18	4	15	6947.9889	6947.9873	0.0016
19	4	15	18	4	14	6953.3603	6953.3602	0.0001
19	1	18	18	1	17	6959.2624	6959.2608	0.0016
19	3	16	18	3	15	6997.8517	6997.8521	-0.0004
19	2	17	18	2	16	7052.4839	7052.4839	0.0000
20	3	18	19	3	17	7305.7473	7305.7469	0.0004

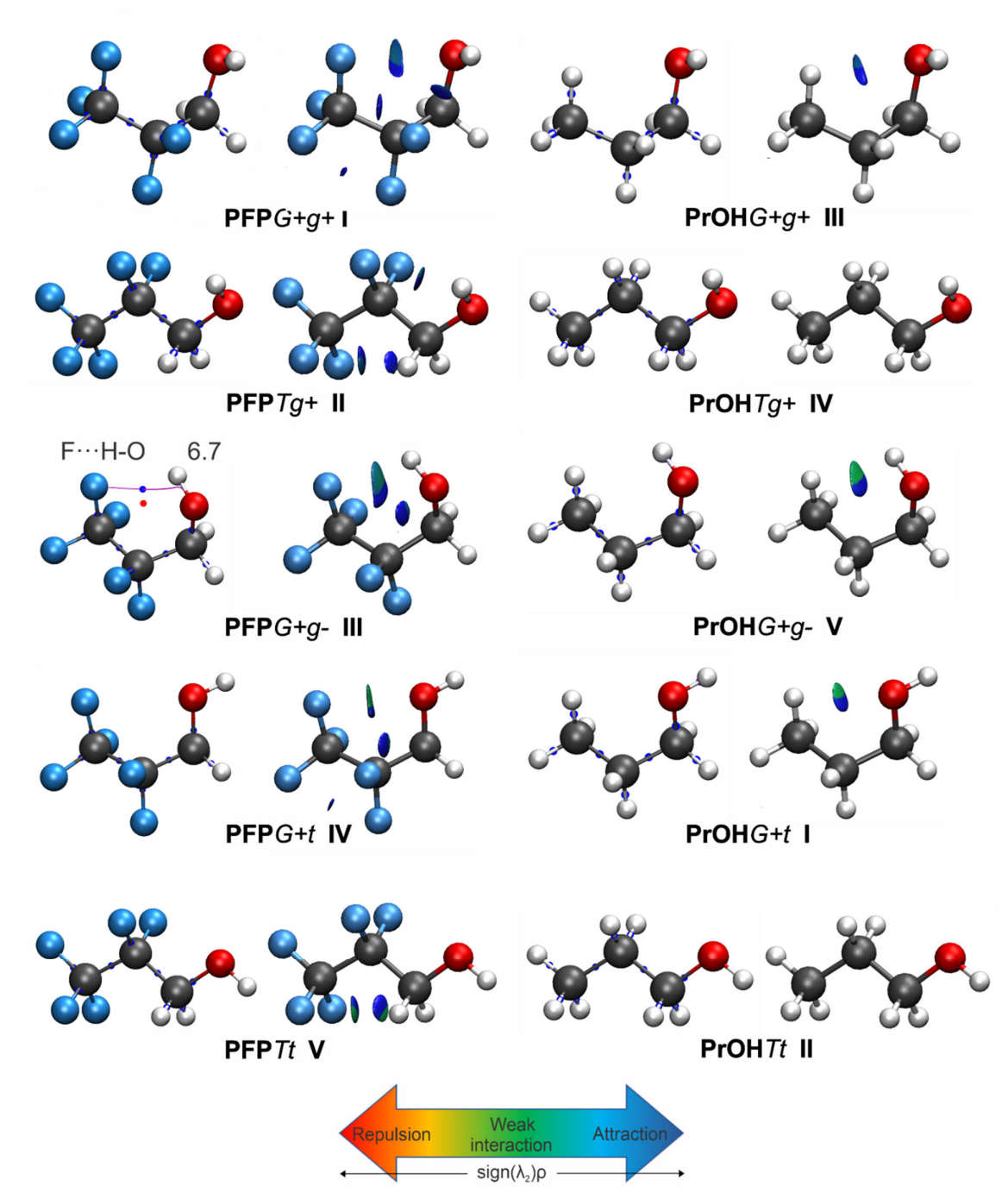

Figure S4. The intramolecular forces for all the non-covalent BCPs identified and non-covalent interaction analyses of the all possible PFP and PrOH monomers calculated at the B3LYP-D3(BJ)/def2-QZVP level of theory. The bond energy is in $kJmol^{-1}$. **I** to **V** indicate the relative stability with **I** being the most stable.

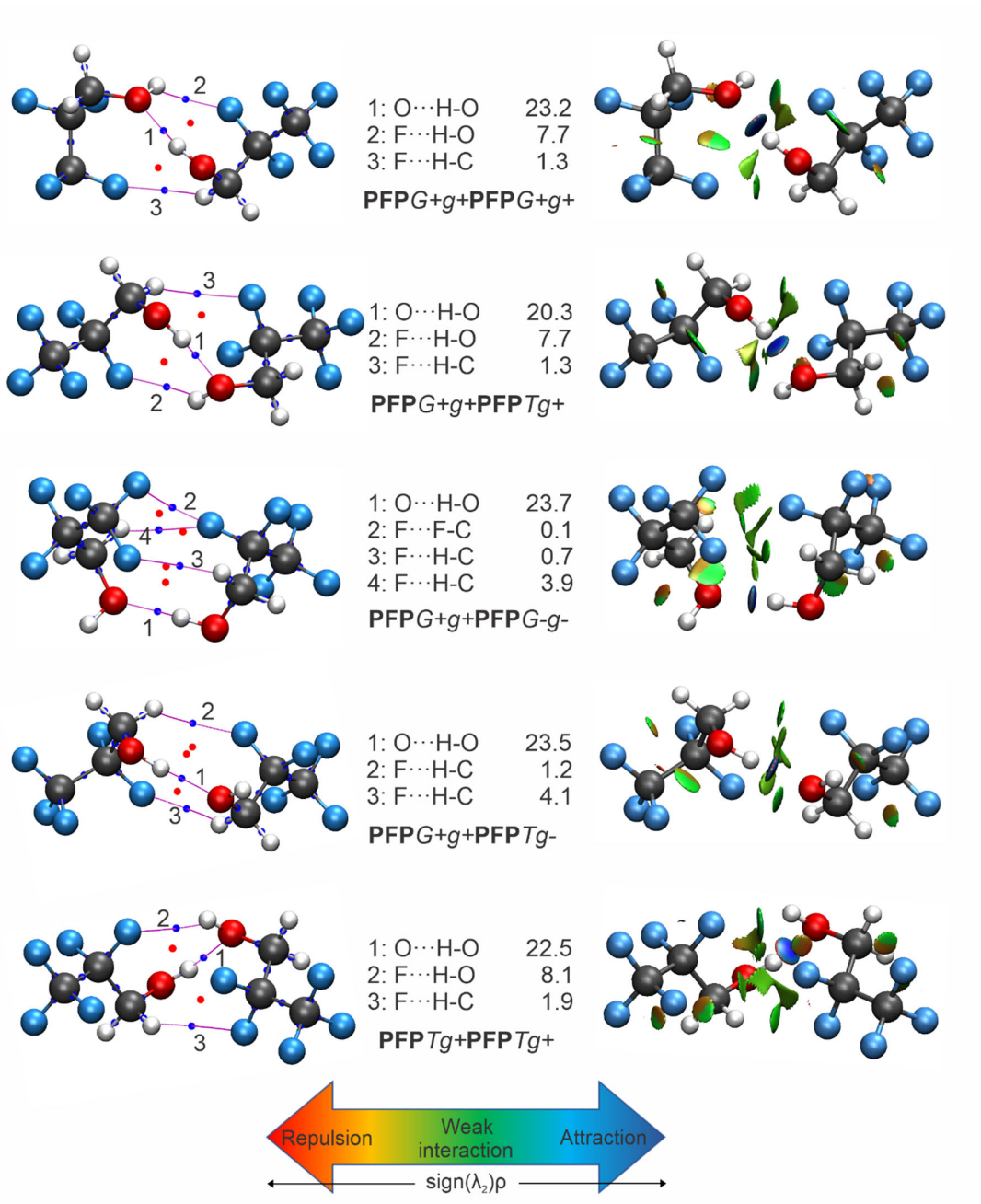

Figure S5. The intermolecular bond energies (in kJmol^{-1}) for all the non-covalent BCPs identified and the NCI analyses of the five observed PFP homodimers calculated at the B3LYP-D3(BJ)/def2-QZVP level of theory.

Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.