

Rotational spectroscopy of hydrogen-bonded binary trifluoropropanol conformers: conformational diversity, preference and abundances in a jet expansion

Alex N. Mort,^a Fan Xie,^{a,b} Arsh S. Hazrah,^a and Yunjie Xu^{a*}

^a*Department of Chemistry, University of Alberta, 11227 Saskatchewan Drive, Edmonton, AB, Canada.*

^b*Present address: Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany.*

* Corresponding Author, Email: yunjie.xu@ualberta.ca, Fax: 1-780-492-8231

Contents

Figure S1. The nine conformations of the TFP monomer and an example binary TFP conformer.....	S2
Figure S2. A zoom-in section of the Q-branch transitions of Dimer 6	S2
Table S1. Spectroscopic properties of the predicted binary TFP conformers.....	S3-S4
Table S2-S6. Rotational transition frequencies of the five binary TFP conformers assigned.....	S4-S24
Table S7. Comparison of the experimental and theoretical rotational constants and planar moments.....	S24
Table S8. Predicted quartic centrifugal distortion constants of the five observed binary conformers.....	S24
Table S9. The binding energies of the selective binary TFP conformers.....	S25

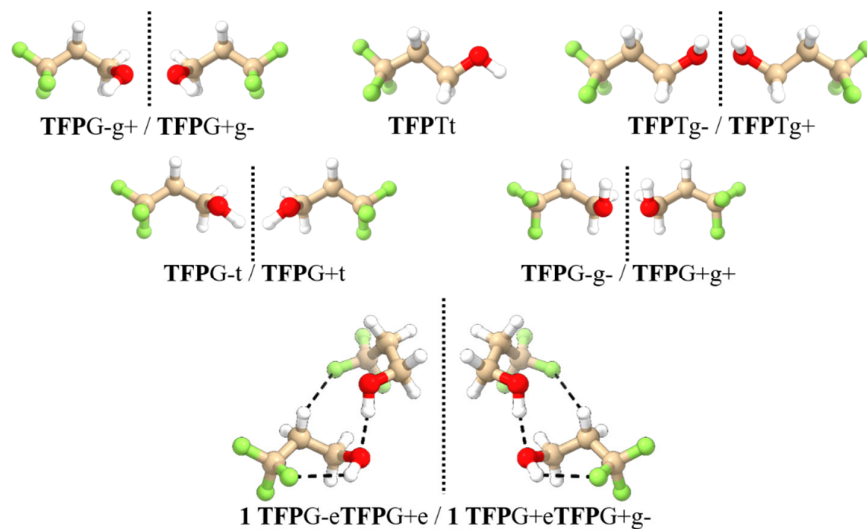


Figure S1. The geometries of nine monomeric conformations of TFP and an example TFP dimer. The mirror-imaged pairs are separated by the dotted lines.

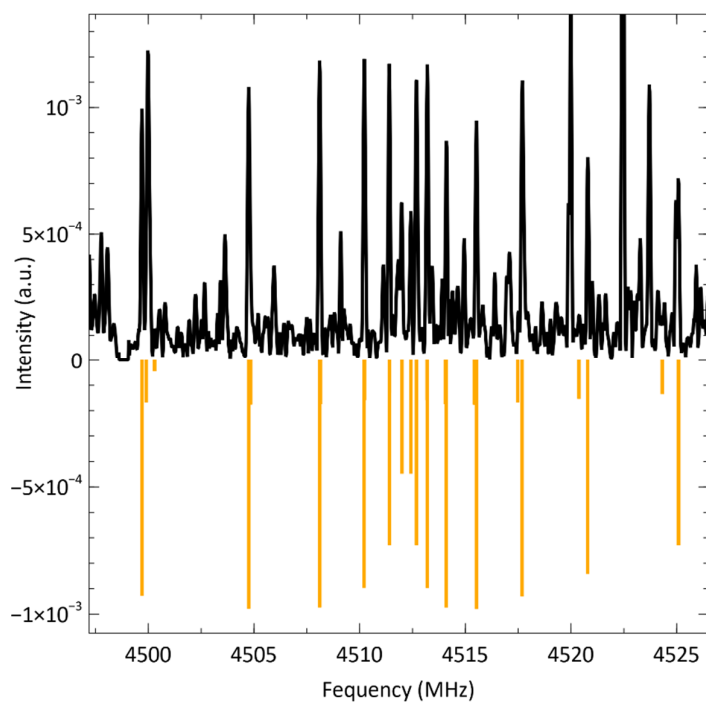


Figure S2. A zoom-in experimental section (top) centring on the Q branch transitions of Dimer **6** to show the signal-to-noise ratio achieved and the corresponding simulated spectrum (bottom). See the main text for the simulation details. Please note that the transitions of Dimer **6** are among the weakest ones assigned.

Table S1. The rotational constants (in MHz), permanent dipole components (in Debye), and the zero-point-energy corrected relative energies, ΔE (in kJ mol⁻¹), of the binary TFP conformers, calculated at the B3LYP-D3BJ/def2-TZVP level.

Dimer ^a	<i>A</i>	<i>B</i>	<i>C</i>	μ_a	μ_b	μ_c	ΔE^{ZPE}
Dimer 1	1113	283	265	1.0	-0.8	1.1	0.0
Dimer 2	1014	308	274	0.0	0.3	-0.1	0.3
Dimer 3	1013	315	287	0.0	-2.2	0.7	0.4
Dimer 4	1083	319	314	1.5	-0.5	0.8	1.5
Dimer 5	972	380	316	-0.4	-1.7	0.2	1.6
Dimer 6	1168	265	256	-0.5	-1.0	2.4	1.7
Dimer 7	943	380	317	0.5	-1.1	2.3	1.8
Dimer 8	1034	334	287	0.4	-1.4	-2.2	2.0
Dimer 9	1235	258	251	1.2	0.5	-0.6	2.2
Dimer 10	1055	336	287	-0.2	-1.3	0.1	2.4
Dimer 11	908	390	318	-1.1	-1.8	-0.6	3.3
Dimer 12	1223	245	234	-2.7	-0.3	1.2	3.9
Dimer 13	1051	288	254	0.7	-0.8	-1.4	3.9
Dimer 14	1590	159	155	-2.5	-1.1	-1.1	3.9
Dimer 15	1107	252	244	-2.3	-0.1	-0.3	3.9
Dimer 16	862	323	264	2.0	-1.0	0.7	4.3
Dimer 17	1764	165	163	-2.2	-1.2	-0.9	4.3
Dimer 18	1068	239	215	3.4	-1.6	0.7	4.3
Dimer 19	1658	174	170	2.0	-1.5	0.7	4.3
Dimer 20	891	404	319	1.6	-2.1	-1.3	4.5
Dimer 21	1465	203	198	-1.4	1.3	-0.1	4.6
Dimer 22	945	286	249	3.3	-1.3	-0.1	4.7
Dimer 23	1124	232	218	3.0	-2.0	-0.3	4.7
Dimer 24	1114	332	316	-0.1	-2.1	0.7	4.7
Dimer 25	1030	271	259	1.0	0.8	-0.5	5.1
Dimer 26	1196	283	274	0.6	-1.6	1.5	5.2
Dimer 27	1142	241	223	1.1	0.6	-0.5	5.5
Dimer 28	886	301	257	1.7	-0.1	1.9	5.7
Dimer 29	1181	237	217	2.2	0.2	-1.8	6.5
Dimer 30	973	345	338	-0.1	1.8	-1.3	6.7
Dimer 31	1801	136	134	-3.0	0.1	0.9	6.9
Dimer 32	1119	200	184	2.6	-0.2	-0.9	7.0
Dimer 33	977	321	270	-0.6	-2.1	-2.2	7.1
Dimer 34	944	311	279	-0.9	-3.0	-0.2	7.2
Dimer 35	1042	333	327	2.2	2.0	-0.9	7.3
Dimer 36	1185	261	239	2.1	1.0	0.8	8.2
Dimer 37	1220	249	230	-1.9	1.1	3.2	8.4
Dimer 38	1067	273	240	1.6	-2.5	3.0	8.4
Dimer 39	918	396	326	-2.2	-3.5	0.4	8.8

Dimer 40	1058	337	314	0.0	0.0	2.5	8.8
Dimer 41	888	385	334	0.0	0.2	0.0	8.9
Dimer 42	1167	235	231	2.3	-1.1	1.9	8.9
Dimer 43	1063	194	177	2.4	-3.7	0.5	9.0
Dimer 44	1587	203	198	0.0	0.0	0.0	9.0
Dimer 45	920	324	285	0.5	-4.3	-1.7	9.0
Dimer 46	945	287	251	3.9	-3.5	-0.9	9.0
Dimer 47	1367	254	236	0.4	-2.3	-0.8	9.1
Dimer 48	1081	243	218	4.4	-3.7	0.8	9.1
Dimer 49	1194	282	274	2.7	-2.2	0.1	9.1
Dimer 50	883	414	324	2.6	-4.0	-1.0	9.2
Dimer 51	1219	294	276	1.6	-2.1	-1.9	9.2
Dimer 52	1132	284	276	0.3	-2.0	2.3	9.4
Dimer 53	1093	253	237	0.0	-2.0	0.0	9.5
Dimer 54	1014	218	205	1.6	-2.8	2.2	9.6
Dimer 55	998	295	272	1.1	-1.9	0.1	9.6
Dimer 56	1124	203	195	1.3	-3.2	1.9	9.6
Dimer 57	1153	180	168	2.7	-3.1	0.8	9.7
Dimer 58	1055	255	235	3.7	-4.0	-1.1	9.9
Dimer 59	1255	252	236	0.8	0.4	0.2	9.9
Dimer 60	1067	214	204	2.2	-3.1	1.4	9.9
Dimer 61	1002	323	310	-1.2	-2.5	-0.4	10.0
Dimer 62	964	301	268	4.2	-3.5	-1.4	10.0

^a The names are given based on the stability ordering according to their relative energy (zero-point energy corrected), with **1** being the most stable one. The observed ones are in red. For the descriptive names of some selected low energy binary TFP conformers, see Table 2.

Table S2. Rotational transition frequencies of Dimer 1.

J'	K_a'	K_c'	J''	K_a''	K_c''	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
13	2	11	13	1	12	2099.3870	2099.3832	0.0038
12	2	10	12	1	11	2102.0940	2102.0963	-0.0023
11	2	9	11	1	10	2119.0050	2119.0116	-0.0066
4	1	4	3	1	3	2124.2210	2124.2214	-0.0004
10	2	8	10	1	9	2147.7210	2147.7157	0.0053
8	2	7	8	1	7	2153.8550	2153.8619	-0.0069
4	0	4	3	0	3	2161.8530	2161.8526	0.0004
4	2	3	3	2	2	2165.2480	2165.2481	-0.0001
4	2	2	3	2	1	2168.9370	2168.9312	0.0058
9	2	7	9	1	8	2185.5750	2185.5725	0.0025
4	1	3	3	1	2	2205.3710	2205.3735	-0.0025

8	2	6	8	1	7	2229.7930	2229.7941	-0.0011
7	2	6	7	1	6	2231.6180	2231.6199	-0.0019
6	0	6	5	1	4	2236.2100	2236.2101	-0.0001
7	2	5	7	1	6	2277.5480	2277.5444	0.0036
6	2	5	6	1	5	2300.4000	2300.4031	-0.0031
6	2	4	6	1	5	2326.0560	2326.0565	-0.0005
5	2	4	5	1	4	2359.8750	2359.8734	0.0016
5	2	3	5	1	4	2372.7470	2372.7450	0.0020
3	1	3	2	0	2	2400.2630	2400.2631	-0.0001
4	2	3	4	1	3	2409.7710	2409.7700	0.0010
4	2	2	4	1	3	2415.2980	2415.2976	0.0004
3	2	2	3	1	2	2449.9020	2449.8954	0.0066
3	2	1	3	1	2	2451.7440	2451.7399	0.0041
2	2	1	2	1	1	2480.1070	2480.1050	0.0020
2	2	0	2	1	1	2480.4750	2480.4741	0.0009
3	1	2	2	0	2	2522.0250	2522.0272	-0.0022
15	1	14	15	0	15	2538.4520	2538.4578	-0.0058
6	0	6	5	1	5	2540.5100	2540.5082	0.0018
2	2	1	2	1	2	2541.0010	2540.9895	0.0115
3	2	2	3	1	3	2571.6570	2571.6596	-0.0026
3	2	1	3	1	3	2573.5000	2573.5041	-0.0041
4	2	3	4	1	4	2612.6830	2612.6863	-0.0033
4	2	2	4	1	4	2618.2160	2618.2139	0.0021
5	1	5	4	1	4	2654.6050	2654.6054	-0.0004
5	2	4	5	1	5	2664.1720	2664.1716	0.0004
5	2	3	5	1	5	2677.0400	2677.0432	-0.0032
5	2	4	4	2	3	2706.0910	2706.0907	0.0003
5	4	1	4	4	0	2707.7270	2707.7274	-0.0004
5	4	2	4	4	1	2707.7270	2707.7271	-0.0001
5	2	3	4	2	2	2713.4360	2713.4346	0.0014
6	2	5	6	1	6	2726.2290	2726.2280	0.0010
6	2	4	6	1	6	2751.8870	2751.8814	0.0056
5	1	4	4	1	3	2755.9910	2755.9872	0.0038
7	2	6	7	1	7	2798.9670	2798.9690	-0.0020
7	2	5	7	1	7	2844.8930	2844.8934	-0.0004
8	2	7	8	1	8	2882.5000	2882.4986	0.0014
4	1	4	3	0	3	2901.8040	2901.8041	-0.0001
8	2	6	8	1	8	2958.4320	2958.4308	0.0012
9	2	8	9	1	9	2976.9010	2976.9004	0.0006
10	2	9	10	1	10	3082.2240	3082.2254	-0.0014

9	2	7	9	1	9	3094.9110	3094.9125	-0.0015
4	1	3	3	0	3	3104.7200	3104.7204	-0.0004
7	0	7	6	1	6	3125.3150	3125.3127	0.0023
8	0	8	7	1	6	3144.9040	3144.9078	-0.0038
6	1	6	5	1	5	3184.5650	3184.5643	0.0007
11	2	10	11	1	11	3198.4830	3198.4816	0.0014
6	0	6	5	0	5	3235.4990	3235.4981	0.0009
6	2	5	5	2	4	3246.6220	3246.6207	0.0013
6	5	1	5	5	0	3249.1990	3249.1958	0.0032
6	5	2	5	5	1	3249.1990	3249.1958	0.0032
6	4	2	5	4	1	3249.5300	3249.5321	-0.0021
6	4	3	5	4	2	3249.5300	3249.5307	-0.0007
6	3	4	5	3	3	3250.1930	3250.1929	0.0001
6	3	3	5	3	2	3250.4260	3250.4274	-0.0014
10	2	8	10	1	10	3256.6830	3256.6839	-0.0009
6	2	4	5	2	3	3259.4030	3259.4025	0.0005
6	1	5	5	1	4	3306.0920	3306.0910	0.0010
10	1	9	9	2	7	3313.1170	3313.1173	-0.0003
12	2	11	12	1	12	3325.6240	3325.6237	0.0003
5	1	5	4	0	4	3394.5570	3394.5570	0.0000
10	1	9	9	2	8	3431.1280	3431.1294	-0.0014
11	2	9	11	1	11	3445.8680	3445.8692	-0.0012
13	2	12	13	1	13	3463.5320	3463.5445	-0.0125
9	0	9	8	1	7	3570.8910	3570.8894	0.0016
2	2	1	1	1	0	3583.1720	3583.1721	-0.0001
2	2	1	1	1	1	3603.4650	3603.4670	-0.0020
2	2	0	1	1	1	3603.8360	3603.8361	-0.0001
14	2	13	14	1	14	3612.0740	3612.0691	0.0049
5	1	4	4	0	4	3698.8540	3698.8551	-0.0011
8	0	8	7	1	7	3712.2560	3712.2568	-0.0008
7	1	7	6	1	6	3714.0350	3714.0352	-0.0002
15	3	12	15	2	13	3741.9610	3741.9629	-0.0019
7	0	7	6	0	6	3769.3690	3769.3688	0.0002
15	2	14	15	1	15	3770.9570	3770.9510	0.0060
14	3	12	14	2	12	3772.4270	3772.4262	0.0008
7	2	6	6	2	5	3786.7760	3786.7762	-0.0002
14	2	12	13	3	10	3787.3700	3787.3649	0.0051
7	5	2	6	5	1	3790.9420	3790.9451	-0.0031
7	5	3	6	5	2	3790.9420	3790.9451	-0.0031
7	4	3	6	4	2	3791.4770	3791.4791	-0.0021

7	4	4	6	4	3	3791.4770	3791.4743	0.0027
7	3	5	6	3	4	3792.4530	3792.4505	0.0025
7	3	4	6	3	3	3792.9790	3792.9775	0.0015
7	2	5	6	2	4	3807.0460	3807.0473	-0.0013
14	2	12	13	3	11	3820.1360	3820.1333	0.0027
14	3	11	14	2	12	3822.6350	3822.6405	-0.0055
7	1	6	6	1	5	3855.5600	3855.5594	0.0006
13	3	11	13	2	11	3863.9500	3863.9563	-0.0063
6	1	6	5	0	5	3879.5540	3879.5542	-0.0002
11	1	10	10	2	8	3896.3580	3896.3593	-0.0013
13	3	10	13	2	11	3896.7250	3896.7247	0.0003
12	3	10	12	2	10	3941.9060	3941.9069	-0.0009
12	3	9	12	2	10	3962.5230	3962.5250	-0.0020
10	0	10	9	1	8	3976.0360	3976.0380	-0.0020
11	3	9	11	2	9	4006.5460	4006.5497	-0.0037
11	3	8	11	2	9	4018.9870	4018.9853	0.0017
10	3	8	10	2	8	4058.5680	4058.5627	0.0053
10	3	7	10	2	8	4065.6990	4065.6971	0.0019
11	1	10	10	2	9	4070.8250	4070.8178	0.0072
9	3	7	9	2	7	4099.0088	4099.0035	0.0053
9	3	6	9	2	7	4102.8570	4102.8566	0.0004
3	2	2	2	1	1	4104.2590	4104.2602	-0.0012
3	2	1	2	1	1	4106.1050	4106.1047	0.0003
8	3	6	8	2	6	4129.2380	4129.2372	0.0008
8	3	5	8	2	6	4131.1690	4131.1680	0.0010
7	3	5	7	2	5	4150.8280	4150.8299	-0.0019
7	3	4	7	2	5	4151.7110	4151.7089	0.0021
3	2	2	2	1	2	4165.1450	4165.1447	0.0003
6	3	4	6	2	4	4165.4300	4165.4267	0.0033
6	3	3	6	2	4	4165.7790	4165.7787	0.0003
3	2	1	2	1	2	4166.9890	4166.9892	-0.0002
5	3	3	5	2	3	4174.6421	4174.6364	0.0057
5	3	2	5	2	3	4174.7510	4174.7538	-0.0028
3	3	1	3	2	1	4182.6090	4182.6085	0.0005
3	3	0	3	2	1	4182.6090	4182.6127	-0.0037
3	3	0	3	2	2	4184.4540	4184.4572	-0.0032
3	3	1	3	2	2	4184.4540	4184.4530	0.0010
4	3	1	4	2	3	4185.4740	4185.4938	-0.0198
4	3	2	4	2	3	4185.4750	4185.4645	0.0105
5	3	3	5	2	4	4187.5160	4187.5080	0.0080

6	3	4	6	2	5	4191.0800	4191.0801	-0.0001
6	3	3	6	2	5	4191.4330	4191.4321	0.0009
7	3	5	7	2	6	4196.7520	4196.7544	-0.0024
7	3	4	7	2	6	4197.6350	4197.6334	0.0016
8	3	6	8	2	7	4205.1690	4205.1694	-0.0004
8	3	5	8	2	7	4207.0990	4207.1001	-0.0011
9	3	7	9	2	8	4217.0160	4217.0156	0.0004
9	3	6	9	2	8	4220.8690	4220.8687	0.0003
10	3	8	10	2	9	4233.0210	4233.0212	-0.0002
10	3	7	10	2	9	4240.1590	4240.1557	0.0033
8	1	8	7	1	7	4242.9650	4242.9660	-0.0010
11	3	9	11	2	10	4253.9460	4253.9373	0.0087
11	3	8	11	2	10	4266.3730	4266.3729	0.0001
12	3	10	12	2	11	4280.5220	4280.5223	-0.0003
9	0	9	8	1	8	4299.5250	4299.5261	-0.0011
8	0	8	7	0	7	4300.9800	4300.9793	0.0007
12	3	9	12	2	11	4301.1430	4301.1404	0.0026
6	1	5	5	0	5	4305.3810	4305.3790	0.0020
13	3	11	13	2	12	4313.5250	4313.5272	-0.0022
8	2	7	7	2	6	4326.5000	4326.4957	0.0043
8	7	1	7	7	0	4332.1260	4332.1264	-0.0004
8	7	2	7	7	1	4332.1260	4332.1264	-0.0004
8	6	2	7	6	1	4332.3730	4332.3765	-0.0035
8	6	3	7	6	2	4332.3740	4332.3765	-0.0025
8	5	3	7	5	2	4332.7950	4332.7944	0.0006
8	5	4	7	5	3	4332.7950	4332.7944	0.0006
8	4	5	7	4	4	4333.5880	4333.5804	0.0076
8	4	4	7	4	3	4333.5880	4333.5934	-0.0054
8	3	6	7	3	5	4334.9110	4334.9107	0.0003
8	3	5	7	3	4	4335.9620	4335.9625	-0.0005
13	3	10	13	2	12	4346.3000	4346.2956	0.0044
14	3	12	14	2	13	4353.6810	4353.6807	0.0003
8	2	6	7	2	5	4356.5020	4356.5034	-0.0014
7	1	7	6	0	6	4358.0890	4358.0913	-0.0023
11	0	11	10	1	9	4359.2940	4359.2925	0.0015
15	3	13	15	2	14	4401.6670	4401.6757	-0.0087
14	3	11	14	2	13	4403.8950	4403.8951	-0.0001
8	1	7	7	1	6	4404.2550	4404.2537	0.0013
15	2	13	14	3	11	4417.8580	4417.8512	0.0068
16	3	14	16	2	15	4458.1610	4458.1564	0.0046

12	1	11	11	2	9	4468.9570	4468.9617	-0.0047
15	3	12	15	2	14	4476.1990	4476.2043	-0.0053
17	3	15	17	2	16	4523.7090	4523.7073	0.0017
16	3	13	16	2	15	4565.6680	4565.6715	-0.0035
18	3	16	18	2	17	4598.8480	4598.8432	0.0048
4	2	3	3	1	2	4615.1440	4615.1435	0.0005
4	2	2	3	1	2	4620.6730	4620.6712	0.0018
12	1	11	11	2	10	4716.3500	4716.3493	0.0007
12	0	12	11	1	10	4720.0620	4720.0584	0.0036
4	2	3	3	1	3	4736.9100	4736.9076	0.0024
4	2	2	3	1	3	4742.4370	4742.4353	0.0017
9	1	9	8	1	8	4771.3190	4771.3171	0.0019
9	0	9	8	0	8	4830.2370	4830.2353	0.0017
8	1	8	7	0	7	4831.6880	4831.6886	-0.0006
9	2	8	8	2	7	4865.7190	4865.7189	0.0001
9	7	2	8	7	1	4873.8140	4873.8104	0.0036
9	7	3	8	7	2	4873.8140	4873.8104	0.0036
9	6	3	8	6	2	4874.1650	4874.1645	0.0005
9	6	4	8	6	3	4874.1660	4874.1645	0.0015
9	5	4	8	5	3	4874.7600	4874.7582	0.0018
9	5	5	8	5	4	4874.7600	4874.7579	0.0021
9	3	7	8	3	6	4877.5680	4877.5650	0.0030
9	3	6	8	3	5	4879.4880	4879.4874	0.0006
10	0	10	9	1	9	4885.3770	4885.3780	-0.0010
9	2	7	8	2	6	4907.8000	4907.7988	0.0012
7	1	6	6	0	6	4925.4430	4925.4403	0.0027
9	1	8	8	1	7	4952.0200	4952.0204	-0.0004
13	1	12	12	2	10	5028.0740	5028.0729	0.0011
13	0	13	12	1	11	5058.3090	5058.3030	0.0060
5	2	4	4	1	3	5115.8590	5115.8607	-0.0017
5	2	3	4	1	3	5128.7290	5128.7323	-0.0033
10	1	10	9	1	9	5299.0600	5299.0616	-0.0016
9	1	9	8	0	8	5302.0240	5302.0263	-0.0023
5	2	4	4	1	4	5318.7740	5318.7770	-0.0030
5	2	3	4	1	4	5331.6490	5331.6486	0.0004
10	0	10	9	0	9	5357.1670	5357.1690	-0.0020
13	1	12	12	2	11	5366.6850	5366.6882	-0.0032
14	0	14	13	1	12	5374.6000	5374.5982	0.0018
10	2	9	9	2	8	5404.3850	5404.3866	-0.0016
10	7	3	9	7	2	5415.5580	5415.5536	0.0044

10	7	4	9	7	3	5415.5580	5415.5536	0.0044
10	4	7	9	4	6	5418.3620	5418.3638	-0.0018
10	4	6	9	4	5	5418.4360	5418.4314	0.0046
10	3	8	9	3	7	5420.3930	5420.3923	0.0007
10	3	7	9	3	6	5423.6730	5423.6736	-0.0006
10	2	8	9	2	7	5460.8350	5460.8330	0.0020
11	0	11	10	1	10	5468.2610	5468.2607	0.0003
10	1	9	9	1	8	5498.6890	5498.6898	-0.0008
8	1	7	7	0	7	5560.3290	5560.3253	0.0037
14	1	13	13	2	11	5571.0500	5571.0574	-0.0074
6	2	5	5	1	4	5606.4950	5606.4942	0.0008
6	2	4	5	1	4	5632.1460	5632.1476	-0.0016
16	4	12	16	3	13	5737.7320	5737.7245	0.0075
15	4	11	15	3	12	5768.6370	5768.6283	0.0087
10	1	10	9	0	9	5770.8550	5770.8526	0.0024
14	4	10	14	3	11	5792.7930	5792.7987	-0.0057
3	3	1	2	2	0	5808.2410	5808.2391	0.0019
3	3	0	2	2	0	5808.2430	5808.2433	-0.0003
3	3	1	2	2	1	5808.6110	5808.6081	0.0029
3	3	0	2	2	1	5808.6110	5808.6123	-0.0013
13	4	10	13	3	10	5810.3960	5810.4013	-0.0053
13	4	9	13	3	10	5811.3530	5811.3544	-0.0014
12	4	8	12	3	9	5825.3350	5825.3294	0.0056
11	1	11	10	1	10	5826.1820	5826.1857	-0.0037
11	4	8	11	3	8	5835.3780	5835.3896	-0.0116
11	4	7	11	3	8	5835.6420	5835.6429	-0.0009
15	4	12	15	3	13	5840.2000	5840.2122	-0.0122
16	4	13	16	3	14	5840.3520	5840.3525	-0.0005
14	4	11	14	3	12	5841.3010	5841.3023	-0.0013
13	4	9	13	3	11	5844.1320	5844.1229	0.0091
12	4	9	12	3	10	5845.4420	5845.4417	0.0003
12	4	8	12	3	10	5845.9460	5845.9474	-0.0014
11	4	8	11	3	9	5847.8230	5847.8252	-0.0022
11	4	7	11	3	9	5848.0820	5848.0785	0.0035
8	4	5	8	3	5	5851.9080	5851.8965	0.0115
8	4	4	8	3	5	5851.9100	5851.9161	-0.0061
8	4	5	8	3	6	5853.8370	5853.8273	0.0097
8	4	4	8	3	6	5853.8370	5853.8468	-0.0098
7	4	3	7	3	4	5854.2830	5854.2851	-0.0021
7	4	4	7	3	4	5854.2850	5854.2786	0.0064

7	4	3	7	3	5	5855.1620	5855.1640	-0.0020
7	4	4	7	3	5	5855.1620	5855.1575	0.0045
6	4	3	6	3	3	5855.7800	5855.7817	-0.0017
6	4	2	6	3	3	5855.7810	5855.7835	-0.0025
6	4	2	6	3	4	5856.1340	5856.1354	-0.0014
6	4	3	6	3	4	5856.1340	5856.1337	0.0003
11	0	11	10	0	10	5881.9420	5881.9443	-0.0023
6	2	5	5	1	5	5910.7920	5910.7923	-0.0003
6	2	4	5	1	5	5936.4430	5936.4457	-0.0027
11	2	10	10	2	9	5942.4480	5942.4419	0.0061
11	8	3	10	8	2	5956.9440	5956.9466	-0.0026
11	8	4	10	8	3	5956.9440	5956.9466	-0.0026
11	7	4	10	7	3	5957.3650	5957.3628	0.0022
11	7	5	10	7	4	5957.3650	5957.3628	0.0022
11	6	5	10	6	4	5958.0080	5958.0053	0.0027
11	6	6	10	6	5	5958.0080	5958.0053	0.0027
11	5	6	10	5	5	5959.0840	5959.0869	-0.0029
11	5	7	10	5	6	5959.0840	5959.0852	-0.0012
11	4	8	10	4	7	5961.0760	5961.0792	-0.0032
11	4	7	10	4	6	5961.2160	5961.2141	0.0019
11	3	9	10	3	8	5963.3590	5963.3580	0.0010
11	3	8	10	3	7	5968.6580	5968.6591	-0.0011
11	2	9	10	2	8	6015.3690	6015.3709	-0.0019
11	1	10	10	1	9	6044.0740	6044.0750	-0.0010
12	0	12	11	1	11	6046.9190	6046.9160	0.0030
7	2	6	6	1	5	6087.1800	6087.1793	0.0007
7	2	5	6	1	5	6133.1040	6133.1038	0.0002
9	1	8	8	0	8	6211.3680	6211.3664	0.0016
11	1	11	10	0	10	6239.8670	6239.8693	-0.0023
4	3	2	3	2	2	6350.7320	6350.7125	0.0195
4	3	1	3	2	2	6350.7330	6350.7419	-0.0089
12	1	12	11	1	11	6352.6850	6352.6882	-0.0032
12	0	12	11	0	11	6404.8380	6404.8410	-0.0030
12	2	11	11	2	10	6479.8270	6479.8302	-0.0032
12	6	6	11	6	5	6500.0770	6500.0770	0.0000
12	6	7	11	6	6	6500.0770	6500.0770	0.0000
12	5	7	11	5	6	6501.4790	6501.4812	-0.0022
12	5	8	11	5	7	6501.4790	6501.4774	0.0016
12	4	9	11	4	8	6504.0340	6504.0317	0.0023
12	4	8	11	4	7	6504.2820	6504.2842	-0.0022

12	3	10	11	3	9	6506.4080	6506.4152	-0.0072
7	2	6	6	1	6	6513.0020	6513.0041	-0.0021
12	3	9	11	3	8	6514.5900	6514.5977	-0.0077
8	2	7	7	1	6	6558.1130	6558.1156	-0.0026
7	2	5	6	1	6	6558.9230	6558.9286	-0.0056
12	2	10	11	2	9	6571.0600	6571.0580	0.0020
12	1	11	11	1	10	6587.9750	6587.9733	0.0017
13	0	13	12	1	12	6620.4460	6620.4457	0.0003
8	2	6	7	1	6	6634.0480	6634.0478	0.0002
12	1	12	11	0	11	6710.6150	6710.6131	0.0019

Table S3. Rotational transition frequencies of Dimer 3.

J'	K_a'	K_c'	J''	K_a''	K_c''	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
7	2	5	7	1	6	1920.7340	1920.7339	0.0001
6	2	4	6	1	5	1969.6230	1969.6288	-0.0058
5	2	3	5	1	4	2020.5140	2020.5167	-0.0027
4	2	2	4	1	3	2069.4380	2069.4358	0.0022
12	1	11	12	0	12	2104.7790	2104.7838	-0.0048
3	2	1	3	1	2	2112.8980	2112.8993	-0.0013
2	2	0	2	1	1	2148.0390	2148.0374	0.0016
2	2	1	2	1	2	2223.8580	2223.8586	-0.0006
3	2	2	3	1	3	2262.5230	2262.5220	0.0010
7	1	6	6	2	5	2294.4210	2294.4210	0.0000
4	2	3	4	1	4	2314.3070	2314.3042	0.0028
5	0	5	4	1	4	2333.3340	2333.3402	-0.0062
13	1	12	13	0	13	2369.4670	2369.4659	0.0011
5	2	4	5	1	5	2379.3740	2379.3714	0.0026
3	1	3	2	0	2	2425.9150	2425.9140	0.0010
6	2	5	6	1	6	2457.8980	2457.8926	0.0054
7	2	6	7	1	7	2550.0200	2550.0174	0.0026
14	1	13	14	0	14	2653.1210	2653.1178	0.0032
8	2	7	8	1	8	2655.8480	2655.8507	-0.0027
9	2	8	9	1	9	2775.4350	2775.4280	0.0070
10	2	9	10	1	10	2908.6940	2908.6931	0.0009
16	3	13	16	2	14	2944.1520	2944.1514	0.0006
15	1	14	15	0	15	2951.9120	2951.8999	0.0121
4	1	4	3	0	3	2967.4760	2967.4782	-0.0022
6	0	6	5	1	5	2968.0990	2968.1023	-0.0033

8	1	7	7	2	6	2977.8210	2977.8159	0.0051
15	3	12	15	2	13	3026.7230	3026.7254	-0.0024
11	2	10	11	1	11	3055.4780	3055.4787	-0.0007
14	3	11	14	2	12	3115.6960	3115.7011	-0.0051
13	3	10	13	2	11	3206.1430	3206.1359	0.0071
12	2	11	12	1	12	3215.4910	3215.4933	-0.0023
4	1	3	3	0	3	3222.3420	3222.3483	-0.0063
16	1	15	16	0	16	3261.7180	3261.7141	0.0039
12	3	9	12	2	10	3293.4930	3293.4912	0.0018
2	2	1	1	1	0	3355.2750	3355.2740	0.0010
2	2	0	1	1	0	3355.9390	3355.9429	-0.0039
11	3	8	11	2	9	3373.9180	3373.9229	-0.0049
2	2	1	1	1	1	3380.7710	3380.7713	-0.0003
2	2	0	1	1	1	3381.4400	3381.4402	-0.0002
13	2	12	13	1	13	3388.3090	3388.3152	-0.0062
10	3	7	10	2	8	3444.5380	3444.5308	0.0072
9	3	7	9	2	7	3493.5230	3493.5291	-0.0061
5	1	5	4	0	4	3498.7684	3498.7667	0.0017
9	3	6	9	2	7	3503.5280	3503.5279	0.0001
8	0	8	7	1	6	3529.0170	3529.0120	0.0050
9	1	8	8	2	6	3535.0370	3535.0284	0.0086
8	3	5	8	2	6	3550.2930	3550.2928	0.0002
14	2	13	14	1	14	3573.3890	3573.3933	-0.0043
7	3	4	7	2	5	3585.2790	3585.2791	-0.0001
7	0	7	6	1	6	3604.7040	3604.7042	-0.0002
6	3	4	6	2	4	3608.8780	3608.8716	0.0064
6	3	3	6	2	4	3609.7900	3609.7902	-0.0002
5	3	2	5	2	3	3625.6700	3625.6706	-0.0006
4	3	1	4	2	2	3634.9840	3634.9832	0.0008
3	3	0	3	2	1	3639.7360	3639.7348	0.0012
3	3	1	3	2	2	3643.0650	3643.0652	-0.0002
4	3	2	4	2	3	3644.9100	3644.9081	0.0019
5	3	3	5	2	4	3648.6040	3648.6008	0.0032
5	3	2	5	2	4	3648.9050	3648.9075	-0.0025
6	3	4	6	2	5	3655.0110	3655.0099	0.0011
6	3	3	6	2	5	3655.9370	3655.9285	0.0085
7	3	5	7	2	6	3665.1170	3665.1169	0.0001
7	3	4	7	2	6	3667.4110	3667.4080	0.0030
9	1	8	8	2	7	3669.7490	3669.7482	0.0008
8	3	6	8	2	7	3679.9890	3679.9891	-0.0001

9	3	7	9	2	8	3700.7470	3700.7480	-0.0010
10	3	8	10	2	9	3728.5360	3728.5355	0.0005
11	3	9	11	2	10	3764.4820	3764.4814	0.0006
15	2	14	15	1	15	3770.0540	3770.0567	-0.0027
13	2	12	12	3	9	3783.8650	3783.8643	0.0007
12	3	10	12	2	11	3809.6740	3809.6717	0.0023
13	3	11	13	2	12	3865.1170	3865.1185	-0.0015
12	2	10	11	3	9	3868.0340	3868.0335	0.0005
5	1	4	4	0	4	3880.8620	3880.8583	0.0037
3	2	2	2	1	1	3920.9780	3920.9791	-0.0011
3	2	1	2	1	1	3924.3170	3924.3205	-0.0035
14	3	12	14	2	13	3931.7370	3931.7349	0.0021
9	0	9	8	1	7	3960.2810	3960.2764	0.0046
3	2	2	2	1	2	3997.4631	3997.4693	-0.0062
3	2	1	2	1	2	4000.8110	4000.8107	0.0003
15	3	13	15	2	14	4010.3130	4010.3115	0.0015
6	1	6	5	0	5	4021.6360	4021.6392	-0.0032
16	3	14	16	2	15	4101.4890	4101.4977	-0.0087
17	2	16	17	1	17	4194.9520	4194.9565	-0.0045
17	3	15	17	2	16	4205.7860	4205.7871	-0.0011
8	0	8	7	1	7	4240.4240	4240.4244	-0.0004
14	2	13	13	3	10	4279.3490	4279.3531	-0.0041
18	3	16	18	2	17	4323.5020	4323.5063	-0.0043
10	1	9	9	2	8	4368.9260	4368.9250	0.0010
4	2	3	3	1	2	4473.8300	4473.8312	-0.0012
4	2	2	3	1	2	4483.8350	4483.8328	0.0022
7	1	7	6	0	6	4538.3690	4538.3725	-0.0035
6	1	5	5	0	5	4556.0380	4556.0413	-0.0033
13	2	11	12	3	10	4578.6900	4578.6942	-0.0042
4	2	3	3	1	3	4626.7970	4626.7953	0.0017
4	2	2	3	1	3	4636.7960	4636.7969	-0.0009
18	4	14	18	3	15	4688.4900	4688.4944	-0.0044
17	4	13	17	3	14	4778.0070	4778.0058	0.0012
16	4	12	16	3	13	4853.8040	4853.7941	0.0099
9	0	9	8	1	8	4872.7880	4872.7873	0.0007
15	4	11	15	3	12	4916.0570	4916.0666	-0.0096
14	4	10	14	3	11	4965.7870	4965.7815	0.0055
13	4	9	13	3	10	5004.3880	5004.3857	0.0023
5	2	4	4	1	3	5013.9040	5013.9071	-0.0031
12	4	8	12	3	9	5033.5640	5033.5628	0.0012

8	1	8	7	0	7	5051.5250	5051.5193	0.0057
11	4	7	11	3	8	5055.0300	5055.0299	0.0001
10	4	6	10	3	7	5070.3940	5070.3945	-0.0005
11	1	10	10	2	9	5073.7690	5073.7670	0.0020
9	4	6	9	3	6	5080.8730	5080.8826	-0.0096
9	4	5	9	3	6	5081.0750	5081.0734	0.0016
13	4	10	13	3	11	5083.9590	5083.9578	0.0012
12	4	9	12	3	10	5084.3990	5084.3997	-0.0007
14	4	11	14	3	12	5085.5120	5085.5084	0.0036
11	4	8	11	3	9	5086.0830	5086.0828	0.0002
8	4	4	8	3	5	5088.2565	5088.2574	-0.0009
10	4	7	10	3	8	5088.3913	5088.3981	-0.0068
9	4	6	9	3	7	5090.8780	5090.8814	-0.0034
7	4	3	7	3	4	5092.9090	5092.9103	-0.0013
8	4	5	8	3	6	5093.2080	5093.2073	0.0007
7	4	4	7	3	5	5095.1780	5095.1769	0.0011
6	4	2	6	3	3	5095.7880	5095.7873	0.0007
6	4	3	6	3	3	5095.7880	5095.7806	0.0074
6	4	3	6	3	4	5096.6990	5096.6991	-0.0001
5	4	1	5	3	2	5097.4620	5097.4623	-0.0003
5	4	2	5	3	3	5097.7680	5097.7676	0.0004
17	4	14	17	3	15	5111.4830	5111.4782	0.0048
18	4	15	18	3	16	5130.8180	5130.8204	-0.0024
7	1	6	6	0	6	5249.7880	5249.7849	0.0031
5	2	4	4	1	4	5268.7730	5268.7772	-0.0042
5	2	3	4	1	4	5292.0130	5292.0141	-0.0011
3	3	1	2	2	0	5416.0060	5416.0069	-0.0009
3	3	0	2	2	1	5416.6820	5416.6868	-0.0048
10	0	10	9	1	9	5499.8010	5499.8022	-0.0012
6	2	5	5	1	4	5541.3730	5541.3746	-0.0016
9	1	9	8	0	8	5563.6950	5563.6972	-0.0022
6	2	4	5	1	4	5587.5120	5587.5129	-0.0009
12	1	11	11	2	10	5782.3910	5782.3893	0.0017
6	2	5	5	1	5	5923.4600	5923.4662	-0.0062
8	1	7	7	0	7	5964.0300	5964.0303	-0.0003
6	2	4	5	1	5	5969.6000	5969.6045	-0.0045
4	3	2	3	2	1	6005.8380	6005.8400	-0.0020
4	3	1	3	2	2	6009.2560	6009.2581	-0.0021
7	2	6	6	1	5	6056.5180	6056.5165	0.0015
10	1	10	9	0	9	6077.3330	6077.3339	-0.0009

11	0	11	10	1	10	6120.1200	6120.1221	-0.0021
7	2	5	6	1	5	6138.6480	6138.6454	0.0026
13	1	12	12	2	11	6492.6010	6492.6075	-0.0065
15	5	11	15	4	12	6521.1480	6521.1480	0.0000
14	5	10	14	4	11	6528.5060	6528.5172	-0.0112
13	5	8	13	4	9	6531.3920	6531.3855	0.0065
12	5	7	12	4	8	6538.3070	6538.3037	0.0033
12	5	8	12	4	9	6540.1550	6540.1573	-0.0023
11	5	6	11	4	7	6543.5300	6543.5331	-0.0031
11	5	7	11	4	8	6544.4670	6544.4670	0.0000
10	5	5	10	4	6	6547.4370	6547.4280	0.0090
10	5	6	10	4	7	6547.8670	6547.8666	0.0004
9	5	4	9	4	5	6550.2700	6550.2725	-0.0025
9	5	5	9	4	6	6550.4530	6550.4614	-0.0084
7	5	2	7	4	3	6553.7000	6553.6860	0.0140
7	5	3	7	4	4	6553.7000	6553.7105	-0.0105
6	5	1	6	4	2	6554.6030	6554.5962	0.0068
6	5	2	6	4	3	6554.6050	6554.6028	0.0022
5	5	0	5	4	1	6555.1500	6555.1536	-0.0036
5	5	1	5	4	2	6555.1500	6555.1549	-0.0049
8	2	7	7	1	6	6559.7590	6559.7606	-0.0016
5	3	3	4	2	2	6593.0720	6593.0721	-0.0001
5	3	2	4	2	2	6593.3750	6593.3788	-0.0038
11	1	11	10	0	10	6594.4370	6594.4271	0.0099
5	3	3	4	2	3	6603.0780	6603.0737	0.0043
5	3	2	4	2	3	6603.3810	6603.3804	0.0006
7	2	5	6	1	6	6673.0540	6673.0476	0.0064
12	0	12	11	1	11	6733.0870	6733.0842	0.0028

Table S4. Rotational transition frequencies of Dimer 6.

J'	K_a'	K_c'	J''	K_a''	K_c''	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
10	2	8	10	1	10	3030.9900	3030.9903	-0.0003
4	1	3	3	0	3	3035.0340	3035.0281	0.0059
9	0	9	8	1	7	3575.4220	3575.4261	-0.0041
5	1	4	4	0	4	3581.2150	3581.2176	-0.0026
2	2	0	1	1	0	3743.3520	3743.3587	-0.0067
2	2	1	1	1	1	3753.4000	3753.3911	0.0089
10	0	10	9	1	8	4039.0140	4039.0124	0.0016
6	1	5	5	0	5	4132.9890	4132.9864	0.0026

3	2	2	2	1	2	4283.9500	4283.9547	-0.0047
12	3	10	12	2	10	4452.8210	4452.8307	-0.0097
10	3	8	10	2	8	4482.6680	4482.6642	0.0038
9	3	7	9	2	7	4492.5210	4492.5113	0.0097
8	3	6	8	2	6	4499.7000	4499.7033	-0.0033
7	3	5	7	2	5	4504.7520	4504.7484	0.0036
6	3	4	6	2	4	4508.1070	4508.1127	-0.0057
5	3	3	5	2	3	4510.2210	4510.2122	0.0088
4	3	2	4	2	2	4511.4010	4511.4078	-0.0068
3	3	0	3	2	1	4511.9950	4512.0019	-0.0069
3	3	0	3	2	2	4512.4240	4512.4272	-0.0032
4	3	1	4	2	3	4512.6890	4512.6865	0.0025
5	3	2	5	2	4	4513.2030	4513.1996	0.0034
6	3	3	6	2	5	4514.1000	4514.0951	0.0049
7	3	4	7	2	6	4515.5260	4515.5295	-0.0035
8	3	5	8	2	7	4517.6990	4517.6890	0.0100
9	3	6	9	2	8	4520.7960	4520.7905	0.0055
10	3	7	10	2	9	4525.0790	4525.0839	-0.0049
11	3	8	11	2	10	4530.8560	4530.8536	0.0024
7	1	6	6	0	6	4690.6120	4690.6180	-0.0060
4	2	2	3	1	2	4760.1280	4760.1324	-0.0044
4	2	3	3	1	3	4819.5550	4819.5599	-0.0049
8	1	7	7	0	7	5254.4470	5254.4494	-0.0024
5	2	3	4	1	3	5262.0200	5262.0173	0.0027
5	2	4	4	1	4	5360.2040	5360.2101	-0.0061
6	2	4	5	1	4	5760.1250	5760.1190	0.0060
6	2	5	5	1	5	5905.9170	5905.9146	0.0024
7	2	5	6	1	5	6254.9680	6254.9634	0.0046

Table S5. Rotational transition frequencies of Dimer **9**.

J'	K_a'	K_c'	J''	K_a''	K_c''	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
5	0	5	4	0	4	2475.5870	2475.5975	-0.0105
5	4	2	4	4	1	2493.6850	2493.6839	0.0011
5	4	1	4	4	0	2494.4540	2494.4649	-0.0109
5	3	3	4	3	2	2495.2890	2495.3034	-0.0144
5	3	2	4	3	1	2513.0970	2513.0981	-0.0011
5	2	3	4	2	2	2970.5730	2970.5732	-0.0002
5	1	4	4	1	3	2991.9360	2991.9306	0.0054
4	1	4	3	0	3	2993.2590	2993.2515	0.0075

11	2	10	11	1	11	2994.7160	2994.7183	-0.0023
7	0	7	6	1	6	3015.5740	3015.5719	0.0021
6	1	6	5	1	5	3465.4710	3465.4717	-0.0007
6	0	6	5	0	5	3489.9140	3489.9113	0.0027
6	2	5	5	2	4	3491.9820	3491.9800	0.0020
6	5	1	5	5	0	3494.3220	3494.3251	-0.0031
6	5	2	5	5	1	3517.9500	3517.9647	-0.0147
6	4	2	5	4	1	3960.2810	3960.2813	-0.0003
6	4	3	5	4	2	3987.6140	3987.5832	0.0308
6	3	4	5	3	3	3990.6430	3990.6409	0.0021
6	3	3	5	3	2	4020.2640	4020.2619	0.0021
6	2	4	5	2	3	4454.9900	4454.9907	-0.0007
6	1	5	5	1	4	4484.9070	4484.9050	0.0020
17	2	16	17	1	17	4489.2260	4489.2244	0.0016
5	1	5	4	0	4	4494.2380	4494.2345	0.0035
8	0	8	7	1	7	4522.4510	4522.4483	0.0027
7	1	7	6	1	6	4949.5930	4949.5891	0.0039
7	0	7	6	0	6	4981.8330	4981.8378	-0.0048
7	2	6	6	2	5	4987.7280	4987.7208	0.0072
7	6	2	6	6	1	4994.5960	4994.5925	0.0035
7	6	1	6	6	0	5024.5070	5024.5082	-0.0012
7	5	2	6	5	1	5444.0630	5444.0663	-0.0033
7	5	3	6	5	2	5478.3400	5478.3456	-0.0056
7	4	3	6	4	2	5486.1210	5486.1206	0.0004
7	4	4	6	4	3	5488.7940	5488.8022	-0.0082
7	3	5	6	3	4	5488.9950	5488.9908	0.0042
7	3	4	6	3	3	5526.4250	5526.4251	-0.0001
7	2	5	6	2	4	5938.4180	5938.4129	0.0051
7	1	6	6	1	5	5974.3940	5974.3962	-0.0022
6	1	6	5	0	5	5996.2250	5996.2318	-0.0068
9	0	9	8	1	8	6028.1870	6028.1816	0.0054

Table S6. Rotational transition frequencies of Dimer 14.

J'	K_a'	K_c'	J''	K_a''	K_c''	Obs/ MHz	Cal/ MHz	Obs - Cal/ MHz
7	1	7	6	1	6	2170.7860	2170.7866	-0.0006
7	0	7	6	0	6	2187.9800	2187.9771	0.0029
7	2	6	6	2	5	2188.6860	2188.6890	-0.0030
7	2	5	6	2	4	2189.4790	2189.4753	0.0037
7	1	6	6	1	5	2206.3870	2206.3888	-0.0018
8	1	8	7	1	7	2480.8200	2480.8198	0.0002

8	0	8	7	0	7	2500.2530	2500.2533	-0.0003
8	2	7	7	2	6	2501.3060	2501.3004	0.0056
8	2	6	7	2	5	2502.4830	2502.4794	0.0036
8	1	7	7	1	6	2521.5010	2521.5028	-0.0018
4	1	4	3	0	3	2606.8120	2606.8025	0.0095
4	1	3	3	0	3	2657.6690	2657.6753	-0.0063
9	1	9	8	1	8	2790.8220	2790.8217	0.0003
9	0	9	8	0	8	2812.4130	2812.4132	-0.0002
9	2	8	8	2	7	2813.8920	2813.8885	0.0035
9	2	7	8	2	6	2815.5710	2815.5718	-0.0008
9	1	8	8	1	7	2836.5840	2836.5825	0.0015
5	1	5	4	0	4	2906.8480	2906.8499	-0.0019
5	1	4	4	0	4	2983.1580	2983.1571	0.0009
10	1	10	9	1	9	3100.7900	3100.7889	0.0011
10	0	10	9	0	9	3124.4410	3124.4427	-0.0017
10	2	9	9	2	8	3126.4510	3126.4502	0.0008
10	2	8	9	2	7	3128.7630	3128.7630	0.0000
10	1	9	9	1	8	3151.6210	3151.6233	-0.0023
6	1	6	5	0	5	3204.4420	3204.4428	-0.0008
6	1	5	5	0	5	3311.2650	3311.2691	-0.0041
11	1	11	10	1	10	3410.7170	3410.7178	-0.0008
11	0	11	10	0	10	3436.3270	3436.3281	-0.0011
11	2	10	10	2	9	3438.9820	3438.9829	-0.0009
11	2	9	10	2	8	3442.0630	3442.0634	-0.0004
11	1	10	10	1	9	3466.6210	3466.6207	0.0003
7	1	7	6	0	6	3499.6270	3499.6306	-0.0036
15	0	15	14	1	14	3548.1600	3548.1646	-0.0046
7	1	6	6	0	6	3642.0580	3642.0590	-0.0010
12	1	12	11	1	11	3720.6060	3720.6052	0.0008
12	0	12	11	0	11	3748.0530	3748.0559	-0.0029
12	2	11	11	2	10	3751.4840	3751.4834	0.0006
12	2	10	11	2	9	3755.4850	3755.4828	0.0022
17	2	16	17	1	16	3761.1230	3761.1150	0.0080
9	3	7	10	2	8	3774.9970	3774.9887	0.0083
9	3	6	10	2	8	3774.9970	3775.0111	-0.0141
12	1	11	11	1	10	3781.5700	3781.5697	0.0003
9	3	7	10	2	9	3781.9440	3781.9334	0.0106
9	3	6	10	2	9	3781.9440	3781.9558	-0.0118
18	2	16	18	1	17	3784.0480	3784.0514	-0.0034
17	2	15	17	1	16	3815.0270	3815.0356	-0.0086

15	2	14	15	1	14	3842.7980	3842.7970	0.0010
16	2	14	16	1	15	3845.7750	3845.7751	-0.0001
15	2	13	15	1	14	3876.0260	3876.0263	-0.0003
14	2	13	14	1	13	3880.1070	3880.1100	-0.0030
16	0	16	15	1	15	3891.3230	3891.3210	0.0020
14	2	12	14	1	13	3905.5480	3905.5560	-0.0080
13	2	12	13	1	12	3915.0370	3915.0361	0.0009
13	2	11	13	1	12	3934.1500	3934.1426	0.0074
12	2	11	12	1	11	3947.5540	3947.5526	0.0014
12	2	10	12	1	11	3961.5750	3961.5773	-0.0023
8	1	7	7	0	7	3975.5830	3975.5847	-0.0017
11	2	10	11	1	10	3977.6510	3977.6389	0.0121
10	2	9	10	1	9	4005.2770	4005.2768	0.0002
10	2	8	10	1	9	4012.2230	4012.2215	0.0015
13	1	13	12	1	12	4030.4470	4030.4477	-0.0007
9	2	7	9	1	8	4035.0830	4035.0819	0.0011
8	2	7	8	1	7	4053.1470	4053.1439	0.0031
8	2	6	8	1	7	4056.0920	4056.0926	-0.0006
13	0	13	12	0	12	4059.6143	4059.6132	0.0012
13	2	12	12	2	11	4063.9524	4063.9490	0.0034
13	2	11	12	2	10	4069.0320	4069.0309	0.0011
7	2	6	7	1	6	4073.3460	4073.3463	-0.0003
7	2	5	7	1	6	4075.1170	4075.1159	0.0011
9	1	9	8	0	8	4083.0380	4083.0417	-0.0037
8	3	5	9	2	7	4089.3260	4089.3367	-0.0107
8	3	6	9	2	7	4089.3260	4089.3255	0.0005
6	2	5	6	1	5	4091.0390	4091.0461	-0.0071
6	2	4	6	1	5	4092.0300	4092.0294	0.0006
8	3	6	9	2	8	4093.9640	4093.9574	0.0066
8	3	5	9	2	8	4093.9640	4093.9686	-0.0046
13	1	12	12	1	11	4096.4650	4096.4655	-0.0005
5	2	4	5	1	4	4106.2380	4106.2340	0.0040
5	2	3	5	1	4	4106.7250	4106.7258	-0.0008
4	2	3	4	1	3	4118.8990	4118.9023	-0.0033
4	2	2	4	1	3	4119.1100	4119.1130	-0.0030
2	2	1	2	1	1	4136.6590	4136.6554	0.0036
2	2	0	2	1	1	4136.6610	4136.6694	-0.0084
2	2	1	2	1	2	4151.9230	4151.9177	0.0053
2	2	0	2	1	2	4151.9230	4151.9318	-0.0088
4	2	3	4	1	4	4169.7760	4169.7751	0.0009

4	2	2	4	1	4	4169.9830	4169.9859	-0.0029
5	2	3	5	1	5	4183.0330	4183.0330	0.0000
6	2	5	6	1	6	4197.8720	4197.8724	-0.0004
6	2	4	6	1	6	4198.8580	4198.8557	0.0023
7	2	6	7	1	7	4215.7760	4215.7747	0.0013
7	2	5	7	1	7	4217.5440	4217.5444	-0.0004
8	2	7	8	1	8	4236.2550	4236.2554	-0.0004
8	2	6	8	1	8	4239.2030	4239.2040	-0.0010
9	2	8	9	1	9	4259.3200	4259.3221	-0.0021
9	2	7	9	1	9	4263.9520	4263.9541	-0.0021
10	2	9	10	1	10	4284.9860	4284.9835	0.0025
10	2	8	10	1	10	4291.9300	4291.9282	0.0018
9	1	8	8	0	8	4311.9140	4311.9139	0.0001
11	2	10	11	1	11	4313.2560	4313.2485	0.0075
11	2	9	11	1	11	4323.2760	4323.2737	0.0023
14	1	14	13	1	13	4340.2440	4340.2423	0.0017
12	2	11	12	1	12	4344.1280	4344.1267	0.0013
16	4	12	17	3	14	4350.1500	4350.1526	-0.0026
16	4	13	17	3	14	4350.1500	4350.1483	0.0017
16	4	13	17	3	15	4351.0960	4351.0852	0.0108
16	4	12	17	3	15	4351.0960	4351.0896	0.0064
14	0	14	13	0	13	4370.9870	4370.9875	-0.0005
10	1	10	9	0	9	4371.4150	4371.4174	-0.0024
14	2	13	13	2	12	4376.3780	4376.3767	0.0013
13	2	12	13	1	13	4377.6310	4377.6280	0.0030
14	2	12	13	2	11	4382.7180	4382.7162	0.0018
13	2	11	13	1	13	4396.7320	4396.7345	-0.0025
7	3	5	8	2	6	4403.2090	4403.2098	-0.0008
7	3	4	8	2	6	4403.2090	4403.2148	-0.0058
7	3	5	8	2	7	4406.1580	4406.1584	-0.0004
7	3	4	8	2	7	4406.1580	4406.1635	-0.0055
14	1	13	13	1	12	4411.3020	4411.3029	-0.0009
14	2	13	14	1	14	4413.7640	4413.7624	0.0016
14	2	12	14	1	14	4439.2120	4439.2084	0.0036
15	2	14	15	1	15	4452.5400	4452.5400	0.0000
15	2	13	15	1	15	4485.7740	4485.7693	0.0047
16	2	15	16	1	16	4493.9740	4493.9709	0.0031
16	2	14	16	1	16	4536.6170	4536.6234	-0.0064
17	2	16	17	1	17	4538.0660	4538.0647	0.0013
18	0	18	17	1	17	4580.6790	4580.6775	0.0015

18	2	17	18	1	18	4584.8340	4584.8309	0.0031
17	2	15	17	1	17	4591.9780	4591.9853	-0.0073
15	1	15	14	1	14	4649.9860	4649.9861	-0.0001
10	1	9	9	0	9	4651.1250	4651.1241	0.0009
11	1	11	10	0	10	4657.6940	4657.6925	0.0015
15	0	15	14	0	14	4682.1670	4682.1675	-0.0005
15	2	14	14	2	13	4688.7630	4688.7637	-0.0007
15	3	13	14	3	12	4691.0640	4691.0673	-0.0033
15	3	12	14	3	11	4691.2220	4691.2169	0.0051
15	2	13	14	2	12	4696.5460	4696.5470	-0.0010
6	3	4	7	2	5	4716.7360	4716.7320	0.0040
6	3	3	7	2	5	4716.7360	4716.7340	0.0020
6	3	3	7	2	6	4718.5000	4718.5037	-0.0037
6	3	4	7	2	6	4718.5000	4718.5017	-0.0017
15	1	14	14	1	13	4726.0790	4726.0767	0.0023
2	2	1	1	1	0	4767.1200	4767.1150	0.0050
2	2	0	1	1	0	4767.1210	4767.1290	-0.0080
2	2	1	1	1	1	4772.2130	4772.2025	0.0105
2	2	0	1	1	1	4772.2130	4772.2165	-0.0035
12	1	12	11	0	11	4941.9670	4941.9695	-0.0025
16	1	16	15	1	15	4959.6780	4959.6763	0.0017
16	0	16	15	0	15	4993.1420	4993.1425	-0.0005
16	2	15	15	2	14	5001.1080	5001.1072	0.0008
16	3	14	15	3	13	5003.8780	5003.8784	-0.0004
16	3	13	15	3	12	5004.0920	5004.0854	0.0066
16	2	14	15	2	13	5010.5300	5010.5303	-0.0003
3	2	2	2	1	2	5089.9877	5089.9858	0.0019
3	2	1	2	1	2	5090.0542	5090.0560	-0.0018
13	1	13	12	0	12	5224.3580	5224.3613	-0.0033
17	1	17	16	1	16	5269.3100	5269.3103	-0.0003
17	0	17	16	0	16	5303.9010	5303.9028	-0.0018
17	2	16	16	2	15	5313.4030	5313.4041	-0.0011
17	3	15	16	3	14	5316.6960	5316.7003	-0.0043
17	3	14	16	3	13	5316.9770	5316.9810	-0.0040
17	2	15	16	2	14	5324.6700	5324.6722	-0.0022
12	1	11	11	0	11	5338.5420	5338.5436	-0.0016
17	1	16	16	1	15	5355.4120	5355.4118	0.0002
4	2	3	3	1	2	5379.7910	5379.7881	0.0029
4	2	2	3	1	2	5379.9910	5379.9989	-0.0079
4	2	3	3	1	3	5410.3130	5410.3124	0.0006

4	2	2	3	1	3	5410.5240	5410.5232	0.0008
14	1	14	13	0	13	5504.9940	5504.9905	0.0035
18	1	18	17	1	17	5578.8870	5578.8857	0.0013
18	0	18	17	0	17	5614.4446	5614.4403	0.0043
18	2	17	17	2	16	5625.6520	5625.6519	0.0001
18	3	16	17	3	15	5629.5340	5629.5324	0.0016
18	3	15	17	3	14	5629.9090	5629.9064	0.0026
18	2	16	17	2	15	5638.9740	5638.9775	-0.0035
18	1	17	17	1	16	5669.9620	5669.9617	0.0003
5	2	4	4	1	3	5682.3000	5682.3100	-0.0100
5	2	3	4	1	3	5682.8100	5682.8017	0.0083
13	1	12	12	0	12	5686.9450	5686.9532	-0.0082
5	2	4	4	1	4	5733.1850	5733.1828	0.0022
5	2	3	4	1	4	5733.6730	5733.6746	-0.0016
15	1	15	14	0	14	5783.9910	5783.9890	0.0020
19	1	19	18	1	18	5888.3980	5888.4001	-0.0021
11	4	7	12	3	9	5915.9910	5915.9963	-0.0053
11	4	8	12	3	9	5915.9910	5915.9961	-0.0051
11	4	8	12	3	10	5916.1150	5916.1173	-0.0023
11	4	7	12	3	10	5916.1150	5916.1176	-0.0026
19	0	19	18	0	18	5924.7490	5924.7480	0.0010
19	2	18	18	2	17	5937.8500	5937.8475	0.0025
19	3	16	18	3	15	5942.8610	5942.8646	-0.0036
19	2	17	18	2	16	5953.4490	5953.4493	-0.0003
6	2	5	5	1	4	5982.2890	5982.2912	-0.0022
6	2	4	5	1	4	5983.2820	5983.2745	0.0075
19	1	18	18	1	17	5984.4240	5984.4252	-0.0012
14	1	13	13	0	13	6038.6420	6038.6429	-0.0009
6	2	5	5	1	5	6058.6030	6058.5983	0.0047
6	2	4	5	1	5	6059.5800	6059.5817	-0.0017
16	1	16	15	0	15	6061.4960	6061.4978	-0.0018
20	1	20	19	1	19	6197.8550	6197.8516	0.0034
20	0	20	19	0	19	6234.8220	6234.8208	0.0012
20	3	18	19	3	17	6255.2290	6255.2252	0.0038
20	3	17	19	3	16	6255.8560	6255.8589	-0.0029
20	2	18	19	2	17	6268.0920	6268.0896	0.0024
7	2	6	6	1	5	6279.7380	6279.7351	0.0029
7	2	5	6	1	5	6281.5060	6281.5047	0.0013
20	1	19	19	1	18	6298.7990	6298.7963	0.0027
17	1	17	16	0	16	6337.6620	6337.6656	-0.0036

7	2	6	6	1	6	6386.5600	6386.5613	-0.0013
7	2	5	6	1	6	6388.3350	6388.3310	0.0040
15	1	14	14	0	14	6393.7320	6393.7321	-0.0001
21	1	21	20	1	20	6507.2390	6507.2383	0.0007
21	0	21	20	0	20	6544.6540	6544.6551	-0.0011
21	2	20	20	2	19	6562.0680	6562.0713	-0.0033
21	2	19	20	2	18	6582.8970	6582.8981	-0.0011
21	1	20	20	1	19	6613.0720	6613.0684	0.0036

Table S7. Comparison of the experimental and calculated^a rotational constants.

Rotational constants	Percentage error ^b				
	Dimer 1	Dimer 3	Dimer 6	Dimer 9	Dimer 14
A	-0.5	1.1	-0.4	1.6	-3.4
B	-0.7	-2.0	0.0	-2.0	-0.1
C	-1.5	-1.6	-0.2	-2.2	-0.6

^a At the B3LYP-D3BJ/def2-TZVP level.

^b Percentage Error = 100% x (Exp. – Calc.) / Exp.

Table S8. Calculated centrifugal distortion constants of the five observed binary TFP conformers at the B3LYP-D3BJ/def2-TZVP level of theory.

	1 TFPG-e TFPG-g+	3 TFPG-g+ TFPG+g-	6 TFPG-g- TFPG+g-	9 TFPG-g+ TFPTt	14 TFPTt TFPG-g+
D_K / kHz	0.513748	0.605328	1.781720	2.547081	5.22448
D_{JK} / kHz	0.038212	-0.172014	-0.539706	-0.683106	-0.33920
D_J / kHz	0.044025	0.114074	0.080929	0.091797	0.019248
d_1 / kHz	-0.004392	-0.021487	-0.005360	0.003424	-0.001240
d_2 / kHz	-0.000241	-0.001789	0.000101	0.000018	0.000015

Table S9. The counterpoise corrected interaction energy and deformation energy (in kJ mol⁻¹) of the selective low-energy binary TFP conformers at the B3LYP-D3BJ/def2-TZVP level of theory.^a

Binary TFP conformers ^b	ΔE_{def} H acceptor (A)	ΔE_{def} H donor (D)	ΔE^{int}
1 TFPG-eTFPG-g+	0.6	9.0	-40.0
2 TFPG-g+TFPG+g-	4.7	0.4	-35.3
3 TFPG-g+TFPG+g-	0.4	2.8	-33.6
4 TFPG-g+TFPG-g+	0.4	2.8	-32.8
5 TFPG-g+TFPG+g-	6.0	0.9	-35.8
6 TFPG-g-TFPG+g-	0.6	0.6	-39.1
7 TFPG-g+TFPG-g+	3.0	0.8	-32.2
8 TFPG-g+TFPG+g-	3.9	0.2	-32.6
9 TFPG-g+TFPTt	3.1	0.4	-34.4
10 TFPG-g+TFPG-g+	5.3	0.3	-34.0
11 TFPG-tTFPG+g-	1.0	0.8	-35.9
12 TFPG-g+TFPTt	5.4	0.5	-35.7
13 TFPG-g-TFPG-g-	0.6	0.6	-36.2
14 TFPTtTFPG-g+	0.4	0.5	-31.3
15 TFPG-g+TFPTg-	4.3	0.4	-35.9
16 TFPTg+TFPG-g+	1.0	0.5	-33.0
17 TFPTg-TFPG-g+	0.4	0.5	-32.6
18 TFPTtTFPG-g+	0.3	0.7	-30.6
19 TFPTg+TFPG-g+	0.5	0.5	-32.9
20 TFPG-g-TFPG-g+	1.0	1.1	-36.4
43 TFPTtTFPTt	0.3	0.4	-28.6
54 TFPTg-TFPTt	0.4	0.4	-30.3
56 TFPTg-TFPTt	0.5	0.4	-30.2
57 TFPTtTFPTg-	0.3	0.3	-29.4
60 TFPTg-TFPTg-	0.4	0.4	-31.3

^a $\Delta E_{\text{def}} = E_{D/A}^{\text{dimer}}(DA) - E_{D/A}^{\text{monomer}}(D/A)$; $E^{\text{int}} = E_{DA}^{\text{dimer}}(DA) - E_A^{\text{dimer}}(DA) - E_D^{\text{dimer}}(DA)$

Here, superscript refers to the molecular system where the calculations were performed while subscript refers to the molecule or the subunits being calculated. *D* stand for the donor fragment and *A* for the acceptor fragment, while *DA* stands for the dimer. Brackets refer to the basis used.