

Examining the gas-phase homodimers of 3,3,3-trifluoro-1,2-epoxypropane using quantum chemistry and microwave spectroscopy

Supporting Information

Mark D. Marshall,^a Helen O. Leung,^a Sérgio Domingos,^{b,†} Anna Krin,^{b,†} Melanie Schnell,^{b,c}

Nathan A. Seifert,^{d,§} Yunjie Xu,^d Wolfgang Jäger^d

^aDepartment of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA, 01002-5000, USA

^bDeutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany

^cInstitut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth-

Str.1, 24118 Kiel, Germany

^dDepartment of Chemistry, University of Alberta, 11227 Saskatchewan Drive, Edmonton, AB,

Canada

[†]Present Address: CFisUC, Department of Physics, University of Coimbra, 3004-516 Coimbra,

Portugal

[†]Present Address: ???

[§]Present Address: Department of Chemistry and Chemical & Biomedical Engineering,

University of New Haven, 300 Boston Post Rd, West Haven, CT, 06516, USA

Address for correspondence: Prof. Mark D. Marshall
Department of Chemistry
Amherst College
P.O. Box 5000
Amherst, MA 01002-5000
Telephone: (413) 542-2006
Fax: (413) 542-2735
E-mail: mdmarshall@amherst.edu

*Corresponding authors. Fax: +1-413-542-2735; *e-mail addresses*: hleung@amherst.edu (H.O. Leung), mdmarshall@amherst.edu (M.D. Marshall).

The authors declare no competing financial interest.

Table S1: Rotational constants, dipole moments, and relative energies of three isomers of homochiral (TFO)₂**B3LYP/6-311++g(p,d)**

	Without BSSE Correction			With BSSE Correction		
	Isomer (i)	Isomer (ii)	Isomer (iii)	Isomer (i)	Isomer (ii)	Isomer (iii)
<i>A</i> /MHz	1280	1190	1369	1287	1196	1395
<i>B</i> /MHz	270	305	285	266	299	276
<i>C</i> /MHz	249	273	272	246	268	264
$ \mu_a $ / D	0.00	2.17	2.06	0.00	2.13	2.04
$ \mu_b $ / D	3.35	3.27	0.11	3.36	3.21	0.20
$ \mu_c $ / D	0.00	0.06	0.74	0.00	0.06	0.67
Equilibrium Energy/ cm ⁻¹	29.39	53.91	0.00	6.94	35.96	0.00
Zero Point Energy/ cm ⁻¹	17.78	41.26	0.00	0.66	26.56	0.00

B3LYP/6-311++g(2p,2d)

	Without BSSE Correction			With BSSE Correction		
	Isomer (i)	Isomer (ii)	Isomer (iii)	Isomer (i)	Isomer (ii)	Isomer (iii)
<i>A</i> /MHz	1285	1168	1334	1295	1185	1379
<i>B</i> /MHz	269	316	294	264	303	278
<i>C</i> /MHz	248	282	280	244	271	266
$ \mu_a $ / D	0.00	1.89	1.92	0.00	1.94	1.93
$ \mu_b $ / D	3.21	3.51	0.10	3.13	3.26	0.10
$ \mu_c $ / D	0.00	0.01	0.80	0.00	0.05	0.69
Equilibrium Energy/ cm ⁻¹	8.45	36.78	0.00	0.00	44.12	28.43
Zero Point Energy/ cm ⁻¹	3.51	21.51	0.00	0.00	27.00	22.39

B3LYP/def2tzvp

	Without BSSE Correction			With BSSE Correction		
	Isomer (i)	Isomer (ii)	Isomer (iii)	Isomer (i)	Isomer (ii)	Isomer (iii)
<i>A</i> /MHz	1290	1171	1375	1290	1178	1383
<i>B</i> /MHz	266	311	282	265	305	278
<i>C</i> /MHz	245	278	269	245	273	266
$ \mu_a $ / D	0.00	1.74	1.87	0.00	1.78	1.87
$ \mu_b $ / D	2.99	3.36	0.12	3.06	3.22	0.13
$ \mu_c $ / D	0.00	0.01	0.63	0.00	0.03	0.63
Equilibrium Energy/ cm ⁻¹	0.00	57.18	40.67	0.00	53.08	38.86
Zero Point Energy/ cm ⁻¹	0.00	38.63	42.36	0.00	38.41	36.43

Table S1: Rotational constants, dipole moments, and relative energies of three isomers of homochiral (TFO)₂**MP2/6-311++g(p,d)**

	Without BSSE Correction			With BSSE Correction		
	Isomer (i)	Isomer (ii)	Isomer (iii)	Isomer (i)	Isomer (ii)	Isomer (iii)
<i>A</i> /MHz	1279	1152	1321	1300	N/A	1408
<i>B</i> /MHz	277	338	304	262	N/A	268
<i>C</i> /MHz	254	298	288	242	N/A	257
$ \mu_a $ / D	0.00	1.93	1.93	0.00	N/A	1.91
$ \mu_b $ / D	3.22	3.83	0.18	3.20	N/A	0.18
$ \mu_c $ / D	0.00	0.09	0.79	0.00	N/A	0.57
Equilibrium Energy/ cm ⁻¹	0.00	72.34	31.21	0.00	N/A	64.83
Zero Point Energy/ cm ⁻¹	0.00	56.62	32.04	0.00	N/A	49.82

MP2/6-311++g(2p,2d)

	Without BSSE Correction			With BSSE Correction		
	Isomer (i)	Isomer (ii)	Isomer (iii)	Isomer (i)	Isomer (ii)	Isomer (iii)
<i>A</i> /MHz	1289	1162	1315	1308	1180	1623
<i>B</i> /MHz	278	353	312	266	306	242
<i>C</i> /MHz	256	313	295	246	274	236
$ \mu_a $ / D	0.00	2.19	1.82	0.00	1.33	2.10
$ \mu_b $ / D	3.09	3.86	0.25	3.07	3.62	1.25
$ \mu_c $ / D	0.00	0.11	0.75	0.00	0.04	0.12
Equilibrium Energy/ cm ⁻¹	0.00	74.39	51.18	0.00	102.48	107.58
Zero Point Energy/ cm ⁻¹	0.00	55.75	52.02	0.00	72.65	73.30

MP2/def2tzvp

	Without BSSE Correction			With BSSE Correction		
	Isomer (i)	Isomer (ii)	Isomer (iii)	Isomer (i)	Isomer (ii)	Isomer (iii)
<i>A</i> /MHz	1299	N/A	1337	1306	N/A	1361
<i>B</i> /MHz	273	N/A	299	265	N/A	285
<i>C</i> /MHz	252	N/A	284	246	N/A	271
$ \mu_a $ / D	0.00	N/A	1.73	0.00	N/A	1.77
$ \mu_b $ / D	2.98	N/A	0.16	2.97	N/A	0.06
$ \mu_c $ / D	0.00	N/A	0.09	0.00	N/A	0.66
Equilibrium Energy/ cm ⁻¹	0.00	N/A	132.04	0.00	N/A	88.46
Zero Point Energy/ cm ⁻¹	0.00	N/A	124.00	0.00	N/A	75.72

Table S2: Rotational constants, dipole moments, and relative energies of three isomers of heterochiral (TFO)₂**B3LYP/6-311++g(p,d)**

	Without BSSE Correction			With BSSE Correction		
	Isomer (iv)	Isomer (v)	Isomer (vi)	Isomer (iv)	Isomer (v)	Isomer (vi)
<i>A</i> /MHz	1713	1422	1164	1710	1433	1251
<i>B</i> /MHz	228	266	314	227	262	276
<i>C</i> /MHz	222	250	281	221	246	254
$ \mu_a $ / D	0.00	1.45	2.46	0.00	1.40	2.65
$ \mu_b $ / D	0.00	0.99	3.24	0.00	0.97	2.11
$ \mu_c $ / D	0.00	0.16	0.55	0.00	0.16	0.12
Equilibrium Energy/ cm ⁻¹	23.56	0.00	149.99	22.95	0.00	154.63
Zero Point Energy/ cm ⁻¹	17.78	0.00	142.00	19.09	0.00	156.49

B3LYP/6-311++g(2p,2d)

	Without BSSE Correction			With BSSE Correction		
	Isomer (iv)	Isomer (v)	Isomer (vi)	Isomer (iv)	Isomer (v)	Isomer (vi)
<i>A</i> /MHz	1721	1462	1157	1717	1452	1165
<i>B</i> /MHz	228	259	319	226	258	310
<i>C</i> /MHz	222	245	284	220	243	278
$ \mu_a $ / D	0.00	1.33	2.32	0.00	1.34	2.31
$ \mu_b $ / D	0.00	1.13	3.25	0.00	1.03	3.20
$ \mu_c $ / D	0.00	0.09	0.60	0.00	0.13	0.57
Equilibrium Energy/ cm ⁻¹	9.01	0.00	123.22	4.42	0.00	143.53
Zero Point Energy/ cm ⁻¹	16.46	0.00	114.57	15.58	0.00	142.44

B3LYP/def2tzvp

	Without BSSE Correction			With BSSE Correction		
	Isomer (iv)	Isomer (v)	Isomer (vi)	Isomer (iv)	Isomer (v)	Isomer (vi)
<i>A</i> /MHz	1719	1475	1163	1719	1460	1168
<i>B</i> /MHz	227	256	313	225	256	308
<i>C</i> /MHz	221	242	280	220	242	276
$ \mu_a $ / D	0.00	1.26	2.27	0.00	1.25	2.26
$ \mu_b $ / D	0.00	1.07	3.07	0.00	0.98	3.03
$ \mu_c $ / D	0.00	0.10	0.56	0.00	0.13	0.54
Equilibrium Energy/ cm ⁻¹	0.00	12.97	147.22	0.00	6.89	141.82
Zero Point Energy/ cm ⁻¹	0.00	3.73	134.98	2.19	0.00	133.88

Table S2: Rotational constants, dipole moments, and relative energies of three isomers of heterochiral (TFO)₂**MP2/6-311++g(p,d)**

	Without BSSE Correction			With BSSE Correction		
	Isomer (iv)	Isomer (v)	Isomer (vi)	Isomer (iv)	Isomer (v)	Isomer (vi)
<i>A</i> /MHz	1741	N/A	1164	1732	N/A	1192
<i>B</i> /MHz	230	N/A	324	223	N/A	294
<i>C</i> /MHz	224	N/A	289	218	N/A	266
$ \mu_a $ / D	0.00	N/A	2.38	0.00	N/A	2.30
$ \mu_b $ / D	0.00	N/A	3.37	0.00	N/A	3.13
$ \mu_c $ / D	0.00	N/A	0.67	0.00	N/A	0.60
Equilibrium Energy/ cm ⁻¹	0.00	N/A	142.67	0.00	N/A	160.64
Zero Point Energy/ cm ⁻¹	0.00	N/A	126.42	0.00	N/A	137.17

MP2/6-311++g(2p,2d)

	Without BSSE Correction			With BSSE Correction		
	Isomer (iv)	Isomer (v)	Isomer (vi)	Isomer (iv)	Isomer (v)	Isomer (vi)
<i>A</i> /MHz	1755	1536	1161	1750	1549	1188
<i>B</i> /MHz	231	255	339	226	245	304
<i>C</i> /MHz	226	243	300	221	234	274
$ \mu_a $ / D	0.00	1.38	2.38	0.00	1.20	2.25
$ \mu_b $ / D	0.00	1.52	3.37	0.00	1.30	3.11
$ \mu_c $ / D	0.00	0.01	0.73	0.00	0.02	0.61
Equilibrium Energy/ cm ⁻¹	0.00	96.93	144.81	0.00	71.62	174.50
Zero Point Energy/ cm ⁻¹	0.00	75.94	127.95	0.00	42.14	146.39

MP2/def2tzvp

	Without BSSE Correction			With BSSE Correction		
	Isomer (iv)	Isomer (v)	Isomer (vi)	Isomer (iv)	Isomer (v)	Isomer (vi)
<i>A</i> /MHz	1759	N/A	1175	1752	N/A	
<i>B</i> /MHz	229	N/A	320	225	N/A	
<i>C</i> /MHz	223	N/A	285	220	N/A	
$ \mu_a $ / D	0.00	N/A	2.24	0.00	N/A	
$ \mu_b $ / D	0.00	N/A	3.14	0.00	N/A	
$ \mu_c $ / D	0.00	N/A	0.66	0.00	N/A	
Equilibrium Energy/ cm ⁻¹	0.00	N/A	191.98	0.00	N/A	155.15
Zero Point Energy/ cm ⁻¹	0.00	N/A	170.09	0.00	N/A	

Table S3: Coordinates in the principal inertial axis system for the theoretical structures (calculated using B3LYP/def2-TZVP with GD3BJ empirical dispersion) of homochiral and heterochiral (TFO)₂

	Isomer (i)			Isomer (ii)			Isomer (iii)		
	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>
O	1.2929	-1.1025	-0.8229	1.1171	-1.0933	-0.9967	1.1574	-1.5544	0.2715
C	1.8384	-1.8288	0.2893	1.5485	-1.8949	0.1158	1.3710	-1.4207	-1.1458
C	1.7714	-0.3716	0.2935	1.5244	-0.4374	0.1917	2.4515	-1.2116	-0.1851
C	2.9967	0.4704	0.0450	2.7927	0.3713	0.0894	2.9302	0.1745	0.1655
H	1.1118	-2.3705	0.8830	0.7580	-2.4418	0.6145	1.3476	-2.3530	-1.6983
H	2.7821	-2.3216	0.0891	2.4922	-2.4052	-0.0347	0.8754	-0.5697	-1.5962
H	1.0191	0.1305	0.8928	0.7453	0.0686	0.7529	3.2225	-1.9637	-0.0465
F	2.6825	1.5844	-0.6432	2.5764	1.5304	-0.5585	3.3029	0.2455	1.4567
F	3.5323	0.8583	1.2195	3.2418	0.6757	1.3242	4.0022	0.4960	-0.5838
F	3.9441	-0.1798	-0.6465	3.7729	-0.2781	-0.5568	1.9912	1.1149	-0.0342
O	-1.2929	-1.1025	0.8229	-1.6479	-1.5219	0.7276	-1.0897	0.7914	-1.1781
C	-1.8384	-1.8288	-0.2893	-2.7601	-1.9220	-0.0845	-1.2365	1.7874	-0.1561
C	-1.7714	-0.3716	-0.2935	-1.9933	-0.7183	-0.3912	-1.5144	0.3791	0.1121
C	-2.9967	0.4704	-0.0450	-2.5261	0.6514	-0.0579	-2.9298	-0.1315	0.1965
H	-1.1118	-2.3705	-0.8830	-2.5960	-2.8071	-0.6886	-0.3090	2.2087	0.2123
H	-2.7821	-2.3216	-0.0891	-3.7282	-1.8346	0.3940	-2.0596	2.4751	-0.3087
H	-1.0191	0.1305	-0.8928	-1.2729	-0.7110	-1.2023	-0.8079	-0.2250	0.6718
F	-2.6825	1.5844	0.6432	-1.5290	1.4629	0.3521	-3.0254	-1.3738	-0.3144
F	-3.5323	0.8583	-1.2195	-3.0786	1.2112	-1.1507	-3.3194	-0.1944	1.4861
F	-3.9441	-0.1798	0.6465	-3.4526	0.6320	0.9112	-3.8060	0.6439	-0.4606

Table S3: Coordinates in the principal inertial axis system for the theoretical structures (calculated using B3LYP/def2-TZVP with GD3BJ empirical dispersion) of homochiral and heterochiral (TFO)₂

Heterochiral (TFO) ₂									
	Isomer (iv)			Isomer (v)			Isomer (vi)		
	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>b</i>	<i>c</i>
O	1.1446	-0.6845	0.7742	1.0211	0.7231	0.8486	-1.2919	1.3717	-0.7680
C	1.3452	-1.4793	-0.4051	1.0839	1.3620	-0.4361	-1.6463	1.8035	0.5550
C	1.8800	-0.1260	-0.3016	1.6936	0.0554	-0.2078	-1.5174	0.3874	0.2260
C	3.3421	0.1208	-0.0323	3.1843	-0.0903	-0.0414	-2.7338	-0.4792	0.0234
H	0.4605	-1.6304	-1.0127	0.1452	1.4061	-0.9759	-0.8452	2.2705	1.1149
H	2.0036	-2.3290	-0.2721	1.7090	2.2460	-0.4712	-2.6320	2.2454	0.6379
H	1.3964	0.6836	-0.8374	1.2102	-0.8397	-0.5841	-0.6458	-0.1695	0.5512
F	3.5101	1.2091	0.7438	3.4779	-1.0610	0.8449	-2.5184	-1.4007	-0.9335
F	3.9900	0.3488	-1.1924	3.7452	-0.4361	-1.2182	-3.0199	-1.1410	1.1638
F	3.9418	-0.9102	0.5802	3.7759	1.0366	0.3817	-3.8221	0.2228	-0.3284
O	-1.1446	0.6845	-0.7742	-1.2136	-1.3075	-0.5685	1.5952	1.5342	0.7609
C	-1.3453	1.4796	0.4049	-1.9614	-2.0437	0.4094	1.8979	1.8279	-0.6139
C	-1.8800	0.1261	0.3016	-1.8732	-0.5874	0.4628	2.7402	0.9379	0.1805
C	-3.3421	-0.1209	0.0323	-3.0187	0.2802	0.0089	2.6850	-0.5583	-0.0004
H	-0.4608	1.6308	1.0125	-1.3658	-2.6232	1.1057	2.2463	2.8379	-0.7980
H	-2.0039	2.3291	0.2718	-2.8622	-2.5137	0.0336	1.1918	1.4195	-1.3248
H	-1.3963	-0.6834	0.8376	-1.2240	-0.0967	1.1801	3.7002	1.2752	0.5596
F	-3.5100	-1.2092	-0.7436	-2.5602	1.3905	-0.6071	2.8717	-1.1931	1.1717
F	-3.9900	-0.3487	1.1924	-3.7450	0.6798	1.0701	3.6610	-0.9569	-0.8380
F	-3.9418	0.9100	-0.5803	-3.8421	-0.3425	-0.8462	1.5120	-0.9771	-0.5030

Table S4: Coordinates in the principal inertial axis system for the lowest energy homochiral (TFO)₂ determined in a structure fit of 4 isotopologues

	<i>a</i>	Δa	<i>b</i>	Δb	<i>c</i>	Δc
O	1.26066	0.00128	-1.05631	0.00103	-0.83345	0.00077
C	1.83484	0.00138	-1.82815	0.00092	0.23455	0.00202
C	1.78394	0.00092	-0.37576	0.00110	0.31544	0.00100
C	2.97921	0.00009	0.45478	0.00009	0.04998	0.00013
H	1.12031	0.00281	-2.39778	0.00236	0.80851	0.00166
H	2.76810	0.00110	-2.30714	0.00003	-0.01637	0.00495
H	1.06529	0.00208	0.11579	0.00268	0.95628	0.00351
F	2.66497	0.00181	1.60488	0.00107	-0.58390	0.00309
F	3.58308	0.00234	0.81844	0.00214	1.20725	0.00044
F	3.89922	0.00131	-0.18576	0.00181	-0.69398	0.00311
O	-1.26066	0.00128	-1.05631	0.00103	0.83345	0.00077
C	-1.83484	0.00138	-1.82815	0.00092	-0.23455	0.00202
C	-1.78394	0.00092	-0.37576	0.00110	-0.31544	0.00100
C	-2.97921	0.00009	0.45478	0.00009	-0.04998	0.00013
H	-1.12031	0.00281	-2.39778	0.00236	-0.80851	0.00166
H	-2.76810	0.00110	-2.30714	0.00003	0.01637	0.00495
H	-1.06529	0.00208	0.11579	0.00268	-0.95628	0.00351
F	-2.66497	0.00181	1.60488	0.00107	0.58390	0.00309
F	-3.58308	0.00234	0.81844	0.00214	-1.20725	0.00044
F	-3.89922	0.00131	-0.18576	0.00181	0.69398	0.00311

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
12	1	11	12	0	12	2039.5359	-0.0052
2	1	2	1	0	1	2046.1116	0.0016
18	3	15	17	4	14	2080.7376	0.0049
5	3	3	6	2	4	2144.9150	-0.0028
6	0	6	5	1	5	2167.5505	0.0005
9	4	6	10	3	7	2189.1502	-0.0004
9	4	5	10	3	8	2193.7170	0.0025
13	5	9	14	4	10	2226.5576	0.0010
13	5	8	14	4	11	2227.4276	-0.0020
13	1	12	13	0	13	2235.0143	-0.0026
17	6	12	18	5	13	2262.3503	0.0010
17	6	11	18	5	14	2262.5044	0.0005
15	2	14	14	3	11	2264.5682	-0.0011
14	2	12	13	3	11	2305.6272	-0.0036
14	1	13	14	0	14	2451.4062	-0.0013
19	3	17	18	4	14	2452.5953	-0.0006
10	1	9	9	2	8	2525.1924	-0.0020
3	1	3	2	0	2	2529.6402	0.0056
14	2	12	14	1	13	2631.8664	0.0054
15	2	13	15	1	14	2635.8058	-0.0019
13	2	11	13	1	12	2643.0885	0.0085
16	2	14	16	1	15	2656.7504	0.0004
4	3	2	5	2	3	2666.6000	0.0017
12	2	10	12	1	11	2667.4288	-0.0013
4	3	1	5	2	4	2676.8790	0.0035
15	1	14	15	0	15	2688.2767	0.0028
17	2	15	17	1	16	2696.3259	0.0015
11	2	9	11	1	10	2702.6703	-0.0101
16	2	15	15	3	12	2716.7055	0.0021
7	0	7	6	1	6	2728.1596	-0.0001
12	5	8	13	4	9	2744.8442	0.0002
12	5	7	13	4	10	2745.3292	-0.0001
10	2	8	10	1	9	2746.4388	0.0021
18	2	16	18	1	17	2755.9923	0.0007
16	6	11	17	5	12	2780.8557	0.0089
16	6	10	17	5	13	2780.9371	0.0028
15	1	15	14	2	12	2794.3015	0.0052
9	2	7	9	1	8	2796.2010	0.0011
19	2	17	19	1	18	2837.0410	-0.0076
8	2	6	8	1	7	2849.4429	0.0001
7	2	5	7	1	6	2903.6946	0.0004
15	2	13	14	3	12	2914.1102	-0.0022

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
20	2	18	20	1	19	2940.6148	-0.0133
16	1	15	16	0	16	2944.6988	0.0066
6	2	4	6	1	5	2956.6166	-0.0032
20	3	18	19	4	15	2961.4341	-0.0007
4	1	4	3	0	3	3003.5051	0.0007
5	2	3	5	1	4	3006.0895	0.0000
4	2	2	4	1	3	3050.2293	-0.0004
3	2	1	3	1	2	3087.4558	-0.0001
2	2	0	2	1	1	3116.4916	-0.0010
11	1	10	10	2	9	3140.2433	0.0013
17	2	16	16	3	13	3154.9315	-0.0044
2	2	1	2	1	2	3177.0121	-0.0005
3	2	2	3	1	3	3207.6065	-0.0042
20	3	17	19	4	16	3216.4829	-0.0050
22	2	20	22	1	21	3218.9002	-0.0059
17	1	16	17	0	17	3219.2739	-0.0090
7	4	4	8	3	5	3224.8785	0.0103
7	4	3	8	3	6	3226.0965	-0.0010
4	2	3	4	1	4	3248.5138	-0.0012
11	5	7	12	4	8	3262.2474	0.0003
11	5	6	12	4	9	3262.5042	0.0000
8	0	8	7	1	7	3292.3825	0.0010
5	2	4	5	1	5	3299.8060	-0.0032
19	7	13	20	6	14	3334.8407	0.0030
19	7	12	20	6	15		
6	2	5	6	1	6	3361.5911	0.0028
7	2	6	7	1	7	3433.9526	-0.0002
21	3	19	20	4	16	3466.1397	-0.0039
5	1	5	4	0	4	3468.3161	-0.0005
18	1	17	18	0	18	3510.2820	0.0115
8	2	7	8	1	8	3517.0017	0.0012
16	2	14	15	3	13	3536.0627	-0.0025
18	2	17	17	3	14	3577.1760	-0.0014
9	2	8	9	1	9	3610.8234	0.0025
10	2	9	10	1	10	3715.4857	0.0006
6	4	3	7	3	4	3740.9975	-0.0017
6	4	2	7	3	5	3741.5589	0.0010
12	1	11	11	2	10	3762.2281	0.0045
10	5	6	11	4	7	3778.9055	0.0002
10	5	5	11	4	8	3779.0342	0.0004
21	3	18	20	4	17	3801.3614	-0.0052
19	1	18	19	0	19	3815.5606	-0.0048

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	2	10	11	1	11	3831.0498	0.0108

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
18	7	12	19	6	13	3852.3407	0.0012
18	7	11	19	6	14		
9	0	9	8	1	8	3858.6275	-0.0003
6	1	6	5	0	5	3924.8972	0.0041
12	2	11	12	1	12	3957.4850	-0.0098
22	3	20	21	4	17	3965.6046	0.0038
19	2	18	18	3	15	3981.2062	-0.0003
10	3	8	11	0	11	4008.6508	0.0042
24	3	21	24	2	22	4079.9661	0.0008
13	2	12	13	1	13	4094.8218	-0.0022
20	1	19	20	0	20	4132.8636	0.0042
2	2	1	1	1	0	4164.1146	0.0015
17	2	15	16	3	14	4171.2244	0.0005
2	2	0	1	1	1	4184.6786	0.0003
22	3	19	22	2	20	4215.2692	0.0041
14	2	13	14	1	14	4242.9504	-0.0008
5	4	2	6	3	3	4256.3573	-0.0026
5	4	1	6	3	4	4256.5787	-0.0048
9	5	5	10	4	6	4294.9340	-0.0054
9	5	4	10	4	7	4295.0015	0.0022
21	3	18	21	2	19	4299.4788	0.0014
13	6	8	14	5	9	4332.3932	-0.0041
13	6	7	14	5	10		
20	2	19	19	3	16	4364.7002	-0.0076
17	7	11	18	6	12	4369.3377	-0.0008
17	7	10	18	6	13		
7	1	7	6	0	6	4374.2718	-0.0009
13	1	12	12	2	11	4390.3976	-0.0044
20	3	17	20	2	18	4390.7983	-0.0038
22	3	19	21	4	18	4399.2771	-0.0010
15	2	14	15	1	15	4401.7463	-0.0021
21	8	14	22	7	15	4406.2194	-0.0076
10	0	10	9	1	9	4425.2829	-0.0005
23	3	21	22	4	18	4458.5275	-0.0033
21	1	20	21	0	21	4459.7251	-0.0060
19	3	16	19	2	17	4486.2405	-0.0062
16	2	15	16	1	16	4571.0319	-0.0005
18	3	15	18	2	16	4582.9000	0.0026
28	2	26	28	1	27	4631.3748	-0.0016
3	2	2	2	1	1	4657.6684	-0.0002
17	3	14	17	2	15	4678.0164	-0.0015
3	2	1	2	1	2	4719.9520	0.0010

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
21	2	20	20	3	17	4725.3186	-0.0038
17	2	16	17	1	17	4750.5606	-0.0024
16	3	13	16	2	14	4769.1450	-0.0016
4	4	1	5	3	2	4771.1599	-0.0047
4	4	0	5	3	3	4771.2389	-0.0002
8	1	8	7	0	7	4817.6963	0.0031
18	2	16	17	3	15	4819.0571	-0.0030
12	6	6	13	5	9	4848.5024	-0.0014
12	6	7	13	5	8		
15	3	12	15	2	13	4854.1880	0.0024
16	7	9	17	6	12	4885.8847	0.0015
16	7	10	17	6	11		
20	8	12	21	7	15	4923.0636	0.0045
20	8	13	21	7	14		
14	3	11	14	2	12	4931.4692	-0.0062
18	2	17	18	1	18	4940.0370	-0.0053
11	0	11	10	1	10	4990.7888	0.0007
13	3	10	13	2	11	4999.8433	-0.0038
23	3	20	22	4	19	5011.3319	0.0040
14	1	13	13	2	12	5023.9143	-0.0008
22	2	21	21	3	18	5060.7196	0.0034
11	3	8	11	2	9	5107.7346	0.0027
19	2	18	19	1	19	5139.1160	-0.0021
4	2	3	3	1	2	5141.0458	0.0021
10	3	7	10	2	8	5147.4081	-0.0037
9	3	6	9	2	7	5178.3917	0.0079
8	3	5	8	2	6	5201.6268	0.0005
7	3	4	7	2	5	5218.2937	0.0013
6	3	3	6	2	4	5229.6029	-0.0035
5	3	2	5	2	3	5236.7721	-0.0021
4	3	1	4	2	2	5240.9147	0.0017
3	3	0	3	2	1	5242.9960	-0.0054
3	3	1	3	2	2	5244.4617	-0.0056
4	3	2	4	2	3	5245.2932	-0.0036
5	3	3	5	2	4	5246.9556	-0.0028
6	3	4	6	2	5	5249.8526	-0.0012
7	3	5	7	2	6	5254.4509	0.0001
9	1	9	8	0	8	5256.5571	0.0001
8	3	6	8	2	7	5261.2753	0.0000
4	2	2	3	1	3	5267.0691	-0.0003
9	3	7	9	2	8	5270.9006	-0.0024
10	3	8	10	2	9	5283.9485	-0.0011

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	3	9	11	2	10	5301.0550	-0.0059
12	3	10	12	2	11	5322.9013	-0.0004
7	5	3	8	4	4		
7	5	2	8	4	5	5325.5492	0.0004
20	2	19	20	1	20	5347.3867	0.0002
13	3	11	13	2	12	5350.1472	0.0019
11	6	6	12	5	7		
11	6	5	12	5	8	5364.1872	0.0023
14	3	12	14	2	13	5383.4625	-0.0005
15	7	9	16	6	10		
15	7	8	16	6	11	5402.0216	0.0022
15	3	13	15	2	14	5423.5178	0.0050
19	8	12	20	7	13		
19	8	11	20	7	14	5439.5075	-0.0022
16	3	14	16	2	15	5470.9246	-0.0053
19	2	17	18	3	16	5478.8218	-0.0061
17	3	15	17	2	16	5526.3092	-0.0078
12	0	12	11	1	11	5553.7351	0.0135
18	3	16	18	2	17	5590.2371	0.0014
5	2	4	4	1	3	5614.2655	-0.0016
24	3	21	23	4	20	5638.4013	-0.0026
24	2	23	23	3	20	5647.1040	-0.0006
15	1	14	14	2	13	5661.7642	-0.0037
19	3	17	19	2	18	5663.1935	-0.0053
10	1	10	9	0	9	5692.3794	-0.0014
20	3	18	20	2	19	5745.6614	-0.0017
22	2	21	22	1	22	5789.6730	0.0079
25	1	24	25	0	25	5816.4861	-0.0025
5	2	3	4	1	4	5827.2153	0.0019
21	3	19	21	2	20	5838.0308	0.0073
6	5	2	7	4	3		
6	5	1	7	4	4	5840.2858	-0.0044
10	6	5	11	5	6		
10	6	4	11	5	7	5879.4966	-0.0007
6	3	4	7	0	7	5883.2761	-0.0064
14	7	8	15	6	9		
14	7	7	15	6	10	5917.7866	-0.0039
22	3	20	22	2	21	5940.6086	0.0007
23	2	22	23	1	23	6022.6746	0.0066
23	3	21	23	2	22	6053.6691	-0.0044
6	2	5	5	1	4	6077.3999	-0.0009
13	0	13	12	1	12	6112.8839	0.0040

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	1	11	10	0	10	6126.7268	0.0009
20	2	18	19	3	17	6149.6126	0.0023
26	1	25	26	0	26	6158.1157	0.0043
24	3	22	24	2	23	6177.4107	0.0078
24	2	23	24	1	24	6262.8627	-0.0027
16	1	15	15	2	14	6302.8279	-0.0001
25	3	23	25	2	24	6311.9039	0.0009
28	4	24	28	3	25	6317.6766	-0.0045
27	3	25	26	4	22	6333.7729	0.0011
5	5	0	6	4	3	6354.7594	-0.0018
5	5	1	6	4	2		
9	6	3	10	5	6	6394.4937	-0.0006
9	6	4	10	5	5		
6	2	4	5	1	5	6401.8484	-0.0014
13	7	6	14	6	9	6433.2365	-0.0009
13	7	7	14	6	8		
27	4	23	27	3	24	6446.6022	0.0064
17	8	9	18	7	12	6471.3967	-0.0039
17	8	10	18	7	11		
25	2	24	25	1	25	6509.7191	0.0170
7	2	6	6	1	5	6530.5470	0.0016
29	2	28	28	3	25	6547.7300	0.0051
12	1	12	11	0	11	6561.1184	0.0002
26	4	22	26	3	23	6568.9881	0.0071
27	3	25	27	2	26	6613.2674	0.0117
14	0	14	13	1	13	6667.3276	-0.0041
25	4	21	25	3	22	6682.9962	0.0018
26	2	25	26	1	26	6762.6176	-0.0006
28	3	26	27	4	23	6769.2207	-0.0032
3	3	1	2	2	0	6785.6403	-0.0030
3	3	0	2	2	1	6785.9365	-0.0033
24	4	20	24	3	21	6787.2804	-0.0060
21	2	19	20	3	18	6830.3507	-0.0061
23	4	19	23	3	20	6881.0115	0.0011
8	6	2	9	5	5	6909.2343	0.0097
8	6	3	9	5	4		
26	3	23	25	4	22	6939.7645	0.0048
17	1	16	16	2	15	6945.8315	0.0021
12	7	5	13	6	8	6948.3983	-0.0004
12	7	6	13	6	7		
22	4	18	22	3	19	6963.8004	-0.0005
8	2	7	7	1	6	6973.8473	0.0005

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
7	2	5	6	1	6	6992.6940	-0.0069
13	1	13	12	0	12	6996.9544	-0.0071
27	2	26	27	1	27	7021.0585	0.0011

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
20	9	11	21	8	14	7025.0982	-0.0056
20	9	12	21	8	13		
21	4	17	21	3	18	7035.7172	-0.0061
20	4	16	20	3	17	7097.1878	-0.0144
19	4	15	19	3	16	7148.9369	0.0009
18	4	14	18	3	15	7191.8087	-0.0008
15	0	15	14	1	14	7216.4424	-0.0026
17	4	13	17	3	14	7226.8100	-0.0017
16	4	12	16	3	13	7254.9709	0.0045
15	4	11	15	3	12	7277.2729	-0.0038
28	2	27	28	1	28	7284.4651	-0.0102
14	4	10	14	3	11	7294.6898	0.0029
4	3	2	3	2	1	7298.8796	-0.0050
4	3	1	3	2	2	7300.3693	-0.0025
13	4	9	13	3	10	7308.0645	0.0081
17	4	14	17	3	15	7321.2308	0.0060
18	4	15	18	3	16	7321.6886	0.0013
16	4	13	16	3	14	7322.0647	0.0032
15	4	12	15	3	13	7323.7824	-0.0001
19	4	16	19	3	17	7323.9254	0.0010
11	4	7	11	3	8	7325.6181	-0.0025
14	4	11	14	3	12	7326.0278	-0.0079
13	4	10	13	3	11	7328.5263	-0.0066
12	4	9	12	3	10	7331.0320	-0.0099
10	4	6	10	3	7		
11	4	8	11	3	9	7333.4079	-0.0054
9	4	5	9	3	6	7334.8620	-0.0057
10	4	7	10	3	8	7335.5119	-0.0041
9	4	6	9	3	7	7337.2940	0.0036
8	4	4	8	3	5	7337.4993	0.0037
8	4	5	8	3	6	7338.7112	-0.0005
7	4	3	7	3	4	7339.2318	-0.0012
7	4	4	7	3	5	7339.7850	-0.0025
6	4	2	6	3	3	7340.3261	-0.0017
6	4	3	6	3	4	7340.5493	-0.0010
5	4	1	5	3	2	7340.9709	-0.0035
5	4	2	5	3	3	7341.0509	0.0023
4	4	1	4	3	2	7341.3325	0.0013
4	4	0	4	3	1		
22	4	19	22	3	20	7346.8476	0.0095
23	4	20	23	3	21	7361.9380	-0.0051
24	4	21	24	3	22	7381.8887	-0.0012

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
25	4	22	25	3	23	7407.3685	0.0017
9	2	8	8	1	7	7407.5055	-0.0002
7	6	2	8	5	3	7423.7268	-0.0070
7	6	1	8	5	4		
14	1	14	13	0	13	7435.4553	-0.0053
11	7	5	12	6	6	7463.3044	-0.0062
11	7	4	12	6	7		
27	4	24	27	3	25	7477.6513	-0.0011
15	8	8	16	7	9	7502.1693	0.0179
15	8	7	16	7	10		
22	2	20	21	3	19	7519.9199	0.0090
28	4	25	28	3	26	7523.7906	-0.0015
19	9	11	20	8	12	7540.5964	-0.0016
19	9	10	20	8	13		
29	2	28	29	1	29	7552.3404	-0.0050
29	4	26	29	3	27	7578.0995	-0.0030
18	1	17	17	2	16	7589.3783	-0.0073
8	2	6	7	1	7	7601.6928	-0.0037
27	3	24	26	4	23	7614.2982	0.0064
16	0	16	15	1	15	7759.8859	0.0017
5	3	3	4	2	2	7810.9953	-0.0005
5	3	2	4	2	3	7815.4716	-0.0012
10	2	9	9	1	8	7831.7911	0.0038
15	1	15	14	0	14	7877.5596	-0.0052
6	6	1	7	5	2	7938.0655	0.0027
6	6	0	7	5	3		
10	7	4	11	6	5	7978.0041	-0.0030
10	7	3	11	6	6		
9	2	7	8	1	8	8230.9156	0.0093
19	1	18	18	2	17	8232.0275	0.0125
11	2	10	10	1	9	8247.0409	0.0078
17	0	17	16	1	16	8297.5789	-0.0001
6	3	4	5	2	3	8321.1654	0.0002
16	1	16	15	0	15	8323.9402	0.0019
6	3	3	5	2	4	8331.6493	0.0022
12	2	11	11	1	10	8653.6787	0.0045
17	1	17	16	0	16	8774.9587	-0.0030
7	3	5	6	2	4	8828.3795	0.0031
18	0	18	17	1	17	8829.6877	0.0097
7	3	4	6	2	5	8849.3908	-0.0141
20	1	19	19	2	18	8872.1689	-0.0121
10	2	8	9	1	9	8882.4553	0.0033

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
13	2	12	12	1	11	9052.2478	0.0033
18	1	18	17	0	17	9230.7708	0.0106
8	3	6	7	2	5	9331.4318	0.0039
19	0	19	18	1	18	9356.5038	0.0120
8	3	5	7	2	6	9369.3733	0.0032
20	5	15	20	4	16	9379.1835	0.0017
21	5	17	21	4	18	9384.6163	0.0205
19	5	14	19	4	15	9391.3206	-0.0042
20	5	16	20	4	17	9392.9837	-0.0029
4	4	1	3	3	0	9397.2318	0.0069
4	4	0	3	3	1		
18	5	13	18	4	14	9401.3241	0.0021
18	5	14	18	4	15	9407.4294	0.0046
17	5	12	17	4	13	9409.5193	0.0065
17	5	13	17	4	14	9413.4106	-0.0128
16	5	11	16	4	12	9416.1761	-0.0085
16	5	12	16	4	13	9418.6276	0.0073
15	5	10	15	4	11	9421.5790	-0.0019
15	5	11	15	4	12	9423.0679	0.0177
14	5	9	14	4	10	9425.9166	0.0090
14	5	10	14	4	11	9426.7658	0.0034
13	5	8	13	4	9	9429.3412	0.0014
13	5	9	13	4	10	9429.8215	0.0049
12	5	7	12	4	8	9432.0384	0.0119
11	5	6	11	4	7	9434.1164	0.0214
9	5	4	9	4	5	9436.8141	0.0004
9	5	5	9	4	6		
8	5	3	8	4	4	9437.6229	0.0031
8	5	4	8	4	5		
7	5	2	7	4	3	9438.1781	0.0085
7	5	3	7	4	4		
6	5	1	6	4	2	9438.5197	-0.0024
6	5	2	6	4	3		
5	5	0	5	4	1	9438.7350	0.0064
5	5	1	5	4	2		
14	2	13	13	1	12	9443.4048	0.0100
21	1	20	20	2	19	9508.3461	0.0015
11	2	9	10	1	10	9558.4083	0.0009
19	1	19	18	0	18	9691.2530	0.0050
15	2	14	14	1	13	9827.9043	-0.0013
9	3	7	8	2	6	9828.9618	-0.0041
20	0	20	19	1	19	9878.4390	-0.0007

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	3	6	8	2	7	9892.2882	-0.0013
5	4	2	4	3	1	9911.1430	0.0022
5	4	1	4	3	2		
20	1	20	19	0	19	10156.1810	-0.0011
16	2	15	15	1	14	10206.6955	-0.0012
12	2	10	11	1	11	10260.6957	0.0029
10	3	8	9	2	7	10319.5223	-0.0147
21	0	21	20	1	20	10395.9982	-0.0018
10	3	7	9	2	8	10419.0479	0.0050
6	4	3	5	3	2	10424.9832	0.0044
6	4	2	5	3	3		
17	2	16	16	1	15	10580.8318	-0.0006
21	1	21	20	0	20	10625.2165	0.0028
23	1	22	22	2	21	10762.8757	-0.0086
11	3	9	10	2	8	10801.6601	0.0028
22	0	22	21	1	21	10909.6772	0.0049
7	4	4	6	3	3	10938.5977	0.0402
7	4	3	6	3	4	10938.7604	-0.0237
11	3	8	10	2	9	10950.6591	0.0049
18	2	17	17	1	16	10951.5167	-0.0030
13	2	11	12	1	12	10990.9699	-0.0070
22	1	22	21	0	21	11097.9373	0.0024
12	3	10	11	2	9	11273.9074	0.0120
19	2	18	18	1	17	11320.0790	-0.0165
23	0	23	22	1	22	11419.9652	0.0162
8	4	5	7	3	4	11451.8472	0.0000
8	4	4	7	3	5	11452.4151	0.0002
12	3	9	11	2	10	11488.3018	-0.0001
19	6	13	19	5	14	11514.8688	-0.0039
19	6	14	19	5	15	11515.1416	0.0110
17	6	11	17	5	12	11522.7594	0.0121
17	6	12	17	5	13		
16	6	10	16	5	11	11525.6707	-0.0372
16	6	11	16	5	12		
15	6	9	15	5	10	11528.1433	-0.0087
15	6	10	15	5	11		
14	6	8	14	5	9	11530.1280	-0.0149
14	6	9	14	5	10		
13	6	7	13	5	8	11531.7294	-0.0097
13	6	8	13	5	9		
12	6	6	12	5	7	11532.9962	0.0007
12	6	7	12	5	8		

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	6	5	11	5	6	11533.9612	-0.0013
11	6	6	11	5	7		
10	6	4	10	5	5	11534.6916	0.0054
10	6	5	10	5	6		
9	6	3	9	5	4	11535.2129	0.0034
9	6	4	9	5	5		
8	6	2	8	5	3	11535.6023	0.0315
8	6	3	8	5	4		
7	6	1	7	5	2	11535.7965	-0.0083
7	6	2	7	5	3		
23	1	23	22	0	22	11573.9077	-0.0077
20	2	19	19	1	18	11688.0204	0.0174
13	3	11	12	2	10	11734.9625	0.0029
14	2	12	13	1	13	11750.6128	0.0126
24	0	24	23	1	23	11927.2926	-0.0027
9	4	6	8	3	5	11964.6300	-0.0001
9	4	5	8	3	6	11965.8870	0.0051
5	5	1	4	4	0	12008.5437	0.0055
5	5	0	4	4	1		
13	3	10	12	2	11	12033.3234	-0.0057
24	1	24	23	0	23	12052.7337	0.0045
21	2	20	20	1	19	12056.7630	0.0105
14	3	12	13	2	11	12183.7902	0.0124
22	2	21	21	1	20	12427.8780	0.0092
25	0	25	24	1	24	12432.1308	-0.0077
10	4	7	9	3	6	12476.6731	0.0039
10	4	6	9	3	7	12479.1792	0.0016
6	5	2	5	4	1	12522.4941	0.0047
6	5	1	5	4	2		
25	1	25	24	0	24	12533.9701	-0.0030
14	3	11	13	2	12	12587.2497	-0.0018
15	3	13	14	2	12	12619.5546	-0.0029
23	2	22	22	1	21	12802.8128	-0.0167
26	0	26	25	1	25	12934.8397	-0.0214
11	4	8	10	3	7	12987.6641	0.0053
11	4	7	10	3	8	12992.3273	0.0021
7	5	3	6	4	2	13036.4028	0.0015
7	5	2	6	4	3		
16	3	14	15	2	13	13041.8290	0.0101
15	3	12	14	2	13	13151.7628	0.0017
27	0	27	26	1	26	13435.7990	-0.0009
17	3	15	16	2	14	13450.3922	-0.0072

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
12	4	9	11	3	8	13497.2337	0.0222
27	1	27	26	0	26	13502.3109	0.0008
12	4	8	11	3	9	13505.3909	0.0026
8	5	4	7	4	3	13550.2419	0.0014
8	5	3	7	4	4	13550.2419	0.0014
22	7	15	22	6	16	13612.0789	-0.0119
22	7	16	22	6	17	13612.0789	-0.0119
21	7	14	21	6	15	13615.8335	0.0005
21	7	15	21	6	16	13615.8335	0.0005
20	7	13	20	6	14	13619.0602	0.0017
20	7	14	20	6	15	13619.0602	0.0017
18	7	11	18	6	12	13624.1601	0.0062
18	7	12	18	6	13	13624.1601	0.0062
17	7	10	17	6	11	13626.1201	0.0056
17	7	11	17	6	12	13626.1201	0.0056
16	7	9	16	6	10	13627.7416	0.0017
16	7	10	16	6	11	13627.7416	0.0017
15	7	8	15	6	9	13629.0736	0.0046
15	7	9	15	6	10	13629.0736	0.0046
14	7	7	14	6	8	13630.1148	-0.0238
14	7	8	14	6	9	13630.1148	-0.0238
13	7	6	13	6	7	13630.9800	-0.0029
13	7	7	13	6	8	13630.9800	-0.0029
12	7	5	12	6	6	13631.6340	0.0000
12	7	6	12	6	7	13631.6340	0.0000
11	7	4	11	6	5	13632.1274	0.0061
11	7	5	11	6	6	13632.1274	0.0061
10	7	3	10	6	4	13632.4683	-0.0039
10	7	4	10	6	5	13632.4683	-0.0039
16	3	13	15	2	14	13728.7511	0.0266
18	3	16	17	2	15	13845.4381	0.0073
13	4	10	12	3	9	14004.8544	0.0099
13	4	9	12	3	10	14018.4851	0.0013
9	5	5	8	4	4	14063.9681	0.0022
9	5	4	8	4	5	14063.9681	0.0022
19	3	17	18	2	16	14227.3028	0.0001
14	4	11	13	3	10	14509.9507	-0.0158
14	4	10	13	3	11	14531.7832	-0.0099
10	5	6	9	4	5	14577.5381	0.0091
10	5	5	9	4	6	14577.5381	0.0091
6	6	1	5	5	0	14619.7070	0.0040
6	6	0	5	5	1	14619.7070	0.0040

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
21	3	19	20	2	18	14954.1311	-0.0167
15	4	12	14	3	11	15011.8604	-0.0041
15	4	11	14	3	12	15045.5836	0.0087
7	6	2	6	5	1	15133.6890	0.0048
7	6	1	6	5	2		
22	3	20	21	2	19	15300.8015	-0.0001
16	4	13	15	3	12	15509.6936	-0.0013
19	3	16	18	2	17	15555.3141	0.0038
16	4	12	15	3	13	15560.1810	0.0030
12	5	8	11	4	7	15603.8877	0.0170
8	6	3	7	5	2	15647.6466	0.0048
8	6	2	7	5	3		
23	8	15	23	7	16	15715.3673	-0.0117
23	8	16	23	7	17		
22	8	14	22	7	15	15717.9491	-0.0167
22	8	15	22	7	16		
18	8	10	18	7	11	15725.0996	0.0096
18	8	11	18	7	12		
17	8	9	17	7	10	15726.2187	0.0026
17	8	10	17	7	11		
16	8	8	16	7	9	15727.1407	0.0056
16	8	9	16	7	10		
15	8	7	15	7	8	15727.8834	0.0115
15	8	8	15	7	9		
14	8	6	14	7	7	15728.4527	0.0029
14	8	7	14	7	8		
13	8	5	13	7	6	15728.8842	-0.0065
13	8	6	13	7	7		
17	4	14	16	3	13	16002.4853	0.0077
13	5	9	12	4	8	16116.5266	0.0127
13	5	8	12	4	9	16116.8022	0.0264
9	6	4	8	5	3	16161.5589	0.0032
9	6	3	8	5	4		
18	4	15	17	3	14	16489.1099	0.0096
18	4	14	17	3	15	16593.7678	0.0008
14	5	10	13	4	9	16628.6741	0.0016
14	5	9	13	4	10	16629.1766	0.0089
10	6	5	9	5	4	16675.4012	-0.0004
10	6	4	9	5	5		
15	5	11	14	4	10	17140.1994	-0.0285
15	5	10	14	4	11	17141.1327	0.0127
11	6	6	10	5	5	17180.1510	-0.0000

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	6	5	10	5	6	17167.1512	-0.0002
7	7	1	6	6	0		
7	7	0	6	6	1	17230.6887	0.0019
20	4	16	19	3	17	17637.6066	-0.0080
16	5	12	15	4	11	17651.0417	0.0033
16	5	11	15	4	12	17652.5782	-0.0019

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
12	6	7	11	5	6	17702.7933	0.0202
12	6	6	11	5	7		
8	7	2	7	6	1	17744.6951	-0.0043
8	7	1	7	6	2		
21	4	18	20	3	17	17899.2267	-0.0170

Table S6: Observed Transition Frequencies (in MHz) for $^{13}\text{CH}_2\text{CH}(\text{CF}_3)\text{O}-\text{CH}_2\text{CH}(\text{CF}_3)\text{O}$

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
3	1	3	2	0	2	2514.2335	0.0008
13	2	11	13	1	12	2613.6140	-0.0031
10	2	8	10	1	9	2712.6787	0.0011
9	2	7	9	1	8	2761.9588	0.0072
6	2	4	6	1	5	2922.7513	0.0049
4	1	4	3	0	3	2986.1912	0.0044
8	0	8	7	1	7	3294.5466	0.0025
6	2	5	6	1	6	3333.3868	0.0031
5	1	5	4	0	4	3448.9725	-0.0004
10	2	9	10	1	10	3692.8940	0.0024
12	1	11	11	2	10	3787.9501	-0.0033
9	0	9	8	1	8	3859.5801	-0.0027
6	1	6	5	0	5	3903.4458	-0.0013
7	1	7	6	0	6	4350.6981	0.0074
10	0	10	9	1	9	4424.8335	-0.0019
3	2	2	2	1	1	4621.6892	-0.0053
3	2	1	2	1	2	4684.9684	-0.0013
8	1	8	7	0	7	4791.9894	-0.0008
11	0	11	10	1	10	4988.7050	-0.0059
14	1	13	13	2	12	5049.3228	-0.0009
10	3	7	10	2	8	5091.0799	-0.0108
4	2	3	3	1	2	5103.2833	0.0007
9	3	6	9	2	7	5123.2031	0.0022
7	3	4	7	2	5	5164.6599	0.0071
6	3	3	6	2	4	5176.4264	0.0053
5	3	2	5	2	3	5183.8792	-0.0017
4	3	2	4	2	3	5192.7557	0.0012
5	3	3	5	2	4	5194.4795	-0.0033
7	3	5	7	2	6	5202.2795	0.0042
8	3	6	8	2	7	5209.3738	0.0025
9	1	9	8	0	8	5228.7963	-0.0034
4	2	2	3	1	3	5231.3576	0.0034
11	3	9	11	2	10	5250.7031	-0.0056
12	3	10	12	2	11	5273.3841	0.0007
12	0	12	11	1	11	5549.7868	0.0114
5	2	4	4	1	3	5574.5691	0.0058
10	1	10	9	0	9	5662.6874	0.0009
6	5	2	7	4	3	5754.7915	0.0051
6	5	1	7	4	4		
10	6	5	11	5	6	5778.1107	0.0026
10	6	4	11	5	7		
5	2	3	4	1	4	5791.0396	0.0012

Table S6: Observed Transition Frequencies (in MHz) for $^{13}\text{CH}_2\text{CH}(\text{CF}_3)\text{O}-\text{CH}_2\text{CH}(\text{CF}_3)\text{O}$

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
6	2	5	5	1	4	6035.5987	-0.0029
11	1	11	10	0	10	6095.2543	-0.0020
6	2	4	5	1	5	6365.5487	0.0012
7	2	6	6	1	5	6486.4998	-0.0032
3	3	1	2	2	0	6729.1020	0.0037
3	3	0	2	2	1	6729.4087	0.0016
7	2	5	6	1	6	6956.6765	0.0062
13	1	13	12	0	12	6962.5333	-0.0027
15	0	15	14	1	14	7205.5990	0.0020
14	4	10	14	3	11	7218.6808	0.0006
13	4	9	13	3	10	7232.7429	-0.0030
4	3	2	3	2	1	7240.9987	0.0032
4	3	1	3	2	2	7242.5386	-0.0061
12	4	8	12	3	9	7243.3423	-0.0152
14	4	11	14	3	12	7252.1062	0.0056
10	4	6	10	3	7	7256.9113	0.0106
12	4	9	12	3	10	7257.1187	-0.0017
11	4	8	11	3	9	7259.5385	0.0112
9	4	5	9	3	6	7260.9239	0.0038
10	4	7	10	3	8	7261.6828	0.0021
9	4	6	9	3	7	7263.5032	-0.0033
8	4	5	8	3	6	7264.9725	-0.0019
7	4	3	7	3	4	7265.4937	-0.0031
7	4	4	7	3	5	7266.0806	-0.0084
6	4	2	6	3	3	7266.6451	0.0013
6	4	3	6	3	4	7266.8759	-0.0054
5	4	1	5	3	2	7267.3069	-0.0142
5	4	2	5	3	3	7267.3968	-0.0037
9	2	8	8	1	7	7358.5727	0.0064
14	1	14	13	0	13	7399.8652	-0.0024
8	2	6	7	1	7	7566.4025	-0.0042
5	3	3	4	2	2	7751.7197	0.0039
5	3	2	4	2	3	7756.3757	-0.0038
10	2	9	9	1	8	7780.2166	-0.0021
15	1	15	14	0	14	7840.9928	0.0029

Table S7: Observed Transition Frequencies (in MHz) for CH₂¹³CH(CF₃)O-CH₂CH(CF₃)O

<i>J'</i>	<i>K_a'</i>	<i>K_c'</i>	<i>J''</i>	<i>K_a''</i>	<i>K_c''</i>	Observed	Obs - Calc
2	1	2	1	0	1	2044.2645	0.0122
10	2	8	10	1	9	2746.1751	-0.0043
9	2	7	9	1	8	2795.9226	-0.0003
7	2	5	7	1	6	2903.2679	-0.0001
6	2	4	6	1	5	2956.0885	0.0017
4	1	4	3	0	3	3000.2452	0.0034
4	2	3	4	1	4	3247.1962	-0.0040
8	0	8	7	1	7	3285.7661	-0.0050
5	1	5	4	0	4	3464.3851	-0.0029
9	2	8	9	1	9	3608.4488	-0.0023
6	1	6	5	0	5	3920.3180	0.0009
7	1	7	6	0	6	4369.0618	-0.0008
13	1	12	12	2	11	4378.7225	-0.0046
10	0	10	9	1	9	4416.9196	-0.0030
3	2	1	2	1	2	4716.4275	0.0000
8	1	8	7	0	7	4811.8543	-0.0012
11	0	11	10	1	10	4981.5868	0.0012
11	3	8	11	2	9	5106.7227	0.0055
4	2	3	3	1	2	5136.9876	-0.0004
10	3	7	10	2	8	5146.2042	-0.0029
8	3	5	8	2	6	5200.1476	-0.0015
7	3	4	7	2	5	5216.7261	-0.0023
6	3	3	6	2	4	5227.9810	-0.0016
5	3	2	5	2	3	5235.1110	-0.0010
4	3	1	4	2	2	5239.2332	0.0047
3	3	1	3	2	2	5242.7516	-0.0119
4	3	2	4	2	3	5243.5862	-0.0025
6	3	4	6	2	5	5248.1195	-0.0018
9	1	9	8	0	8	5250.0913	-0.0002
8	3	6	8	2	7	5259.4831	0.0008
4	2	2	3	1	3	5262.6406	0.0001
9	3	7	9	2	8	5269.0696	0.0100
11	3	9	11	2	10	5299.0641	0.0027
13	3	11	13	2	12	5347.8941	-0.0028
14	3	12	14	2	13	5381.0509	0.0026
5	2	4	4	1	3	5609.5225	-0.0033
10	1	10	9	0	9	5685.2801	0.0003
5	2	3	4	1	4	5821.8388	0.0043
6	2	5	5	1	4	6071.9993	-0.0033
13	0	13	12	1	12	6102.0827	0.0055
11	1	11	10	0	10	6118.9750	-0.0007
6	2	4	5	1	5	6395.4707	0.0023

Table S7: Observed Transition Frequencies (in MHz) for CH₂¹³CH(CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
7	2	6	6	1	5	6524.5225	0.0041
12	1	12	11	0	11	6552.7000	0.0006
3	3	0	2	2	1	6781.8239	-0.0046
8	2	7	7	1	6	6967.2170	-0.0013
7	2	5	6	1	6	6985.2640	0.0079
15	0	15	14	1	14	7204.1533	0.0026
14	4	10	14	3	11	7292.5895	-0.0050
4	3	2	3	2	1	7293.9781	0.0024
4	3	1	3	2	2	7295.4542	-0.0005
13	4	10	13	3	11	7326.1958	0.0004
10	4	6	10	3	7	7328.7145	-0.0008
9	4	5	9	3	6	7332.5195	-0.0022
10	4	7	10	3	8	7333.1574	-0.0008
8	4	4	8	3	5	7335.1310	-0.0027
8	4	5	8	3	6	7336.3450	0.0048
7	4	3	7	3	4	7336.8587	-0.0021
6	4	2	6	3	3	7337.9528	0.0036
6	4	3	6	3	4	7338.1762	0.0064
5	4	1	5	3	2	7338.5929	0.0010
9	2	8	8	1	7	7400.3007	-0.0008
14	1	14	13	0	13	7425.6304	-0.0044
8	2	6	7	1	7	7593.1138	-0.0040
5	3	3	4	2	2	7805.2905	-0.0033
5	3	2	4	2	3	7809.7458	-0.0005
10	2	9	9	1	8	7824.0355	0.0039
15	1	15	14	0	14	7867.0001	0.0004

Table S8: Observed Transition Frequencies (in MHz) for CH₂CH(¹³CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
2	1	2	1	0	1	2042.1413	0.0015
10	2	8	10	1	9	2749.7014	-0.0053
6	2	4	6	1	5	2959.3020	-0.0083
4	1	4	3	0	3	2995.3988	0.0028
11	1	10	10	2	9	3108.5296	0.0004
8	0	8	7	1	7	3271.8452	-0.0073
5	1	5	4	0	4	3458.2516	0.0164
10	2	9	10	1	10	3712.4348	0.0034
12	1	11	11	2	10	3727.4660	-0.0023
9	0	9	8	1	8	3835.5774	0.0038
6	1	6	5	0	5	3912.8854	-0.0013
13	1	12	12	2	11	4352.5996	0.0012
7	1	7	6	0	6	4360.3693	-0.0038
10	0	10	9	1	9	4399.7572	-0.0073
3	2	1	2	1	2	4714.0881	-0.0025
8	1	8	7	0	7	4801.9110	-0.0020
14	1	13	13	2	12	4983.0776	0.0029
11	3	8	11	2	9	5112.0856	0.0034
4	2	3	3	1	2	5133.5679	-0.0057
10	3	7	10	2	8	5151.2170	0.0058
8	3	5	8	2	6	5204.6385	0.0055
7	3	4	7	2	5	5221.0444	-0.0015
6	3	3	6	2	4	5232.1872	0.0019
9	1	9	8	0	8	5238.8867	-0.0023
5	3	2	5	2	3	5239.2332	-0.0079
4	3	1	4	2	2	5243.3144	-0.0004
3	3	1	3	2	2	5246.8045	-0.0083
4	3	2	4	2	3	5247.6281	-0.0013
5	3	3	5	2	4	5249.2655	0.0003
6	3	4	6	2	5	5252.1185	0.0029
4	2	2	3	1	3	5258.5941	0.0025
8	3	6	8	2	7	5263.3605	-0.0006
9	3	7	9	2	8	5272.8459	0.0042
10	3	8	10	2	9	5285.6900	-0.0006
11	3	9	11	2	10	5302.5431	-0.0016
12	3	10	12	2	11	5324.0625	0.0020
14	3	12	14	2	13	5383.7500	0.0134
15	3	13	15	2	14	5423.2020	-0.0097
12	0	12	11	1	11	5523.5102	0.0034
5	2	4	4	1	3	5604.7737	0.0003
15	1	14	14	2	13	5617.9240	0.0023
10	1	10	9	0	9	5672.7976	0.0009

Table S8: Observed Transition Frequencies (in MHz) for CH₂CH(¹³CF₃)O-CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
5	2	3	4	1	4	5815.9956	0.0010
6	2	5	5	1	4	6065.9640	0.0033
6	2	4	5	1	5	6387.7452	0.0015
7	2	6	6	1	5	6517.2357	0.0015
12	1	12	11	0	11	6537.5567	0.0084
3	3	1	2	2	0	6780.9799	-0.0020
3	3	0	2	2	1	6781.2700	-0.0037
8	2	7	7	1	6	6958.7371	-0.0003
13	1	13	12	0	12	6971.2980	0.0006
7	2	5	6	1	6	6975.5384	0.0028
15	0	15	14	1	14	7179.7948	-0.0101
15	4	11	15	3	12	7281.7692	-0.0047
4	3	1	3	2	2	7293.3631	0.0043
12	4	8	12	3	9	7321.8801	0.0132
15	4	12	15	3	13	7327.2052	0.0023
11	4	7	11	3	8	7329.2060	0.0052
14	4	11	14	3	12	7329.4649	-0.0046
13	4	10	13	3	11	7331.9551	-0.0081
10	4	6	10	3	7	7334.5057	-0.0125
8	4	4	8	3	5	7340.8545	-0.0049
8	4	5	8	3	6	7342.0496	0.0029
7	4	3	7	3	4	7342.5705	0.0044
7	4	4	7	3	5	7343.1089	0.0014
6	4	2	6	3	3	7343.6432	0.0013
6	4	3	6	3	4	7343.8607	0.0017
5	4	1	5	3	2	7344.2774	0.0002
5	4	2	5	3	3	7344.3584	0.0087
4	4	0	4	3	1	7344.6212	-0.0065
4	4	1	4	3	2	7344.6212	-0.0065
9	2	8	8	1	7	7390.6595	-0.0074
14	1	14	13	0	13	7407.6248	-0.0039
8	2	6	7	1	7	7581.2703	-0.0022
16	0	16	15	1	15	7721.2357	0.0000
5	3	3	4	2	2	7801.6946	-0.0019
5	3	2	4	2	3	7806.1020	-0.0002
10	2	9	9	1	8	7813.2839	0.0012
15	1	15	14	0	14	7847.5008	0.0062

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
6	0	6	5	1	4	2217.8421	-0.0121
2	1	1	1	0	1	2223.3415	-0.0018
4	1	4	3	1	3	2238.7268	0.0016
4	0	4	3	0	3	2265.6110	0.0029
4	2	3	3	2	2	2266.9403	0.0028
4	2	2	3	2	1	2268.3134	0.0016
4	1	3	3	1	2	2294.7208	0.0000
13	2	12	13	1	12	2591.1470	-0.0023
7	0	7	6	1	5	2735.9455	-0.0018
5	1	5	4	1	4	2798.1186	0.0034
3	1	2	2	0	2	2811.1510	0.0005
5	0	5	4	0	4	2830.9412	0.0014
5	2	4	4	2	3	2833.4599	0.0018
5	3	3	4	3	2	2834.3357	0.0039
5	3	2	4	3	1	2836.2042	0.0003
5	2	3	4	2	2	2836.2042	0.0003
5	1	4	4	1	3	2868.0969	0.0043
5	2	4	5	1	4	3102.0934	-0.0031
4	2	3	4	1	3	3136.7290	-0.0019
3	2	2	3	1	2	3164.5154	0.0011
8	0	8	7	1	6	3243.9479	-0.0093
3	2	1	3	1	3	3249.2043	-0.0050
4	2	2	4	1	4	3278.7955	-0.0003
5	2	3	5	1	5	3316.8869	0.0023
6	1	6	5	1	5	3357.3170	0.0018
6	0	6	5	0	5	3395.5636	0.0001
6	2	5	5	2	4	3399.8377	0.0015
6	4	3	5	4	2	3401.1998	0.0040
6	4	2	5	4	1	3401.1998	0.0040
6	3	3	5	3	2	3401.3354	0.0095
6	3	4	5	3	3	3401.3354	0.0095
6	2	4	5	2	3	3404.6341	0.0013
4	1	3	3	0	3	3406.1678	0.0031
7	2	5	7	1	7	3421.6031	-0.0033
6	1	5	5	1	4	3441.2548	0.0010
13	1	13	12	2	11	3500.4699	-0.0146
9	0	9	8	1	7	3741.1149	-0.0050
7	1	7	6	1	6	3916.2958	0.0043
7	0	7	6	0	6	3959.3477	0.0007
7	2	6	6	2	5	3966.0402	-0.0027
7	4	4	6	4	3	3968.1214	0.0045
7	4	3	6	4	2	3968.1214	0.0045

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
7	3	5	6	3	4	3968.3374	0.0011
7	3	4	6	3	3	3968.4400	-0.0025
7	2	5	6	2	4	3973.6957	0.0001
5	1	4	4	0	4	4008.6511	0.0018
7	1	6	6	1	5	4014.1576	0.0001
12	1	11	11	2	9	4021.0267	-0.0025
10	0	10	9	1	8	4226.6329	-0.0030
2	2	0	1	1	0	4333.0566	0.0011
2	2	1	1	1	1	4346.9159	-0.0041
8	1	8	7	1	7	4475.0132	0.0001
8	0	8	7	0	7	4522.1652	-0.0022
8	2	7	7	2	6	4532.0437	-0.0057
8	4	5	7	4	4	4535.0555	-0.0069
8	4	4	7	4	3		
8	6	2	7	6	1	4535.2007	-0.0057
8	6	3	7	6	2		
8	3	6	7	3	5	4535.4303	0.0032
8	3	5	7	3	4	4535.6371	-0.0022
8	2	6	7	2	5	4543.4822	0.0022
8	1	7	7	1	6	4586.7503	-0.0034
6	1	5	5	0	5	4618.9604	-0.0029
3	2	1	2	1	1	4886.3856	0.0004
3	2	2	2	1	2	4927.7030	0.0002
9	1	9	8	1	8	5033.4470	-0.0040
9	0	9	8	0	8	5083.9177	0.0014
9	2	8	8	2	7	5097.8288	0.0019
9	5	4	8	5	3	5101.9249	0.0014
9	5	5	8	5	4		
9	4	5	8	4	4	5102.0393	0.0040
9	4	6	8	4	5		
9	7	2	8	7	1	5102.3631	0.0072
9	7	3	8	7	2		
9	3	7	8	3	6	5102.5769	0.0026
9	8	1	8	8	0	5102.7463	0.0116
9	8	2	8	8	1		
9	3	6	8	3	5	5102.9632	0.0004
9	2	7	8	2	6	5114.0603	0.0018
9	1	8	8	1	7	5158.9927	0.0032
13	3	11	13	2	11	5215.7226	-0.0017
7	1	6	6	0	6	5237.5538	-0.0034
12	3	10	12	2	10	5249.0476	0.0042
10	3	8	10	2	8	5296.4275	-0.0131

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	3	7	9	2	7	5312.1455	-0.0038
8	3	6	8	2	6	5323.6309	-0.0025
7	3	5	7	2	5	5331.6772	-0.0091
6	3	4	6	2	4	5337.0314	-0.0142
5	3	3	5	2	3	5340.3614	-0.0147
5	3	2	5	2	4	5345.2174	0.0101
6	3	3	6	2	5	5346.7231	0.0024
7	3	4	7	2	6	5349.1221	0.0018
8	3	5	8	2	7	5352.7067	-0.0035
9	3	6	9	2	8	5357.8457	-0.0003
10	3	7	10	2	9	5364.9258	-0.0125
12	3	9	12	2	11	5386.9313	0.0021
13	3	10	13	2	12	5402.9550	-0.0001
14	3	11	14	2	13	5423.2018	0.0020
4	2	2	3	1	2	5433.5125	-0.0011
4	2	3	3	1	3	5515.4485	-0.0108
10	1	10	9	1	9	5591.5782	-0.0011
10	0	10	9	0	9	5644.5035	-0.0022
10	2	9	9	2	8	5663.3358	-0.0107
10	5	5	9	5	4	5668.8133	0.0053
10	5	6	9	5	5	5668.9228	0.0068
10	6	4	9	6	3	5669.0404	0.0024
10	6	5	9	6	4	5669.2199	0.0144
10	4	7	9	4	6	5669.7770	0.0030
10	4	6	9	4	5	5670.4363	-0.0024
10	7	4	9	7	3	5685.4792	-0.0034
10	7	3	9	7	2	5730.8089	0.0005
10	3	8	9	3	7	5842.6821	0.0024
10	3	7	9	3	6	5864.9642	0.0003
10	2	8	9	2	7	5974.9984	0.0017
10	1	9	9	1	8	6110.1881	-0.0041
15	1	14	14	2	12	6149.3743	-0.0010
8	1	7	7	0	7	6203.8722	-0.0009
5	2	3	4	1	3	6228.5779	-0.0014
5	2	4	4	1	4	6235.6913	0.0000
11	1	11	10	1	10	6235.7426	-0.0026
11	0	11	10	0	10		
11	2	10	10	2	9		
11	5	7	10	5	6		
11	5	6	10	5	5		
11	6	6	10	6	5		
11	6	5	10	6	4		

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	4	8	10	4	7	6236.0640	-0.0019
11	4	7	10	4	6	6236.0802	-0.0004
11	3	9	10	3	8	6237.0148	-0.0040
11	3	8	10	3	7	6238.0969	0.0002
11	2	9	10	2	8	6257.7738	-0.0038
11	1	10	10	1	9	6302.1480	-0.0015
12	1	12	11	1	11	6706.8191	0.0000
12	0	12	11	0	11	6761.9865	-0.0012
12	2	11	11	2	10	6793.4945	-0.0021
12	6	7	11	6	6	6802.5521	-0.0013
12	6	6	11	6	5	6802.5521	-0.0013
12	5	8	11	5	7	6802.5717	-0.0005
12	5	7	11	5	6	6802.5717	-0.0005
12	4	9	11	4	8	6803.1280	-0.0012
12	4	8	11	4	7	6803.1547	-0.0019
12	3	10	11	3	9	6804.2979	0.0001
12	3	9	11	3	8	6805.9684	-0.0016
12	2	10	11	2	9	6830.9346	-0.0016
12	1	11	11	1	10	6872.9491	0.0011
7	2	5	6	1	5	7043.9821	0.0034
13	1	13	12	1	12	7263.8969	0.0022
13	0	13	12	0	12	7318.8557	0.0020
7	2	6	6	1	6	7320.6420	0.0011
13	2	12	12	2	11	7358.0690	-0.0007
13	5	9	12	5	8	7369.4475	-0.0013
13	5	8	12	5	7	7369.4475	-0.0013
13	4	10	12	4	9	7370.2220	-0.0023
13	4	9	12	4	8	7370.2727	-0.0003
13	3	11	12	3	10	7371.5970	0.0012
13	3	10	12	3	9	7374.0929	-0.0027
13	2	11	12	2	10	7404.9133	-0.0016
13	1	12	12	1	11	7443.1330	-0.0012
6	4	3	6	3	3	7480.3653	-0.0051
6	4	2	6	3	4	7480.4437	0.0023
8	2	6	7	1	6	7573.3026	0.0013
4	3	1	3	2	1	7610.5758	0.0010
4	3	2	3	2	2	7611.2521	-0.0043
11	1	10	10	0	10	7806.3184	-0.0036
14	1	14	13	1	13	7820.5893	0.0005
14	0	14	13	0	13	7874.5122	0.0003
14	2	13	13	2	12	7922.2727	0.0025
14	5	10	13	5	9	7936.3176	-0.0015

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
14	5	9	13	5	8	7936.4011	0.0023
8	2	7	7	1	7	7937.3505	-0.0002
14	4	11	13	4	10	7937.4344	0.0010
14	4	10	13	4	9	7938.8943	0.0002
14	3	12	13	3	11	7942.5148	-0.0002
14	3	11	13	3	10	7979.6331	0.0007
14	2	12	13	2	11	8012.6333	-0.0001
5	3	2	4	2	2	8176.6049	0.0013
5	3	3	4	2	3	8178.6417	-0.0002
15	1	15	14	1	14	8376.8914	-0.0004
15	0	15	14	0	14	8429.0379	0.0005
15	2	14	14	2	13	8486.0721	0.0019
15	5	11	14	5	10	8503.1824	0.0015
15	5	10	14	5	9	8504.5094	0.0026
15	4	12	14	4	11	8504.6435	0.0017
15	3	13	14	3	12	8506.1715	0.0015
15	3	12	14	3	11	8511.2756	0.0024
15	2	13	14	2	12	8554.9713	-0.0004
9	2	8	8	1	8	8559.2121	-0.0004
15	1	14	14	1	13	8581.3666	0.0001
10	2	8	9	1	8	8627.1015	0.0023
6	3	3	5	2	3	8741.7495	0.0002
6	3	4	5	2	4	8746.4857	-0.0004
16	1	16	15	1	15	8932.7980	0.0011
16	0	16	15	0	15	8982.5336	-0.0006
16	2	15	15	2	14	9049.4446	0.0025
16	3	14	15	3	13	9073.4001	0.0031
16	3	13	15	3	12	9080.4201	0.0010
16	2	14	15	2	13	9130.7839	-0.0009
16	1	15	15	1	14	9149.2507	0.0004
11	2	9	10	1	9	9154.0703	0.0018
10	2	9	9	1	9	9189.1094	0.0014
7	3	4	6	2	4	9305.5611	0.0021
7	3	5	6	2	5	9314.9879	0.0017
17	1	17	16	1	16	9488.3010	0.0006
17	0	17	16	0	16	9535.1266	-0.0009
17	2	16	16	2	15	9612.3625	0.0037
17	3	15	16	3	14	9640.5466	0.0017
12	2	10	11	1	10	9682.8564	0.0013
17	2	15	16	2	14	9706.8976	-0.0029

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
17	1	16	16	1	15	9716.1984	0.0009
4	4	0	3	3	0	9747.9665	-0.0005
4	4	1	3	3	1		
11	2	10	10	1	10	9826.1080	0.0000
14	1	13	13	0	13	9850.3222	-0.0009
8	3	5	7	2	5	9867.5020	-0.0006
8	3	6	7	2	6	9884.3707	0.0003
18	1	18	17	1	17	10043.3991	-0.0018
18	0	18	17	0	17	10086.9514	-0.0019
13	2	11	12	1	11	10214.8252	0.0032
18	1	17	17	1	16	10282.1139	-0.0049
5	4	1	4	3	1	10314.8681	0.0003
5	4	2	4	3	2		
9	3	6	8	2	6	10426.9845	-0.0008
9	3	7	8	2	7	10454.8951	-0.0002
12	2	11	11	1	11	10470.2297	0.0004
6	4	2	5	3	2	10881.7210	0.0008
6	4	3	5	3	3	10881.7469	0.0033
10	3	7	9	2	7	10983.3664	0.0008
10	3	8	9	2	8	11026.8431	0.0007
13	2	12	12	1	12	11121.4789	-0.0010
15	2	13	14	1	13	11293.6622	0.0037
7	4	3	6	3	3	11448.4894	0.0016
7	4	4	6	3	4	11448.5568	-0.0010
11	3	9	10	2	9	11600.5148	0.0000
14	2	13	13	1	13	11779.8595	0.0040
8	4	4	7	3	4	12015.1107	0.0023
8	4	5	7	3	5	12015.2822	-0.0010
12	3	9	11	2	9	12084.1721	0.0000
5	5	0	4	4	0	12451.4299	0.0005
5	5	1	4	4	1		
9	4	5	8	3	5	12581.5067	0.0007
9	4	6	8	3	6	12581.8885	-0.0011
13	3	10	12	2	10	12627.3318	0.0003
13	3	11	12	2	11	12754.3333	0.0009
6	5	1	5	4	1	13018.4021	-0.0030
6	5	2	5	4	2		
10	4	6	9	3	6	13147.5841	-0.0009
10	4	7	9	3	7	13148.3490	-0.0007
7	5	2	6	4	2	13585.3645	0.0004
7	5	3	6	4	3		
11	4	7	10	3	7	13713.2263	-0.0006

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	4	8	10	3	8	13714.6400	-0.0016
8	5	3	7	4	3	14152.2870	0.0009
8	5	4	7	4	4	14278.2851	-0.0016
12	4	8	11	3	8	14280.7508	-0.0011

Table S9: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O-CH₂CH(CF₃)O in an excited state

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	5	4	8	4	4	14719.1474	0.0002
9	5	5	8	4	5		
13	4	9	12	3	9	14842.5880	-0.0017
13	4	10	12	3	10	14846.6763	-0.0021
6	6	0	5	5	0	15154.3955	0.0017
6	6	1	5	5	1		
10	5	5	9	4	5	15285.9188	-0.0012
10	5	6	9	4	6		
14	4	10	13	3	10	15405.9266	-0.0009
14	4	11	13	3	11	15412.4317	-0.0017
7	6	1	6	5	1	15721.4550	0.0021
7	6	2	6	5	2		
15	4	12	14	3	12	15978.0449	-0.0011
8	6	3	7	5	3	16288.5061	0.0017
8	6	2	7	5	2		
9	6	4	8	5	4	16855.5358	0.0015
9	6	3	8	5	3		
10	6	5	9	5	5	17422.5289	0.0021
10	6	4	9	5	4		
11	6	6	10	5	6	17989.4647	0.0007
11	6	5	10	5	5		
8	7	2	7	6	2	18423.9360	-0.0018
8	7	1	7	6	1		
9	7	3	8	6	3	18991.0861	-0.0012
9	7	2	8	6	2		
10	7	3	9	6	3	19558.2237	-0.0003
10	7	4	9	6	4		

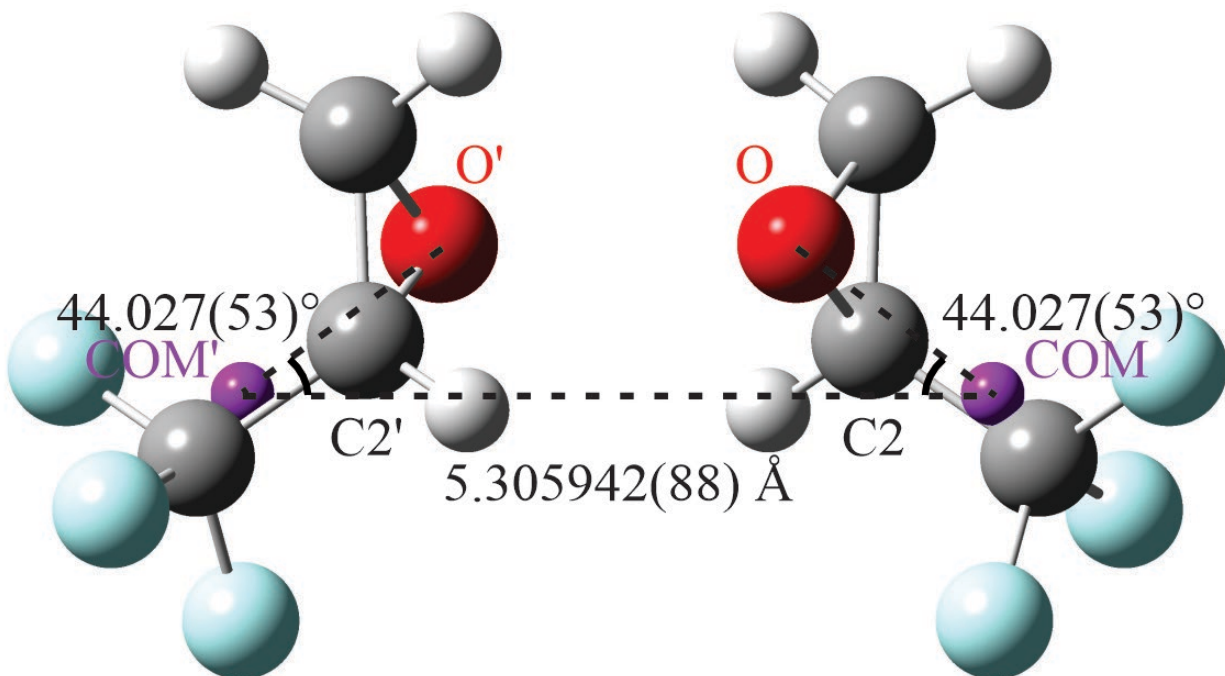


Figure S1: Structural parameters used in the fitting of intermolecular geometric parameters of (TFO)₂ Isomer (i) using STRFIT. In addition to the parameters shown in the figure, namely the distance between the centers of mass of the two subunits (COM–COM') and the two symmetrically equivalent angles (COM'–COM–O and COM–COM'–O'), two symmetrically equivalent dihedral angles (not shown for clarity) are fit (COM'–COM–O–C2 and COM–COM'–O'–C2') and share the common value $-42.78(16)^\circ$. A third dihedral angle (O'–COM'–COM–O), also not shown, is fixed at a value of 74.9° , which is found to minimize the rms deviation of the fit. The geometry of each subunit is fixed at its zero-point average structure.

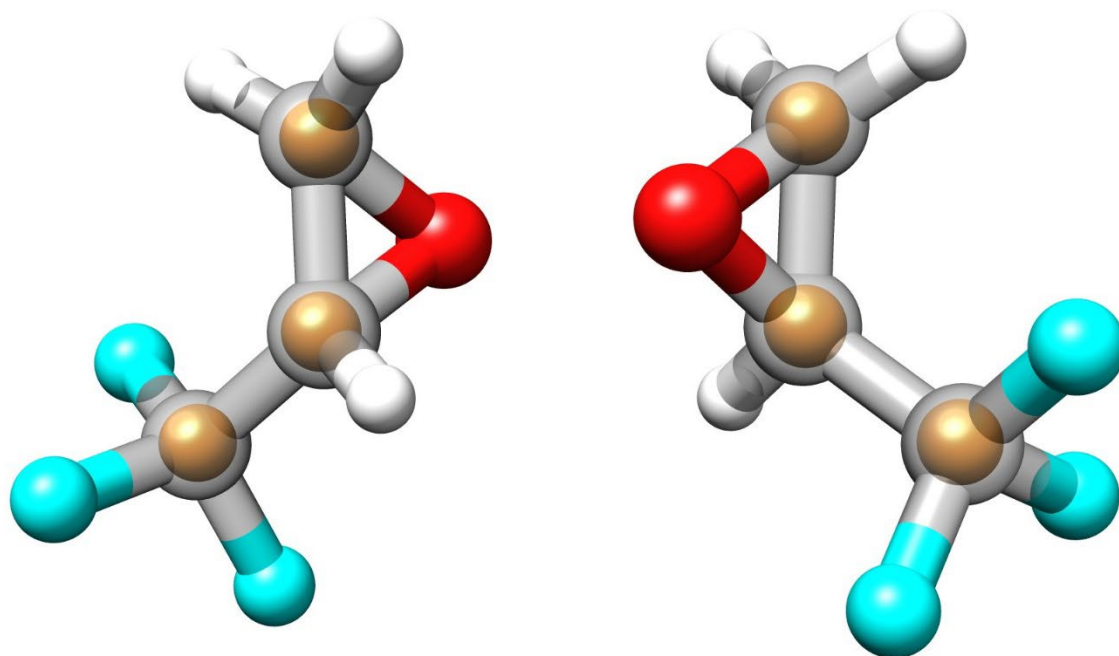


Figure S2: A comparison of the theoretically predicted structure of the lowest energy homochiral TFO dimer and the experimentally determined locations of the two sets of three symmetrically equivalent carbon atoms (in orange). Atom colors (theoretical structure): C, gray; H, white; F, blue, O, red.