

**Microwave Spectrum and Molecular Structure of the Chiral Tagging Candidate,
3,3,3-Trifluoro-1,2-Epoxypropane and Its Complex with the Argon Atom**

Mark D. Marshall, Helen O. Leung, Kevin Wang, Mbatang Desmond Acha

Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000

Supporting Information

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).

Table S1 presents the atomic coordinates in the appropriate principal inertial axis system for each of the theoretical structures presented in Figures 1 and 4 of the manuscript.

Tables S2 through S10 contain the quantum number assignments, observed transition frequencies (in MHz), and the residuals (obs. - calc., also in MHz) from the least squares fits. The quantum numbers are J , K_a , and K_c , the usual asymmetric top rotational quantum numbers for the initial and final levels of the transition.

Table S11 presents the spectroscopic constants in the S reduction for all isotopologues studied of argon-3,3,3-trifluoro-1,2-epoxypropane. (A reduction constants are presented in Table 5 of the manuscript.)

The complete reference for Gaussian 16 (reference 16) is given here.

Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A. V., Bloino, J., Janesko, B. G., Gomperts, R., Mennucci, B., Hratchian, H. P., Ortiz, J. V., Izmaylov, A. F., Sonnenberg, J. L., Williams-Young, F., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V. G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M. J., Heyd, J. J., Brothers, E. N., Kudin, K. N., Staroverov, V. N., Keith, T. A., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A. P., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Millam, J. M., Klene, M., Adamo, C., Cammi, R., Ochterski, J. W., Martin, R. L., Morokuma, K., Farkas, O., Foresman, J. B. and Fox, D. J. *Gaussian 16*, Revision A.03; Gaussian, Inc.: Wallingford, CT, 2016.

Table S1: Coordinates in the principal inertial axis system for the theoretical structures of 3,3,3-trifluoro-1,2-epoxypropane and its argon complex

3,3-difluoro-1,2-epoxypropane

	<i>a</i>	<i>b</i>	<i>c</i>
C1	-1.8857	-0.7140	0.0071
C2	-0.7754	-0.0231	0.6609
C3	0.5819	-0.0090	0.0248
O	-1.7739	0.7297	-0.0228
F _O	1.2114	1.1543	0.2560
F _C	1.3402	-0.9912	0.5502
F _a	0.5284	-0.1890	-1.2998
H1	-2.6868	-1.0921	0.6232
H2	-1.7168	-1.1966	-0.9427
H3	-0.7475	0.0805	1.7367

Ar-3,3,3-trifluoro-1,2-epoxypropane

No BSSE Correction

	Structure (a)			Structure (b)			Structure (c)		
	<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>
C1	0.1937	-1.4405	-0.6012	0.0338	-1.7905	0.1162	-0.0510	1.7611	-0.6639
C2	-0.2234	-0.1039	-0.2036	0.7630	-0.7789	-0.6345	-1.1278	1.1506	0.1018
C3	-1.6517	0.2385	-0.0264	1.1394	0.5147	-0.0229	-1.4275	-0.2944	-0.0038
O	0.2978	-1.0198	0.7693	1.4496	-1.9175	-0.0968	0.1242	1.4580	0.7302
F _O	-1.8423	1.0978	0.9976	2.3461	0.9439	-0.4505	-1.8053	-0.8202	1.1812
F _C	-2.1422	0.8556	-1.1287	0.2560	1.4852	-0.3605	-2.4577	-0.5144	-0.8561
F _a	-2.4191	-0.8437	0.1976	1.1756	0.4604	1.3209	-0.3798	-1.0083	-0.4542
H1	1.1401	-1.5516	-1.1077	-0.5661	-2.5007	-0.4317	-0.1159	2.8147	-0.8874
H2	-0.5579	-2.1936	-0.7782	-0.2445	-1.5863	1.1381	0.5344	1.1455	-1.3286
H3	0.3888	0.7564	-0.4357	0.6818	-0.7262	-1.7112	-1.9825	1.7347	0.4134
Ar	3.4055	0.3481	-0.0314	-2.9543	0.1322	-0.0158	2.9796	-0.3992	-0.0155

Table S1: Coordinates in the principal inertial axis system for the theoretical structures of 3,3,3-trifluoro-1,2-epoxypropane and its argon complex

	Structure (d)			Structure (e)			Structure (f)		
	<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>
C1	-1.0601	2.0726	0.3337	2.1081	1.4564	-0.7091	2.9647	0.3599	0.7477
C2	-0.5430	0.7338	0.5758	0.9007	0.8593	-0.1575	2.0709	-0.4817	-0.0342
C3	-1.2127	-0.4642	0.0233	0.7647	-0.6059	-0.0037	0.6062	-0.2737	-0.0212
O	0.0714	1.5816	-0.4043	1.8705	1.4647	0.7085	2.8187	0.5656	-0.6673
F _O	-0.3261	-1.4110	-0.3521	0.0847	-0.9357	1.1153	0.0521	-0.5043	-1.2307
F _C	-2.0097	-1.0454	0.9524	0.0670	-1.1386	-1.0360	0.0027	-1.1319	0.8365
F _a	-1.9852	-0.1803	-1.0410	1.9537	-1.2341	0.0383	0.2640	0.9715	0.3564
H1	-0.8262	2.8480	1.0468	2.0307	2.4238	-1.1809	3.9199	-0.0453	1.0442
H2	-1.9563	2.1904	-0.2548	2.9165	0.8135	-1.0196	2.5464	1.1464	1.3558
H3	0.0370	0.5188	1.4624	-0.0523	1.3624	-0.2443	2.3485	-1.4957	-0.2863
Ar	2.9404	-0.2230	0.0343	-3.0061	0.3572	-0.0165	-3.1962	0.2183	0.0239

With BSSE Correction

	Structure (a)			Structure (b)			Structure (c)		
	<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>
C1	0.1499	-1.4400	-0.6063	0.0346	-1.7667	0.1436	-0.0655	1.7311	-0.6666
C2	-0.2613	-0.1047	-0.1979	0.7654	-0.7714	-0.6270	-1.1616	1.1472	0.0926
C3	-1.6886	0.2451	-0.0262	1.1995	0.5072	-0.0223	-1.4873	-0.2927	-0.0047
O	0.2479	-1.0337	0.7690	1.4379	-1.9322	-0.1199	0.0895	1.4361	0.7317
F _O	-1.8802	1.0952	1.0052	2.4022	0.9049	-0.4899	-1.8872	-0.8017	1.1803
F _C	-2.1681	0.8762	-1.1252	0.3327	1.5044	-0.3233	-2.5126	-0.5002	-0.8660
F _a	-2.4642	-0.8344	0.1821	1.2814	0.4435	1.3191	-0.4487	-1.0298	-0.4385
H1	1.0987	-1.5520	-1.1079	-0.6041	-2.4563	-0.3866	-0.1082	2.7840	-0.8991
H2	-0.6054	-2.1864	-0.7955	-0.2017	-1.5612	1.1758	0.5149	1.0993	-1.3202
H3	0.3578	0.7539	-0.4174	0.6478	-0.7096	-1.6999	-2.0082	1.7498	0.3905
Ar	3.5159	0.3387	-0.0294	-3.0813	0.1462	-0.0177	3.1247	-0.3848	-0.0140

Table S1: Coordinates in the principal inertial axis system for the theoretical structures of 3,3,3-trifluoro-1,2-epoxypropane and its argon complex

	Structure (d)			Structure (e)			Structure (f)		
	<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>
C1	-1.0864	2.0673	0.3510	2.0893	1.5130	-0.7088	3.0198	0.4321	0.7263
C2	-0.5674	0.7245	0.5659	0.9113	0.8642	-0.1519	2.1391	-0.4694	-0.0018
C3	-1.2580	-0.4662	0.0235	0.8366	-0.6060	-0.0045	0.6717	-0.2802	-0.0048
O	0.0206	1.5786	-0.4249	1.8616	1.5047	0.7104	2.8749	0.5450	-0.6993
F _O	-0.3867	-1.4128	-0.3864	0.1786	-0.9688	1.1174	0.1239	-0.5949	-1.1981
F _C	-2.0289	-1.0526	0.9712	0.1540	-1.1620	-1.0347	0.0771	-1.0896	0.9049
F _a	-2.0610	-0.1702	-1.0146	2.0506	-1.1851	0.0262	0.3124	0.9820	0.2917
H1	-0.8282	2.8356	1.0634	1.9690	2.4786	-1.1751	3.9794	0.0592	1.0498
H2	-1.9994	2.1934	-0.2093	2.9212	0.9052	-1.0281	2.5897	1.2503	1.2820
H3	0.0382	0.4998	1.4328	-0.0620	1.3282	-0.2296	2.4305	-1.4937	-0.1880
Ar	3.0647	-0.2166	0.0343	-3.1521	0.3235	-0.0150	-3.3726	0.2158	0.0105

Table S2: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
3	1	2	2	2	0	5635.8406	-0.0086
3	1	2	2	2	1	5639.8034	-0.0067
9	1	8	9	0	9	5884.2253	-0.0084
2	0	2	1	1	0	5946.7176	0.0014
2	0	2	1	1	1	6061.0605	-0.0041
9	2	7	9	1	8	6197.8043	0.0004
10	2	8	10	1	9	6237.8610	-0.0013
8	2	6	8	1	7	6245.2131	0.0012
6	2	5	6	1	5	6257.5406	0.0002
7	2	5	7	1	6	6362.1030	0.0004
11	2	9	11	1	10	6380.6829	-0.0037
6	2	4	6	1	5	6528.0499	0.0003
5	2	4	5	1	4	6584.2955	-0.0018
12	2	10	12	1	11	6639.1549	-0.0001
1	1	1	0	0	0	6659.2280	0.0014
5	2	3	5	1	4	6721.1989	0.0003
1	1	0	0	0	0	6773.5733	-0.0016
10	1	9	10	0	10	6784.2599	0.0024
4	2	3	4	1	3	6860.7604	0.0009
4	2	2	4	1	3	6919.8556	-0.0007
13	2	11	13	1	12	7023.9471	-0.0015
3	2	2	3	1	2	7084.3858	0.0001
3	2	1	3	1	2	7104.1602	0.0014
2	2	1	2	1	1	7253.4117	-0.0026
2	2	0	2	1	1	7257.3774	0.0021
14	2	12	14	1	13	7543.2802	0.0002
2	2	1	2	1	2	7596.4556	-0.0027
2	2	0	2	1	2	7600.4208	0.0016
3	2	2	3	1	3	7770.3861	0.0013
11	1	10	11	0	11	7789.8159	0.0056
3	2	1	3	1	3	7790.1573	-0.0006
4	2	3	4	1	4	8003.6246	-0.0025
4	2	2	4	1	4	8062.7236	-0.0002
6	3	4	5	4	1	8153.7618	-0.0391
6	3	3	5	4	2	8160.9587	-0.0346
5	2	4	5	1	5	8297.0902	0.0023
2	1	2	1	1	1	8368.4791	0.0006
5	2	3	5	1	5	8433.9925	0.0033
2	0	2	1	0	1	8478.8742	0.0025
2	1	1	1	1	0	8597.1728	-0.0013
6	2	5	6	1	6	8651.6060	0.0017
5	2	4	4	3	1	8809.4991	0.0028
5	2	4	4	3	2	8810.1054	0.0087
12	1	11	12	0	12	8885.5464	0.0035
6	2	4	6	1	6	8922.1148	0.0013

Table S2: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
4	1	4	3	2	1	8939.0834	0.0005
5	2	3	4	3	1	8946.3972	-0.0004
5	2	3	4	3	2	8947.0060	0.0080
4	1	4	3	2	2	8958.8572	0.0012
16	2	14	16	1	15	9000.3758	-0.0068
14	3	12	14	2	12	9016.2929	0.0114
7	2	6	7	1	7	9067.7838	0.0027
16	3	13	16	2	14	9501.0150	0.0025
8	2	7	8	1	8	9545.8257	0.0042
11	7	5	10	8	2	9571.7458	-0.0027
11	7	4	10	8	3		
13	3	11	13	2	11	9647.1742	0.0072
15	3	12	15	2	13	9686.6494	0.0012
14	3	11	14	2	12	9952.3181	0.0018
13	1	12	13	0	13	10052.1807	0.0028
3	0	3	2	1	1	10057.9626	-0.0012
4	1	3	3	2	1	10081.9506	0.0002
9	2	8	9	1	9	10085.3742	0.0027
4	1	3	3	2	2	10101.7254	0.0019
12	3	10	12	2	10	10221.3536	-0.0059
13	3	10	13	2	11	10273.1057	0.0010
10	6	5	9	7	2	10280.3364	0.0018
10	6	4	9	7	3		
8	2	6	8	1	8	10322.4050	0.0000
3	0	3	2	1	2	10401.0059	-0.0019
12	3	9	12	2	10	10622.8568	-0.0031
10	2	9	10	1	10	10685.3949	-0.0009
11	3	9	11	2	9	10730.2999	-0.0024
2	1	2	1	0	1	10786.2853	-0.0004
11	3	8	11	2	9	10976.0657	-0.0056
9	5	5	8	6	2	10989.8001	0.0004
9	5	4	8	6	3		
2	1	1	1	0	1	11129.3320	0.0023
10	3	8	10	2	8	11167.3503	-0.0027
9	2	7	9	1	9	11265.4910	0.0048
14	1	13	14	0	14	11268.6064	0.0043
10	3	7	10	2	8	11309.9241	-0.0015
11	2	10	11	1	11	11344.1059	0.0043
9	3	7	9	2	7	11528.6106	0.0043
9	3	6	9	2	7	11606.2273	-0.0050
8	4	5	7	5	2	11700.9336	0.0174
8	4	4	7	5	3	11701.6873	0.0090
8	3	6	8	2	6	11813.8055	0.0001
8	3	5	8	2	6	11852.9310	0.0033
7	3	5	7	2	5	12026.9460	0.0026

Table S2: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
7	3	4	7	2	5	12044.8272	0.0028
12	2	11	12	1	12	12058.9188	0.0013
6	3	4	6	2	4	12176.1257	-0.0047
6	3	3	6	2	4	12183.3084	-0.0005
5	3	3	5	2	3	12272.5653	-0.0040
5	3	2	5	2	3	12274.9667	-0.0009
4	3	2	4	2	2	12328.9124	-0.0011
4	3	1	4	2	2	12329.5128	-0.0011
3	3	0	3	2	1	12357.6149	-0.0166
3	3	1	3	2	2	12377.3398	0.0212
10	2	8	10	1	10	12383.8642	0.0039
4	3	2	4	2	3	12388.0093	-0.0010
4	3	1	4	2	3	12388.6160	0.0054
5	3	3	5	2	4	12409.4732	0.0026
5	3	2	5	2	4	12411.8727	0.0038
7	3	4	6	4	3	12427.3912	0.0304
6	3	4	6	2	5	12446.6396	-0.0001
6	3	3	6	2	5	12453.8218	0.0037
7	3	5	7	2	6	12505.0028	-0.0024
15	1	14	15	0	15	12514.0898	-0.0001
7	3	4	7	2	6	12522.8929	0.0067
3	1	3	2	1	2	12550.2716	0.0022
8	3	6	8	2	7	12590.3955	0.0067
8	3	5	8	2	7	12629.5025	-0.0087
3	0	3	2	0	2	12708.4250	0.0033
3	2	2	2	2	1	12724.1957	-0.0001
3	2	1	2	2	0	12740.0072	-0.0008
9	3	6	9	2	8	12786.3381	-0.0088
13	2	12	13	1	13	12826.5424	0.0068
5	1	5	4	2	2	12841.9280	0.0057
10	3	8	10	2	9	12865.8207	0.0032
3	1	2	2	1	1	12893.2255	0.0011
5	1	5	4	2	3	12901.0164	-0.0027
10	3	7	10	2	9	13008.3944	0.0043
6	2	5	5	3	2	13018.5495	0.0076
6	2	5	5	3	3	13020.9461	0.0059
11	3	9	11	2	10	13067.1830	0.0147
6	2	4	5	3	2	13289.0582	0.0070
6	2	4	5	3	3	13291.4510	0.0016
11	3	8	11	2	10	13312.9416	0.0044
12	3	10	12	2	11	13317.7416	-0.0049
13	3	11	13	2	12	13621.8270	-0.0163
14	2	13	14	1	14	13643.0026	-0.0053
11	2	9	11	1	11	13680.9605	-0.0071
12	3	9	12	2	11	13719.2291	-0.0178

Table S2: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
16	1	15	16	0	16	13770.3342	0.0033
12	7	6	11	8	3	13823.5976	0.0027
14	3	12	14	2	13	13982.9359	0.0042
4	0	4	3	1	2	14091.0340	0.0031
13	3	10	13	2	12	14247.7976	0.0166
15	3	13	15	2	14	14403.5876	0.0275
15	2	14	15	1	15	14503.8821	-0.0083
11	6	6	10	7	3	14533.7214	-0.0008
5	1	4	4	2	2	14554.7193	0.0064
5	1	4	4	2	3	14613.8151	0.0055
4	0	4	3	1	3	14777.0329	0.0030
3	1	3	2	0	2	14857.6807	-0.0026
16	3	14	16	2	15	14885.2967	0.0195
14	3	11	14	2	13	14918.9467	-0.0197
12	2	10	12	1	12	15155.3047	0.0002
16	2	15	16	1	16	15404.4130	-0.0027
3	1	2	2	0	2	15543.6799	-0.0025
16	4	12	16	3	13	15764.3131	0.0047
2	2	1	1	1	0	15850.5887	0.0002
2	2	0	1	1	0	15854.5506	0.0011
9	4	6	8	5	3	15960.4001	-0.0177
9	4	5	8	5	4	15962.4003	0.0035
2	2	1	1	1	1	15964.9367	-0.0001
2	2	0	1	1	1	15968.8955	-0.0023
15	4	11	15	3	12	16135.9322	-0.0151
14	4	11	14	3	11	16381.2770	0.0113
14	4	10	14	3	11	16446.0725	-0.0429
6	1	6	5	2	3	16641.9046	-0.0007
8	3	6	7	4	3	16668.2276	-0.0024
8	3	5	7	4	4	16707.6023	-0.0039
4	1	4	3	1	3	16729.2350	-0.0057
6	1	6	5	2	4	16778.8106	0.0041
13	2	11	13	1	13	16801.1993	-0.0125
12	4	9	12	3	9	16867.3802	0.0037
12	4	8	12	3	9	16886.8014	-0.0038
4	0	4	3	0	3	16926.2873	-0.0043
4	2	3	3	2	2	16962.4884	0.0054
4	3	2	3	3	1	16973.1700	-0.0047
4	3	1	3	3	0	16973.6782	-0.0109
4	2	2	3	2	1	17001.8071	0.0004
11	4	8	11	3	8	17019.9327	0.0105
11	4	7	11	3	8	17029.7013	0.0029
10	4	7	10	3	7	17127.7799	-0.0031
10	4	6	10	3	7	17132.3730	0.0057
4	1	3	3	1	2	17186.1099	0.0007

Table S2: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	4	6	9	3	6	17201.6145	0.0060
9	4	5	9	3	6	17203.5747	-0.0056
7	2	6	6	3	3	17204.9420	0.0094
7	2	6	6	3	4	17212.1130	0.0019
8	4	5	8	3	5	17250.4434	0.0086
8	4	4	8	3	5	17251.2003	0.0051
11	4	8	11	3	9	17265.6836	-0.0076
12	4	9	12	3	10	17268.8806	0.0037
10	4	7	10	3	8	17270.3491	-0.0065
10	4	6	10	3	8	17274.9486	0.0087
11	4	7	11	3	9	17275.4598	-0.0075
9	4	6	9	3	7	17279.2206	-0.0138
9	4	5	9	3	7	17281.2024	-0.0039
7	4	3	7	3	4	17281.7810	0.0030
13	4	10	13	3	11	17284.3667	0.0038
12	4	8	12	3	10	17288.3070	0.0014
8	4	5	8	3	6	17289.5612	0.0040
8	4	4	8	3	6	17290.3276	0.0100
7	4	4	7	3	5	17299.4031	-0.0019
6	4	2	6	3	3	17300.5475	0.0203
6	4	3	6	3	4	17307.6097	-0.0267
5	4	1	5	3	2	17311.3826	0.0019
5	4	2	5	3	3	17313.7563	-0.0088
4	4	0	4	3	1	17317.1974	-0.0089
4	4	1	4	3	2	17317.7975	-0.0076
13	4	9	13	3	11	17320.7728	0.0088
15	4	12	15	3	13	17373.3736	-0.0007
14	4	10	14	3	12	17382.1553	0.0052
16	4	13	16	3	14	17458.5961	-0.0011
7	2	5	6	3	3	17682.9839	-0.0105
7	2	5	6	3	4	17690.1690	-0.0039
5	0	5	4	1	3	18034.0791	-0.0012
13	7	7	12	8	4	18077.7078	-0.0018

Table S3: Observed Transition Frequencies (in MHz) for $^{13}\text{CH}_2\text{CH}(\text{CF}_3)\text{O}$

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	2	7	9	1	8	6231.6722	0.0140
8	2	6	8	1	7	6279.5333	0.0009
7	2	5	7	1	6	6397.1744	0.0023
6	2	4	6	1	5	6564.0498	-0.0044
1	1	1	0	0	0	6605.5667	0.0003
5	2	4	5	1	4	6620.7452	-0.0025
1	1	0	0	0	0	6720.4663	-0.0001
5	2	3	5	1	4	6758.2219	-0.0023
4	2	3	4	1	3	6898.5514	0.0027
4	2	2	4	1	3	6957.8938	0.0005
3	2	2	3	1	2	7123.2560	0.0001
3	2	1	3	1	2	7143.1104	-0.0015
2	2	0	2	1	1	7297.0714	-0.0070
2	2	1	2	1	2	7637.7955	-0.0041
2	2	0	2	1	2	7641.7738	-0.0034
3	2	1	3	1	3	7832.4337	0.0135
4	2	3	4	1	4	8046.9434	0.0135
4	2	2	4	1	4	8106.2774	0.0029
2	1	2	1	1	1	8234.1539	0.0041
5	2	4	5	1	5	8341.8073	0.0040
2	0	2	1	0	1	8345.0784	0.0006
5	2	4	4	3	1	8407.4605	0.0171
2	1	1	1	1	0	8463.9478	-0.0008
4	1	4	3	2	1	8628.1399	0.0055
4	1	4	3	2	2	8647.9940	0.0037
6	2	5	6	1	6	8698.0177	-0.0077
6	2	4	6	1	6	8969.6791	0.0040
7	2	6	7	1	7	9116.2134	0.0090
4	1	3	3	2	1	9776.5008	-0.0149
4	1	3	3	2	2	9796.3742	0.0026
3	0	3	2	1	1	9842.8886	0.0046
3	0	3	2	1	2	10187.5841	0.0013
2	1	2	1	0	1	10665.1856	-0.0001
2	1	1	1	0	1	11009.8840	-0.0005
8	3	5	8	2	6	11918.1985	-0.0047
7	3	4	7	2	5	12110.9440	0.0005
6	3	4	6	2	4	12242.8328	0.0116
6	3	3	6	2	4	12250.0148	-0.0103
5	3	3	5	2	3	12339.6672	0.0010
5	3	2	5	2	3	12342.0673	-0.0057
3	1	3	2	1	2	12348.7712	0.0040
4	3	2	4	2	2	12396.2538	0.0081
4	3	1	4	2	2	12396.8516	0.0035
3	3	0	3	2	1	12425.0612	-0.0214
3	3	1	3	2	2	12444.8708	0.0185

Table S3: Observed Transition Frequencies (in MHz) for $^{13}\text{CH}_2\text{CH}(\text{CF}_3)\text{O}$

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
4	3	2	4	2	3	12455.5881	-0.0022
4	3	1	4	2	3	12456.1902	-0.0025
5	3	3	5	2	4	12477.1478	0.0051
5	3	2	5	2	4	12479.5448	-0.0047
3	0	3	2	0	2	12507.6889	-0.0017
6	3	4	6	2	5	12514.4794	0.0085
3	2	2	2	2	1	12523.5366	0.0047
3	2	1	2	2	0	12539.4041	-0.0061
6	2	5	5	3	2	12549.4694	-0.0016
6	2	5	5	3	3	12551.8717	-0.0061
7	3	5	7	2	6	12573.0857	-0.0007
7	3	4	7	2	6	12591.0378	0.0070
8	3	6	8	2	7	12658.8432	0.0068
3	1	2	2	1	1	12693.3815	0.0049
8	3	5	8	2	7	12698.0764	-0.0214
9	3	7	9	2	8	12777.6632	-0.0147
10	3	8	10	2	9	12935.4591	0.0057
10	3	7	10	2	9	13078.5357	-0.0002
4	0	4	3	1	2	13808.0868	0.0040
5	1	4	4	2	2	14183.5354	-0.0085
5	1	4	4	2	3	14242.8918	0.0034
4	0	4	3	1	3	14497.3899	-0.0013
3	1	3	2	0	2	14668.8767	0.0017
3	1	2	2	0	2	15358.1795	-0.0038
2	2	1	1	1	0	15757.0492	-0.0003
2	2	0	1	1	0	15761.0254	-0.0016
2	2	1	1	1	1	15871.9397	-0.0097
2	2	0	1	1	1	15875.9276	0.0007
6	1	6	5	2	3	16193.5220	0.0034
4	1	4	3	1	3	16460.5554	0.0008
4	0	4	3	0	3	16658.5627	-0.0127
4	2	3	3	2	2	16694.9355	0.0153
4	3	2	3	3	1	16705.6556	-0.0026
4	3	1	3	3	0	16706.1699	-0.0047
4	2	2	3	2	1	16734.4076	-0.0013
4	1	3	3	1	2	16919.6213	-0.0063
7	4	3	7	3	4	17376.1464	0.0004
6	4	2	6	3	3	17394.9952	0.0284
6	4	3	6	3	4	17402.0777	-0.0234
5	4	1	5	3	2	17405.8476	-0.0134
5	4	2	5	3	3	17408.2676	0.0137

Table S4: Observed Transition Frequencies (in MHz) for CH₂¹³CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	2	7	9	1	8	6174.0404	-0.0188
8	2	6	8	1	7	6232.5308	-0.0079
6	2	5	6	1	5	6270.6827	0.0144
7	2	5	7	1	6	6354.8983	0.0021
6	2	4	6	1	5	6521.6176	0.0175
5	2	4	5	1	4	6585.0648	-0.0107
1	1	1	0	0	0	6636.2899	0.0000
5	2	3	5	1	4	6711.9683	0.0008
1	1	0	0	0	0	6746.0936	-0.0002
4	2	3	4	1	3	6850.8944	-0.0070
4	2	2	4	1	3	6905.6542	0.0036
3	2	2	3	1	2	7065.8262	0.0044
2	2	1	2	1	1	7228.2205	0.0009
2	2	0	2	1	1	7231.8878	0.0000
2	2	1	2	1	2	7557.6314	0.0015
3	2	2	3	1	3	7724.5616	-0.0007
3	2	1	3	1	3	7742.8806	0.0046
4	2	3	4	1	4	7948.3924	0.0063
5	2	4	5	1	5	8229.9517	0.0012
2	1	2	1	1	1	8343.9487	0.0017
5	2	3	5	1	5	8356.8351	-0.0073
2	0	2	1	0	1	8450.0893	0.0013
2	1	1	1	1	0	8563.5530	-0.0006
6	2	5	6	1	6	8570.0525	-0.0027
5	2	4	4	3	1	8791.8386	0.0038
5	2	4	4	3	2	8792.3681	-0.0029
6	2	4	6	1	6	8820.9995	0.0127
4	1	4	3	2	1	8937.8564	-0.0032
7	2	6	7	1	7	8969.3060	0.0054
8	2	7	8	1	8	9427.9386	0.0058
9	2	8	9	1	9	9945.7056	0.0054
3	0	3	2	1	1	10033.2955	0.0004
4	1	3	3	2	1	10035.3369	-0.0075
4	1	3	3	2	2	10053.6600	0.0019
3	0	3	2	1	2	10362.7365	0.0312
10	2	9	10	1	10	10521.7265	-0.0089
2	1	2	1	0	1	10753.3561	0.0005
2	1	1	1	0	1	11082.7671	0.0010
8	3	5	8	2	6	11834.3392	-0.0088
7	3	5	7	2	5	11998.3235	-0.0031
7	3	4	7	2	5	12014.2938	-0.0102
6	3	4	6	2	4	12137.1492	-0.0095
6	3	3	6	2	4	12143.5662	-0.0052
5	3	3	5	2	3	12226.7136	0.0094
5	3	2	5	2	3	12228.8501	0.0037

Table S4: Observed Transition Frequencies (in MHz) for CH₂¹³CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
4	3	2	4	2	2	12278.9483	0.0015
4	3	1	4	2	2	12279.4888	0.0057
3	3	0	3	2	1	12305.5510	-0.0005
3	3	1	3	2	2	12323.7991	0.0105
4	3	2	4	2	3	12333.6578	-0.0383
4	3	1	4	2	3	12334.2323	0.0000
5	3	3	5	2	4	12353.5978	0.0016
5	3	2	5	2	4	12355.7382	-0.0001
7	3	5	7	2	6	12442.3120	0.0064
7	3	4	7	2	6	12458.2747	-0.0084
3	1	3	2	1	2	12513.6342	-0.0162
8	3	6	8	2	7	12521.7071	0.0055
9	3	7	9	2	8	12631.8658	-0.0009
3	0	3	2	0	2	12665.9715	-0.0016
3	2	2	2	2	1	12680.5838	0.0011
3	2	1	2	2	0	12695.2262	-0.0021
5	1	5	4	2	2	12841.3685	0.0011
3	1	2	2	1	1	12842.9824	0.0018
5	1	5	4	2	3	12896.1282	0.0115
6	2	5	5	3	2	12988.7415	-0.0165
6	2	4	5	3	3	13241.8588	0.0270
4	0	4	3	1	2	14061.3357	-0.0039
5	1	4	4	2	2	14486.2335	-0.0089
5	1	4	4	2	3	14540.9629	-0.0288
4	0	4	3	1	3	14720.0792	-0.0009
3	1	3	2	0	2	14816.9179	-0.0002
3	1	2	2	0	2	15475.6602	0.0016
2	2	1	1	1	0	15791.7760	0.0029
2	2	0	1	1	0	15795.4425	0.0012
2	2	1	1	1	1	15901.5778	0.0008
2	2	0	1	1	1	15905.2486	0.0035
4	1	4	3	1	3	16680.7313	-0.0043
4	0	4	3	0	3	16871.0248	-0.0003
4	2	3	3	2	2	16904.5589	-0.0006
4	3	2	3	3	1	16914.4605	-0.0065
4	3	1	3	3	0	16914.9280	0.0015
4	2	2	3	2	1	16940.9964	0.0014
4	1	3	3	1	2	17119.4853	0.0055
7	4	3	7	3	4	17210.5719	0.0181
7	4	4	7	3	5	17226.2916	-0.0210
7	4	3	7	3	5	17226.5672	0.0359
6	4	2	6	3	3	17227.7737	0.0275
6	4	3	6	3	4	17234.0739	-0.0253
5	4	1	5	3	2	17237.7121	-0.0098
5	4	2	5	3	3	17239.8577	0.0057

Table S4: Observed Transition Frequencies (in MHz) for CH₂¹³CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
4	4	0	4	3	1	17243.0822	-0.0078
4	4	1	4	3	2	17243.6154	-0.0095
5	0	5	4	1	3	18003.9969	0.0105

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(¹³CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	2	7	9	1	8	6206.1479	0.0027
8	2	6	8	1	7	6254.9355	-0.0027
6	2	5	6	1	5	6270.3196	0.0039
7	2	5	7	1	6	6372.6945	0.0003
6	2	4	6	1	5	6539.0508	-0.0008
5	2	4	5	1	4	6596.2548	-0.0036
1	1	1	0	0	0	6656.9104	0.0011
5	2	3	5	1	4	6732.2500	-0.0002
1	1	0	0	0	0	6770.9487	0.0009
4	2	3	4	1	3	6872.0125	0.0021
4	2	2	4	1	3	6930.7117	0.0004
3	2	2	3	1	2	7095.0533	0.0026
3	2	1	3	1	2	7114.6897	-0.0012
2	2	1	2	1	1	7263.6199	-0.0110
2	2	0	2	1	1	7267.5635	-0.0017
2	2	1	2	1	2	7605.7343	-0.0106
3	2	2	3	1	3	7779.1835	-0.0068
3	2	1	3	1	3	7798.8302	-0.0001
4	2	3	4	1	4	8011.7800	-0.0027
4	2	2	4	1	4	8070.4968	0.0132
5	2	4	5	1	5	8304.4177	-0.0025
2	1	2	1	1	1	8357.3444	0.0007
5	2	3	5	1	5	8440.4123	0.0003
2	0	2	1	0	1	8467.4537	0.0002
2	1	1	1	1	0	8585.4196	0.0002
6	2	5	6	1	6	8657.9346	-0.0025
5	2	4	4	3	1	8764.7834	-0.0113
5	2	4	4	3	2	8765.3917	0.0032
5	2	3	4	3	2	8901.3657	-0.0146
4	1	4	3	2	1	8908.2074	0.0117
6	2	4	6	1	6	8926.6954	0.0224
4	1	4	3	2	2	8927.8430	0.0072
7	2	6	7	1	7	9072.9327	-0.0062
7	2	5	7	1	7	9547.9406	0.0120
8	2	7	8	1	8	9549.6384	0.0043
3	0	3	2	1	1	10038.1548	0.0101
4	1	3	3	2	2	10067.6083	0.0002
9	2	8	9	1	9	10087.6641	-0.0162
3	0	3	2	1	2	10380.2608	0.0021
10	2	9	10	1	10	10686.0685	0.0087
2	1	2	1	0	1	10778.5589	0.0025
2	1	1	1	0	1	11120.6690	-0.0015
8	3	6	8	2	6	11833.5738	0.0417
8	3	5	8	2	6	11872.2191	-0.0165
7	3	4	7	2	5	12063.0990	-0.0118

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(¹³CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
6	3	4	6	2	4	12193.6746	-0.0100
6	3	3	6	2	4	12200.7846	-0.0012
5	3	3	5	2	3	12289.5042	0.0023
5	3	2	5	2	3	12291.8705	-0.0037
4	3	2	4	2	2	12345.4716	-0.0024
4	3	1	4	2	2	12346.0661	-0.0018
3	3	0	3	2	1	12373.9867	-0.0127
3	3	1	3	2	2	12393.5635	0.0089
4	3	2	4	2	3	12404.1743	-0.0006
4	3	1	4	2	3	12404.7692	0.0004
5	3	3	5	2	4	12425.4962	0.0026
5	3	2	5	2	4	12427.8780	0.0120
6	3	3	6	2	5	12469.5170	-0.0047
7	3	5	7	2	6	12520.4339	0.0223
3	1	3	2	1	2	12533.5848	0.0000
8	3	6	8	2	7	12605.2733	0.0161
3	0	3	2	0	2	12691.3644	0.0028
3	2	2	2	2	1	12707.0288	-0.0014
3	2	1	2	2	0	12722.7343	-0.0017
5	1	5	4	2	2	12806.4504	0.0082
5	1	5	4	2	3	12865.1711	0.0280
3	1	2	2	1	1	12875.6217	0.0114
10	3	8	10	2	9	12878.9959	-0.0126
5	1	4	4	2	2	14514.6078	0.0038
5	1	4	4	2	3	14573.2980	-0.0069
4	0	4	3	1	3	14750.3357	-0.0059
3	1	3	2	0	2	14844.6862	-0.0014
3	1	2	2	0	2	15528.8276	0.0004
2	2	1	1	1	0	15849.0484	-0.0018
2	2	0	1	1	0	15852.9873	0.0028
2	2	1	1	1	1	15963.0845	-0.0041
2	2	0	1	1	1	15967.0215	-0.0014
6	1	6	5	2	3	16602.2842	0.0003
4	1	4	3	1	3	16707.0232	-0.0029
6	1	6	5	2	4	16738.2678	-0.0078
4	0	4	3	0	3	16903.6670	-0.0007
4	2	3	3	2	2	16939.6150	-0.0036
4	3	2	3	3	1	16950.2330	-0.0059
4	3	1	3	3	0	16950.7291	-0.0187
4	2	2	3	2	1	16978.6739	-0.0054
4	1	3	3	1	2	17162.6589	0.0002
7	4	3	7	3	4	17304.8405	-0.0161
8	4	5	8	3	6	17312.4599	-0.0164
7	4	4	7	3	5	17322.2998	0.0045
6	4	2	6	3	3	17323.4782	0.0202

Table S5: Observed Transition Frequencies (in MHz) for CH₂CH(¹³CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
5	4	1	5	3	2	17334.2351	0.0064
5	4	2	5	3	3	17336.5618	-0.0257
4	4	1	4	3	2	17340.6174	0.0134
7	2	5	6	3	4	17631.5006	0.0039
5	0	5	4	1	3	18004.6096	-0.0006

Table S6: Observed Transition Frequencies (in MHz) for CH₂CH(CF₃)¹⁸O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
1	1	1	0	0	0	6559.4215	0.0036
1	1	0	0	0	0	6675.8437	0.0045
10	1	9	10	0	10	6887.4745	0.0005
3	2	2	3	1	2	7129.9751	-0.0001
4	2	3	4	1	4	8065.9285	0.0008
2	1	2	1	1	1	8134.3756	-0.0005
2	0	2	1	0	1	8246.7214	-0.0043
5	2	4	5	1	5	8364.7783	-0.0071
2	1	1	1	1	0	8367.2107	-0.0069
4	1	3	3	2	1	9575.6164	-0.0010
3	0	3	2	1	1	9688.9883	0.0029
2	1	1	1	0	1	10917.6511	-0.0007
3	1	3	2	1	2	12199.0471	0.0042
5	3	2	5	2	3	12358.3469	0.0159
3	0	3	2	0	2	12359.9034	-0.0080
3	2	2	2	2	1	12376.1511	0.0014
3	2	1	2	2	0	12392.4349	0.0089
4	3	2	4	2	3	12474.6310	-0.0080
5	3	3	5	2	4	12496.7237	0.0012
3	1	2	2	1	1	12548.2118	-0.0012
7	3	5	7	2	6	12594.9811	-0.0062
4	0	4	3	1	2	13601.8276	-0.0218
4	0	4	3	1	3	14300.2908	0.0086
3	1	3	2	0	2	14520.7125	0.0062
3	1	2	2	0	2	15219.1437	0.0047
2	2	1	1	1	0	15669.2562	0.0002
2	2	0	1	1	0	15673.3279	-0.0055
2	2	1	1	1	1	15785.6721	-0.0051
2	2	0	1	1	1	15789.7557	0.0011
4	1	4	3	1	3	16260.8098	0.0022
4	0	4	3	0	3	16461.0802	0.0032
4	2	3	3	2	2	16498.3318	0.0043
4	2	2	3	2	1	16538.8011	0.0002
4	1	3	3	1	2	16725.9450	-0.0012

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
5	1	5	4	1	4	5783.2539	-0.0018
5	0	5	4	0	4	5852.5868	-0.0073
5	2	4	4	2	3	5857.2362	0.0038
5	2	3	4	2	2	5862.3612	0.0057
5	1	4	4	1	3	5929.9771	-0.0012
3	1	2	2	0	2	6122.1905	-0.0019
11	1	10	10	2	8	6140.9682	0.0045
13	2	12	13	1	12	6261.7871	0.0031
13	1	13	12	2	11	6292.5728	0.0124
8	0	8	7	1	6	6395.0791	-0.0034
12	2	11	12	1	11	6441.6162	0.0002
11	2	10	11	1	10	6609.3248	0.0053
10	2	9	10	1	9	6764.4102	-0.0023
9	2	8	9	1	8	6906.4850	0.0015
6	1	6	5	1	5	6939.0671	-0.0010
6	0	6	5	0	5	7020.1329	-0.0013
6	2	5	5	2	4	7028.0353	0.0006
8	2	7	8	1	7	7035.1807	-0.0034
6	2	4	5	2	3	7036.9864	0.0007
4	1	4	3	0	3	7059.3564	-0.0028
6	1	5	5	1	4	7115.0531	-0.0005
7	2	6	7	1	6	7150.2242	0.0034
6	2	5	6	1	5	7251.3454	-0.0039
6	2	4	6	1	5	7269.2717	0.0012
5	2	4	5	1	4	7338.3692	0.0010
5	2	3	5	1	4	7347.3298	-0.0085
4	1	3	3	0	3	7352.9442	0.0028
4	2	3	4	1	3	7411.1113	-0.0028
4	2	2	4	1	3	7414.9496	-0.0115
9	0	9	8	1	7	7423.7181	0.0009
3	2	2	3	1	2	7469.4530	-0.0043
3	2	1	3	1	2	7470.7464	0.0063
2	2	1	2	1	1	7513.2974	-0.0008
2	2	0	2	1	2	7601.6466	0.0019
3	2	2	3	1	3	7645.6225	-0.0026
3	2	1	3	1	3	7646.9079	0.0000
4	2	2	4	1	4	7708.5450	0.0018
5	2	4	5	1	5	7778.6736	0.0006
5	2	3	5	1	5	7787.6432	0.0001
6	2	5	6	1	6	7867.6165	-0.0230
6	2	4	6	1	6	7885.5596	-0.0012
8	2	7	8	1	8	8090.9089	-0.0126
7	1	7	6	1	6	8094.4383	0.0021
8	2	6	8	1	8	8144.4761	-0.0044
5	1	5	4	0	4	8158.9037	-0.0059

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
15	1	15	14	2	13	8184.7485	-0.0142
7	0	7	6	0	6	8186.0699	-0.0012
7	2	6	6	2	5	8198.4888	0.0027
7	4	3	6	4	2	8202.1003	-0.0041
7	4	4	6	4	3	8202.8433	-0.0001
7	3	4	6	3	3	8212.7751	0.0028
7	2	5	6	2	4	8225.4449	0.0096
9	2	8	9	1	9	8299.6124	-0.0022
7	1	6	6	1	5	8309.3438	0.0019
9	2	7	9	1	9	8375.3299	0.0032
10	2	9	10	1	10	8428.8984	-0.0030
10	0	10	9	1	8	8500.6781	0.0030
10	2	8	10	1	10	8540.6574	-0.0250
11	2	10	11	1	11	8599.2150	0.0007
5	1	4	4	0	4	8698.3395	-0.0037
13	1	12	12	2	10	8720.7933	0.0017
11	2	9	11	1	11	8972.0670	0.0047
12	2	10	12	1	12	9245.3862	0.0027
6	1	6	5	0	5	9249.2962	-0.0007
8	1	8	7	1	7	9256.8599	0.0074
13	2	11	13	1	13	9350.1649	-0.0006
8	0	8	7	0	7	9368.5303	0.0014
8	2	7	7	2	6	9373.8569	0.0000
8	4	4	7	4	3	9374.7447	0.0204
8	4	5	7	4	4	9375.0241	-0.0520
8	3	6	7	3	5	9389.8828	0.0023
8	3	5	7	3	4	9409.0628	-0.0003
8	2	6	7	2	5	9483.5657	0.0002
11	0	11	10	1	9	9577.4574	0.0069
8	1	7	7	1	6	9747.8571	0.0039
14	2	12	14	1	14	9770.9693	0.0014
10	0	10	9	1	9	9861.6727	-0.0010
10	5	5	11	4	7	9886.1269	0.0025
6	1	5	5	0	5	9915.2269	-0.0054
2	2	0	1	1	0	9935.9985	0.0016
2	2	1	1	1	1	9967.8303	-0.0044
15	2	13	15	1	15	10403.5936	0.0021
14	1	13	13	2	11	10512.2033	0.0031
9	1	9	8	1	8	10538.1090	0.0037
9	0	9	8	0	8	10545.1761	-0.0023
9	2	8	8	2	7	10545.6187	0.0001
9	5	4	8	5	3		
9	5	5	8	5	4		
9	4	6	8	4	5		
9	4	5	8	4	4		

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
9	3	7	8	3	6	10546.8543	0.0023
9	3	6	8	3	5	10547.4977	0.0016
9	2	7	8	2	6	10568.4521	-0.0007
9	1	8	8	1	7	10666.8069	0.0010
9	5	5	10	4	7	10943.4701	-0.0013
11	0	11	10	1	10	11019.9875	0.0102
3	2	2	2	1	1	11028.1074	0.0009
3	2	1	2	1	1	11029.3874	-0.0020
3	2	2	2	1	2	11116.1939	-0.0025
3	2	1	2	1	2	11117.4764	-0.0028
7	1	6	6	0	6	11141.1575	0.0034
15	1	14	14	2	12	11227.2471	-0.0084
13	0	13	12	1	11	11288.1846	-0.0034
8	1	8	7	0	7	11382.9069	-0.0043
10	1	10	9	1	9	11557.2710	0.0039
10	0	10	9	0	9	11671.9938	0.0036
10	2	9	9	2	8	11707.1628	0.0043
10	4	7	9	4	6	11717.3893	-0.0008
10	4	6	9	4	5	11719.0488	0.0065
10	3	8	9	3	7	11720.1488	0.0041
10	3	7	9	3	6	11748.6050	0.0047
10	2	8	9	2	7	11849.2290	-0.0005
10	1	9	9	1	8	12071.7915	0.0250
16	3	14	16	2	14	12155.5949	0.0001
4	2	3	3	1	2	12159.4401	-0.0016
4	2	2	3	1	2	12181.9844	0.0086
15	3	13	15	2	13	12184.3642	-0.0030
14	0	14	13	1	12	12294.0293	0.0180
12	0	12	11	1	11	12331.7626	0.0000
4	2	3	3	1	3	12335.6108	0.0013
4	2	2	3	1	3	12352.6570	0.0072
13	3	11	13	2	11	12415.7582	0.0046
12	3	10	12	2	10	12436.3367	-0.0006
9	1	9	8	0	8	12438.6529	0.0044
8	1	7	7	0	7	12466.0566	0.0050
11	3	9	11	2	9	12470.2478	0.0166
11	3	8	11	2	9	12473.6456	-0.0206
16	1	15	15	2	13	12534.7161	-0.0046
9	3	7	9	2	7	12556.3227	0.0012
8	3	6	8	2	6	12556.9798	0.0127
8	3	5	8	2	6	12571.4777	-0.0001
7	3	5	7	2	5	12571.7851	0.0136
7	3	4	7	2	5	12581.5884	0.0055
6	3	4	6	2	4	12587.8745	-0.0101
5	3	3	5	2	3		

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
4	3	2	4	2	2	12591.4646	-0.0022
3	3	1	3	2	1	12593.2377	-0.0015
3	3	0	3	2	2	12594.5290	0.0056
4	3	1	4	2	3	12595.3342	0.0107
5	3	2	5	2	4	12596.9034	0.0095
6	3	3	6	2	5	12599.6139	-0.0078
7	3	4	7	2	6	12603.9799	0.0010
8	3	6	8	2	7	12609.9008	0.0202
8	3	5	8	2	7	12610.5262	0.0001
9	3	7	9	2	8	12618.6145	-0.0127
9	3	6	9	2	8	12619.9167	-0.0003
10	3	8	10	2	9	12630.4944	-0.0167
10	3	7	10	2	9	12632.9017	-0.0015
11	3	8	11	2	10	12650.3403	-0.0001
12	3	9	12	2	11	12673.1975	0.0033
13	3	10	13	2	12	12702.5475	0.0012
11	1	11	10	1	10	12710.2809	0.0050
14	3	11	14	2	13	12739.6019	0.0010
15	3	12	15	2	14	12785.7018	0.0104
11	0	11	10	0	10	12829.3960	0.0049
11	2	10	10	2	9	12875.6217	-0.0099
11	5	6	10	5	5	12888.1422	-0.0236
11	4	8	10	4	7	12889.1738	0.0014
11	4	7	10	4	6	12891.2859	0.0045
11	3	9	10	3	8	12930.3972	0.0048
11	2	9	10	2	8	13030.7264	0.0019
11	1	10	10	1	9	13050.0960	-0.0014
15	0	15	14	1	13	13268.3452	-0.0013
5	2	4	4	1	3	13277.3184	0.0018
5	2	3	4	1	3	13287.6983	0.0168
7	5	2	8	4	4	13481.3959	-0.0082
7	5	3	8	4	5	13561.9321	0.0035
10	1	10	9	0	9	13570.8907	-0.0080
5	2	4	4	1	4	13755.2888	-0.0002
5	2	3	4	1	4	13862.5762	-0.0007
9	1	8	8	0	8	13984.3165	0.0066
12	1	12	11	1	11	14043.4731	0.0042
12	0	12	11	0	11	14059.1477	-0.0133
12	2	11	11	2	10	14059.5734	-0.0012
12	6	6	11	6	5	14060.9706	0.0041
12	6	7	11	6	6		
12	5	7	11	5	6		
12	5	8	11	5	7		
12	4	8	11	4	7		
12	4	9	11	4	8		

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
12	3	10	11	3	9	14063.5545	0.0050
12	3	9	11	3	8	14066.3035	-0.0191
12	2	10	11	2	9	14113.8526	0.0050
12	1	11	11	1	10	14211.1742	0.0019
6	2	5	5	1	4	14366.4017	-0.0011
6	2	4	5	1	4	14384.3243	0.0003
6	5	2	7	4	4	14459.5506	0.0124
11	1	11	10	0	10	14519.6902	0.0004
6	2	5	5	1	5	14806.7100	0.0024
6	2	4	5	1	5	14824.6185	-0.0104
13	1	13	12	1	12	15014.1339	-0.0009
10	1	9	9	0	9	15092.3241	0.0058
13	0	13	12	0	12	15136.7166	0.0048
13	2	12	12	2	11	15210.6154	0.0003
13	6	7	12	6	6	15230.2820	-0.0087
13	6	8	12	6	7		
13	5	8	12	5	7	15230.9259	0.0066
13	5	9	12	5	8		
13	3	11	12	3	10	15235.8290	0.0080
13	3	10	12	3	9	15239.9734	0.0062
13	2	11	12	2	10	15298.9319	0.0070
13	1	12	12	1	11	15390.4450	-0.0022
7	2	6	6	1	5	15449.8514	0.0160
7	2	5	6	1	5	15482.0455	0.0027
12	1	12	11	0	11	15552.8926	0.0171
7	2	6	6	1	6	16066.1225	-0.0031
7	2	5	6	1	6	16098.3306	-0.0025
14	1	14	13	1	13	16164.9250	0.0041
14	0	14	13	0	13	16286.6248	-0.0016
14	2	13	13	2	12	16377.0141	-0.0024
14	6	8	13	6	7	16401.3046	-0.0029
14	6	9	13	6	8		
14	5	9	13	5	8	16402.1986	0.0043
14	5	10	13	5	9		
14	4	10	13	4	9	16404.5941	0.0009
14	4	11	13	4	10		
14	3	12	13	3	11	16408.0698	0.0058
14	3	11	13	3	10	16414.0730	0.0019
11	1	10	10	0	10	16451.0546	0.0019
14	2	12	13	2	11	16485.5197	0.0008
8	2	7	7	1	6	16518.7588	0.0091
14	1	13	13	1	12	16568.4167	0.0003
8	2	6	7	1	6	16572.3088	0.0001
13	1	13	12	0	12	16582.6797	-0.0207
4	3	1	3	2	1	17280.1685	-0.0097

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
15	1	15	14	1	14	17314.9112	-0.0018
8	2	7	7	1	7	17340.2185	0.0002
8	2	6	7	1	7	17393.7694	-0.0080
15	0	15	14	0	14	17434.1450	-0.0016
15	2	14	14	2	13	17542.6163	-0.0039
15	6	9	14	6	8	17572.1985	-0.0040
15	5	10	14	5	9	17573.3868	-0.0072
15	5	11	14	5	10	17576.5326	0.0056
15	4	11	14	4	10	17580.2612	0.0209
15	3	13	14	3	12	17588.7217	0.0110
15	3	12	14	3	11	17595.8156	-0.0232
14	4	11	14	3	11	17605.3763	-0.0013
13	4	10	13	3	10	17609.5163	0.0103
15	4	11	15	3	13	17612.6001	-0.0075
12	4	9	12	3	9	17613.2153	-0.0039
14	4	10	14	3	12	17616.6195	-0.0097
13	4	9	13	3	11	17617.9588	-0.0251
11	4	8	11	3	8	17619.6404	-0.0008
12	4	8	12	3	10	17621.8915	0.0003
10	4	7	10	3	7	17622.2010	-0.0030
11	4	7	11	3	9	17624.2970	-0.0053
10	4	6	10	3	8	17624.6432	-0.0080
9	4	6	9	3	6	17625.9468	-0.0022
9	4	5	9	3	7	17626.5267	-0.0046
8	4	5	8	3	5	17627.1753	-0.0047
8	4	4	8	3	6	17627.7550	0.0035
7	4	4	7	3	4	17628.0353	-0.0110
7	4	3	7	3	5	17628.4907	-0.0002
6	4	3	6	3	3	17657.1982	0.0022
9	2	7	8	1	7	17673.4514	-0.0080
15	2	13	14	2	12	17744.9560	0.0162
15	1	14	14	1	13	17832.8270	-0.0068
12	1	11	11	0	11		

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
6	1	6	5	1	5	6925.8649	0.0006
6	0	6	5	0	5	7009.5236	-0.0008
6	1	5	5	1	4	7108.3307	-0.0004
4	1	3	3	0	3	7308.3140	0.0004
7	1	7	6	1	6	8078.9502	0.0002
7	0	7	6	0	6	8173.3408	0.0023
7	2	6	6	2	5	8186.9040	0.0000
7	3	5	6	3	4	8191.4609	-0.0008
7	3	4	6	3	3	8191.6640	-0.0010
7	1	6	6	1	5	8291.6766	0.0011
5	1	4	4	0	4	8555.7992	0.0009
8	1	8	7	1	7	9231.4930	-0.0004
8	0	8	7	0	7	9335.1557	0.0005
8	2	7	7	2	6	9355.2142	-0.0009
8	3	6	7	3	5	9361.9693	-0.0006
8	3	5	7	3	4	9362.3764	0.0004
8	2	6	7	2	5	9378.5555	0.0004
8	1	7	7	1	6	9474.3617	-0.0008
2	2	0	1	1	0	9751.6023	-0.0007
2	2	1	1	1	1	9781.7712	0.0017
6	1	5	5	0	5	9820.1619	0.0020
9	1	9	8	1	8	10383.4337	0.0005
9	0	9	8	0	8	10494.7432	-0.0013
9	2	8	8	2	7	10523.0297	0.0002
9	3	7	8	3	6	10532.5636	-0.0017
9	3	6	8	3	5	10533.3112	0.0024
9	2	7	8	2	6	10556.1883	0.0017
9	1	8	8	1	7	10656.2815	-0.0009
3	2	2	2	1	2	10982.1884	0.0003
7	1	6	6	0	6	11102.3096	-0.0014
10	0	10	9	0	9	11651.9127	-0.0020
10	3	8	9	3	7	11703.2403	0.0010
10	3	7	9	3	6	11704.5117	0.0001
10	1	9	9	1	8	11837.3194	-0.0003
4	2	2	3	1	2	12019.2924	0.0005
4	2	3	3	1	3	12197.7457	-0.0012
9	3	7	9	2	7	12311.1789	0.0003
8	3	6	8	2	6	12334.8010	0.0011
7	3	5	7	2	5	12351.3837	-0.0016
6	3	4	6	2	4	12362.4501	0.0006
5	3	3	5	2	3	12369.3537	0.0003
5	3	2	5	2	4	12379.2123	0.0008
6	3	3	6	2	5	12382.1891	0.0006
7	3	4	7	2	6	12386.9483	-0.0013
8	3	5	8	2	7	12394.1099	-0.0005

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

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
8	1	7	7	0	7	12403.3347	-0.0003
11	1	11	10	1	10	12685.2885	0.0013
11	0	11	10	0	10	12806.5198	-0.0029
11	1	10	10	1	9	13017.3514	-0.0001
5	2	3	4	1	3	13133.8528	0.0013
5	2	4	4	1	4	13428.4435	-0.0018
9	1	8	8	0	8	13724.4647	0.0024
12	1	12	11	1	11	13835.1115	0.0009
12	0	12	11	0	11	13958.4848	-0.0006
12	1	11	11	1	10	14196.2490	0.0016
6	2	4	5	1	4	14237.3654	-0.0004
6	2	5	5	1	5	14674.2983	-0.0011
10	1	9	9	0	9	15067.0358	-0.0017
7	2	5	6	1	5	15331.5605	-0.0003
7	2	6	6	1	6	15935.3393	0.0003
8	2	7	7	1	7	17211.6044	0.0003

Table S9: Observed Transition Frequencies (in MHz) for Ar-CH₂¹³CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
6	0	6	5	0	5	7020.3762	0.0017
6	1	5	5	1	4	7115.2195	-0.0009
4	1	3	3	0	3	7352.0548	-0.0021
7	1	7	6	1	6	8094.7852	-0.0004
7	0	7	6	0	6	8186.3545	-0.0017
7	2	6	6	2	5	8198.7592	0.0018
7	2	5	6	2	4	8213.0272	-0.0005
5	1	4	4	0	4	8598.3090	-0.0028
8	1	8	7	1	7	9249.6971	-0.0006
8	0	8	7	0	7	9350.4993	0.0021
8	2	7	7	2	6	9368.8407	0.0004
8	2	6	7	2	5	9390.1672	-0.0011
6	1	5	5	0	5	9860.7397	-0.0008
2	2	0	1	1	0	9883.4335	0.0038
2	2	1	1	1	1	9912.5166	0.0007
9	1	9	8	1	8	10404.0449	0.0005
9	0	9	8	0	8	10512.5809	0.0001
9	2	8	8	2	7	10538.4572	-0.0003
9	2	7	8	2	6	10568.7708	-0.0006
9	1	8	8	1	7	10667.0645	0.0011
3	2	1	2	1	1	11026.7553	0.0014
3	2	2	2	1	2	11113.4976	0.0013
7	1	6	6	0	6	11140.1780	0.0012
10	1	10	9	1	9	11557.7739	0.0012
10	0	10	9	0	9	11672.4235	0.0014
10	3	8	9	3	7	11719.4236	0.0003
10	3	7	9	3	6	11720.5265	0.0024
4	2	2	3	1	2	12156.8745	-0.0005
8	1	7	7	0	7	12437.6121	-0.0005
9	3	7	9	2	7	12530.1524	0.0022
8	3	6	8	2	6	12551.7252	-0.0013
7	3	5	7	2	5	12566.8637	-0.0017
6	3	4	6	2	4	12576.9586	-0.0002
5	3	3	5	2	3	12583.2522	-0.0008
5	3	2	5	2	4	12592.2532	0.0010
8	3	5	8	2	7	12605.8712	0.0007
9	3	6	9	2	8	12615.2513	-0.0001
11	1	11	10	1	10	12710.8340	-0.0009
11	0	11	10	0	10	12829.8754	-0.0014
5	2	3	4	1	3	13274.8266	-0.0002
5	2	4	4	1	4	13559.2275	-0.0011
9	1	8	8	0	8	13754.1814	0.0026
12	1	12	11	1	11	13863.1916	0.0017
12	0	12	11	0	11	13984.8498	-0.0018
12	1	11	11	1	10	14211.5282	-0.0015

Table S9: Observed Transition Frequencies (in MHz) for Ar-CH₂¹³CH(CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
6	2	4	5	1	4	14381.9162	-0.0016
6	2	5	5	1	5	14803.9926	0.0012
7	2	5	6	1	5	15479.7246	-0.0006
7	2	6	6	1	6	16063.3808	-0.0016
8	2	7	7	1	7	17337.4357	-0.0014

Table S10: Observed Transition Frequencies (in MHz) for Ar-CH₂CH(¹³CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
6	1	6	5	1	5	6916.6455	-0.0017
6	1	5	5	1	4	7091.7318	-0.0003
4	1	3	3	0	3	7337.8594	-0.0005
7	1	7	6	1	6	8068.2894	-0.0001
7	0	7	6	0	6	8159.5139	-0.0007
7	2	6	6	2	5	8171.8023	0.0014
7	3	5	6	3	4	8175.9420	0.0010
7	3	4	6	3	3	8176.1121	-0.0022
7	1	6	6	1	5	8272.4183	-0.0006
5	1	4	4	0	4	8579.9257	-0.0013
8	1	8	7	1	7	9219.4279	-0.0009
8	0	8	7	0	7	9319.8685	-0.0007
8	2	7	7	2	6	9338.0442	0.0018
8	3	6	7	3	5	9344.1751	-0.0011
8	3	5	7	3	4	9344.5233	0.0009
8	2	6	7	2	5	9359.1710	0.0011
8	1	7	7	1	6	9452.5007	-0.0008
6	1	5	5	0	5	9838.0906	0.0015
2	2	0	1	1	0	9881.3865	0.0022
2	2	1	1	1	1	9910.3488	0.0043
9	0	9	8	0	8	10478.1859	0.0014
9	2	8	8	2	7	10503.8217	-0.0001
9	3	6	8	3	5	10513.1161	0.0010
9	2	7	8	2	6	10533.8525	0.0002
9	1	8	8	1	7	10631.8806	-0.0002
3	2	1	2	1	1	11020.9702	-0.0032
3	2	2	2	1	2	11107.3405	-0.0022
7	1	6	6	0	6	11113.1709	-0.0014
10	1	10	9	1	9	11519.9736	0.0014
10	0	10	9	0	9	11634.2769	0.0009
10	3	8	9	3	7	11680.8502	0.0024
10	3	7	9	3	6	11681.9336	0.0010
10	1	9	9	1	8	11810.4508	-0.0011
4	2	2	3	1	2	12147.4094	-0.0002
4	2	3	3	1	3	12318.8694	0.0008
8	1	7	7	0	7	12406.1598	0.0005
9	3	7	9	2	7	12540.0604	-0.0002
8	3	6	8	2	6	12561.4310	-0.0007
7	3	5	7	2	5	12576.4240	-0.0013
6	3	4	6	2	4	12586.4230	0.0020
5	3	3	5	2	3	12592.6532	-0.0006
5	3	2	5	2	4	12601.5691	0.0015
8	3	5	8	2	7	12615.0637	0.0015
9	3	6	9	2	8	12624.3533	-0.0021
11	1	11	10	1	10	12669.2756	-0.0008

Table S10: Observed Transition Frequencies (in MHz) for Ar-CH₂CH(¹³CF₃)O

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Obs - Calc
11	1	10	10	1	9	12988.1032	-0.0007
5	2	3	4	1	3	13261.7182	0.0012
5	2	4	4	1	4	13544.9184	-0.0015
9	1	8	8	0	8	13718.1720	0.0011
12	1	12	11	1	11	13817.8772	-0.0014
12	0	12	11	0	11	13939.2627	0.0004
12	1	11	11	1	10	14164.7182	-0.0014
6	2	4	5	1	4	14365.1911	-0.0008
6	2	5	5	1	5	14785.5081	-0.0015
7	2	5	6	1	5	15459.3971	0.0006
7	2	6	6	1	6	16040.6637	0.0005

Table S11. Spectroscopic constants in the S reduction (in MHz, unless as otherwise noted) for four isotopologues of the Ar-2-(trifluoromethyl)oxirane complex.^a

	Ar-CH ₂ CH(CF ₃)O	Ar- ¹³ CH ₂ CH(CF ₃)O	Ar-CH ₂ ¹³ CH(CF ₃)O	Ar-CH ₂ CH(¹³ CF ₃)O
A	3105.06579(36)	3060.66881(21)	3104.15794(27)	3104.09773(25)
B	600.48745(10)	600.214146(41)	600.495554(55)	598.504193(51)
C	571.12240(10)	569.766337(42)	571.152552(57)	569.289591(54)
$D_J / 10^{-3}$	0.66135(28)	0.65471(17)	0.66047(24)	0.65745(22)
$D_{JK} / 10^{-3}$	-2.0838(20)	-2.1163(25)	-2.0876(32)	-2.1000(29)
$D_K / 10^{-3}$	31.798(15)	31.760(22)	31.872(30)	31.854(29)
$d_1 / 10^{-3}$	-0.07320(12)	-0.07502(10)	-0.07284(15)	-0.07270(13)
$d_2 / 10^{-3}$	-0.001303(40)	-0.001327(80)	-0.001252(84)	-0.001245(86)
No. of rotational transitions	258	61	50	56
No. of a type	104	33	24	30
No. of b type	41	0	0	0
No. of c type	113	28	26	26
J range	1 – 16	1 – 12	1 – 12	1 – 12
K_a range	0 – 6	0 – 3	0 – 3	0 – 3
rms/kHz	8.23	1.14	1.41	1.39

^a1 σ standard deviations in the parameters are given in parentheses.