

Supplementary Table 1. Observed and assigned transitions for the gauche and trans conformers of 1H-heptafluoropropane.

J'	K <sub>p</sub> '	K <sub>o</sub> '	←	J''	K <sub>p</sub> ''	K <sub>o</sub> ''	Gauche Freq/MHz	Gauche (Obs- Calc)/kHz	Trans Freq/MHz	Trans (Obs- Calc)/kHz
a-types										
4	0	4		3	0	3	8271.8813	0.4	9257.7763	-0.1
5	0	5		4	0	4	10257.4942	-3.6	11553.0458	-0.8
6	0	6		5	0	5	12219.2199	0.4		
7	0	7		6	0	6	14171.5208	0.4		
4	1	3		3	1	2			9374.1207	-0.5
5	1	4		4	1	3			11711.5802	-0.3
4	1	4		3	1	3	8109.8122	0.1		
5	1	5		4	1	4	10115.4563	0.0		
6	1	6		5	1	5	12110.9545	0.9		
7	1	7		6	1	6	14097.5409	-0.1		
4	2	2		3	2	1			9311.0208	0.7
5	2	3		4	2	2			11654.3509	0.4
4	2	3		3	2	1			9283.2838	0.5
5	2	4		4	2	3			11600.5447	0.0
4	3	2		3	3	1			9290.8261	0.3
5	3	3		4	3	2			11615.4784	-0.3
3	2	1		2	0	2			9348.2797	-2.6
4	2	2		3	0	3			11706.4242	1.1
b-types										
4	1	4		3	0	3			9647.7934	1.1
5	1	5		4	0	4			11867.2882	-0.1
3	2	1		2	1	2	9420.9505	-1.2		
4	2	2		3	1	3	11867.5765	1.0	11244.1661	0.3
5	2	3		4	1	4			13712.9829	1.6
3	2	2		2	1	1	8934.5772	0.7		
4	2	3		3	1	2	10829.4948	0.3	10918.5964	-1.2
5	2	4		4	1	3			13145.0215	0.3
3	3	1		2	2	0	11022.7468	0.8	9922.0559	1.0
4	3	2		3	2	1	13094.1046	-0.8	12237.4867	-1.0
3	3	0		2	2	1	11038.7443	-1.1	9924.9952	0.7
4	3	1		3	2	2	13174.9626	-0.7	12252.3286	-1.2
11	9	2		10	8	3			10047.9244	1.4
12	9	3		11	8	4			10044.9070	1.3
13	9	4		12	8	5			10041.1173	3.0
14	9	5		13	8	6			10036.4164	-4.6
4	0	4		3	1	3	7675.7466	0.3		
5	0	5		4	1	4	9823.4325	0.4	11163.0289	-1.8
6	0	6		5	1	5	11927.1952	0.0	13524.3707	-1.0
5	1	4		4	2	3	8606.5753	-0.3	10167.1039	-0.2
6	1	5		5	2	4	11006.6988	0.0	12610.9590	-0.6
6	2	4		5	3	3	8576.4345	0.0	11117.3594	0.6
7	2	5		6	3	4	11051.1536	-0.8	13537.0984	-1.2
6	3	3		5	4	2			9814.3443	0.9

7	3	4	6	4	3		12156.4483	0.3
7	4	3	6	5	2		10945.9649	0.3
8	4	4	7	5	3		13227.7959	-1.1
8	6	2	7	7	1		10894.9202	4.8
9	6	3	8	7	2		13221.5676	-2.0
10	6	5	10	5	6	10265.9605		0.5
11	6	6	11	5	7	10226.6561		0.2
12	6	7	12	5	8	10179.8824		0.3
c-types								
3	1	2	2	0	2	7670.6820		1.1
4	1	3	3	0	3	10074.3087		0.0
4	2	2	3	1	2	11043.3012		0.3
5	2	3	4	1	3	13128.2254		0.1
3	2	2	2	1	2	9347.2279		0.0
4	2	3	3	1	3	11653.7700		0.9
3	3	0	2	2	0	11023.7700		-2.0
4	3	1	3	2	1	13101.2391		-0.4
3	3	1	2	2	1	11037.7213		2.0
4	3	2	3	2	2	13167.8296		0.4
7	0	7	6	1	5	11181.7455		0.0
8	0	8	7	1	6	12360.9606		0.1
7	1	7	6	2	5	9747.0534		-1.3
8	1	8	7	2	6	11217.2498		1.4
7	2	5	6	3	3	10968.6913		0.2
8	2	6	7	3	4	13392.1149		-0.3
7	2	6	6	3	4	9640.9176		-0.5
8	2	7	7	3	5	11498.0450		0.1
6	6	1	6	5	1	10348.3078		-1.8
7	6	2	7	5	2	10336.9126		-1.0
8	6	3	8	5	3	10319.6089		0.2
9	6	4	9	5	4	10294.1767		0.9
10	6	5	10	5	5	10257.3890		-1.0
11	6	6	11	5	6	10204.3173		-0.2
12	6	7	12	5	7	10127.2570		0.1
13	6	8	13	5	8	10014.3781		-1.5
14	6	9	14	5	9	9848.4528		0.0
15	6	10	15	5	10	9606.6497		-0.6
6	6	0	6	5	2	10348.3440		1.5
7	6	1	7	5	3	10337.1090		-1.9
8	6	2	8	5	4	10320.4614		-0.4
9	6	3	9	5	5	10297.1463		0.9
10	6	4	10	5	6	10266.2175		1.4
11	6	5	11	5	7	10227.5176		1.1
12	6	6	12	5	8	10182.4249		0.7
13	6	7	13	5	9	10134.8843		0.5
14	6	8	14	5	10	10092.7006		3.5
15	6	9	15	5	11	10068.9828		-2.4
16	6	10	16	5	12	10083.6851		-0.7
6	0	6	5	1	4	9892.1192		0.4
7	0	7	6	1	5	11181.7450		-0.5

9	5	5	8	6	3	8704.5955	0.8
10	5	6	9	6	4	10860.7858	-0.6
9	5	4	8	6	2	8707.5955	0.1
10	5	5	9	6	3	10869.2914	-0.4