

**SIX-FOLD SYMMETRY INTERNAL ROTATION IN TOLUENES:  
THE LOW BARRIER CHALLENGE OF 2,6- AND 3,5-DIFLUOROTOLUENE**

**ELECTRONIC SUPPLEMENTARY INFORMATION**

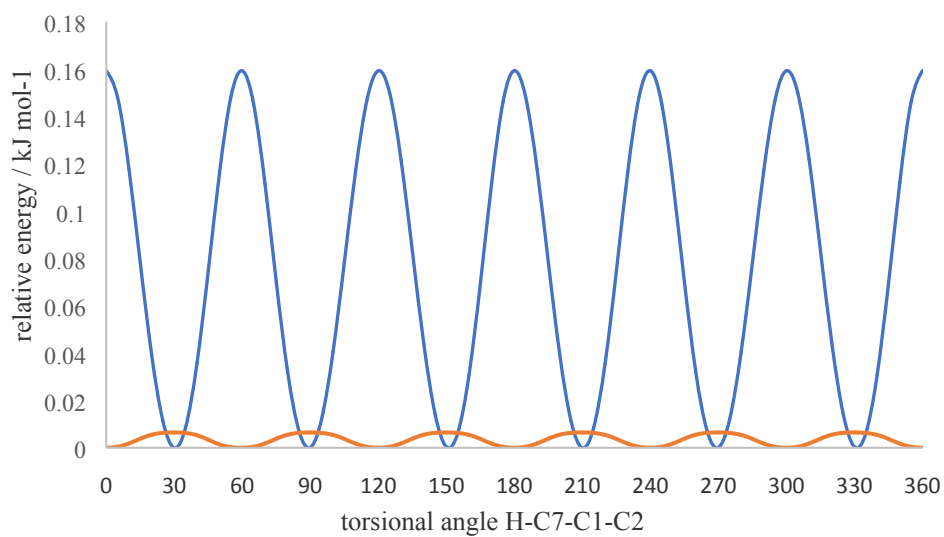
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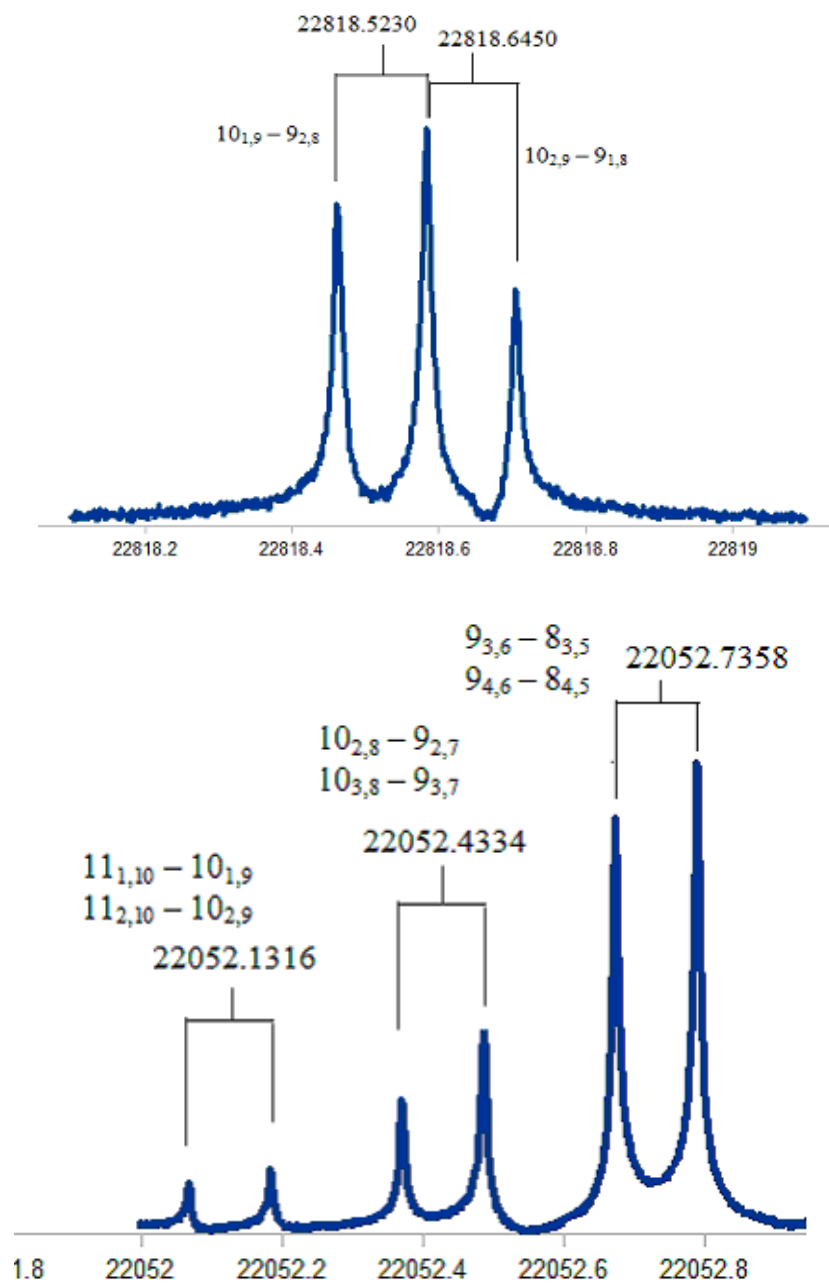
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**Figure S1.** Torsional potential function for 2,6- and 3,5-difluorotoluene (torsion dihedral angle defined as H-C7-C1-C2; torsion origin for a methyl C-H bond coplanar with the benzyl ring).



**Figure S2.** Illustration of rotational transitions in 2,6- and 3,5-difluorotoluene (top and down traces, respectively).



**Table S1.** Rotational parameters for the  $^{13}\text{C}$  isotopic species of 2,6-difluorotoluene.

	$^{13}\text{C}(1)$	$^{13}\text{C}(2), ^{13}\text{C}(6)$	$^{13}\text{C}(3), ^{13}\text{C}(5)$	$^{13}\text{C}(4)$	$^{13}\text{C}(7)$
<i>A</i> (MHz)	2265.24743(25)	2270.4559(15)	2250.6222(11)	2226.00964(20)	2221.48138(22)
<i>B</i> (MHz)	1743.06740(12)	1734.8370(15)	1734.0077(11)	1742.99541(21)	1742.99796(19)
<i>C</i> (MHz)	991.045912(22)	989.368957(29)	985.316430(22)	983.436666(38)	982.547947(37)
<i>N</i>	53	61	68	57	47
$\sigma$ (kHz)	1.0	1.6	1.2	1.8	1.8

**Table S2.** Rotational parameters for the  $^{13}\text{C}$  isotopic species of 3,5-difluorotoluene.

	$^{13}\text{C}(1)$	$^{13}\text{C}(2), ^{13}\text{C}(6)$	$^{13}\text{C}(3), ^{13}\text{C}(5)$	$^{13}\text{C}(4)$	$^{13}\text{C}(7)$
<i>A</i> (MHz)	1751.37601(58)	1762.02786(65)	1762.57786(68)	1752.76720(21)	1745.19054(20)
<i>B</i> (MHz)	1745.21262(55)	1735.31944(66)	1736.21712(68)	1745.28119(29)	1711.98540(19)
<i>C</i> (MHz)	878.855314(37)	878.999347(21)	879.365172(17)	879.224262(44)	868.815129(27)
<i>N</i>	36	42	43	42	27
$\sigma$ (kHz)	1.8	1.1	1.0	1.6	1.1

**Table S3.** Atomic coordinates for the substitution ( $r_s$ ) and ab initio ( $r_e$ ) structures of 2,6-difluorotoluene (Principal inertial axes labeled as  $a$ ,  $b$ ,  $c$ ; all coordinates in ångstrom).

	$r_s$			<i>Ab initio</i>		
	$a$	$b$	$c$	$a$	$b$	$c$
C1	[0] <sup>a</sup>	-0.71232(2)	[0]	0.000	-0.714	0.005
C2	-1.16907(9)	[0]	[0]	-1.174	0.032	0.000
C3	-1.20860(5)	1.41761(4)	[0]	-1.207	1.416	-0.001
C4	[0]	2.11167(1)	[0]	0.001	2.108	0.001
C5	1.20860(5)	1.41761(4)	[0]	1.207	1.416	0.001
C6	1.16907(9)	[0.000]	[0]	1.174	0.032	0.000
C7	[0]	-2.21867(1)	[0]	-0.001	-2.210	0.003
F				-2.343	-0.636	-0.003
F				2.342	-0.637	-0.003
H				-2.162	1.927	-0.001
H				0.001	3.192	0.000
H				2.163	1.926	0.000
H				0.003	-2.600	-1.019
H				-0.892	-2.593	0.501
H				0.884	-2.597	0.509

<sup>a</sup>Values in squared brackets were kept fixed to zero.

**Table S4.** Atomic coordinates for the substitution ( $r_s$ ) and ab initio ( $r_e$ ) structures of 3,5-difluorotoluene (Principal inertial axes labeled as  $a$ ,  $b$ ,  $c$ ; all coordinates in angstrom).

	$r_s$			$Ab\ initio$		
	$a$	$b$	$c$	$A$	$B$	$C$
C1	[0]	1.45130(3)	[0]	-0.007	-1.456	-0.013
C2	-1.21040(3)	0.73822(8)	[0]	1.200	-0.755	-0.009
C3	-1.17228(4)	-0.6289(1)	[0]	1.181	0.629	0.001
C4	[0]	-1.36711(2)	[0]	0.006	1.362	0.007
C5	1.17228(4)	-0.6289(1)	[0]	-1.175	0.639	0.001
C6	1.21040(3)	0.73822(8)	[0]	-1.207	-0.744	-0.010
C7	[0]	2.96304(2)	[0]	-0.014	-2.957	0.012
F				2.348	1.295	0.001
F				-2.336	1.316	0.002
H				2.153	-1.273	-0.016
H				0.011	2.445	0.009
H				-2.165	-1.253	-0.018
H				-0.030	-3.326	1.042
H				0.874	-3.365	-0.473
H				-0.894	-3.356	-0.495

<sup>a</sup>Values in squared brackets were kept fixed to zero.

**Table S5.** Rotational transitions of the parent species of 2,6-difluorotoluene, sorted by branch, together with fit residuals (o.-c., frequencies in MHz). Rotational transitions labeled with symmetry species, free rotor quantum number ( $m$ ), and asymmetric rotor quantum numbers ( $J$ ,  $K_a$ ,  $K_c$ ).

Upper level				Lower level				Measured(Unc. )	o.-c. (MHz)		
Sym'	m'	J'	Ka'	Kc'	Sym	m	J	Ka	Kc		
B1	0	2	1	2	B2	0	1	0	1	5246.3820(0.002)	-0.0011
A2	0	3	1	3	A1	0	2	0	2	7058.6730(0.002)	-0.0022
B1	0	4	1	4	B2	0	3	0	3	8956.8990(0.002)	0.0016
A2	0	5	1	5	A1	0	4	0	4	10918.4910(0.002)	0.0007
B1	0	6	1	6	B2	0	5	0	5	12897.7080(0.002)	0.0008
A2	0	7	1	7	A1	0	6	0	6	14880.6620(0.002)	-0.0001
B1	0	8	1	8	B2	0	7	0	7	16864.3640(0.002)	0.0007
A2	0	9	1	9	A1	0	8	0	8	18848.2310(0.002)	0.0023
B1	0	5	1	4	B2	0	5	0	5	8780.3766(0.002)	0.0043
A2	0	6	1	5	A1	0	6	0	6	10805.0584(0.002)	-0.0007
B1	0	7	1	6	B2	0	7	0	7	12802.7847(0.002)	-0.0046
A2	0	8	1	7	A1	0	8	0	8	14792.8227(0.002)	-0.0012
B1	0	9	1	8	B2	0	9	0	9	16780.3770(0.002)	-0.0021
B1	0	10	0	10	B2	0	9	0	9	20832.1420(0.002)	-0.0002
B2	0	11	0	11	B1	0	10	0	10	22816.0760(0.002)	0.0005
B1	0	12	0	12	B2	0	11	0	11	24800.0180(0.002)	-0.0010
B2	0	2	2	1	B1	0	1	1	0	7803.1620(0.002)	0.0002
B2	0	4	2	3	B1	0	3	1	2	11434.7910(0.002)	-0.0070
A1	0	5	2	4	A2	0	4	1	3	13095.0120(0.002)	0.0010
B2	0	6	2	5	B1	0	5	1	4	14938.3040(0.002)	0.0017
A1	0	7	2	6	A2	0	6	1	5	16881.5600(0.002)	0.0007
B2	0	8	2	7	B1	0	7	1	6	18854.9850(0.002)	0.0003
A1	0	9	2	8	A2	0	8	1	7	20835.8880(0.002)	0.0008
B2	0	10	2	9	B1	0	9	1	8	22818.6450(0.002)	0.0007
A1	0	11	2	10	A2	0	10	1	9	24801.9540(0.002)	-0.0011
A1	0	6	2	4	A2	0	6	1	5	8472.9084(0.002)	-0.0001
B2	0	7	2	5	B1	0	7	1	6	10616.8335(0.002)	-0.0024
A1	0	8	2	6	A2	0	8	1	7	12662.0328(0.002)	-0.0002
A1	0	10	2	8	A2	0	10	1	9	16669.4469(0.002)	0.0039
A1	0	5	2	4	A2	0	5	1	5	8852.1951(0.002)	-0.0001
B2	0	6	2	5	B1	0	6	1	6	10820.9657(0.002)	-0.0016
A1	0	7	2	6	A2	0	7	1	7	12805.9550(0.002)	-0.0013
B2	0	8	2	7	B1	0	8	1	8	14793.4083(0.002)	-0.0024
A1	0	9	2	8	A2	0	9	1	9	16780.4813(0.002)	-0.0010
A1	0	2	0	2	A2	0	1	1	1	4556.3270(0.002)	0.0003
B2	0	3	0	3	B1	0	2	1	2	6833.5910(0.002)	-0.0010
A1	0	4	0	4	A2	0	3	1	3	8904.6180(0.002)	-0.0001
B2	0	5	0	5	B1	0	4	1	4	10908.3320(0.002)	0.0010
A1	0	6	0	6	A2	0	5	1	5	12895.9170(0.002)	0.0003
B2	0	7	0	7	B1	0	6	1	6	14880.3660(0.002)	0.0007



A1	0	8	0	8	A2	0	7	1	7	16864.3170 (0.002)	0.0009
B2	0	9	0	9	B1	0	8	1	8	18848.2190 (0.002)	-0.0025
A1	0	10	1	10	A2	0	9	1	9	20832.1420 (0.002)	0.0009
A2	0	11	1	11	A1	0	10	1	10	22816.0760 (0.002)	0.0004
A1	0	12	1	12	A2	0	11	1	11	24800.0180 (0.002)	-0.0010
A2	0	4	1	3	A1	0	3	2	2	10361.0980 (0.002)	-0.0029
B1	0	5	1	4	B2	0	4	2	3	12741.5330 (0.002)	-0.0039
A2	0	6	1	5	A1	0	5	2	4	14848.7810 (0.002)	0.0004
B1	0	7	1	6	B2	0	6	2	5	16862.1880 (0.002)	0.0007
A2	0	8	1	7	A1	0	7	2	6	18851.1840 (0.002)	0.0003
B1	0	9	1	8	B2	0	8	2	7	20835.1910 (0.002)	0.0012
A2	0	10	1	9	A1	0	9	2	8	22818.5230 (0.002)	0.0005
B1	0	11	1	10	B2	0	10	2	9	24801.9380 (0.002)	0.0034
A2	0	5	3	3	A1	0	4	2	2	16169.8604 (0.002)	-0.0034
A2	0	7	3	5	A1	0	6	2	4	19112.5030 (0.002)	0.0041
B1	0	8	3	6	B2	0	7	2	5	20920.8190 (0.002)	0.0020
A2	0	9	3	7	A1	0	8	2	6	22849.9580 (0.002)	0.0016
B1	0	3	3	0	B2	0	2	2	1	13151.1520 (0.002)	0.0000
B1	0	5	3	2	B2	0	4	2	3	22601.1060 (0.002)	0.0012
A2	0	5	3	3	A1	0	5	2	4	7041.0404 (0.002)	0.0031
B1	0	6	3	4	B2	0	6	2	5	8786.5790 (0.002)	-0.0017
A2	0	7	3	5	A1	0	7	2	6	10703.8475 (0.002)	-0.0006
B1	0	8	3	6	B2	0	8	2	7	12682.6678 (0.002)	-0.0004
A2	0	9	3	7	A1	0	9	2	8	14676.1063 (0.002)	0.0040
A2	0	8	3	5	A1	0	8	2	6	10255.0970 (0.002)	0.0044
B2	0	4	4	1	B1	0	3	3	0	17221.0370 (0.002)	0.0030
A1	0	5	4	2	A2	0	4	3	1	19528.7730 (0.002)	-0.0047
B2	0	6	4	3	B1	0	5	3	2	21198.5720 (0.002)	-0.0018
A1	0	7	4	4	A2	0	6	3	3	22431.1230 (0.002)	-0.0010
B2	0	8	4	5	B1	0	7	3	4	23620.4100 (0.002)	0.0012
A1	0	10	2	8	A2	0	9	3	7	24811.8650 (0.002)	0.0017
A1	0	7	4	4	A2	0	7	3	5	8797.5426 (0.002)	0.0020
A1	0	9	4	6	A2	0	9	3	7	12522.2201 (0.002)	0.0027
B2	0	5	4	1	B1	0	4	3	2	21069.6850 (0.002)	0.0000
B1	0	5	5	0	B2	0	4	4	1	21939.2140 (0.002)	-0.0012
A2	0	6	3	3	A1	0	5	4	2	15423.1802 (0.002)	-0.0033
A2	0	8	3	5	A1	0	7	4	4	22266.9196 (0.002)	-0.0011
A2	0	7	5	3	A1	0	7	4	4	7902.3806 (0.002)	0.0041
A2	0	5	5	1	A1	0	4	4	0	21847.3400 (0.002)	-0.0001
B1	0	6	5	2	B2	0	5	4	1	24435.4050 (0.002)	0.0018
A1	0	6	6	0	A2	0	6	5	1	8487.5639 (0.002)	-0.0059
B2	0	7	4	3	B1	0	6	5	2	16845.8636 (0.002)	0.0018
A1	0	8	4	4	A2	0	7	5	3	21406.7351 (0.002)	-0.0035
B2	0	8	6	3	B1	0	8	5	4	8780.1893 (0.002)	0.0031

E2	1	2	1	2	E2	1	1	0	1	6087.2890 (0.002)	-0.0037
E2	1	4	1	4	E2	1	3	0	3	10389.3220 (0.002)	-0.0006
E1	1	5	1	5	E1	1	4	0	4	11892.4451 (0.002)	0.0011
E2	1	6	1	6	E2	1	5	0	5	13340.4850 (0.002)	0.0003
E1	1	7	1	7	E1	1	6	0	6	15051.2920 (0.002)	0.0000
E2	1	8	1	8	E2	1	7	0	7	16944.4190 (0.002)	-0.0003
E1	1	9	1	9	E1	1	8	0	8	18897.8165 (0.002)	0.0000
E2	1	10	1	10	E2	1	9	0	9	20868.2258 (0.002)	-0.0009
E1	1	11	1	11	E1	1	10	0	10	22844.2687 (0.002)	-0.0010
E2	1	12	1	12	E2	1	11	0	11	24822.8419 (0.002)	-0.0001
E2	1	7	1	6	E2	1	7	0	7	10859.7707 (0.002)	0.0012
E2	1	9	1	8	E2	1	9	0	9	15842.5178 (0.002)	0.0014
E1	1	4	0	4	E1	1	3	1	3	6987.3722 (0.002)	0.0026
E2	1	5	0	5	E2	1	4	1	4	10198.5916 (0.002)	0.0003
E1	1	6	0	6	E1	1	5	1	5	12752.1919 (0.002)	0.0001
E2	1	7	0	7	E2	1	6	1	6	14902.3230 (0.002)	-0.0001
E1	1	8	0	8	E1	1	7	1	7	16913.1750 (0.002)	0.0000
E2	1	9	0	9	E2	1	8	1	8	18891.9408 (0.002)	-0.0002
E1	1	10	0	10	E1	1	9	1	9	20867.1995 (0.002)	0.0015
E2	1	11	0	11	E2	1	10	1	10	22844.0972 (0.002)	-0.0012
E1	1	12	0	12	E1	1	11	1	11	24822.8125 (0.002)	-0.0021
E2	1	2	2	1	E2	1	1	1	0	6962.2023 (0.002)	0.0028
E2	1	4	2	3	E2	1	3	1	2	12784.9210 (0.002)	0.0040
E1	1	5	2	4	E1	1	4	1	3	15456.4180 (0.002)	0.0005
E2	1	6	2	5	E2	1	5	1	4	17562.2300 (0.002)	-0.0006
E1	1	7	2	6	E1	1	6	1	5	18881.1076 (0.002)	-0.0010
E2	1	8	2	7	E2	1	7	1	6	19905.6965 (0.002)	-0.0015
E1	1	9	2	8	E1	1	8	1	7	21286.8131 (0.002)	-0.0009
E2	1	10	2	9	E2	1	9	1	8	23040.1202 (0.002)	-0.0005
E1	1	11	2	10	E1	1	10	1	9	24940.9032 (0.002)	-0.0013
E2	1	4	2	3	E2	1	4	1	4	8518.5291 (0.002)	-0.0050
E2	1	6	2	5	E2	1	6	1	6	10200.2775 (0.002)	0.0028
E1	1	7	2	6	E1	1	7	1	7	11847.1561 (0.002)	0.0035
E2	1	8	2	7	E2	1	8	1	8	13821.0498 (0.002)	0.0016
E2	1	10	2	9	E2	1	10	1	10	18014.4116 (0.002)	0.0012
E2	1	3	2	1	E2	1	3	1	2	8779.6542 (0.002)	0.0095
E2	1	9	2	7	E2	1	9	1	8	12161.1180 (0.002)	-0.0027
E2	1	11	2	9	E2	1	11	1	10	17531.4598 (0.002)	-0.0042
E2	1	5	1	4	E2	1	4	1	4	16177.1212 (0.002)	0.0011
E2	1	4	3	2	E2	1	4	2	3	9742.6611 (0.002)	0.0003
E1	1	5	3	3	E1	1	5	2	4	10239.5750 (0.002)	0.0027
E1	1	7	3	5	E1	1	7	2	6	11066.0051 (0.002)	0.0001
E2	1	8	3	6	E2	1	8	2	7	12048.2467 (0.002)	-0.0025
E1	1	7	3	5	E1	1	6	2	4	22311.8156 (0.002)	-0.0021
E2	1	8	3	6	E2	1	7	2	5	24499.3116 (0.002)	-0.0043
E1	1	6	1	5	E1	1	5	2	4	11682.5470 (0.002)	-0.0014
E2	1	7	1	6	E2	1	6	2	5	15561.8180 (0.002)	0.0001
E1	1	8	1	7	E1	1	7	2	6	18589.6372 (0.002)	0.0010
E2	1	9	1	8	E2	1	8	2	7	20913.4104 (0.002)	0.0012
E1	1	10	1	9	E1	1	9	2	8	22954.5080 (0.002)	-0.0008
E2	1	11	1	10	E2	1	10	2	9	24923.4842 (0.002)	-0.0019

E2	1	5	3	2	E2	1	5	2	3	10651.2463 (0.002)	0.0022
E1	1	6	3	3	E1	1	6	2	4	10984.7166 (0.002)	0.0027
E2	1	7	3	4	E2	1	7	2	5	10585.9296 (0.002)	0.0023
E2	1	3	3	0	E2	1	2	2	1	18038.7706 (0.010)	-0.0012
E2	1	7	2	5	E2	1	6	2	5	23016.4464 (0.002)	-0.0029
E2	1	5	4	1	E2	1	5	3	2	10227.8840 (0.002)	-0.0020
E1	1	6	4	2	E1	1	6	3	3	11676.2812 (0.002)	0.0005
E2	1	7	4	3	E2	1	7	3	4	12501.1035 (0.002)	0.0006
E2	1	9	4	5	E2	1	9	3	6	12377.0149 (0.002)	0.0001
E2	1	4	4	1	E2	1	3	3	0	15275.7366 (0.002)	0.0038
E1	1	5	4	2	E1	1	4	3	1	17658.5800 (0.002)	0.0041
E2	1	6	4	3	E2	1	5	3	2	20526.8258 (0.002)	0.0010
E1	1	7	4	4	E1	1	6	3	3	23452.8368 (0.002)	-0.0034
E1	1	8	2	6	E1	1	7	3	5	16697.9088 (0.002)	-0.0001
E2	1	9	2	7	E2	1	8	3	6	21026.2843 (0.002)	0.0036
E1	1	10	2	8	E1	1	9	3	7	24428.2364 (0.002)	0.0040
E1	1	5	4	2	E1	1	5	3	3	10722.8960 (0.002)	-0.0039
E2	1	6	4	3	E2	1	6	3	4	11615.4529 (0.002)	0.0014
E1	1	7	4	4	E1	1	7	3	5	12125.7369 (0.002)	0.0004
E2	1	8	4	5	E2	1	8	3	6	12457.7841 (0.002)	-0.0041
E2	1	7	5	2	E2	1	7	4	3	12353.8773 (0.002)	-0.0011
E1	1	5	5	1	E1	1	4	4	0	19887.0356 (0.002)	-0.0055
E2	1	6	5	2	E2	1	5	4	1	21669.6732 (0.002)	-0.0015
E1	1	7	5	3	E1	1	6	4	2	24413.9916 (0.002)	-0.0037
E2	1	6	5	2	E2	1	6	4	3	11370.7300 (0.002)	-0.0059
E2	1	8	5	4	E2	1	8	4	5	13447.5100 (0.002)	0.0019
E2	1	5	4	1	E2	1	4	4	1	18149.8765 (0.002)	0.0112
E1	1	6	4	2	E1	1	5	4	2	21016.3692 (0.002)	0.0025
E2	1	7	4	3	E2	1	6	4	3	23920.2723 (0.002)	-0.0032
E2	1	9	3	6	E2	1	8	4	5	17494.5451 (0.002)	-0.0018
E2	1	5	5	0	E2	1	4	4	1	24858.5476 (0.002)	-0.0013
E2	1	7	5	2	E2	1	6	5	2	24903.4203 (0.002)	0.0024
E2	2	9	1	9	E2	2	8	0	8	19463.1213 (0.002)	0.0025
E2	2	5	2	4	E2	2	4	1	3	15600.9320 (0.002)	-0.0083
E2	2	6	1	5	E2	2	5	1	5	17778.5195 (0.002)	0.0029
E2	2	5	3	3	E2	2	4	2	2	16485.5760 (0.002)	0.0055
E2	2	7	3	5	E2	2	6	2	4	22266.4936 (0.010)	-0.0026
E2	2	6	2	4	E2	2	5	2	4	18922.8913 (0.002)	-0.0072
E2	2	8	2	6	E2	2	7	2	6	24575.8030 (0.002)	0.0032
E2	2	6	3	3	E2	2	5	3	3	19835.7953 (0.002)	0.0017

E2 2 7 4 4 E2 2 6 3 3 23197.7720(0.002) 0.0001

**Table S6.** Rotational transitions of the parent species of 3,5-difluorotoluene sorted by branch, together with fit residuals (o.-c., frequencies in MHz). Rotational transitions labeled with symmetry species, free rotor quantum number ( $m$ ), and asymmetric rotor quantum numbers ( $J, K_a, K_c$ ).

Upper level				Lower level				Measured(Unc. )	o.-c. (MHz)		
Sym'	m'	J'	Ka'	Kc'	Sym m	J	Ka	Kc			
B2	0	3	0	3	B1	0	2	0	2	6174.6440 (0.002)	0.0008
B1	0	4	0	4	B2	0	3	0	3	7938.7798 (0.002)	-0.0003
B2	0	5	0	5	B1	0	4	0	4	9702.9157 (0.002)	-0.0003
B1	0	6	0	6	B2	0	5	0	5	11467.0502 (0.002)	-0.0006
B2	0	7	0	7	B1	0	6	0	6	13231.1836 (0.002)	-0.0006
B1	0	8	0	8	B2	0	7	0	7	14995.3156 (0.002)	-0.0004
B2	0	9	0	9	B1	0	8	0	8	16759.4461 (0.002)	0.0000
B1	0	10	0	10	B2	0	9	0	9	18523.5742 (0.002)	0.0000
B2	0	11	0	11	B1	0	10	0	10	20287.7001 (0.002)	0.0001
B1	0	12	0	12	B2	0	11	0	11	22051.8236 (0.002)	0.0001
B2	0	13	0	13	B1	0	12	0	12	23815.9443 (0.002)	0.0000
B1	0	7	1	6	B2	0	7	0	7	11468.9288 (0.002)	-0.0017
B2	0	8	1	7	B1	0	8	0	8	13233.3680 (0.002)	-0.0036
B1	0	9	1	8	B2	0	9	0	9	14997.8102 (0.002)	0.0006
A2	0	3	1	3	A1	0	2	1	2	6174.6440 (0.002)	0.0009
A1	0	4	1	4	A2	0	3	1	3	7938.7798 (0.002)	-0.0003
A2	0	5	1	5	A1	0	4	1	4	9702.9157 (0.002)	-0.0003
A1	0	6	1	6	A2	0	5	1	5	11467.0502 (0.002)	-0.0006
A2	0	7	1	7	A1	0	6	1	6	13231.1836 (0.002)	-0.0006
A1	0	8	1	8	A2	0	7	1	7	14995.3156 (0.002)	-0.0004
A2	0	9	1	9	A1	0	8	1	8	16759.4461 (0.002)	0.0000
A1	0	10	1	10	A2	0	9	1	9	18523.5742 (0.002)	0.0000
A2	0	11	1	11	A1	0	10	1	10	20287.7001 (0.002)	0.0001
A1	0	12	1	12	A2	0	11	1	11	22051.8236 (0.002)	0.0001
A2	0	13	1	13	A1	0	12	1	12	23815.9443 (0.002)	0.0000
B1	0	5	1	4	B2	0	4	1	3	11467.3651 (0.002)	-0.0003
B2	0	6	1	5	B1	0	5	1	4	13231.4976 (0.002)	-0.0001
B1	0	7	1	6	B2	0	6	1	5	14995.6283 (0.002)	0.0000
B2	0	8	1	7	B1	0	7	1	6	16759.7571 (0.002)	-0.0001
B1	0	9	1	8	B2	0	8	1	7	18523.8840 (0.002)	-0.0001
B2	0	10	1	9	B1	0	9	1	8	20288.0096 (0.002)	0.0009
B1	0	11	1	10	B2	0	10	1	9	22052.1316 (0.002)	0.0007
B1	0	3	3	0	B2	0	2	1	1	11468.2560 (0.002)	-0.0023
B1	0	8	2	6	B2	0	8	1	7	11468.8906 (0.002)	0.0010
B2	0	9	2	7	B1	0	9	1	8	13233.3186 (0.002)	0.0000
B1	0	10	2	8	B2	0	10	1	9	14997.7447 (0.002)	0.0019
A1	0	7	2	6	A2	0	7	1	7	11468.9288 (0.002)	-0.0017
A2	0	8	2	7	A1	0	8	1	8	13233.3680 (0.002)	-0.0036
A1	0	9	2	8	A2	0	9	1	9	14997.8102 (0.002)	0.0006

B1	0	9	3	6	B2	0	9	2	7	11468.8455 (0.002)	0.0018
B2	0	10	3	7	B1	0	10	2	8	13233.2581 (0.002)	-0.0016
B1	0	11	3	8	B2	0	11	2	9	14997.6697 (0.002)	0.0003
B2	0	5	2	3	B1	0	4	2	2	13231.8111 (0.002)	-0.0012
B1	0	6	2	4	B2	0	5	2	3	14995.9396 (0.002)	-0.0001
B2	0	7	2	5	B1	0	6	2	4	16760.0662 (0.002)	0.0000
B1	0	8	2	6	B2	0	7	2	5	18524.1909 (0.002)	0.0002
B2	0	9	2	7	B1	0	8	2	6	20288.3136 (0.002)	0.0005
B1	0	10	2	8	B2	0	9	2	7	22052.4334 (0.002)	0.0005
A1	0	8	3	6	A2	0	8	2	7	11468.8906 (0.002)	0.0010
A2	0	9	3	7	A1	0	9	2	8	13233.3186 (0.002)	0.0000
A1	0	10	3	8	A2	0	10	2	9	14997.7447 (0.002)	0.0019
A1	0	5	2	4	A2	0	4	2	3	11467.3651 (0.002)	-0.0003
A2	0	6	2	5	A1	0	5	2	4	13231.4976 (0.002)	-0.0001
A1	0	7	2	6	A2	0	6	2	5	14995.6283 (0.002)	0.0000
A2	0	8	2	7	A1	0	7	2	6	16759.7571 (0.002)	-0.0001
A1	0	9	2	8	A2	0	8	2	7	18523.8840 (0.002)	-0.0001
A2	0	10	2	9	A1	0	9	2	8	20288.0096 (0.002)	0.0009
A1	0	11	2	10	A2	0	10	2	9	22052.1316 (0.002)	0.0007
A1	0	4	4	0	A2	0	3	2	1	14997.0908 (0.002)	0.0041
A1	0	4	3	2	A2	0	3	2	1	11468.1892 (0.002)	0.0032
B1	0	10	4	6	B2	0	10	3	7	11468.7896 (0.002)	-0.0030
B2	0	11	4	7	B1	0	11	3	8	13233.1946 (0.002)	-0.0004
B1	0	12	4	8	B2	0	12	3	9	14997.5889 (0.002)	-0.0005
B1	0	7	3	4	B2	0	6	3	3	18524.5003 (0.002)	0.0003
B2	0	8	3	5	B1	0	7	3	4	20288.6189 (0.002)	0.0001
B1	0	9	3	6	B2	0	8	3	5	22052.7358 (0.002)	0.0006
A2	0	5	3	3	A1	0	4	3	2	13231.8111 (0.002)	0.0007
A1	0	6	3	4	A2	0	5	3	3	14995.9396 (0.002)	-0.0001
A2	0	7	3	5	A1	0	6	3	4	16760.0662 (0.002)	0.0000
A1	0	8	3	6	A2	0	7	3	5	18524.1909 (0.002)	0.0002
A2	0	9	3	7	A1	0	8	3	6	20288.3136 (0.002)	0.0005
A1	0	10	3	8	A2	0	9	3	7	22052.4334 (0.002)	0.0005
B1	0	5	4	2	B2	0	4	3	1	14997.0908 (0.002)	0.0015
A2	0	6	4	3	A1	0	5	3	2	16760.3832 (0.002)	0.0020
A1	0	9	4	6	A2	0	9	3	7	11468.8455 (0.002)	0.0018
A2	0	10	4	7	A1	0	10	3	8	13233.2581 (0.002)	-0.0016
A1	0	11	4	8	A2	0	11	3	9	14997.6697 (0.002)	0.0003
A1	0	7	4	4	A2	0	6	4	3	18524.5003 (0.002)	0.0003
A2	0	8	4	5	A1	0	7	4	4	20288.6189 (0.002)	0.0001
A1	0	9	4	6	A2	0	8	4	5	22052.7358 (0.002)	0.0006
A1	0	10	5	6	A2	0	10	4	7	11468.7896 (0.002)	-0.0030
A2	0	11	5	7	A1	0	11	4	8	13233.1946 (0.002)	-0.0004
A1	0	12	5	8	A2	0	12	4	9	14997.5889 (0.002)	-0.0005
B2	0	6	3	3	B1	0	5	4	2	16760.3739 (0.002)	-0.0029
B1	0	11	5	6	B2	0	11	4	7	11468.7355 (0.002)	-0.0010
B2	0	12	5	7	B1	0	12	4	8	13233.1250 (0.002)	0.0007

B1	0	13	5	8	B2	0	13	4	9	14997.5024(0.002)	-0.0002
A1	0	11	6	6	A2	0	11	5	7	11468.7355(0.002)	-0.0010
A2	0	12	6	7	A1	0	12	5	8	13233.1250(0.002)	0.0007
A1	0	13	6	8	A2	0	13	5	9	14997.5024(0.002)	-0.0002
B1	0	12	6	6	B2	0	12	5	7	11468.6757(0.002)	0.0005
B2	0	13	6	7	B1	0	13	5	8	13233.0476(0.002)	-0.0001
B1	0	14	6	8	B2	0	14	5	9	14997.4095(0.002)	0.0003
A1	0	12	7	6	A2	0	12	6	7	11468.6757(0.002)	0.0005
A2	0	13	7	7	A1	0	13	6	8	13233.0476(0.002)	-0.0001
A1	0	14	7	8	A2	0	14	6	9	14997.4095(0.002)	0.0003
B1	0	13	7	6	B2	0	13	6	7	11468.6080(0.002)	-0.0009
B1	0	15	7	8	B2	0	15	6	9	14997.3089(0.002)	-0.0002
A1	0	13	8	6	A2	0	13	7	7	11468.6080(0.002)	-0.0009
A1	0	15	8	8	A2	0	15	7	9	14997.3089(0.002)	-0.0002
B1	0	14	8	6	B2	0	14	7	7	11468.5383(0.002)	0.0009
B2	0	15	8	7	B1	0	15	7	8	13232.8769(0.002)	-0.0001
A1	0	14	9	6	A2	0	14	8	7	11468.5383(0.002)	0.0009
A2	0	15	9	7	A1	0	15	8	8	13232.8769(0.002)	-0.0001
B1	0	15	9	6	B2	0	15	8	7	11468.4613(0.002)	0.0005
A1	0	15	10	6	A2	0	15	9	7	11468.4613(0.002)	0.0005
E2	1	10	0	10	E2	1	9	0	9	18545.9842(0.002)	-0.0006
E2	1	11	0	11	E2	1	10	0	10	20305.6635(0.002)	0.0001
E2	1	12	0	12	E2	1	11	0	11	22066.5509(0.002)	-0.0024
E2	1	13	0	13	E2	1	12	0	12	23828.2453(0.002)	0.0002
E1	1	3	1	3	E1	1	2	0	2	7157.5945(0.002)	0.0008
E2	1	4	1	4	E2	1	3	0	3	8719.2607(0.002)	0.0004
E1	1	5	1	5	E1	1	4	0	4	9997.5114(0.002)	0.0027
E2	1	6	1	6	E2	1	5	0	5	11564.5157(0.002)	0.0009
E1	1	7	1	7	E1	1	6	0	6	13286.2219(0.002)	-0.0006
E2	1	8	1	8	E2	1	7	0	7	15033.8052(0.002)	0.0031
E1	1	9	1	9	E1	1	8	0	8	16788.2340(0.002)	-0.0012
E2	1	7	1	6	E2	1	7	0	7	10682.6720(0.002)	0.0060
E2	1	9	1	8	E2	1	9	0	9	14464.7536(0.002)	-0.0018
E2	1	10	1	9	E2	1	10	0	10	16300.7707(0.002)	0.0019
E1	1	10	1	10	E1	1	9	1	9	18545.9842(0.002)	-0.0006
E1	1	11	1	11	E1	1	10	1	10	20305.6635(0.002)	0.0001
E1	1	12	1	12	E1	1	11	1	11	22066.5509(0.002)	-0.0024
E1	1	13	1	13	E1	1	12	1	12	23828.2453(0.002)	0.0002
E2	1	6	2	5	E2	1	6	1	6	8769.3315(0.002)	0.0019
E2	1	8	2	7	E2	1	8	1	8	12601.6664(0.002)	0.0021
E1	1	9	2	8	E1	1	9	1	9	14464.7654(0.002)	-0.0039
E1	1	10	2	9	E1	1	10	1	10	16300.7707(0.002)	0.0022
E2	1	10	1	9	E2	1	9	1	8	20381.9976(0.002)	-0.0006
E2	1	11	1	10	E2	1	10	1	9	22124.4842(0.002)	0.0001
E1	1	4	0	4	E1	1	3	1	3	7359.0809(0.002)	-0.0030

E2	1	5	0	5	E2	1	4	1	4	9709.1838 (0.002)	-0.0025
E1	1	6	0	6	E1	1	5	1	5	11538.7194 (0.002)	-0.0019
E2	1	7	0	7	E2	1	6	1	6	13284.9587 (0.002)	-0.0008
E1	1	8	0	8	E1	1	7	1	7	15033.7583 (0.002)	-0.0036
E2	1	9	0	9	E2	1	8	1	8	16788.2340 (0.002)	-0.0003
E1	1	7	2	6	E1	1	6	1	5	15408.4296 (0.002)	0.0032
E2	1	8	2	7	E2	1	7	1	6	16952.8008 (0.002)	0.0004
E1	1	9	2	8	E1	1	8	1	7	18651.8641 (0.002)	-0.0005
E2	1	9	2	7	E2	1	9	1	8	12420.9640 (0.002)	-0.0006
E2	1	10	3	8	E2	1	10	1	9	14335.9283 (0.002)	-0.0013
E1	1	10	2	9	E1	1	9	2	8	20381.9866 (0.002)	0.0027
E1	1	11	2	10	E1	1	10	2	9	22124.4842 (0.002)	-0.0002
E2	1	7	1	6	E2	1	6	2	5	15198.2922 (0.002)	-0.0038
E1	1	8	1	7	E1	1	7	2	6	16938.9423 (0.002)	-0.0008
E2	1	9	1	8	E2	1	8	2	7	18651.3250 (0.002)	-0.0004
E1	1	10	2	8	E1	1	10	2	9	14335.8159 (0.002)	0.0003
E2	1	8	3	6	E2	1	8	2	7	10453.9947 (0.002)	-0.0002
E1	1	9	3	7	E1	1	9	2	8	12424.6128 (0.002)	-0.0012
E2	1	8	4	5	E2	1	8	3	6	8542.5154 (0.002)	0.0013
E1	1	10	2	8	E1	1	9	3	7	22293.1862 (0.002)	0.0007
E2	1	6	5	2	E2	1	6	4	3	10678.2273 (0.002)	-0.0007
E1	1	8	3	5	E1	1	7	4	4	17636.3211 (0.002)	0.0006
E2	2	9	1	9	E2	2	8	0	8	16912.6245 (0.002)	0.0008
E2	2	6	2	4	E2	2	5	2	4	16011.6707 (0.002)	-0.0009
E2	2	6	3	3	E2	2	5	3	3	16425.3845 (0.002)	0.0016



**Table S7.** Rotational transitions of the  $^{13}\text{C}$  (2) and  $^{13}\text{C}$ (6) isotopologues of 2,6-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
A1	0	10	0	10	A2	0	9	0	9	20776.9300 (0.002)	-0.0007
A2	0	11	0	11	A1	0	10	0	10	22755.6030 (0.002)	-0.0005
A1	0	12	0	12	A2	0	11	0	11	24734.2880 (0.002)	0.0013
A1	0	4	1	4	A2	0	3	0	3	8934.7930 (0.002)	0.0008
A2	0	5	1	5	A1	0	4	0	4	10890.0030 (0.002)	-0.0016
A1	0	6	1	6	A2	0	5	0	5	12863.6408 (0.002)	0.0002
A2	0	7	1	7	A1	0	6	0	6	14841.2580 (0.002)	0.0010
A1	0	8	1	8	A2	0	7	0	7	16819.6780 (0.002)	-0.0011
A2	0	9	1	9	A1	0	8	0	8	18798.2808 (0.002)	0.0016
A2	0	3	0	3	A1	0	2	1	2	6810.8930 (0.002)	-0.0008
A1	0	4	0	4	A2	0	3	1	3	8879.5760 (0.002)	-0.0002
A2	0	5	0	5	A1	0	4	1	4	10879.0750 (0.002)	-0.0005
A1	0	6	0	6	A2	0	5	1	5	12861.6780 (0.002)	-0.0007
A2	0	7	0	7	A1	0	6	1	6	14840.9260 (0.002)	0.0002
A1	0	8	0	8	A2	0	7	1	7	16819.6250 (0.002)	-0.0005
A2	0	9	0	9	A1	0	8	1	8	18798.2697 (0.002)	-0.0011
A1	0	10	1	10	A2	0	9	1	9	20776.9300 (0.002)	0.0003
A2	0	11	1	11	A1	0	10	1	10	22755.6030 (0.002)	-0.0004
A1	0	12	1	12	A2	0	11	1	11	24734.2880 (0.002)	0.0013
A1	0	5	2	4	A2	0	4	1	3	13070.7745 (0.002)	-0.0004
A2	0	6	2	5	A1	0	5	1	4	14902.6939 (0.002)	0.0001
A1	0	7	2	6	A2	0	6	1	5	16838.0810 (0.002)	-0.0001
A2	0	8	2	7	A1	0	7	1	6	18805.4380 (0.002)	-0.0003
A1	0	9	2	8	A2	0	8	1	7	20780.8510 (0.002)	0.0009
A2	0	3	3	1	A1	0	2	2	0	12514.6220 (0.002)	0.0003
A2	0	5	3	3	A1	0	4	2	2	16164.2806 (0.002)	-0.0016
A1	0	6	3	4	A2	0	5	2	3	17539.6200 (0.002)	-0.0009
A2	0	7	3	5	A1	0	6	2	4	19079.0945 (0.002)	0.0047
A1	0	8	3	6	A2	0	7	2	5	20872.0644 (0.002)	-0.0002
A1	0	3	3	0	A2	0	2	2	1	13135.7850 (0.002)	-0.0038
A2	0	4	3	1	A1	0	3	2	2	17249.9736 (0.002)	0.0032
A1	0	5	1	4	A2	0	4	2	3	12698.3172 (0.002)	-0.0022
A2	0	6	1	5	A1	0	5	2	4	14806.5420 (0.002)	-0.0010
A1	0	7	1	6	A2	0	6	2	5	16816.8817 (0.002)	0.0009
A2	0	8	1	7	A1	0	7	2	6	18801.2000 (0.002)	-0.0007
A1	0	9	1	8	A2	0	8	2	7	20780.0600 (0.002)	0.0018
A1	0	6	2	4	A2	0	5	3	3	16203.3522 (0.002)	-0.0014
A2	0	7	2	5	A1	0	6	3	4	18629.5000 (0.002)	-0.0007
A1	0	8	2	6	A2	0	7	3	5	20750.3864 (0.002)	-0.0005
E	1	5	1	5	E	1	4	0	4	11875.7050 (0.002)	0.0017
E	1	6	1	6	E	1	5	0	5	13316.5432 (0.002)	0.0017
E	1	7	1	7	E	1	6	0	6	15016.3250 (0.002)	0.0018
E	1	8	1	8	E	1	7	0	7	16901.2020 (0.002)	0.0003
E	1	6	0	6	E	1	5	1	5	12708.6909 (0.002)	-0.0018

E	1	7	0	7	E	1	6	1	6	14859.8670 (0.002)	0.0002
E	1	8	0	8	E	1	7	1	7	16867.8428 (0.002)	-0.0009
E	1	9	0	9	E	1	8	1	8	18841.9953 (0.002)	0.0002
E	1	4	2	3	E	1	3	1	2	12761.5351 (0.002)	-0.0025
E	1	5	2	4	E	1	4	1	3	15426.7443 (0.002)	-0.0015
E	1	6	2	5	E	1	5	1	4	17537.7435 (0.002)	0.0013
E	1	7	2	6	E	1	6	1	5	18866.6509 (0.002)	0.0006
E	1	8	2	7	E	1	7	1	6	19885.4907 (0.002)	0.0004
E	1	9	2	8	E	1	8	1	7	21246.5109 (0.002)	0.0002
E	1	3	1	2	E	1	2	1	2	9467.0763 (0.002)	0.0009
E	1	4	1	3	E	1	3	1	3	12479.2290 (0.002)	0.0008
E	1	5	1	4	E	1	4	1	4	16117.3107 (0.002)	0.0027
E	1	3	2	1	E	1	2	2	1	10343.6873 (0.002)	0.0000
E	1	4	2	2	E	1	3	2	2	13265.8853 (0.002)	-0.0043
E	1	5	2	3	E	1	4	2	3	16192.2560 (0.002)	-0.0017
E	1	6	2	4	E	1	5	2	4	19265.3411 (0.002)	0.0023
E	1	7	1	6	E	1	6	2	5	15465.9853 (0.002)	0.0016
E	1	8	1	7	E	1	7	2	6	18513.4255 (0.002)	-0.0020
E	1	9	1	8	E	1	8	2	7	20849.5412 (0.002)	-0.0032
E	1	4	3	2	E	1	3	2	1	13729.7239 (0.002)	0.0018

**Table S8.** Rotational transitions of the  $^{13}\text{C}$  (1) isotopologue of 2,6-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
B1	0	4	1	4	B2	0	3	0	3	8947.5178 (0.002)	0.0007
A2	0	5	1	5	A1	0	4	0	4	10907.7892 (0.002)	-0.0003
B1	0	6	1	6	B2	0	5	0	5	12885.2636 (0.002)	0.0004
A2	0	7	1	7	A1	0	6	0	6	14866.3536 (0.002)	0.0012
B1	0	8	1	8	B2	0	7	0	7	16848.1568 (0.002)	-0.0017
A2	0	9	1	9	A1	0	8	0	8	18830.1239 (0.002)	0.0018
B1	0	10	0	10	B2	0	9	0	9	20812.1316 (0.002)	-0.0006
B2	0	11	0	11	B1	0	10	0	10	22794.1617 (0.002)	0.0003
B2	0	6	2	5	B1	0	5	1	4	14922.0739 (0.002)	-0.0005
A1	0	7	2	6	A2	0	6	1	5	16864.7469 (0.002)	-0.0016
B2	0	8	2	7	B1	0	7	1	6	18836.6690 (0.002)	0.0003
A1	0	9	2	8	A2	0	8	1	7	20815.7814 (0.002)	0.0013
A1	0	10	1	10	A2	0	9	1	9	20812.1316 (0.002)	0.0004
A2	0	11	1	11	A1	0	10	1	10	22794.1617 (0.002)	0.0002
B2	0	3	0	3	B1	0	2	1	2	6829.2246 (0.002)	-0.0006
A1	0	4	0	4	A2	0	3	1	3	8896.7455 (0.002)	0.0002
B2	0	5	0	5	B1	0	4	1	4	10898.0122 (0.002)	-0.0001
A1	0	6	0	6	A2	0	5	1	5	12883.5573 (0.002)	0.0017
B2	0	7	0	7	B1	0	6	1	6	14866.0721 (0.002)	0.0002
A1	0	8	0	8	A2	0	7	1	7	16848.1139 (0.002)	-0.0004
B2	0	9	0	9	B1	0	8	1	8	18830.1129 (0.002)	-0.0025
B1	0	5	1	4	B2	0	4	2	3	12733.7656 (0.002)	-0.0005
A2	0	6	1	5	A1	0	5	2	4	14835.8523 (0.002)	-0.0018
B1	0	7	1	6	B2	0	6	2	5	16846.2624 (0.002)	-0.0002
A2	0	8	1	7	A1	0	7	2	6	18833.0750 (0.002)	0.0003
A2	0	5	3	3	A1	0	4	2	2	16136.2159 (0.010)	-0.0001
B1	0	6	3	4	B2	0	5	2	3	17522.4218 (0.010)	0.0027
A2	0	7	3	5	A1	0	6	2	4	19085.9826 (0.010)	0.0023
B1	0	8	3	6	B2	0	7	2	5	20897.5882 (0.002)	0.0000
A1	0	6	2	4	A2	0	5	3	3	16281.2322 (0.002)	0.0002
B2	0	7	2	5	B1	0	6	3	4	18680.7407 (0.002)	0.0005
A1	0	8	2	6	A2	0	7	3	5	20791.1189 (0.002)	0.0006
E1	1	5	1	5	E1	1	4	0	4	11873.7329 (0.002)	0.0008
E2	1	6	1	6	E2	1	5	0	5	13322.1086 (0.002)	0.0008
E1	1	7	1	7	E1	1	6	0	6	15034.4638 (0.002)	-0.0008
E2	1	8	1	8	E2	1	7	0	7	16927.3320 (0.002)	0.0000
E1	1	9	1	9	E1	1	8	0	8	18879.3532 (0.002)	-0.0001
E2	1	4	2	3	E2	1	3	1	2	12767.5067 (0.002)	-0.0002
E1	1	5	2	4	E1	1	4	1	3	15436.0087 (0.002)	-0.0013
E2	1	6	2	5	E2	1	5	1	4	17534.4046 (0.002)	0.0000
E1	1	7	2	6	E1	1	6	1	5	18845.4116 (0.002)	-0.0001
E2	1	8	2	7	E2	1	7	1	6	19870.7551 (0.002)	0.0005
E2	1	3	1	2	E2	1	2	1	2	9470.0591 (0.002)	0.0007
E1	1	4	1	3	E1	1	3	1	3	12497.4798 (0.002)	0.0000

E2	1	5	0	5	E2	1	4	1	4	10199.1274 (0.002)	0.0011
E1	1	6	0	6	E1	1	5	1	5	12744.6144 (0.002)	-0.0012
E2	1	7	0	7	E2	1	6	1	6	14889.4069 (0.002)	0.0000
E1	1	8	0	8	E1	1	7	1	7	16897.1535 (0.002)	-0.0004
E2	1	9	0	9	E2	1	8	1	8	18873.7246 (0.002)	-0.0001
E2	1	7	1	6	E2	1	6	2	5	15573.4168 (0.002)	-0.0001
E1	1	8	1	7	E1	1	7	2	6	18584.6388 (0.002)	0.0005
E1	1	4	2	2	E1	1	3	2	2	13268.1832 (0.002)	-0.0002
E2	1	5	2	3	E2	1	4	2	3	16205.8536 (0.002)	0.0008
E2	1	4	3	2	E2	1	3	2	1	13725.8127 (0.002)	-0.0010
E1	1	4	3	1	E1	1	3	3	1	14225.7354 (0.002)	0.0007

**Table S9.** Rotational transitions of the  $^{13}\text{C}$  (3) and  $^{13}\text{C}$  (5) isotopologues of 2,6-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
A1	0	4	1	4	A2	0	3	0	3	8895.3999(0.002)	0.0003
A2	0	5	1	5	A1	0	4	0	4	10844.6241(0.002)	0.0005
A1	0	6	1	6	A2	0	5	0	5	12810.7441(0.002)	0.0001
A2	0	7	1	7	A1	0	6	0	6	14780.3983(0.002)	-0.0007
A1	0	8	1	8	A2	0	7	0	7	16750.7517(0.002)	-0.0008
A2	0	9	1	9	A1	0	8	0	8	18721.2602(0.002)	0.0008
A1	0	10	0	10	A2	0	9	0	9	20691.8105(0.002)	-0.0009
A2	0	11	0	11	A1	0	10	0	10	22662.3826(0.002)	0.0000
A1	0	12	0	12	A2	0	11	0	11	24632.9633(0.002)	0.0001
A2	0	3	0	3	A1	0	2	1	2	6790.8584(0.002)	-0.0012
A1	0	4	0	4	A2	0	3	1	3	8845.6556(0.002)	0.0000
A2	0	5	0	5	A1	0	4	1	4	10835.0878(0.002)	-0.0015
A1	0	6	0	6	A2	0	5	1	5	12809.0860(0.002)	-0.0005
A2	0	7	0	7	A1	0	6	1	6	14780.1274(0.002)	-0.0006
A1	0	8	0	8	A2	0	7	1	7	16750.7096(0.002)	-0.0004
A2	0	9	0	9	A1	0	8	1	8	18721.2514(0.002)	-0.0015
A1	0	10	1	10	A2	0	9	1	9	20691.8105(0.002)	-0.0002
A2	0	11	1	11	A1	0	10	1	10	22662.3826(0.002)	0.0001
A1	0	12	1	12	A2	0	11	1	11	24632.9633(0.002)	0.0002
A2	0	4	2	3	A1	0	3	1	2	11345.0875(0.002)	-0.0011
A1	0	5	2	4	A2	0	4	1	3	12999.3101(0.002)	0.0001
A2	0	6	2	5	A1	0	5	1	4	14834.8717(0.002)	0.0002
A1	0	7	2	6	A2	0	6	1	5	16766.9593(0.002)	0.0000
A2	0	8	2	7	A1	0	7	1	6	18727.6750(0.002)	0.0009
A1	0	9	2	8	A2	0	8	1	7	20695.3989(0.002)	0.0001
A2	0	10	2	9	A1	0	9	1	8	22664.8554(0.002)	0.0017
A1	0	5	1	4	A2	0	4	2	3	12662.4075(0.002)	-0.0008
A2	0	6	1	5	A1	0	5	2	4	14750.7597(0.002)	-0.0005
A1	0	7	1	6	A2	0	6	2	5	16749.0127(0.002)	0.0008
A2	0	8	1	7	A1	0	7	2	6	18724.2014(0.002)	0.0002
A1	0	9	1	8	A2	0	8	2	7	20694.7697(0.002)	-0.0007
A2	0	10	1	9	A1	0	9	2	8	22664.7481(0.002)	0.0026
A2	0	3	3	1	A1	0	2	2	0	12407.7668(0.002)	0.0004
A2	0	5	3	3	A1	0	4	2	2	16033.7073(0.002)	0.0008
A1	0	6	3	4	A2	0	5	2	3	17413.4098(0.002)	0.0004
A2	0	7	3	5	A1	0	6	2	4	18971.5497(0.002)	0.0005
A1	0	8	3	6	A2	0	7	2	5	20775.2226(0.002)	0.0004
A1	0	3	3	0	A2	0	2	2	1	13048.4905(0.002)	-0.0022
A1	0	6	2	4	A2	0	5	3	3	16195.3042(0.002)	-0.0004
A2	0	7	2	5	A1	0	6	3	4	18575.8856(0.002)	-0.0003
A1	0	8	2	6	A2	0	7	3	5	20671.7948(0.002)	0.0013
E	1	4	1	4	E	1	3	0	3	10310.2779(0.002)	-0.0014
E	1	5	1	5	E	1	4	0	4	11800.9316(0.002)	-0.0020
E	1	6	1	6	E	1	5	0	5	13241.9621(0.002)	-0.0022
E	1	7	1	7	E	1	6	0	6	14946.2324(0.002)	-0.0011
E	1	8	1	8	E	1	7	0	7	16829.0236(0.002)	0.0003

E	1	9	1	9	E	1	8	0	8	18770.0331 (0.002)	-0.0010
E	1	10	1	10	E	1	9	0	9	20727.4036 (0.002)	-0.0011
E	1	5	0	5	E	1	4	1	4	10146.0171 (0.002)	0.0021
E	1	6	0	6	E	1	5	1	5	12673.5276 (0.002)	0.0016
E	1	7	0	7	E	1	6	1	6	14804.0827 (0.002)	0.0002
E	1	8	0	8	E	1	7	1	7	16799.5786 (0.002)	-0.0009
E	1	9	0	9	E	1	8	1	8	18764.5659 (0.002)	-0.0007
E	1	10	0	10	E	1	9	1	9	20726.4576 (0.002)	-0.0020
E	1	4	2	3	E	1	3	1	2	12690.8254 (0.002)	-0.0006
E	1	5	2	4	E	1	4	1	3	15343.6783 (0.002)	-0.0003
E	1	6	2	5	E	1	5	1	4	17426.8345 (0.002)	0.0026
E	1	7	2	6	E	1	6	1	5	18726.5735 (0.002)	0.0004
E	1	8	2	7	E	1	7	1	6	19747.0967 (0.002)	0.0033
E	1	9	2	8	E	1	8	1	7	21131.5390 (0.002)	0.0006
E	1	3	1	2	E	1	2	1	2	9412.8464 (0.002)	-0.0011
E	1	4	1	3	E	1	3	1	3	12424.8396 (0.002)	-0.0021
E	1	5	1	4	E	1	4	1	4	16081.6829 (0.002)	-0.0005
E	1	7	1	6	E	1	6	2	5	15498.1552 (0.002)	0.0016
E	1	8	1	7	E	1	7	2	6	18484.2001 (0.002)	0.0008
E	1	9	1	8	E	1	8	2	7	20778.5214 (0.002)	0.0000
E	1	10	1	9	E	1	9	2	8	22800.7052 (0.002)	0.0007
E	1	3	2	1	E	1	2	2	1	10270.7840 (0.002)	0.0015
E	1	4	2	2	E	1	3	2	2	13187.7304 (0.002)	0.0006
E	1	5	2	3	E	1	4	2	3	16109.7445 (0.002)	-0.0006
E	1	6	2	4	E	1	5	2	4	19189.1987 (0.002)	-0.0022

**Table S10.** Rotational transitions of the  $^{13}\text{C}$  (4) isotopologue of 2,6-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
B1	0	10	0	10	B2	0	9	0	9	20652.3100 (0.002)	0.0002
B2	0	11	0	11	B1	0	10	0	10	22619.1275 (0.002)	0.0003
B1	0	4	1	4	B2	0	3	0	3	8873.4636 (0.002)	-0.0001
A2	0	5	1	5	A1	0	4	0	4	10822.6136 (0.002)	-0.0013
B1	0	6	1	6	B2	0	5	0	5	12785.9606 (0.002)	-0.0001
A2	0	7	1	7	A1	0	6	0	6	14752.0878 (0.002)	-0.0006
B1	0	8	1	8	B2	0	7	0	7	16718.7398 (0.002)	-0.0008
A2	0	9	1	9	A1	0	8	0	8	18685.5072 (0.002)	-0.0003
B2	0	3	0	3	B1	0	2	1	2	6792.3986 (0.002)	-0.0004
B2	0	5	0	5	B1	0	4	1	4	10815.3739 (0.002)	-0.0004
B2	0	7	0	7	B1	0	6	1	6	14751.9075 (0.002)	-0.0006
A1	0	8	0	8	A2	0	7	1	7	16718.7141 (0.002)	-0.0001
B2	0	9	0	9	B1	0	8	1	8	18685.5035 (0.002)	-0.0003
A1	0	5	2	4	A2	0	4	1	3	12942.1351 (0.002)	-0.0005
B2	0	6	2	5	B1	0	5	1	4	14794.9248 (0.002)	-0.0008
A1	0	7	2	6	A2	0	6	1	5	16731.3808 (0.002)	-0.0011
B2	0	8	2	7	B1	0	7	1	6	18690.7127 (0.002)	0.0002
A1	0	9	2	8	A2	0	8	1	7	20655.3449 (0.002)	0.0024
B2	0	10	2	9	B1	0	9	1	8	22621.2534 (0.002)	-0.0031
A1	0	10	1	10	A2	0	9	1	9	20652.3100 (0.002)	0.0008
A2	0	11	1	11	A1	0	10	1	10	22619.1275 (0.002)	0.0002
B1	0	5	1	4	B2	0	4	2	3	12666.6844 (0.002)	-0.0006
A2	0	6	1	5	A1	0	5	2	4	14730.7300 (0.002)	0.0008
B1	0	7	1	6	B2	0	6	2	5	16718.5778 (0.002)	-0.0002
A2	0	8	1	7	A1	0	7	2	6	18688.3962 (0.002)	0.0009
B1	0	9	1	8	B2	0	8	2	7	20654.9498 (0.002)	-0.0005
A2	0	10	1	9	A1	0	9	2	8	22621.1940 (0.002)	0.0007
B1	0	4	3	2	B2	0	3	2	1	14316.9244 (0.002)	-0.0006
A2	0	5	3	3	A1	0	4	2	2	15879.0585 (0.002)	0.0038
A2	0	7	3	5	A1	0	6	2	4	18884.0148 (0.002)	0.0007
B1	0	8	3	6	B2	0	7	2	5	20716.6311 (0.002)	-0.0008
B1	0	3	3	0	B2	0	2	2	1	12961.4930 (0.002)	-0.0042
A1	0	6	2	4	A2	0	5	3	3	16268.5440 (0.002)	0.0015
B2	0	7	2	5	B1	0	6	3	4	18578.6965 (0.002)	0.0005
A1	0	8	2	6	A2	0	7	3	5	20642.2954 (0.002)	-0.0013
B2	0	9	2	7	B1	0	8	3	6	22628.6021 (0.002)	0.0036
E2	1	6	1	6	E2	1	5	0	5	13180.1624 (0.002)	0.0058
E2	1	8	1	8	E2	1	7	0	7	16791.8338 (0.002)	0.0003
E1	1	9	1	9	E1	1	8	0	8	18732.2495 (0.002)	0.0008
E2	1	10	1	10	E2	1	9	0	9	20686.8141 (0.002)	0.0018
E2	1	3	1	2	E2	1	2	1	2	9365.7105 (0.002)	0.0025
E2	1	5	0	5	E2	1	4	1	4	10195.2446 (0.002)	-0.0029
E1	1	6	0	6	E1	1	5	1	5	12679.4353 (0.002)	-0.0019
E2	1	7	0	7	E2	1	6	1	6	14784.4713 (0.002)	-0.0010

E1	1	8	0	8	E1	1	7	1	7	16768.7438 (0.002)	0.0005
E2	1	9	0	9	E2	1	8	1	8	18728.2076 (0.002)	-0.0007
E1	1	10	0	10	E1	1	9	1	9	20686.1544 (0.002)	-0.0005
E2	1	4	2	3	E2	1	3	1	2	12631.4652 (0.002)	0.0005
E1	1	5	2	4	E1	1	4	1	3	15276.1589 (0.002)	-0.0024
E1	1	9	2	8	E1	1	8	1	7	21042.9387 (0.002)	-0.0033
E2	1	3	2	1	E2	1	2	2	1	10193.0762 (0.002)	0.0029
E1	1	4	2	2	E1	1	3	2	2	13116.8323 (0.002)	-0.0006
E2	1	5	2	3	E2	1	4	2	3	16048.4324 (0.002)	-0.0014
E1	1	6	2	4	E1	1	5	2	4	19161.2358 (0.002)	0.0025
E2	1	7	1	6	E2	1	6	2	5	15644.2909 (0.002)	0.0015
E1	1	8	1	7	E1	1	7	2	6	18530.1675 (0.002)	-0.0001
E2	1	9	1	8	E2	1	8	2	7	20762.3243 (0.002)	-0.0006
E2	1	4	3	2	E2	1	3	2	1	13553.5092 (0.002)	-0.0021
E1	1	4	3	1	E1	1	3	3	1	14035.1509 (0.002)	-0.0002



**Table S11.** Rotational transitions of the  $^{13}\text{C}$  (7) isotopologue of 2,6-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
B1	0	4	1	4	B2	0	3	0	3	8864.8711 (0.002)	0.0015
A2	0	5	1	5	A1	0	4	0	4	10812.6858 (0.002)	0.0002
B1	0	6	1	6	B2	0	5	0	5	12774.3670 (0.002)	0.0001
B1	0	8	1	8	B2	0	7	0	7	16703.6238 (0.002)	-0.0003
A2	0	9	1	9	A1	0	8	0	8	18668.6170 (0.002)	0.0013
B1	0	10	0	10	B2	0	9	0	9	20633.6422 (0.002)	0.0007
B2	0	11	0	11	B1	0	10	0	10	22598.6834 (0.002)	0.0012
B2	0	3	0	3	B1	0	2	1	2	6787.9855 (0.002)	0.0008
A1	0	6	0	6	A2	0	5	1	5	12773.2400 (0.002)	-0.0009
B2	0	7	0	7	B1	0	6	1	6	14738.5710 (0.002)	-0.0011
A1	0	8	0	8	A2	0	7	1	7	16703.5993 (0.002)	0.0001
B2	0	9	0	9	B1	0	8	1	8	18668.6111 (0.002)	-0.0011
A1	0	5	2	4	A2	0	4	1	3	12926.6478 (0.002)	-0.0016
B2	0	6	2	5	B1	0	5	1	4	14780.2427 (0.002)	0.0003
A1	0	7	2	6	A2	0	6	1	5	16715.8623 (0.002)	-0.0009
B2	0	8	2	7	B1	0	7	1	6	18673.6816 (0.002)	0.0001
A1	0	9	2	8	A2	0	8	1	7	20636.6068 (0.002)	-0.0004
A1	0	10	1	10	A2	0	9	1	9	20633.6422 (0.002)	0.0012
A2	0	11	1	11	A1	0	10	1	10	22598.6834 (0.002)	0.0011
B1	0	3	3	0	B2	0	2	2	1	12942.3609 (0.002)	-0.0021
B1	0	4	3	2	B2	0	3	2	1	14289.4578 (0.010)	-0.0052
A2	0	5	3	3	A1	0	4	2	2	15849.4187 (0.002)	0.0040
B1	0	6	3	4	B2	0	5	2	3	17251.6115 (0.010)	-0.0026
A2	0	7	3	5	A1	0	6	2	4	18861.0975 (0.002)	-0.0008
B1	0	8	3	6	B2	0	7	2	5	20695.8175 (0.002)	-0.0014
A2	0	4	1	3	A1	0	3	2	2	10359.4458 (0.002)	0.0010
B1	0	5	1	4	B2	0	4	2	3	12658.5041 (0.002)	0.0002
A2	0	6	1	5	A1	0	5	2	4	14718.3035 (0.002)	0.0007
B1	0	7	1	6	B2	0	6	2	5	16703.6115 (0.002)	-0.0055
A2	0	8	1	7	A1	0	7	2	6	18671.4835 (0.002)	-0.0008
B1	0	9	1	8	B2	0	8	2	7	20636.2404 (0.002)	0.0018
A1	0	6	2	4	A2	0	5	3	3	16265.9046 (0.002)	0.0015
B2	0	7	2	5	B1	0	6	3	4	18566.1329 (0.002)	0.0015
A1	0	8	2	6	A2	0	7	3	5	20624.6596 (0.002)	0.0000
E2	1	6	1	6	E2	1	5	0	5	13163.2474 (0.002)	0.0027
E2	1	8	1	8	E2	1	7	0	7	16775.9843 (0.002)	-0.0007
E1	1	9	1	9	E1	1	8	0	8	18715.0439 (0.002)	0.0001
E1	1	6	0	6	E1	1	5	1	5	12671.8644 (0.002)	-0.0025
E2	1	7	0	7	E2	1	6	1	6	14772.1260 (0.002)	-0.0009
E1	1	8	0	8	E1	1	7	1	7	16753.6781 (0.002)	0.0018
E2	1	9	0	9	E2	1	8	1	8	18711.1702 (0.002)	-0.0006
E1	1	5	2	4	E1	1	4	1	3	15257.2248 (0.002)	-0.0019
E1	1	7	2	6	E1	1	6	1	5	18536.9928 (0.002)	-0.0002
E2	1	8	2	7	E2	1	7	1	6	19573.9891 (0.002)	0.0014

E2	1	5	1	4	E2	1	4	1	4	16107.4937 (0.002)	0.0009
E2	1	5	2	3	E2	1	4	2	3	16030.3808 (0.002)	-0.0030
E1	1	6	2	4	E1	1	5	2	4	19146.0954 (0.002)	0.0032
E2	1	7	1	6	E2	1	6	2	5	15653.4238 (0.002)	0.0005
E1	1	8	1	7	E1	1	7	2	6	18523.4712 (0.002)	-0.0015

**Table S12.** Rotational transitions of the  $^{13}\text{C}$  (1) isotopologue of 3,5-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
A2	0	3	0	3	A1	0	2	0	2	6152.2218 (0.002)	0.0018
B2	0	5	0	5	B1	0	4	0	4	9667.5582 (0.002)	-0.0016
B1	0	6	0	6	B2	0	5	0	5	11425.2657 (0.002)	-0.0004
B2	0	7	0	7	B1	0	6	0	6	13182.9704 (0.002)	-0.0009
B1	0	8	0	8	B2	0	7	0	7	14940.6743 (0.002)	-0.0007
B2	0	9	0	9	B1	0	8	0	8	16698.3762 (0.002)	-0.0007
B1	0	10	0	10	B2	0	9	0	9	18456.0750 (0.002)	-0.0019
B2	0	11	0	11	B1	0	10	0	10	20213.7740 (0.002)	-0.0006
B1	0	12	0	12	B2	0	11	0	11	21971.4691 (0.002)	-0.0009
A1	0	4	1	4	A2	0	3	0	3	7909.8542 (0.002)	0.0007
A2	0	5	1	5	A1	0	4	1	4	9667.5582 (0.002)	-0.0016
A1	0	6	1	6	A2	0	5	1	5	11425.2657 (0.002)	-0.0004
A2	0	7	1	7	A1	0	6	1	6	13182.9704 (0.002)	-0.0009
A1	0	8	1	8	A2	0	7	1	7	14940.6743 (0.002)	-0.0007
A2	0	9	1	9	A1	0	8	1	8	16698.3762 (0.002)	-0.0007
A1	0	10	1	10	A2	0	9	1	9	18456.0750 (0.002)	-0.0019
A2	0	11	1	11	A1	0	10	1	10	20213.7740 (0.002)	-0.0006
A1	0	12	1	12	A2	0	11	1	11	21971.4691 (0.002)	-0.0009
B1	0	4	0	4	B2	0	3	1	3	7909.8542 (0.002)	0.0017
B2	0	6	1	5	B1	0	5	1	4	13183.2880 (0.002)	0.0001
B1	0	7	1	6	B2	0	6	1	5	14940.9871 (0.002)	0.0002
B2	0	8	1	7	B1	0	7	1	6	16698.6873 (0.002)	0.0014
B1	0	9	1	8	B2	0	8	1	7	18456.3853 (0.002)	0.0016
B2	0	10	1	9	B1	0	9	1	8	20214.0790 (0.002)	-0.0007
B1	0	11	1	10	B2	0	10	1	9	21971.7748 (0.002)	0.0013
A1	0	6	3	4	A2	0	5	2	3	14941.3739 (0.002)	0.0008
B2	0	7	2	5	B1	0	6	2	4	16699.0217 (0.002)	0.0001
B1	0	8	2	6	B2	0	7	2	5	18456.7048 (0.002)	0.0009
A2	0	6	2	5	A1	0	5	2	4	13183.2880 (0.002)	0.0001
A1	0	7	2	6	A2	0	6	2	5	14940.9871 (0.002)	0.0002
A2	0	8	2	7	A1	0	7	2	6	16698.6873 (0.002)	0.0014
A1	0	9	2	8	A2	0	8	2	7	18456.3853 (0.002)	0.0016
A2	0	10	2	9	A1	0	9	2	8	20214.0790 (0.002)	-0.0007
A1	0	11	2	10	A2	0	10	2	9	21971.7748 (0.002)	0.0013
A2	0	7	3	5	A1	0	6	3	4	16699.0217 (0.002)	-0.0001
A1	0	8	3	6	A2	0	7	3	5	18456.7048 (0.002)	0.0009
B2	0	6	3	3	B1	0	5	3	2	16702.3679 (0.002)	-0.0009
B1	0	7	3	4	B2	0	6	3	3	18457.2307 (0.002)	0.0071
B1	0	6	2	4	B2	0	5	3	3	14941.3446 (0.002)	-0.0007
A1	0	7	4	4	A2	0	6	4	3	18457.1361 (0.002)	-0.0044
E2	1	8	0	8	E2	1	7	0	7	14978.5998 (0.002)	0.0013
E2	1	9	0	9	E2	1	8	0	8	16726.7689 (0.002)	0.0016
E2	1	10	0	10	E2	1	9	0	9	18478.1874 (0.002)	0.0012

E2	1	6	1	6	E2	1	5	0	5	11519.2833 (0.002)	0.0004
E1	1	7	1	7	E1	1	6	0	6	13237.0093 (0.002)	-0.0002
E1	1	8	1	8	E1	1	7	1	7	14978.5747 (0.002)	0.0017
E1	1	9	1	9	E1	1	8	1	8	16726.7689 (0.002)	0.0011
E1	1	10	1	10	E1	1	9	1	9	18478.1874 (0.002)	0.0012
E2	1	8	2	7	E2	1	7	1	6	16886.0915 (0.002)	-0.0012
E1	1	6	0	6	E1	1	5	1	5	11497.3759 (0.002)	-0.0003
E2	1	7	0	7	E2	1	6	1	6	13236.0594 (0.002)	0.0005
E1	1	6	1	5	E1	1	5	2	4	13007.5134 (0.002)	0.0000
E2	1	7	1	6	E2	1	6	2	5	15151.0855 (0.002)	-0.0027
E1	1	8	1	7	E1	1	7	2	6	16875.6367 (0.002)	-0.0015
E2	1	6	3	4	E2	1	5	2	3	16886.6626 (0.002)	-0.0018

**Table S13.** Rotational transitions of the  $^{13}\text{C}$  (2) and  $^{13}\text{C}$  (6) isotopologue of 3,5-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
A2	0	8	1	7	A1	0	8	0	8	13187.1966 (0.002)	0.0000
A2	0	3	0	3	A1	0	2	0	2	6153.2213 (0.002)	0.0025
A2	0	5	0	5	A1	0	4	0	4	9669.1423 (0.002)	-0.0001
A1	0	6	0	6	A2	0	5	0	5	11427.1360 (0.002)	-0.0008
A2	0	7	0	7	A1	0	6	0	6	13185.1294 (0.002)	-0.0007
A1	0	8	0	8	A2	0	7	0	7	14943.1210 (0.002)	-0.0008
A2	0	9	0	9	A1	0	8	0	8	16701.1114 (0.002)	-0.0004
A1	0	10	0	10	A2	0	9	0	9	18459.0996 (0.002)	-0.0002
A2	0	11	0	11	A1	0	10	0	10	20217.0855 (0.002)	-0.0001
A1	0	12	0	12	A2	0	11	0	11	21975.0689 (0.002)	-0.0001
A2	0	3	1	3	A1	0	2	0	2	6153.2213 (0.002)	0.0016
A2	0	6	1	5	A1	0	5	1	4	13185.4415 (0.002)	-0.0009
A1	0	7	1	6	A2	0	6	1	5	14943.4301 (0.002)	0.0003
A2	0	8	1	7	A1	0	7	1	6	16701.4169 (0.002)	-0.0001
A1	0	9	1	8	A2	0	8	1	7	18459.4020 (0.002)	-0.0009
A1	0	5	2	4	A2	0	4	1	3	11427.4644 (0.002)	0.0031
A2	0	3	1	3	A1	0	2	1	2	6153.0885 (0.002)	-0.0009
A2	0	5	1	5	A1	0	4	1	4	9669.1423 (0.002)	-0.0001
A1	0	6	1	6	A2	0	5	1	5	11427.1360 (0.002)	-0.0008
A2	0	7	1	7	A1	0	6	1	6	13185.1294 (0.002)	-0.0007
A1	0	8	1	8	A2	0	7	1	7	14943.1210 (0.002)	-0.0008
A2	0	9	1	9	A1	0	8	1	8	16701.1114 (0.002)	-0.0004
A1	0	10	1	10	A2	0	9	1	9	18459.0996 (0.002)	-0.0002
A2	0	11	1	11	A1	0	10	1	10	20217.0855 (0.002)	-0.0001
A1	0	12	1	12	A2	0	11	1	11	21975.0689 (0.002)	-0.0001
A2	0	3	0	3	A1	0	2	1	2	6153.0885 (0.002)	-0.0001
A2	0	8	2	7	A1	0	8	1	8	13187.1966 (0.002)	0.0000
A2	0	5	3	3	A1	0	4	2	2	13186.9203 (0.002)	-0.0007
A2	0	6	2	5	A1	0	5	2	4	13185.4415 (0.002)	-0.0009
A1	0	7	2	6	A2	0	6	2	5	14943.4301 (0.002)	0.0003
A2	0	8	2	7	A1	0	7	2	6	16701.4169 (0.002)	-0.0001
A1	0	9	2	8	A2	0	8	2	7	18459.4020 (0.002)	-0.0009
A1	0	5	1	4	A2	0	4	2	3	11427.4545 (0.002)	-0.0008
A1	0	6	2	4	A2	0	5	2	3	14943.8045 (0.002)	0.0008
A2	0	7	2	5	A1	0	6	2	4	16701.7461 (0.002)	0.0000
A1	0	8	2	6	A2	0	7	2	5	18459.7177 (0.002)	0.0002
A2	0	6	4	3	A1	0	5	3	2	16704.8618 (0.002)	0.0002
A1	0	7	4	4	A2	0	6	3	3	18460.2113 (0.002)	0.0003
A2	0	5	3	3	A1	0	4	3	2	13184.9686 (0.002)	0.0002
A1	0	6	3	4	A2	0	5	3	3	14943.7805 (0.002)	0.0006
A2	0	7	3	5	A1	0	6	3	4	16701.7461 (0.002)	0.0003

A1	0	8	3	6	A2	0	7	3	5	18459.7177 (0.002)	0.0002
A2	0	5	2	3	A1	0	4	3	2	13184.9446 (0.002)	0.0002
A1	0	7	3	4	A2	0	6	4	3	18460.1390 (0.002)	0.0010
E	1	10	0	10	E	1	9	0	9	18481.5238 (0.002)	0.0022
E	1	11	0	11	E	1	10	0	10	20235.0570 (0.002)	0.0022
E	1	6	1	6	E	1	5	0	5	11525.6794 (0.002)	0.0005
E	1	7	1	7	E	1	6	0	6	13240.3303 (0.002)	0.0004
E	1	8	1	8	E	1	7	0	7	14981.6522 (0.002)	0.0006
E	1	9	1	9	E	1	8	0	8	16729.9222 (0.002)	0.0005
E	1	4	2	3	E	1	3	1	2	10862.4063 (0.002)	0.0004
E	1	8	2	7	E	1	7	1	6	16896.0825 (0.002)	-0.0027
E	1	5	0	5	E	1	4	1	4	9671.2324 (0.002)	-0.0026
E	1	6	0	6	E	1	5	1	5	11498.1621 (0.002)	-0.0011
E	1	7	0	7	E	1	6	1	6	13238.9102 (0.002)	-0.0007
E	1	8	0	8	E	1	7	1	7	14981.6033 (0.002)	0.0004
E	1	9	0	9	E	1	8	1	8	16729.9222 (0.002)	0.0017
E	1	10	1	10	E	1	9	1	9	18481.5238 (0.002)	0.0022
E	1	11	1	11	E	1	10	1	10	20235.0570 (0.002)	0.0022
E	1	6	3	4	E	1	5	2	3	16905.7556 (0.002)	-0.0007
E	1	4	2	2	E	1	3	2	2	11110.5527 (0.002)	-0.0004
E	1	8	1	7	E	1	7	2	6	16880.5285 (0.002)	-0.0024

**Table S14.** Rotational transitions of the  $^{13}\text{C}$  (3) and  $^{13}\text{C}$  (5) isotopologues of 3,5-difluorotoluene.

Upper level				Lower level				Measured(Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
A1	0	4	0	4	A2	0	3	0	3	7914.4425 (0.002)	-0.0006
A1	0	6	0	6	A2	0	5	0	5	11431.8950 (0.002)	-0.0009
A2	0	7	0	7	A1	0	6	0	6	13190.6206 (0.002)	-0.0002
A1	0	8	0	8	A2	0	7	0	7	14949.3442 (0.002)	0.0000
A2	0	9	0	9	A1	0	8	0	8	16708.0665 (0.002)	0.0007
A1	0	10	0	10	A2	0	9	0	9	18466.7859 (0.002)	0.0004
A2	0	11	0	11	A1	0	10	0	10	20225.5039 (0.002)	0.0009
A1	0	12	0	12	A2	0	11	0	11	21984.2180 (0.002)	-0.0001
A2	0	3	1	3	A1	0	2	0	2	6155.7679 (0.010)	0.0014
A2	0	8	1	7	A1	0	8	0	8	13192.7490 (0.002)	-0.0006
A1	0	9	1	8	A2	0	9	0	9	14951.7794 (0.002)	0.0007
A1	0	4	1	4	A2	0	3	1	3	7914.4425 (0.002)	0.0000
A1	0	6	1	6	A2	0	5	1	5	11431.8950 (0.002)	-0.0009
A2	0	7	1	7	A1	0	6	1	6	13190.6206 (0.002)	-0.0002
A1	0	8	1	8	A2	0	7	1	7	14949.3442 (0.002)	0.0000
A2	0	9	1	9	A1	0	8	1	8	16708.0665 (0.002)	0.0007
A1	0	10	1	10	A2	0	9	1	9	18466.7859 (0.002)	0.0004
A2	0	11	1	11	A1	0	10	1	10	20225.5039 (0.002)	0.0009
A1	0	12	1	12	A2	0	11	1	11	21984.2180 (0.002)	-0.0001
A2	0	6	1	5	A1	0	5	1	4	13190.9384 (0.002)	0.0003
A1	0	7	1	6	A2	0	6	1	5	14949.6576 (0.002)	-0.0003
A2	0	8	1	7	A1	0	7	1	6	16708.3774 (0.002)	0.0002
A1	0	9	1	8	A2	0	8	1	7	18467.0947 (0.002)	-0.0002
A1	0	5	2	4	A2	0	4	1	3	11432.2202 (0.002)	-0.0021
A2	0	8	2	7	A1	0	8	1	8	13192.7490 (0.002)	-0.0006
A1	0	9	2	8	A2	0	9	1	9	14951.7794 (0.002)	0.0007
A1	0	10	3	8	A2	0	10	1	9	14951.6555 (0.002)	-0.0007
A2	0	3	0	3	A1	0	2	1	2	6155.6668 (0.010)	-0.0007
A2	0	9	2	7	A1	0	9	1	8	13192.6355 (0.002)	-0.0014
A1	0	5	1	4	A2	0	4	2	3	11432.2202 (0.002)	0.0018
A2	0	6	2	5	A1	0	5	2	4	13190.9384 (0.002)	0.0003
A1	0	7	2	6	A2	0	6	2	5	14949.6576 (0.002)	-0.0003
A2	0	8	2	7	A1	0	7	2	6	16708.3774 (0.002)	0.0002
A1	0	9	2	8	A2	0	8	2	7	18467.0947 (0.002)	-0.0002
A1	0	6	2	4	A2	0	5	2	3	14950.0192 (0.002)	-0.0009
A2	0	7	2	5	A1	0	6	2	4	16708.7059 (0.002)	-0.0001
A2	0	5	3	3	A1	0	4	2	2	13192.1363 (0.002)	-0.0004
A1	0	6	3	4	A2	0	5	2	3	14950.0192 (0.002)	-0.0011

A2	0	10	3	7	A1	0	10	2	8	13192.4975 (0.002)	0.0013
A1	0	11	3	8	A2	0	11	2	9	14951.5101 (0.002)	0.0014
A1	0	10	2	8	A2	0	10	2	9	14951.6555 (0.002)	-0.0007
A2	0	9	3	7	A1	0	9	2	8	13192.6355 (0.002)	-0.0014
A2	0	10	4	7	A1	0	10	3	8	13192.4975 (0.002)	0.0013
A1	0	11	4	8	A2	0	11	3	9	14951.5101 (0.002)	0.0014
A2	0	11	4	7	A1	0	11	3	8	13192.3233 (0.002)	0.0007
A1	0	6	3	4	A2	0	5	3	3	14950.0047 (0.002)	0.0003
A2	0	7	3	5	A1	0	6	3	4	16708.7059 (0.002)	0.0000
A1	0	6	2	4	A2	0	5	3	3	14950.0047 (0.002)	0.0004
A2	0	6	4	3	A1	0	5	4	2	16707.6946 (0.002)	-0.0009
A2	0	6	3	3	A1	0	5	4	2	16707.6481 (0.002)	0.0001
A2	0	11	5	7	A1	0	11	4	8	13192.3233 (0.002)	0.0007
E	1	6	1	6	E	1	5	0	5	11530.5876 (0.002)	0.0018
E	1	7	1	7	E	1	6	0	6	13245.8748 (0.002)	0.0006
E	1	8	1	8	E	1	7	0	7	14987.9075 (0.002)	0.0000
E	1	9	1	9	E	1	8	0	8	16736.9005 (0.002)	0.0000
E	1	10	0	10	E	1	9	0	9	18489.2285 (0.002)	0.0017
E	1	6	0	6	E	1	5	1	5	11502.9366 (0.002)	-0.0003
E	1	6	0	6	E	1	5	1	5	11502.9352 (0.002)	-0.0017
E	1	7	0	7	E	1	6	1	6	13244.4449 (0.002)	-0.0001
E	1	8	0	8	E	1	7	1	7	14987.8587 (0.002)	0.0003
E	1	9	0	9	E	1	8	1	8	16736.9005 (0.002)	0.0012
E	1	7	2	6	E	1	6	1	5	15371.8603 (0.002)	0.0014
E	1	8	2	7	E	1	7	1	6	16903.2970 (0.002)	-0.0008
E	1	10	1	10	E	1	9	1	9	18489.2285 (0.002)	0.0018
E	1	5	2	3	E	1	4	2	3	14112.4503 (0.002)	0.0016
E	1	8	1	7	E	1	7	2	6	16887.6304 (0.002)	-0.0028
E	1	6	3	4	E	1	5	2	3	16913.0595 (0.002)	-0.0021
E	1	6	3	3	E	1	5	3	3	17217.2153 (0.002)	-0.0006



**Table S15.** Rotational transitions of the  $^{13}\text{C}$  (4) isotopologue of 3,5-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
A2	0	3	0	3	A1	0	2	0	2	6154.7863 (0.002)	0.0000
B2	0	5	0	5	B1	0	4	0	4	9671.6170 (0.002)	0.0003
B1	0	6	0	6	B2	0	5	0	5	11430.0609 (0.002)	-0.0001
B2	0	7	0	7	B1	0	6	0	6	13188.5037 (0.002)	-0.0004
B1	0	8	0	8	B2	0	7	0	7	14946.9457 (0.002)	0.0001
B2	0	9	0	9	B1	0	8	0	8	16705.3854 (0.002)	-0.0001
B1	0	10	0	10	B2	0	9	0	9	18463.8242 (0.002)	0.0009
A1	0	4	1	4	A2	0	3	0	3	7913.1716 (0.002)	-0.0005
B2	0	3	1	3	B1	0	2	1	2	6154.6709 (0.002)	0.0007
A2	0	5	1	5	A1	0	4	1	4	9671.6170 (0.002)	0.0003
A1	0	6	1	6	A2	0	5	1	5	11430.0609 (0.002)	-0.0001
A2	0	7	1	7	A1	0	6	1	6	13188.5037 (0.002)	-0.0004
A1	0	8	1	8	A2	0	7	1	7	14946.9457 (0.002)	0.0001
A2	0	9	1	9	A1	0	8	1	8	16705.3854 (0.002)	-0.0001
A1	0	10	1	10	A2	0	9	1	9	18463.8242 (0.002)	0.0009
B1	0	5	1	4	B2	0	4	1	3	11430.3852 (0.002)	0.0012
B2	0	6	1	5	B1	0	5	1	4	13188.8160 (0.002)	-0.0003
B1	0	7	1	6	B2	0	6	1	5	14947.2538 (0.002)	0.0000
B2	0	8	1	7	B1	0	7	1	6	16705.6905 (0.002)	-0.0006
B1	0	9	1	8	B2	0	8	1	7	18464.1279 (0.002)	0.0009
B1	0	4	0	4	B2	0	3	1	3	7913.1716 (0.002)	0.0002
A2	0	5	2	3	A1	0	4	2	2	13190.1502 (0.002)	-0.0034
B2	0	7	2	5	B1	0	6	2	4	16706.0183 (0.002)	0.0005
B1	0	8	2	6	B2	0	7	2	5	18464.4408 (0.002)	0.0001
A2	0	4	2	3	A1	0	3	2	2	9671.6797 (0.002)	0.0019
A1	0	5	2	4	A2	0	4	2	3	11430.3781 (0.002)	-0.0008
A2	0	6	2	5	A1	0	5	2	4	13188.8160 (0.002)	-0.0002
A1	0	7	2	6	A2	0	6	2	5	14947.2538 (0.002)	0.0000
A2	0	8	2	7	A1	0	7	2	6	16705.6905 (0.002)	-0.0006
A1	0	9	2	8	A2	0	8	2	7	18464.1279 (0.002)	0.0009
A1	0	6	3	4	A2	0	5	2	3	14947.6200 (0.002)	-0.0006
A2	0	7	3	5	A1	0	6	3	4	16706.0183 (0.002)	0.0004
A1	0	8	3	6	A2	0	7	3	5	18464.4408 (0.002)	0.0001
B1	0	6	2	4	B2	0	5	3	3	14947.5997 (0.002)	-0.0007
B1	0	7	3	4	B2	0	6	3	3	18464.9123 (0.002)	-0.0003
A2	0	6	4	3	A1	0	5	4	2	16704.7622 (0.002)	0.0015
A1	0	7	4	4	A2	0	6	4	3	18464.8516 (0.002)	-0.0007
E2	1	6	1	6	E2	1	5	0	5	11524.4453 (0.002)	0.0018
E1	1	7	1	7	E1	1	6	0	6	13242.6559 (0.002)	0.0015
E2	1	8	0	8	E2	1	7	0	7	14984.9347 (0.002)	-0.0005
E2	1	9	0	9	E2	1	8	0	8	16733.8241 (0.002)	0.0002
E2	1	10	0	10	E2	1	9	0	9	18485.9705 (0.002)	0.0003

E1	1	8	1	8	E1	1	7	1	7	14984.9068 (0.002)	-0.0016
E1	1	9	1	9	E1	1	8	1	8	16733.8241 (0.002)	-0.0003
E1	1	10	1	10	E1	1	9	1	9	18485.9705 (0.002)	0.0003
E2	1	4	2	3	E2	1	3	1	2	10848.1099 (0.002)	0.0041
E2	1	8	2	7	E2	1	7	1	6	16893.6937 (0.002)	-0.0003
E1	1	6	0	6	E1	1	5	1	5	11502.1428 (0.002)	-0.0013
E2	1	7	0	7	E2	1	6	1	6	13241.6734 (0.002)	-0.0004
E1	1	8	1	7	E1	1	7	2	6	16882.9112 (0.002)	-0.0016
E1	1	4	2	2	E1	1	3	2	2	11086.8810 (0.002)	0.0052
E2	1	5	2	3	E2	1	4	2	3	14112.6284 (0.002)	-0.0008
E2	1	4	3	2	E2	1	3	2	1	11204.2460 (0.002)	0.0017
E2	1	6	3	4	E2	1	5	2	3	16894.8808 (0.002)	0.0019
E2	1	5	3	2	E2	1	4	3	2	14183.4562 (0.002)	0.0007
E1	1	5	4	2	E1	1	4	3	1	14267.1507 (0.002)	-0.0043
E2	1	6	4	3	E2	1	5	3	2	17229.7887 (0.002)	-0.0026

**Table S16.** Rotational transitions of the  $^{13}\text{C}$  (7) isotopologue of 3,5-difluorotoluene.

Upper level				Lower level				Measured (Unc. ) o.-c. (MHz)			
Sym'm'	J'	Ka'	Kc'	Sym m	J	Ka	Kc				
A1	0	4	0	4	A2	0	3	0	3	7819.5593 (0.002)	0.0012
B1	0	6	0	6	B2	0	5	0	5	11294.7554 (0.002)	-0.0008
B2	0	7	0	7	B1	0	6	0	6	13032.3756 (0.002)	-0.0023
B1	0	8	0	8	B2	0	7	0	7	14769.9988 (0.002)	-0.0007
B1	0	10	0	10	B2	0	9	0	9	18245.2385 (0.002)	-0.0004
B2	0	11	0	11	B1	0	10	0	10	19982.8561 (0.002)	0.0003
B1	0	12	0	12	B2	0	11	0	11	21720.4709 (0.002)	0.0005
B1	0	4	1	4	B2	0	3	1	3	7819.4935 (0.002)	0.0008
A1	0	6	1	6	A2	0	5	1	5	11294.7554 (0.002)	-0.0008
A2	0	7	1	7	A1	0	6	1	6	13032.3756 (0.002)	-0.0023
A1	0	8	1	8	A2	0	7	1	7	14769.9988 (0.002)	-0.0007
A1	0	10	1	10	A2	0	9	1	9	18245.2385 (0.002)	-0.0004
A2	0	11	1	11	A1	0	10	1	10	19982.8561 (0.002)	0.0003
A1	0	12	1	12	A2	0	11	1	11	21720.4709 (0.002)	0.0005
B1	0	5	1	4	B2	0	4	1	3	11295.5862 (0.002)	0.0002
B2	0	6	1	5	B1	0	5	1	4	13032.8384 (0.002)	-0.0026
B1	0	7	1	6	B2	0	6	1	5	14770.3970 (0.002)	-0.0002
A1	0	5	2	4	A2	0	4	2	3	11295.1334 (0.002)	0.0010
A2	0	6	2	5	A1	0	5	2	4	13032.8294 (0.002)	0.0022
A1	0	7	2	6	A2	0	6	2	5	14770.3970 (0.002)	0.0001
A1	0	4	2	2	A2	0	3	2	1	11419.6888 (0.002)	-0.0010
A1	0	6	2	4	A2	0	5	2	3	14772.7029 (0.002)	0.0008
B1	0	6	3	4	B2	0	5	3	3	14770.9076 (0.002)	0.0014
E2	1	8	0	8	E2	1	7	0	7	14806.2779 (0.002)	-0.0012
E2	1	9	0	9	E2	1	8	0	8	16534.8410 (0.002)	0.0001
E2	1	10	0	10	E2	1	9	0	9	18266.4664 (0.002)	0.0012
E2	1	6	1	6	E2	1	5	0	5	11379.6033 (0.002)	0.0008
E1	1	7	1	7	E1	1	6	0	6	13083.6264 (0.002)	-0.0001
E1	1	8	1	8	E1	1	7	1	7	14806.2779 (0.002)	0.0024
E1	1	9	1	9	E1	1	8	1	8	16534.8410 (0.002)	0.0001
E1	1	10	1	10	E1	1	9	1	9	18266.4664 (0.002)	0.0012
E1	1	7	2	6	E1	1	6	1	5	15098.9608 (0.002)	-0.0011
E2	1	8	2	7	E2	1	7	1	6	16680.6163 (0.002)	-0.0003
E1	1	6	0	6	E1	1	5	1	5	11367.2708 (0.002)	0.0006
E2	1	7	0	7	E2	1	6	1	6	13083.3024 (0.002)	-0.0011
E1	1	6	1	5	E1	1	5	2	4	12995.5886 (0.002)	0.0000
E1	1	6	3	3	E1	1	5	3	3	16959.0156 (0.002)	-0.0006

**Table S17.** Stark effect measurements on several rotational transitions of 2,6-difluorotoluene.

For each electric field (V cm<sup>-1</sup>) the Table presents the observed (Obs.), calculated (Calc.) and observed minus calculated (Obs.-Calc.) frequencies (MHz).

$J' - J''$	Electric field	Obs.	Calc.	Obs.-Calc.
$2_{0,2} - 1_{1,1}$	0.0	4556.32700	4556.3261	0.0009
$M_{F'} - M_{F''}=2 - 1$	33.6504	4556.30987	4556.3118	-0.0019
	37.0090	4556.30744	4556.3088	-0.0014
	42.0469	4556.30297	4556.3038	-0.0008
	50.4433	4556.29244	4556.2940	-0.0016
$2_{2,1} - 1_{1,0}$	0.0	7803.16250	7803.1616	0.00090
$M_{F'} - M_{F''}=2 - 1$	16.8575	7803.15403	7803.1522	0.00185
	33.6504	7803.12560	7803.1241	0.00151
	42.0469	7803.10199	7803.1030	-0.00105
	50.4433	7803.07728	7803.0773	-0.00004
	58.8396	7803.04852	7803.0469	0.00159
	67.2361	7803.01066	7803.0119	-0.00122
$3_{0,3} - 2_{1,2}$	0.0	6833.59115	6833.5914	-0.0003
$M_{F'} - M_{F''}=3 - 2$	16.8575	6833.59133	6833.5917	-0.0004
	33.6504	6833.59258	6833.5927	-0.0001
	50.4433	6833.59376	6833.5943	-0.0005
	67.2361	6833.59574	6833.5965	-0.0007
	75.6325	6833.59707	6833.5978	-0.0007
	84.0290	6833.59855	6833.5993	-0.0007
	92.4253	6833.60022	6833.6010	-0.0007
	100.8219	6833.60211	6833.6028	-0.0007
	109.2182	6833.60401	6833.6048	-0.0007
	117.6147	6833.60632	6833.6069	-0.0006
	126.0111	6833.60820	6833.6092	-0.0010
134.4076	6833.61098	6833.6116	-0.0007	
$3_{3,0} - 2_{2,1}$	0.0000	13151.15224	13151.1513	0.00094
$M_{F'} - M_{F''}=3 - 2$	16.8575	13151.15292	13151.1534	-0.00049
	50.4433	13151.17130	13151.1702	0.00105
	67.2361	13151.18333	13151.1850	-0.00164
	84.0290	13151.20291	13151.2039	-0.00098
	92.4253	13151.21580	13151.2149	0.00088
$4_{0,4} - 3_{1,3}$	0.0	8904.61834	8904.6175	0.0008
$M_{F'} - M_{F''}=4 - 3$	50.4433	8904.62216	8904.6228	-0.0006
	84.0290	8904.63111	8904.6321	-0.0009
	92.4353	8904.63531	8904.6351	0.0002
	100.8219	8904.63882	8904.6384	0.0004
	109.2182	8904.64245	8904.6421	0.0004
	117.6147	8904.64600	8904.6460	0.0001
	126.0111	8904.65015	8904.6502	-0.0000
$4_{0,4} - 3_{1,3}$	0.0	8904.61834	8904.6175	0.0008
$M_{F'} - M_{F''}=3 - 2$	50.4433	8904.61720	8904.6176	-0.00044
	84.0290	8904.61882	8904.6178	-0.001
	92.4353	8904.61779	8904.6179	-0.0001
	100.8219	8904.61699	8904.6180	-0.001
	109.2182	8904.61681	8904.6181	-0.001
	117.6147	8904.61845	8904.6181	0.0003
	126.0111	8904.61869	8904.6182	0.0004

**Table S18.** Stark effect measurements on several rotational transitions of 3,5-difluorotoluene.

For each electric field (V cm<sup>-1</sup>) the Table presents the observed (Obs.), calculated (Calc.) and observed minus calculated (Obs.-Calc.) frequencies (MHz).

$J' - J''$	Electric field	Obs.	Calc.	Obs.-Calc.
$3_{0,3} - 2_{1,2}$	0.0	6174.64400	6174.6419	0.0021
$M_{F'} - M_{F''}=3 - 2$	16.8575	6174.65011	6174.6505	-0.0003
	33.6504	6174.67665	6174.6761	0.0005
	42.0468	6174.69567	6174.6953	0.0004
	50.4433	6174.71940	6174.7188	0.0006
	58.8396	6174.74740	6174.7465	0.0009
	67.2361	6174.77970	6174.7784	0.0013
	75.6325	6174.81581	6174.8147	0.0011
	84.0290	6174.85491	6174.8552	-0.0002
	92.4253	6174.90086	6174.8999	0.0009
	100.8219	6174.94958	6174.9489	0.0007
$3_{0,3} - 2_{1,2}$	33.6504	6174.63820	6174.6380	0.0002
$M_{F'} - M_{F''}=2 - 1$	42.0468	6174.63548	6174.6358	-0.0003
	50.4433	6174.63351	6174.6331	0.0004
	58.8396	6174.63078	6174.6300	0.0008
	67.2361	6174.62793	6174.6263	0.0016
	75.6325	6174.62291	6174.6222	0.00074
	84.0290	6174.61847	6174.6176	0.00092
	100.8219	6174.60837	6174.6069	0.00015
	$3_{0,3} - 2_{1,2}$	58.8396	6174.61513	6174.6132
$M_{F'} - M_{F''}=1 - 0$	67.2361	6174.60510	6174.6044	0.00072
	75.6325	6174.59830	6174.5944	0.0039
	84.0290	6174.58567	6174.5833	0.00236
	100.8219	6174.55995	6174.5576	0.00238
$4_{1,4} - 3_{0,3}$	0.0	7938.78039	7938.7790	0.0014
$M_{F'} - M_{F''}=4 - 3$	16.8575	7938.78096	7938.7827	-0.0018
	33.6504	7938.79291	7938.7939	-0.0010
	42.0468	7938.80211	7938.8022	-0.00013
	50.4433	7938.81164	7938.8124	-0.00081
	58.8396	7938.82512	7938.8245	0.00061
	67.2361	7938.83746	7938.8384	-0.0010
	75.6325	7938.85237	7938.8542	-0.0018
	84.0290	7938.87196	7938.8718	0.000120
	$4_{1,4} - 3_{0,3}$	0.0000	7938.78039	7938.7790
$M_{F'} - M_{F''}=3 - 2$	33.6504	7938.78274	7938.7806	0.0021
	42.0468	7938.78194	7938.7815	0.0004
	50.4433	7938.78257	7938.7826	-0.0000
	58.8396	7938.78371	7938.7839	-0.0002
	67.2361	7938.78643	7938.7854	0.0010
	75.6325	7938.78796	7938.7871	0.0009
	84.0290	7938.78941	7938.7890	0.00041
	$4_{1,4} - 3_{0,3}$	50.4433	7938.77058	7938.7682
$M_{F'} - M_{F''}=2 - 1$	58.8396	7938.76526	7938.7643	0.00093

