

Supplementary information for:

Shape and Interactions of the Synthetic Repellent DEET

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N,N-diethyl-3-methylbenzamide (DEET) is the most widely used insect repellent, exhibiting high efficiency against a wide variety of species. In this work, a comprehensive isolated-molecule investigation of DEET was conducted using chirp-excitation Fourier transform microwave (CP-FTMW) spectroscopy within the frequency range of 7 - 14 GHz. Four out of the eight theoretically predicted conformers were detected and grouped in pairs based on their rotational constants and planar moments of inertia. We also studied the non-covalent interactions of DEET by characterizing the attractive and repulsive forces, which could explain the energetic ordering of the four conformers. In addition, DEET has a methyl top bound to the benzyl ring which is predicted to rotate almost freely with respect to the molecular framework.

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Figure S1. Theoretically predicted 8 chiral pairs of conformations of DEET (B3LYP-GD3BJ/def2-TZVP)

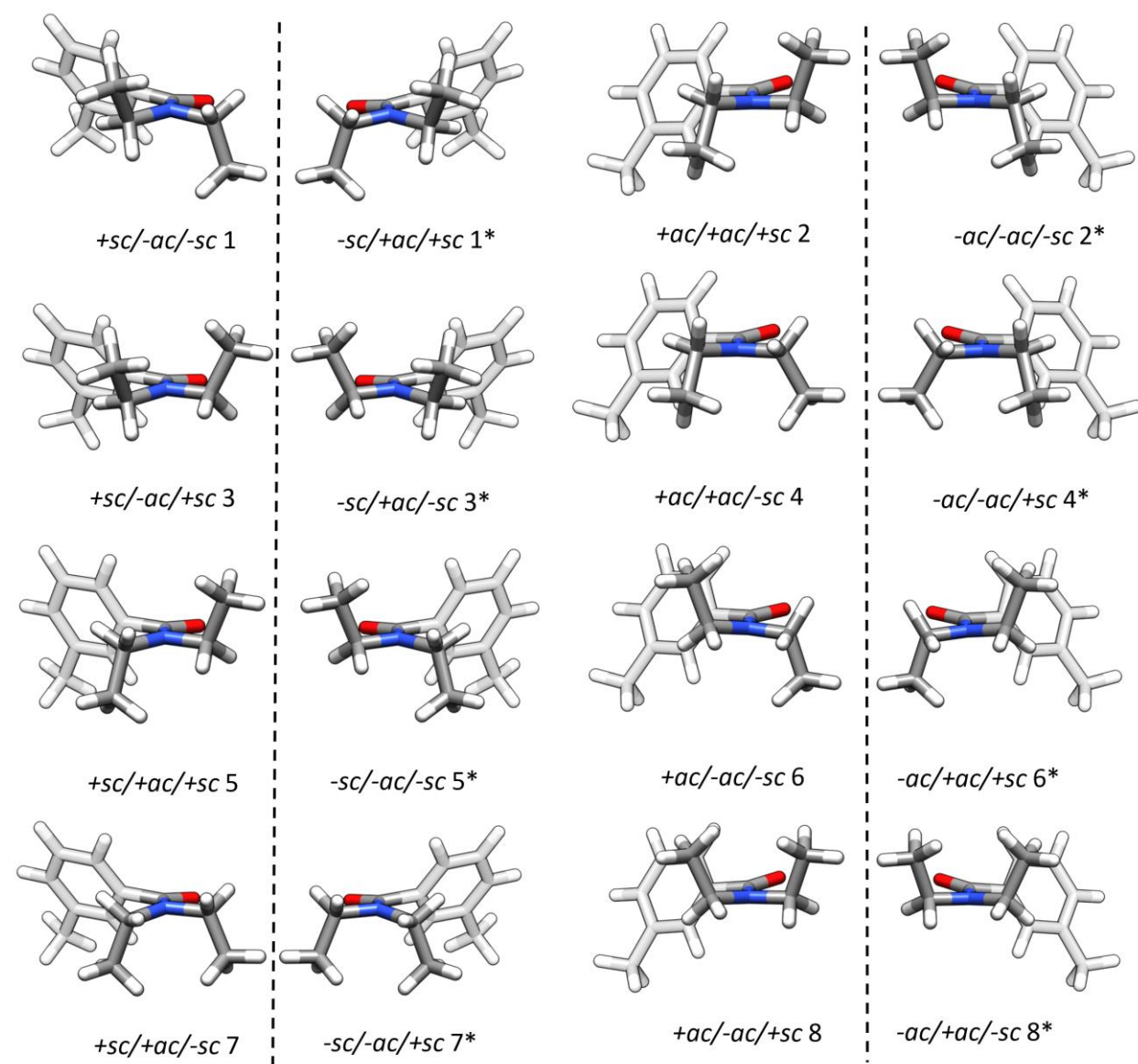


Figure S2. Predicted conformations of DEET (B3LYP-GD3BJ/def2-TZVP) showing the conversion pathways. The eight stable conformers of DEET connected through the changes in the δ (blue arrows), ϕ (green arrows), and θ (red arrows) dihedral angles.

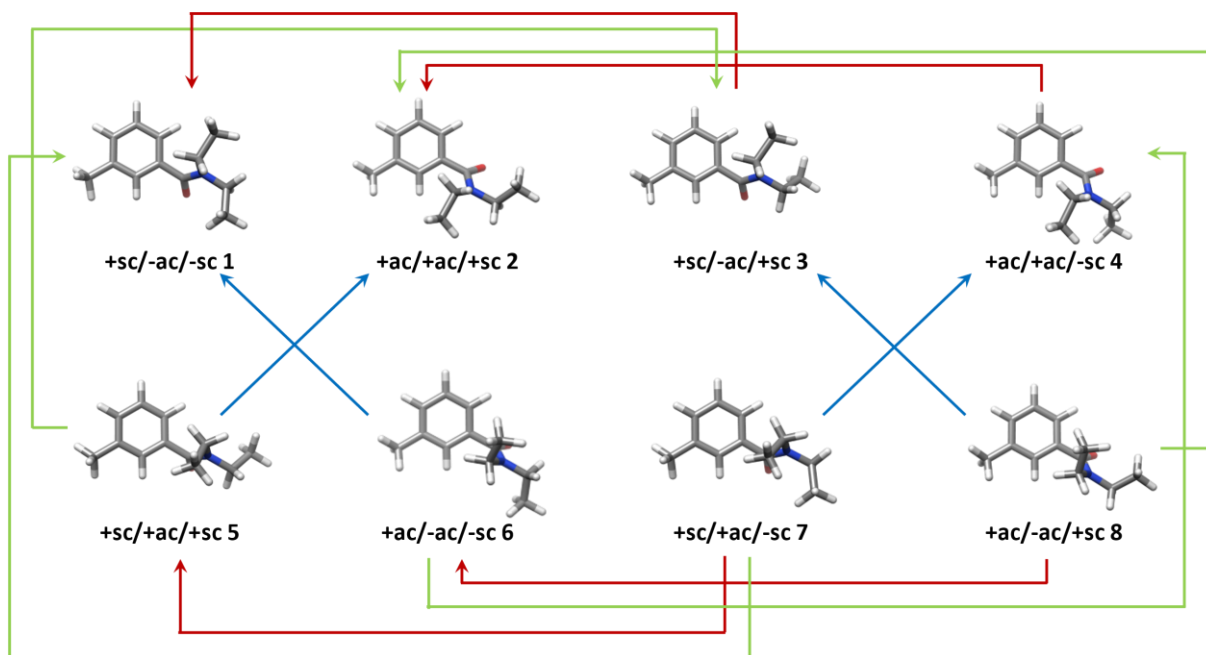


Figure S3. Potential energy surface scan of the δ (C6-C1-C8-O1) dihedral angle. The scans were performed in steps of 10° at the B3LYP-D3BJ/def2-TZVP level of theory. Each conformer is illustrated in the plot close to their minima position in the scan. See figure 1 for atom labelling.

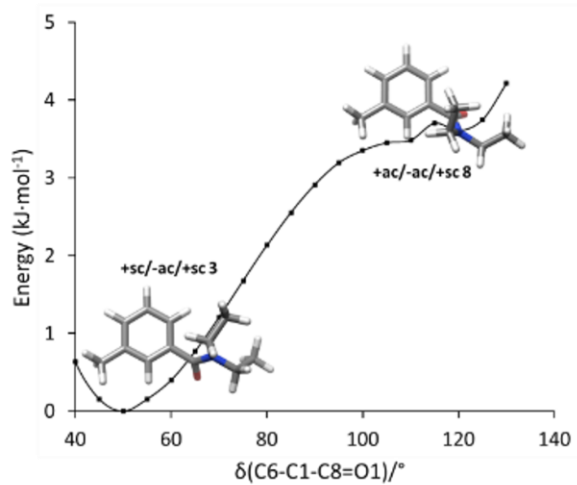
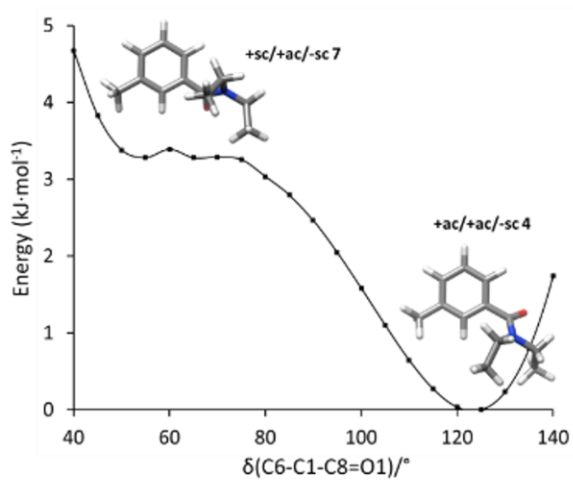
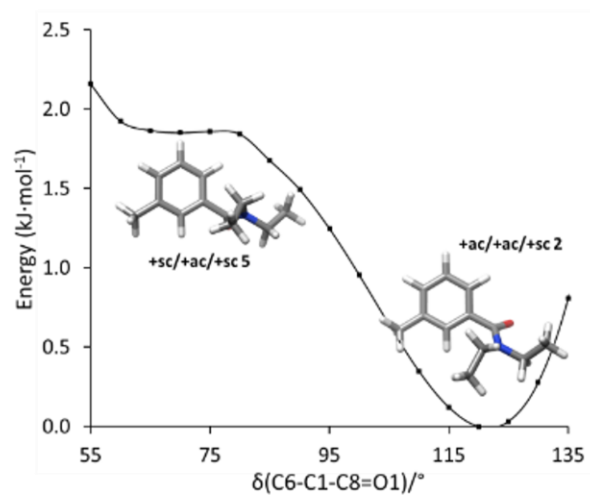
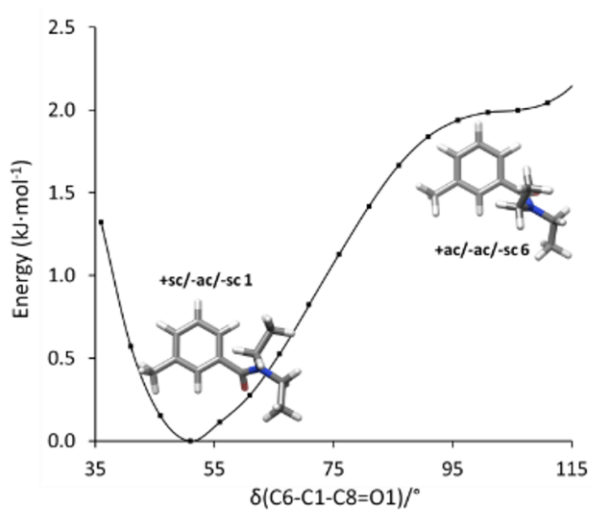


Figure S4. Potential energy surface scan of the θ (C8-N1-C10-C12) dihedral angle. The scan was performed in steps of 10° at the B3LYP-D3BJ/def2-TZVP level of theory. Each conformer is illustrated in the plot close to their minima position in the scan. See figure 1 for atom labelling.

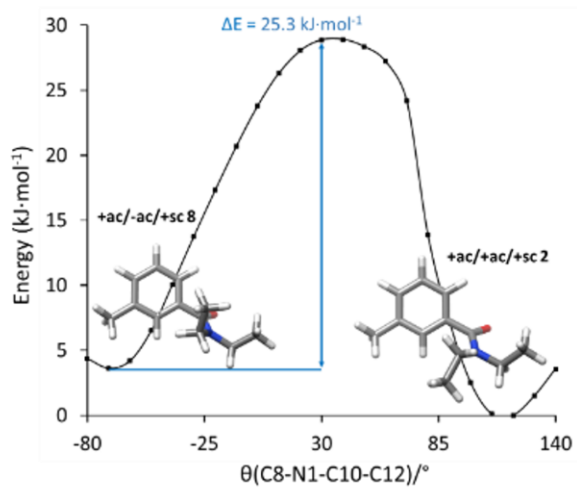
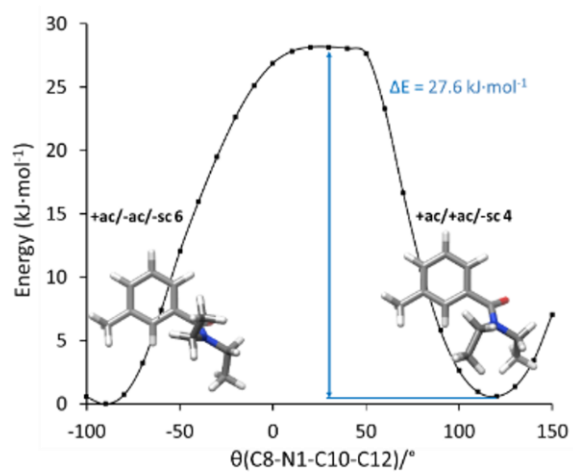
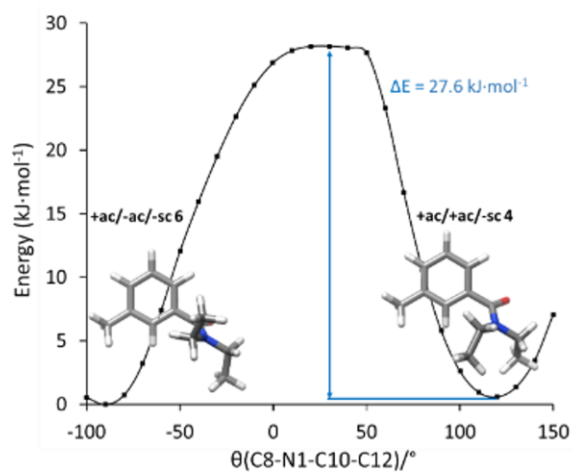
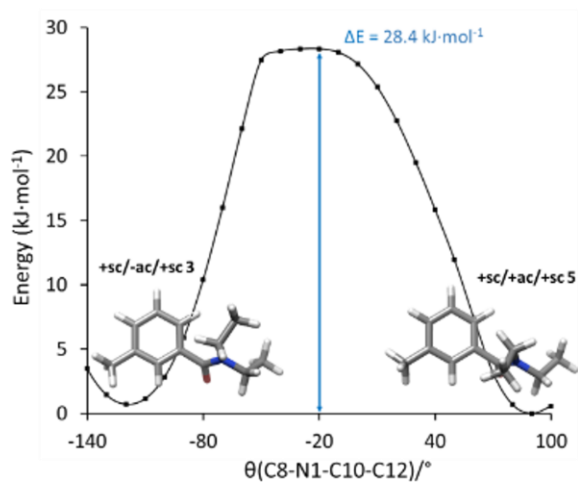


Figure S5. Potential energy surface scan of the ϕ (C8-N1-C9-C11) dihedral angle. The scan was performed in steps of 10° at the B3LYP-D3BJ/def2-TZVP level of theory. Each conformer is illustrated in the plot close to their minima position in the scan. See figure 1 for atom labelling.

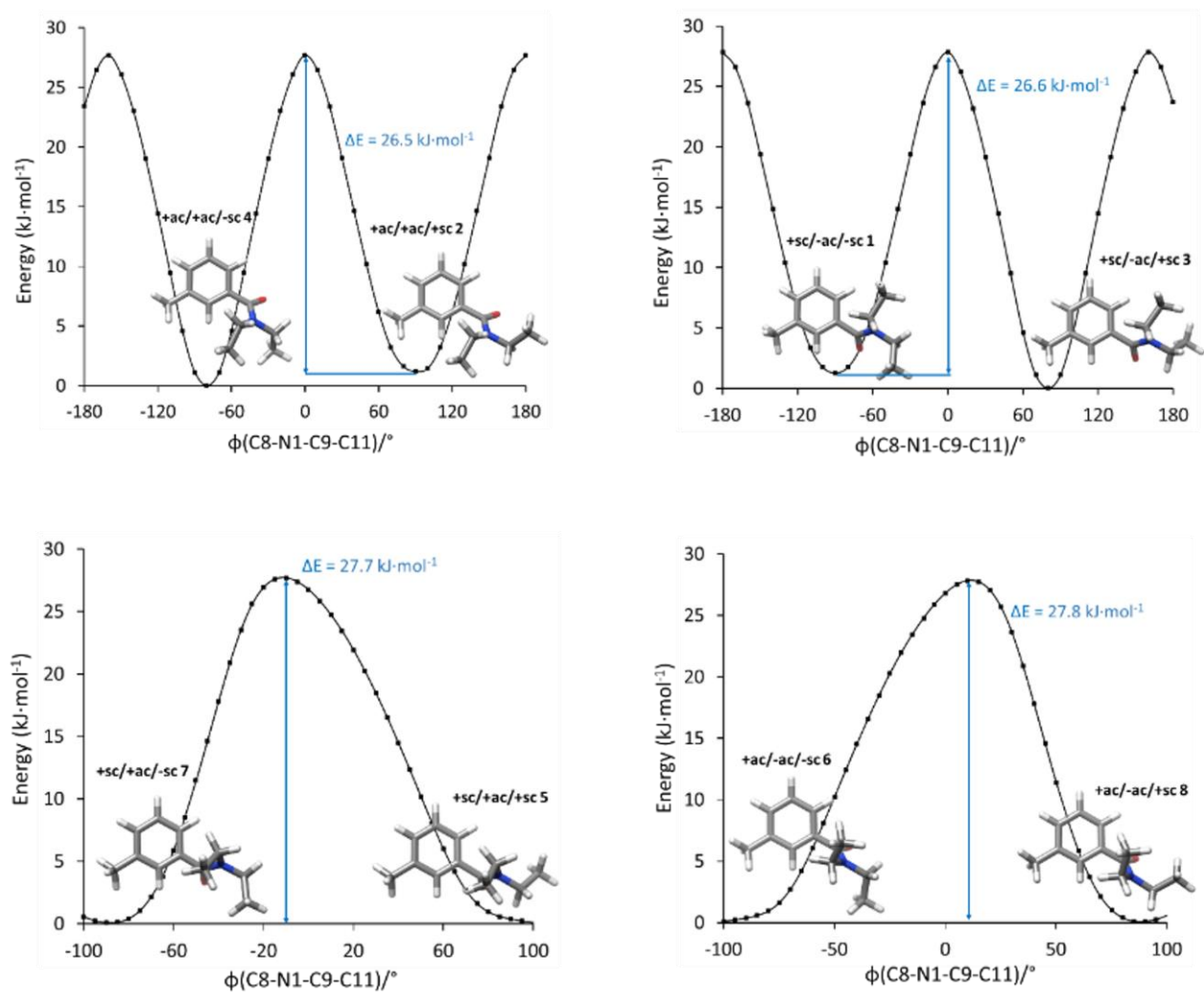


Figure S6. Full frequency range of the recorded rotational spectrum of DEET, experimental (upwards black trace) and simulations based on the experimental rotational parameters for the four observed conformers (downwards coloured traces).

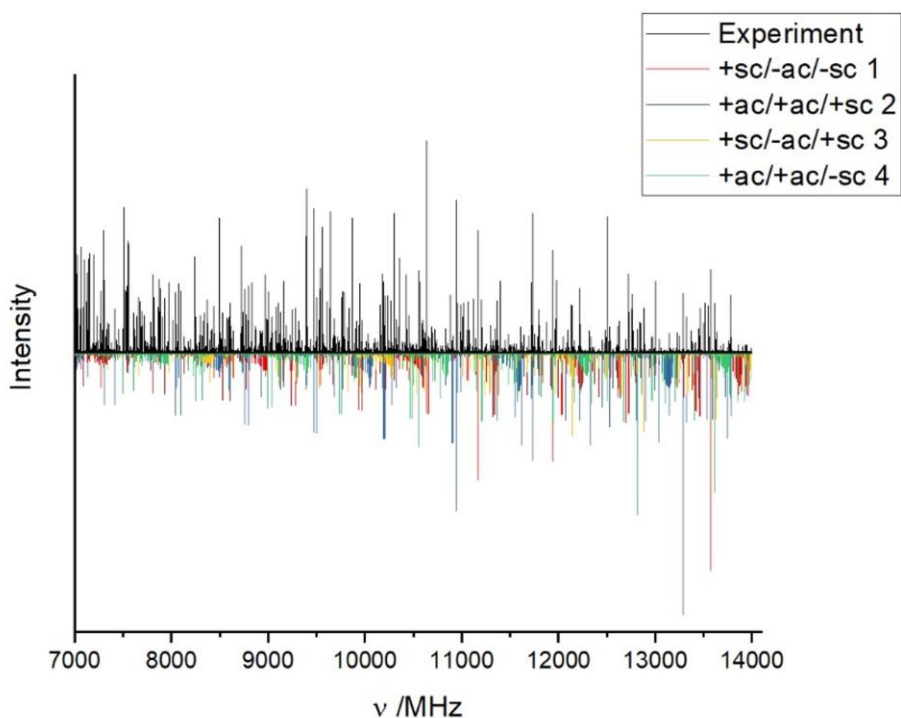


Figure S7. Excerpt of the DEET spectrum. The observed experimental spectrum is shown in the upward black trace, and the fitted spectra are displayed in the downward coloured trace. The hyperfine structure of the lines is shown for two different conformations of DEET, +sc/-ac/-sc 1 (red) and +sc/-ac/+sc 3 (green) for $J'_{K_a K_c} \leftarrow J''_{K_a K_c}$ and $F' \leftarrow F''$ transitions.

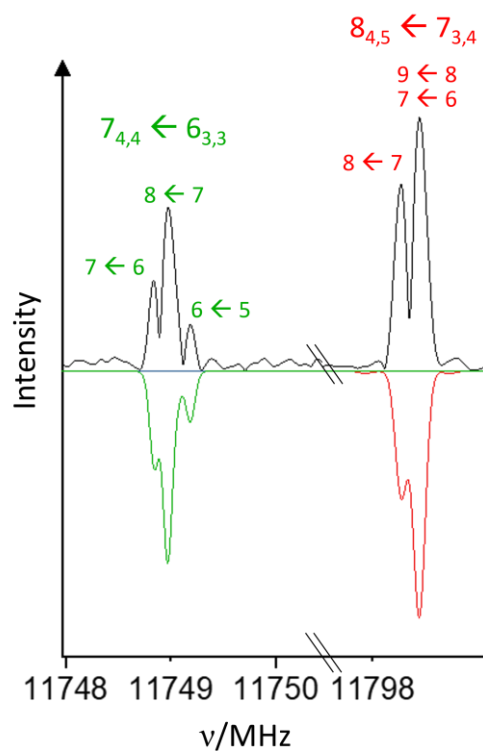


Table S1. Theoretical rotational parameters (A , B , C , D_J , D_{JK} , D_K), ^{14}N quadrupole coupling constants (χ_{ii}), dipole moment components (μ_i) and planar moments of inertia (P_{ii}) of DEET conformers at B3LYP-D3BJ/def2-TZVP from Gaussian computations. The energies (ΔE_{ZPE}) represent the difference of energy relative to the most stable conformer considering the zero-point energy correction.

	<i>+sc/-ac/-sc 1</i>	<i>+ac/+ac/+sc 2</i>	<i>+sc/-ac/+sc 3</i>	<i>+ac/+ac/-sc 4</i>	<i>+sc/+ac/+sc 5</i>	<i>+ac/-ac/-sc 6</i>	<i>+sc/+ac/-sc 7</i>	<i>+ac/-ac/+sc 8</i>
A [MHz]	1201	1178	1313	1134	1253	1129	1289	1283
B [MHz]	415	436	399	440	393	405	398	405
C [MHz]	348	356	346	368	379	394	385	385
D_J [kHz]	0.018	0.013	0.01	0.016	0.044	0.02	0.019	0.014
D_{JK} [kHz]	0.167	0.084	0.154	0.027	0.373	0.249	0.034	0.122
D_K [kHz]	0.015	0.031	0.026	0.112	-0.173	0.084	0.321	-0.050
χ_{aa} [MHz]	2.1	1.7	1.9	2.1	1.9	2.1	2.1	1.5
χ_{bb} [MHz]	-0.6	-0.3	0.6	0.2	-0.7	-3.9	0.2	0.7
χ_{cc} [MHz]	-1.4	-1.4	-2.5	-1.9	-1.2	1.8	-2.3	-2.2
$ \mu_a / \mu_b / \mu_c $ [D]	0.0/2.7/2.3	0.6/3.2/1.9	0.0/3.1/1.6	0.4/3.4/1.7	0.1/2.9/2.4	0.4/0.6/3.8	0.1/3.0/2.0	0.6/3.5/1.4
$P_{aa}/\mu\text{\AA}^2$	1124	1074	1171	1038	1107	1041	1095	1084
$P_{bb}/\mu\text{\AA}^2$	327	344	289	335	225	241	218	230
$P_{cc}/\mu\text{\AA}^2$	93	84	95	110	178	206	174	164
ΔE_{ZPE} [kJ/mol]	0	0.1	0.7	0.8	1.6	1.6	4.1	4.2

Table S2. Relative energies ΔE , ΔE_{ZPE} , and ΔG_{423} (all the values in kJ/mol) for the eight conformers of DEET at B3LYP-D3BJ/def2-TZVP calculated both with Gaussian and Orca. The relative populations (in percentage, %) have been estimated from the relative Gibbs free energies.

Gaussian	<i>+sc/-ac/-sc 1</i>	<i>+ac/+ac/+sc 2</i>	<i>+sc/-ac/+sc 3</i>	<i>+ac/+ac/-sc 4</i>	<i>+sc/+ac/+sc 5</i>	<i>+ac/-ac/-sc 6</i>	<i>+sc/+ac/-sc 7</i>	<i>+ac/-ac/+sc 8</i>
ΔE	0.0	0.0	0.7	0.7	1.9	2.0	4.0	4.2
ΔE_{ZPE}	0.0	0.1	0.8	0.8	1.1	1.3	4.1	4.3
ΔG_{423}	1.3	4.4	2.6	5.4	0.0	3.6	7.1	7.7
N_i^a	23.3	6.7	13.6	4.4	39.0	9.1	2.2	1.7
$N_{i,\text{relax}}^b$	32.3	45.7	15.3	6.6	-	-	-	-
$N_{i,\text{exp}}^c$	34.4(0.8)	34.4(0.7)	17.2(0.6)	13.9(0.5)	-	-	-	-
Orca	<i>+sc/-ac/-sc 1</i>	<i>+ac/+ac/+sc 2</i>	<i>+sc/-ac/+sc 3</i>	<i>+ac/+ac/-sc 4</i>	<i>+sc/+ac/+sc 5</i>	<i>+ac/-ac/-sc 6</i>	<i>+sc/+ac/-sc 7</i>	<i>+ac/-ac/+sc 8</i>
ΔE	0.0	0.1	0.7	0.7	1.9	1.9	3.9	4.1
ΔE_{ZPE}	0.0	0.1	0.7	0.7	1.6	1.6	4.1	4.2
ΔG_{423}	0.1	1.0	1.4	2.0	0.0	0.7	4.7	5.1
N_i	20.7	14.4	12.2	9.5	21.4	15.9	3.2	2.7
$N_{i,\text{relax}}$	36.6	35.8	14.9	12.7	-	-	-	-
$N_{i,\text{exp}}$	34.4(0.8)	34.4(0.7)	17.2(0.6)	13.9(0.5)	-	-	-	-

^a Estimated relative populations based on the Gibbs free energies for each conformer. ^b Estimated relative populations considering the described pathways for collisional relaxations. According to the scans and barriers reported in this work, the population of *+sc/+ac/+sc 5* is added to *+ac/+ac/+sc 2*; *+ac/-ac/-sc 6* to *+sc/-ac/-sc 1*; *+sc/+ac/-sc 7* to *+ac/+ac/-sc 4* and *+ac/-ac/+sc 8* to *+sc/-ac/+sc 3*. ^c Experimental relative populations from the observed intensities and the most intense dipole moment component.

Table S3. Observed frequencies and residuals (MHz) for $+sc/-ac/-sc$ 1 for $J_{K_a'K_c'} \leftarrow J_{K_a''K_c''}$ and $F' \leftarrow F''$ transitions.

J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res	J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res	J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res
7	2	6	6	1	5	7	6	7073.3208	-0.0090	7	2	5	6	1	5	6	5	7556.2343	-0.0568	9	2	8	8	1	7	8	7	8128.8932	-0.0172
						6	5	7073.3208	-0.0090							7	6	7556.2343	0.0421							9	8	8128.8932	-0.0508
						8	7	7073.3208	0.0030							8	7	7556.2343	-0.0322	8	2	6	7	1	6	8	7	8365.3712	0.0512
10	0	10	9	1	9	10	9	7087.6702	0.0000	8	2	7	7	1	6	7	6	7610.1778	-0.0266							7	6	8365.3712	-0.0424
						11	10	7087.6702	0.0084							9	8	7610.1778	-0.0194							9	8	8365.3712	-0.0223
						9	8	7087.6702	-0.0002							8	7	7610.1778	-0.0481	8	1	7	7	0	7	8	7	8391.5032	-0.0012
4	3	2	3	2	1	4	3	7127.5511	-0.0089	11	0	11	10	1	10	12	11	7812.3403	0.0082							9	8	8391.6904	-0.0036
						5	4	7127.7908	0.0009							10	9	7812.3403	0.0011							7	6	8391.6904	-0.0422
						3	2	7127.7908	-0.0562							11	10	7812.3403	0.0000	12	1	11	11	2	10	12	11	8434.1408	0.0025
4	3	1	3	2	1	4	3	7128.7640	0.0049	6	2	4	5	1	5	6	5	7821.7545	-0.0058							13	12	8434.1408	0.0041
						5	4	7129.0010	0.0113							5	4	7822.1127	-0.0362							11	10	8434.1408	-0.0011
						3	2	7129.0010	-0.0461							7	6	7822.1127	0.0425	7	2	6	6	1	6	7	6	8505.4919	-0.0030
4	3	2	3	2	2	4	3	7149.1662	0.0055	13	2	11	12	3	10	14	13	7833.9479	-0.0119							8	7	8505.7205	0.0113
						5	4	7149.4281	0.0192							12	11	7833.9479	-0.0156							6	5	8505.7205	-0.0390
						3	2	7149.4281	-0.0444							13	12	7833.9479	-0.0133	12	0	12	11	1	11	11	10	8526.8638	0.0015
4	3	1	3	2	2	4	3	7150.3641	0.0044	5	3	3	4	2	2	5	4	7864.1335	0.0039							12	11	8526.8638	-0.0002
						5	4	7150.6312	0.0225							6	5	7864.3005	-0.0128							13	12	8526.8638	0.0075
						3	2	7150.6312	-0.0414							5	4	7868.9121	0.0066	6	3	4	5	2	3	6	5	8573.4713	-0.0141
7	1	6	6	0	6	7	6	7260.4371	-0.0009	5	3	2	4	2	2	6	5	7869.0627	-0.0288							7	6	8573.5989	-0.0192
						8	7	7260.6351	0.0076							5	5	7869.1701	0.0188							6	5	8587.7106	0.0057
						6	5	7260.6351	-0.0388	5	3	3	4	2	3	5	4	7928.1716	0.0054	6	3	3	5	2	3	7	6	8587.8275	-0.0151
10	1	10	9	0	9	11	10	7272.0142	0.0203							4	3	7928.4101	-0.0321	12	1	12	11	0	11	11	10	8605.6781	0.0016
						9	8	7272.0142	0.0127							6	5	7928.4101	0.0268							13	12	8605.6781	0.0072
						10	9	7272.0142	0.0008	5	3	2	4	2	3	5	4	7932.9506	0.0085							12	11	8605.6781	-0.0052
11	1	10	10	2	9	12	11	7539.3848	0.0064							4	3	7933.1782	-0.0426	10	2	9	9	1	8	11	10	8638.3795	-0.0104
						11	10	7539.3848	0.0040							6	5	7933.1782	0.0168							9	8	8638.3795	-0.0134
						10	9	7539.3848	0.0004	11	1	11	10	0	10	10	9	7933.9516	0.0122							10	9	8638.3795	-0.0525
6	2	5	5	1	5	6	5	7539.7503	-0.0015							11	10	7933.9516	0.0032	6	3	4	5	2	4	6	5	8719.6019	0.0031
						7	6	7540.0279	0.0352							12	11	7933.9516	0.0187							7	6	8719.7698	-0.0123
						5	4	7540.0279	-0.0319	9	2	8	8	1	7	10	9	8128.8932	-0.0127							5	4	8719.7698	-0.0581

J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res
6	3	3	5	2	4	6	5	8733.8229	0.0047	7	3	4	6	2	4	7	6	9280.7863	0.0170	8	3	6	7	2	5	7	6	9873.6847	0.0007
						7	6	8733.9920	-0.0145							6	5	9280.8773	-0.0150							7	8	9873.6847	0.0713
						5	4	8733.9920	-0.0612							8	7	9280.8773	0.0100							9	8	9873.6847	0.0163
4	4	1	3	3	0	3	2	8774.6021	-0.0391	13	1	13	12	0	12	12	11	9284.5819	0.0076	14	0	14	13	1	13	14	13	9936.6794	0.0075
						3	2	8774.6021	-0.0447							13	12	9284.5819	0.0023							13	12	9936.6794	0.0098
						4	3	8774.6021	0.0304							14	13	9284.5819	0.0125							15	14	9936.6794	0.0142
4	4	1	3	3	0	4	3	8774.6021	0.036	13	1	12	12	2	11	13	12	9293.3185	-0.0041	8	3	5	7	2	5	9	8	9949.4617	-0.0088
						5	4	8774.7308	0.0422							14	13	9293.3185	-0.0014							8	7	9949.4617	0.0591
4	4	0	3	3	1	4	3	8774.7308	-0.0124							12	11	9293.3185	-0.0058							7	6	9949.4617	-0.0263
						5	4	8774.8641	-0.0019	8	2	7	7	1	7	8	7	9503.6857	0.0042	14	1	14	13	0	13	14	13	9968.4700	-0.0008
						3	2	8774.8641	0.0453							7	6	9503.8679	-0.0484							15	14	9968.4700	0.0077
4	4	1	3	3	1	4	3	8774.7308	-0.0068							9	8	9503.8679	-0.0089							13	12	9968.4700	0.0033
						5	4	8774.8641	0.0036	7	3	5	6	2	5	7	6	9527.6749	0.0082	14	1	13	13	2	12	13	12	10116.9886	-0.0075
						3	2	8774.8641	0.0509							8	7	9527.8009	-0.0232							15	14	10116.9886	-0.0038
4	4	0	3	3	0	5	4	8774.7308	0.0365							6	5	9527.8009	-0.0586							14	13	10116.9886	-0.0082
7	2	5	6	1	6	7	6	8988.3472	-0.0100	5	4	2	4	3	1	5	4	9537.3581	0.0309	10	2	8	9	1	8	9	8	10155.1125	-0.0099
						8	7	8988.7026	0.0446							4	3	9537.5356	0.0076							11	10	10155.1126	0.0057
						6	5	8988.7026	-0.0182							6	5	9537.5356	0.0305	13	2	12	12	1	11	12	11	10214.5908	-0.0107
11	2	10	10	1	9	11	10	9149.1186	-0.0440	5	4	1	4	3	2	5	4	9538.5645	-0.0122							14	13	10214.5908	-0.0088
						10	9	9149.1186	-0.0042							4	3	9538.7451	-0.0335							13	12	10214.5908	-0.0433
						12	11	9149.1186	-0.0020							6	5	9538.7451	-0.0104	8	2	6	7	1	7	8	7	10258.7677	-0.0076
9	2	7	8	1	7	10	9	9229.3838	-0.0117	7	3	4	6	2	5	7	6	9562.7812	0.0033							9	8	10259.1032	0.0301
						9	8	9229.3838	0.0656							8	7	9562.9190	-0.0256							7	6	10259.1032	-0.0222
						8	7	9229.3838	-0.0291							6	5	9562.9190	-0.0623	6	4	3	5	3	2	6	5	10297.6346	0.0006
13	0	13	12	1	12	14	13	9234.2158	0.0033	9	1	8	8	0	8	9	8	9574.6846	0.0019							5	4	10297.8586	0.0255
						12	11	9234.2158	-0.0018							8	7	9574.8684	-0.0348							7	6	10297.8586	0.0560
						13	12	9234.2158	-0.0039							10	9	9574.8684	-0.0021	6	4	2	5	3	2	6	5	10297.8586	-0.0275
7	3	5	6	2	4	7	6	9245.7219	0.0636	12	2	11	11	1	10	13	12	9671.6306	-0.0149							5	6	10298.0631	-0.0103
						8	7	9245.7219	-0.0249							11	10	9671.6306	-0.0168							7	6	10298.0631	0.0081
						6	5	9245.7219	-0.0486							12	11	9671.6306	-0.0540	6	4	3	5	3	3	6	5	10302.4138	0.0039

J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res
						5	4	10302.6368	0.0251							9	8	10797.0672	-0.0065							5	4	11172.7016	0.0722
						7	6	10302.6368	0.0561	15	1	14	14	2	13	16	15	10908.6694	0.0269	5	5	1	4	4	1	5	4	11172.7016	0.0668
6	4	2	5	3	3	6	5	10302.6368	-0.0251							15	14	10908.6694	0.0209							4	3	11172.7016	0.0165
						7	6	10302.8307	-0.0023							14	13	10908.6694	0.0237							6	5	11172.7016	-0.0181
						5	4	10302.8307	-0.0333	10	3	8	9	2	7	10	9	10990.3165	0.0027	9	3	7	8	2	7	9	8	11209.7659	-0.0034
8	3	6	7	2	6	8	7	10356.4783	0.0001							11	10	10990.3165	0.0010							8	7	11209.9134	-0.0049
						9	8	10356.6356	0.0183							9	8	10990.3165	-0.0051							10	9	11209.9134	0.0179
						7	6	10356.6356	-0.0096	7	4	4	6	3	3	7	6	11052.5924	-0.0003	10	3	7	9	2	7	10	9	11253.4984	0.0350
8	3	5	7	2	6	8	7	10432.2646	-0.0002							8	7	11052.7379	-0.0004							11	10	11253.4984	-0.0008
						7	6	10432.4266	-0.0228							6	5	11052.7379	-0.0273							9	8	11253.4984	-0.0105
						9	8	10432.4266	0.0072	7	4	3	6	3	3	7	6	11053.5176	0.0038	16	0	16	15	1	15	16	15	11332.8943	0.0043
9	3	7	8	2	6	10	9	10454.6898	-0.0093							8	7	11053.6640	0.0042							17	16	11332.8943	0.0100
						8	7	10454.6898	-0.0193							6	5	11053.6640	-0.0226							15	14	11332.8943	0.0065
						9	8	10454.6898	0.0144	7	4	4	6	3	4	7	6	11066.8134	0.0012	16	1	16	15	0	15	16	15	11345.2173	0.0006
9	2	8	8	1	8	9	8	10532.7738	0.0061							6	5	11066.9772	-0.0133							17	16	11345.2173	0.0069
						8	7	10532.9582	-0.0227							8	7	11066.9772	0.0143							15	14	11345.2173	0.0035
						10	9	10532.9582	0.0092	7	4	3	6	3	4	7	6	11067.7359	0.0026	9	3	6	8	2	7	9	8	11357.1561	-0.0039
9	3	6	8	2	6	10	9	10602.1399	0.0261							8	7	11067.8927	0.0085							8	7	11357.3276	-0.0078
						8	7	10602.1399	0.0135							6	5	11067.8927	-0.0192							10	9	11357.3276	0.0176
15	0	15	14	1	14	16	15	10635.8568	0.0112	11	2	9	10	1	9	11	10	11147.9386	-0.0148	15	2	14	14	1	13	15	14	11377.9994	-0.0055
						15	14	10635.8568	0.0050							10	9	11148.0474	-0.0123							16	15	11377.9994	0.0189
						14	13	10635.8568	0.0073							12	11	11148.0474	0.0021							14	13	11377.9994	0.0169
15	1	15	14	0	14	15	14	10655.7347	0.0012	5	5	0	4	4	1	4	3	11172.7016	0.0163	11	3	9	10	2	8	10	9	11485.0379	0.0093
						16	15	10655.7347	0.0085							5	4	11172.7016	0.0666							11	10	11485.0379	-0.0018
						14	13	10655.7347	0.0047							6	5	11172.7016	-0.0183							12	11	11485.0379	0.0130
14	2	13	13	1	12	13	12	10783.0433	-0.0003	5	5	1	4	4	0	4	3	11172.7016	0.0221	16	1	15	15	2	14	16	15	11673.5809	-0.0340
						15	14	10783.0433	0.0015							5	4	11172.7016	0.0724							17	16	11673.5809	-0.0269
						14	13	10783.0433	-0.0278							6	5	11172.7016	-0.0125							15	14	11673.5809	-0.0296
10	1	9	9	0	9	10	9	10796.8591	-0.0033	5	5	0	4	4	0	4	3	11172.7016	0.0219	8	4	5	7	3	4	8	7	11797.7076	-0.0023
						11	10	10797.0672	0.0214							6	5	11172.7016	-0.0126							9	8	11797.8430	0.0119

J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	
						7	6	11797.8430	-0.0097								16	15	12028.5491	0.0028							6	5	12699.4349	-0.0317
8	4	4	7	3	4	8	7	11800.4558	-0.0006	17	1	17	16	0	16	16	15	12036.1226	-0.0108	7	5	2	6	4	2	7	6	12699.0946	0.0274	
						7	6	11800.5911	-0.0088								17	16	12036.1226	-0.0133							6	5	12699.2451	0.0198
						9	8	11800.5911	0.0128								18	17	12036.1226	-0.0077							8	7	12699.2451	0.0373
8	4	5	7	3	5	8	7	11832.8182	-0.0028	10	3	8	9	2	8	10	9	12090.6699	-0.0179	7	5	2	6	4	3	7	6	12699.2451	-0.0742	
						9	8	11832.9763	0.0248								11	10	12090.8246	0.0195							8	7	12699.4349	-0.0251
						7	6	11832.9763	0.0018								9	8	12090.8246	0.0003							6	5	12699.4349	-0.0427
8	4	4	7	3	5	8	7	11835.5748	0.0072	12	2	10	11	1	10	13	12	12211.3889	-0.0073	10	4	7	9	3	6	10	9	13230.5989	0.0647	
						9	8	11835.7113	0.0126								11	10	12211.3889	-0.0209							11	10	13230.5989	-0.0107
						7	6	11835.7113	-0.0103	10	3	7	9	2	8	10	9	12353.8314	-0.0059							9	8	13230.5989	-0.0236	
11	3	8	10	2	8	11	10	11921.7517	0.0343								11	10	12354.0030	0.0141	10	4	6	9	3	6	9	8	13246.9096	-0.0307
						10	9	11921.7517	-0.0046								9	8	12354.0030	-0.0083							11	10	13246.9096	-0.0176
						12	11	11921.7517	0.0032	9	4	6	8	3	5	8	7	12526.6102	-0.0193							10	9	13246.9096	0.0608	
6	5	2	5	4	2	6	5	11936.1619	-0.0385								10	9	12526.6102	-0.0024	12	1	11	11	0	11	12	11	13295.8323	0.0224
						7	6	11936.3168	-0.0198								8	7	12533.7011	0.0085							11	10	13295.9990	0.0011
						5	4	11936.3168	-0.0278	9	4	5	8	3	5	10	9	12533.7011	0.0085							13	12	13295.9990	0.0217	
6	5	2	5	4	1	6	5	11936.1619	0.0120	9	4	6	8	3	6	9	8	12602.3082	0.0064	10	4	7	9	3	7	11	10	13378.0146	-0.0097	
						5	4	11936.3168	0.0227								8	7	12602.4337	0.0000							10	9	13378.0146	0.0897
						7	6	11936.3168	0.0307								10	9	12602.4337	0.0188							9	8	13378.0146	-0.0252
6	5	1	5	4	1	6	5	11936.1619	0.0101	9	4	5	8	3	6	9	8	12609.3802	0.0001	10	4	6	9	3	7	10	9	13394.2317	-0.0077	
						7	6	11936.3168	0.0289								8	7	12609.5096	-0.0040							9	8	13394.3463	-0.0112
						5	4	11936.3168	0.0209								10	9	12609.5096	0.0149							11	10	13394.3463	0.0046
6	5	1	5	4	2	6	5	11936.1619	-0.0403	12	3	9	11	2	9	11	10	12624.9903	-0.0197	11	3	8	10	2	9	11	10	13438.2930	-0.0151	
						5	4	11936.3168	-0.0296								13	12	12624.9903	-0.0127							12	11	13438.4705	0.0051
						7	6	11936.3168	-0.0216								12	11	12624.9903	0.0186							10	9	13438.4705	-0.0154
12	3	10	11	2	9	11	10	11945.2888	-0.0207	7	5	3	6	4	2	7	6	12699.0946	0.0384	8	5	4	7	4	3	8	7	13460.6787	0.0074	
						12	11	11945.2888	-0.0456								6	5	12699.2451	0.0308							8	7	13460.6787	-0.0399
						13	12	11945.2888	-0.0186								8	7	12699.2451	0.0483							9	8	13460.8645	0.0625
17	0	17	16	1	16	18	17	12028.5491	0.0059	7	5	3	6	4	3	7	6	12699.2451	-0.0633	8	5	3	7	4	3	7	6	13460.8645	-0.0030	
						17	16	12028.5491	0.0008								8	7	12699.4349	-0.0141							9	8	13460.8645	0.0151

J	K _a	K _c	J	K _a	K _c	F	F''	Obs	Res
						7	6	13460.8645	0.0444
8	5	4	7	4	4	8	7	13461.5949	0.0025
						8	7	13461.5949	-0.0448
						9	8	13461.7719	0.0011
8	5	4	7	4	4	9	8	13461.7719	0.0486
						7	6	13461.7719	-0.0169
						7	6	13461.7719	0.0304
6	6	0	5	5	1	6	5	13570.5202	-0.0299
						5	4	13570.6291	0.0430
						7	6	13570.6291	0.0166
6	6	0	5	5	0	6	5	13570.5202	-0.0297
						5	4	13570.6291	0.0432
						7	6	13570.6291	0.0168
6	6	1	5	5	0	6	5	13570.5202	-0.0297
						5	4	13570.6291	0.0432
						7	6	13570.6291	0.0168
6	6	1	5	5	1	6	5	13570.5202	-0.0299
						5	4	13570.6291	0.0430
						7	6	13570.6291	0.0166
11	4	7	10	3	7	10	9	13934.3757	-0.0023
						12	11	13934.3757	0.0077
12	3	10	11	2	10	12	11	13944.1225	-0.0026
						11	10	13944.2289	-0.0175
						13	12	13944.2289	-0.0032
13	5	8	13	4	9	12	12	7138.3616	-0.0233
						14	14	7138.3616	-0.0161
12	5	8	12	4	8	11	11	7205.0791	-0.0058
						13	13	7205.0791	0.0037
12	5	7	12	4	8	12	12	7208.0902	-0.0121
						11	11	7208.2270	0.0006

J	K _a	K _c	J	K _a	K _c	F	F''	Obs	Res
						13	13	7208.2270	0.0102
13	5	9	13	4	10	14	14	7254.7222	-0.0003
						12	12	7254.7222	-0.0084
11	5	6	11	4	7	11	11	7257.2083	0.0058
						10	10	7257.3425	-0.0126
						12	12	7257.3425	0.0001
12	5	8	12	4	9	12	12	7272.1903	-0.0101
						11	11	7272.3280	-0.0048
						13	13	7272.3280	0.0054
11	5	7	11	4	8	10	10	7290.4013	-0.0333
						12	12	7290.4013	-0.0201
10	5	5	10	4	6	10	10	7291.1560	-0.0126
						9	9	7291.3373	-0.0199
						11	11	7291.3373	-0.0027
10	5	6	10	4	7	10	10	7306.9802	-0.0098
						11	11	7307.1649	0.0006
						9	9	7307.1649	-0.0168
10	5	5	10	4	7	10	10	7307.4892	0.0059
						11	11	7307.6686	0.0110
						9	9	7307.6686	-0.0064
9	5	5	9	4	5	9	9	7314.1646	-0.0104
						8	8	7314.4185	0.0078
						10	10	7314.4185	0.0315
9	5	4	9	4	5	9	9	7314.3212	-0.0191
						8	8	7314.582	0.0060
						10	10	7314.582	0.0297
9	5	5	9	4	6	9	9	7321.2426	-0.0108
						8	8	7321.4738	-0.0168
						10	10	7321.4738	0.0070
9	5	4	9	4	6	8	8	7321.6636	0.0076

J	K _a	K _c	J	K _a	K _c	F	F''	Obs	Res
						10	10	7321.6636	0.0315
5	5	1	5	4	1	5	5	7350.5989	0.0226
						6	6	7351.2276	0.0209
						4	4	7351.3666	0.0317
5	5	1	5	4	2	5	5	7350.5989	-0.0279
						6	6	7351.2276	-0.0296
						4	4	7351.3666	-0.0189
5	5	0	5	4	1	5	5	7350.5989	0.0224
						6	6	7351.2276	0.0208
						4	4	7351.3666	0.0315
5	5	0	5	4	2	5	5	7350.5989	-0.0281
						6	6	7351.2276	-0.0297
						4	4	7351.3666	-0.019
7	6	1	7	5	2	7	7	8981.8041	0.0083
						8	8	8982.2305	0.0144
						6	6	8982.2305	-0.0461
7	6	1	7	5	3	7	7	8981.8041	-0.0026
						8	8	8982.2305	0.0034
						6	6	8982.2305	-0.0570
7	6	2	7	5	2	7	7	8981.8041	0.0083
						8	8	8982.2305	0.0145
						6	6	8982.2305	-0.0460
7	6	2	7	5	3	7	7	8981.8041	-0.0025
						8	8	8982.2305	0.0035
						6	6	8982.2305	-0.0570
6	6	1	6	5	1	6	6	8984.9828	0.0081
						7	7	8985.5486	0.0173
						5	5	8985.5486	-0.0765
6	6	1	6	5	2	6	6	8984.9828	0.0063
						7	7	8985.5486	0.0155

J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res
						5	5	8985.5486	-0.0783
6	6	0	6	5	1	6	6	8984.9828	0.0081
						5	5	8985.5486	-0.0765
						7	7	8985.5486	0.0173
6	6	0	6	5	2	6	6	8984.9828	0.0063
						5	5	8985.5486	-0.0783
						7	7	8985.5486	0.0155
11	7	4	11	6	6	11	11	10599.1931	-0.0293
						12	12	10599.4186	-0.0174
						10	10	10599.4186	-0.0369
11	7	4	11	6	5	11	11	10599.1931	-0.0009
						10	10	10599.4186	-0.0085
						12	12	10599.4186	0.0109
11	7	5	11	6	6	11	11	10599.1931	-0.0289
						10	10	10599.4186	-0.0365
						12	12	10599.4186	-0.0170
11	7	5	11	6	5	11	11	10599.1931	-0.0005
						10	10	10599.4186	-0.0082
						12	12	10599.4186	0.0112
10	7	3	10	6	4	10	10	10606.7172	0.0060
						9	9	10606.9872	-0.0058
						11	11	10606.9872	0.0199
10	7	3	10	6	5	10	10	10606.7172	-0.0023
						11	11	10606.9872	0.0115
						9	9	10606.9872	-0.0141
10	7	4	10	6	4	10	10	10606.7172	0.0061
						9	9	10606.9872	-0.0057
						11	11	10606.9872	0.0200
10	7	4	10	6	5	10	10	10606.7172	-0.0022
						11	11	10606.9872	0.0116

J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res
						9	9	10606.9872	-0.014
9	7	2	9	6	3	9	9	10612.3329	0.0059
						10	10	10612.6646	0.0253
						8	8	10612.6646	-0.0096
9	7	2	9	6	4	9	9	10612.3329	0.0038
						10	10	10612.6646	0.0232
						8	8	10612.6646	-0.0117
9	7	3	9	6	3	9	9	10612.3329	0.0059
						8	8	10612.6646	-0.0096
						10	10	10612.6646	0.0253
9	7	3	9	6	4	9	9	10612.3329	0.0038
						8	8	10612.6646	-0.0117
						10	10	10612.6646	0.0232
7	7	0	7	6	1	7	7	10619.2166	0.0137
						6	6	10619.7264	-0.0457
						8	8	10619.7264	0.0259
7	7	0	7	6	2	7	7	10619.2166	0.0136
						8	8	10619.7264	0.0258
						6	6	10619.7264	-0.0458
7	7	1	7	6	1	7	7	10619.2166	0.0137
						6	6	10619.7264	-0.0457
						8	8	10619.7264	0.0259
7	7	1	7	6	2	7	7	10619.2166	0.0136
						6	6	10619.7264	-0.0458
						8	8	10619.7264	0.0258

Table S4. Observed frequencies and residuals (MHz) for $+ac/+ac/+sc$ 2 for $J_{K_a'K_c'} \leftarrow J_{K_a''K_c''}$ and $F' \leftarrow F''$ transitions.

J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res	J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res	J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res
7	2	6	6	1	5	6	5	7021.6049	0.0190							6	5	7661.3157	-0.0222							7	6	8096.5694	0.0332
						8	7	7021.6049	0.0159	6	2	5	5	1	5	6	5	7688.6738	0.0018	11	1	11	10	0	10	12	11	8101.4138	0.0077
						7	6	7021.6049	-0.0688							7	6	7688.9879	0.0456							11	10	8101.4138	-0.0106
4	3	2	3	2	1	4	3	7031.1347	-0.0041							5	4	7688.9879	-0.0236							10	9	8101.4138	0.0021
						5	4	7031.2945	-0.0034	7	2	5	6	1	5	7	6	7706.1053	0.0657	6	3	4	5	2	3	5	4	8499.2031	-0.0225
						3	2	7031.2945	-0.0407							6	5	7706.1053	-0.0300							7	6	8499.2031	-0.0045
4	3	1	3	2	1	4	3	7033.3914	-0.0069							8	7	7706.1053	-0.0099							6	5	8499.2031	0.0540
						5	4	7033.5519	-0.0077	5	3	3	4	2	2	5	4	7784.6297	0.0030	10	2	9	9	1	8	9	8	8593.2274	0.0283
						3	2	7033.5519	-0.0457							4	3	7784.7485	-0.0197							10	9	8593.2274	-0.0575
4	3	2	3	2	2	4	3	7063.4255	-0.0021							6	5	7784.7485	0.0107							11	10	8593.2274	0.0253
						3	2	7063.6455	-0.0296	5	3	2	4	2	2	5	4	7793.6068	0.0031	4	4	1	3	3	0	4	3	8600.1028	0.0094
						5	4	7063.6455	0.0209							4	3	7793.7154	-0.0375							5	4	8600.1851	-0.0010
4	3	1	3	2	2	4	3	7065.6852	-0.0018							6	5	7793.7156	-0.0055							3	2	8600.1859	0.0365
						5	4	7065.8929	0.0066	5	3	3	4	2	3	5	4	7879.7243	0.0010	4	4	0	3	3	1	4	3	8600.4419	0.0114
						3	2	7065.8929	-0.0445							6	5	7879.9117	0.0101							3	2	8600.4419	-0.0453
10	1	9	9	2	8	9	8	7141.2372	-0.0115							4	3	7879.9117	-0.0377							5	4	8600.5457	0.0218
						10	9	7141.2372	0.0158	5	3	2	4	2	3	5	4	7888.7013	0.0010	8	2	6	7	1	6	8	7	8602.4003	-0.0033
						11	10	7141.2372	-0.0036							4	5	7888.8977	0.0190							9	8	8602.5109	0.0150
10	0	10	9	1	9	9	8	7306.9802	-0.0001							4	3	7888.8977	-0.0362							7	6	8602.5109	-0.0039
						11	10	7306.9802	0.0075	11	0	11	10	1	10	11	10	8036.8568	-0.0081	6	3	4	5	2	4	6	5	8713.6755	-0.0012
						10	9	7306.9802	-0.0018							10	9	8036.8568	-0.0048							7	6	8713.8262	-0.0091
10	1	10	9	0	9	9	8	7412.4976	-0.0011							12	11	8036.8568	0.0015							5	4	8713.8262	-0.0474
						10	9	7412.4976	-0.0189	11	1	10	10	2	9	10	9	8057.0674	-0.0135	7	2	6	6	1	6	7	6	8720.9436	0.0041
						11	10	7412.4976	0.0050							12	11	8057.0674	-0.0073							6	5	8721.2261	-0.0174
8	2	7	7	1	6	7	6	7553.8429	0.0141							11	10	8057.0674	0.0050							8	7	8721.2261	0.0361
						9	8	7553.8429	0.0100	9	2	8	8	1	7	10	9	8073.0850	0.0119	6	3	3	5	2	4	6	5	8740.2799	-0.0022
22	3	19	21	5	16	23	22	7643.8373	0.0130							9	8	8073.0850	-0.0781							7	6	8740.4442	-0.0097
						22	21	7643.9586	-0.0140							8	7	8073.0850	0.0158	12	0	12	11	1	11	11	10	8759.1525	0.0001
7	1	6	6	0	6	7	6	7661.0103	-0.0007	6	2	4	5	1	5	6	5	8096.1296	-0.0042							13	12	8759.1525	0.0054
						8	7	7661.3157	0.0335							5	4	8096.5694	-0.0583							12	11	8759.1525	-0.0040

J	K _a	K _c	J''	K _a ''	K _c ''	F	F''	Obs	Res	J	K _a	K _c	J''	K _a ''	K _c ''	F	F''	Obs	Res	J	K _a	K _c	J''	K _a ''	K _c ''	F	F''	Obs	Res
12	1	12	11	0	11	13	12	8797.9796	0.0102	13	1	13	12	0	12	13	12	9499.5727	-0.0107	6	4	3	5	3	2	6	5	10180.589	-0.0081
						12	11	8797.9796	-0.0041							12	11	9499.5727	-0.0034							5	6	10180.7391	0.0026
						11	10	8797.9796	0.0053							14	13	9499.5727	0.0009							5	5	10180.7391	0.0338
12	1	11	11	2	10	12	11	8929.1757	-0.0013	9	2	7	8	1	7	9	8	9570.3744	-0.0060	6	4	2	5	3	2	6	5	10181.1869	-0.0076
						13	12	8929.1757	-0.0060							8	7	9570.5126	0.0028							5	4	10181.3286	-0.0119
						11	10	8929.1757	-0.0108							10	9	9570.5126	0.0214							7	6	10181.3286	0.0101
11	2	10	10	1	9	10	9	9128.2228	0.0340	7	3	5	6	2	5	7	6	9570.7917	0.0110	6	4	3	5	3	3	6	5	10189.5660	-0.0082
						12	11	9128.2228	0.0321							6	5	9570.9213	-0.0351							7	6	10189.7137	0.0096
						11	10	9128.2228	-0.0396							8	7	9570.9213	-0.0042							5	4	10189.7137	-0.0135
7	3	5	6	2	4	7	6	9163.3456	0.0268	7	3	4	6	2	5	7	6	9635.9779	0.0036	6	4	2	5	3	3	6	5	10190.1678	-0.0037
						8	7	9163.3456	0.0139							6	5	9636.1342	-0.0436							7	6	10190.3227	0.0207
						6	5	9163.3456	0.0054							8	7	9636.1342	-0.0092							5	4	10190.3227	-0.0024
5	4	2	4	3	1	5	4	9392.4796	-0.0082	12	2	11	11	1	10	11	10	9688.8168	0.0244	14	0	14	13	1	13	13	12	10190.8758	0.0036
						4	3	9392.6313	-0.0065							12	11	9688.8168	-0.0355							15	14	10190.8758	0.0075
						6	5	9392.6313	0.0099							13	12	9688.8168	0.0237							14	13	10190.8758	-0.0005
5	4	1	4	3	1	5	4	9392.6313	0.0234	13	1	12	12	2	11	14	13	9759.9459	0.0042	14	1	14	13	0	13	14	13	10204.3824	-0.0017
						4	3	9392.7676	0.0097							13	12	9759.9459	0.0024							15	14	10204.3824	0.0080
						6	5	9392.7676	0.0262							12	11	9759.9459	0.0005							13	12	10204.3824	0.0041
5	4	2	4	3	2	5	4	9394.7300	-0.0173	8	3	6	7	2	5	7	6	9771.7035	0.0210	13	2	12	12	1	11	12	11	10280.1152	0.0024
						4	3	9394.8641	-0.0361							9	8	9771.7035	0.0235							14	13	10280.1152	0.0025
						6	5	9394.8641	-0.0190							8	7	9771.7035	-0.0001							13	12	10280.1152	-0.0447
5	4	1	4	3	2	5	4	9394.8641	-0.0032	8	2	7	7	1	7	8	7	9789.9622	0.0126	9	3	7	8	2	6	8	7	10325.2290	0.0136
						6	5	9395.0227	0.0195							7	6	9790.1922	-0.0362							10	9	10325.2290	0.0124
						4	3	9395.0227	0.0024							9	8	9790.1922	0.0068							9	8	10325.2290	-0.0384
7	2	5	6	1	6	7	6	9405.3013	-0.0040	8	3	5	7	2	5	7	6	9910.7830	0.0078	8	3	6	7	2	6	8	7	10456.0678	-0.0016
						6	5	9405.7681	-0.0249							8	7	9910.7830	0.0312							7	6	10456.2199	-0.0120
						8	7	9405.7681	0.0517							9	8	9910.7830	0.0152							9	8	10456.2199	0.0136
13	0	13	12	1	12	12	11	9476.5423	-0.0049	9	1	8	8	0	8	9	8	10166.9792	0.0047	14	1	13	13	2	12	15	14	10555.7529	0.0150
						13	12	9476.5423	-0.0092							8	7	10167.2414	-0.0375							13	12	10555.7529	0.0121
						14	13	9476.5423	-0.0003							10	9	10167.2414	0.0024							14	13	10555.7529	0.0086

J'	K _a '	K _c '	J''	K _a ''	K _c ''	F'	F''	Obs	Res
8	3	5	7	2	6	8	7	10595.1175	-0.0001
						7	6	10595.2972	-0.0275
						9	8	10595.2972	0.0030
15	0	15	14	1	14	16	15	10903.3128	0.0015
						14	13	10903.3128	-0.0019
						15	14	10903.3128	-0.0058
5	5	1	4	4	0	6	5	10944.1852	-0.0085
						5	4	10944.1852	0.0560
						4	3	10944.1852	0.0181
7	4	4	6	3	3	7	6	10959.3697	-0.0051
						8	7	10959.5000	0.0234
						6	5	10959.5000	0.0048
7	4	3	6	3	3	7	6	10961.5529	0.0016
						6	5	10961.6810	0.0081
						8	7	10961.6810	0.0269
7	4	4	6	3	4	7	6	10985.9716	-0.0086
						8	7	10986.1214	0.0261
						6	5	10986.1214	0.0053
7	4	3	6	3	4	7	6	10988.1506	-0.0060
						8	7	10988.2992	0.0264
						6	5	10988.2992	0.0054
9	3	6	8	2	7	9	8	11639.4808	-0.0071
						8	7	11639.6889	-0.0194
						10	9	11639.6889	0.0090
8	4	5	7	3	4	9	8	11721.0318	-0.0048
						8	7	11721.0318	0.0719
						7	8	11721.0318	0.0152
8	4	4	7	3	4	7	6	11727.4988	-0.0208
						8	7	11727.4988	0.0727
						9	8	11727.4988	-0.0065

J'	K _a '	K _c '	J''	K _a ''	K _c ''	F'	F''	Obs	Res
6	5	2	5	4	1	7	6	11737.9623	0.0025
						6	5	11737.9623	0.1055
						5	4	11737.9623	-0.0032
8	4	5	7	3	5	8	7	11786.1493	-0.0043
						9	8	11786.2796	0.0249
						7	6	11786.2796	0.0074
8	4	4	7	3	5	8	7	11792.6148	-0.0049
						9	8	11792.7468	0.0236
						7	6	11792.7468	0.0057
7	5	3	6	4	2	7	6	12530.5284	-0.0284
						8	7	12530.6311	-0.0314
						6	5	12530.6311	-0.0444
7	5	2	6	4	3	7	6	12531.1905	0.0035
						8	7	12531.3167	0.0236
						6	5	12531.3167	0.0106
8	5	4	7	4	3	8	7	13321.0594	-0.0150
						7	6	13321.1628	-0.0221
						9	8	13321.1628	-0.0088
8	5	3	7	4	4	8	7	13323.3645	-0.0275
						7	6	13323.4911	-0.0126
						9	8	13323.4911	0.0007

Table S5. Observed frequencies and residuals (MHz) for $+sc/-ac/+sc$ 3 for $J_{K_a K_c}' \leftarrow J_{K_a K_c}''$ and $F' \leftarrow F''$ transitions.

J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res	J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res	J'	K_a'	K_c'	J''	K_a''	K_c''	F'	F''	Obs	Res	
6	2	4	5	1	4	5	4	7019.1823	0.0111							11	10	7971.1690	0.0077							6	5	8828.1072	0.0040	
						7	6	7019.1823	-0.0085	8	2	7	7	1	6	9	8	8016.8051	-0.0082		10	2	9	9	1	8	11	10	9087.4705	0.0292
						6	5	7019.3304	0.0066							7	6	8016.8051	0.0445							10	9	9087.8741	0.0025	
10	1	10	9	0	9	9	8	7334.7758	-0.0059							8	7	8017.2565	-0.0003		6	3	4	5	2	3	5	4	9090.2098	-0.0060
						11	10	7334.7758	-0.0098	5	3	2	4	2	2	5	4	8376.9805	-0.0049							7	6	9090.2098	0.0029	
						10	9	7334.9513	-0.0044							4	3	8377.1038	-0.0132							6	5	9090.2098	0.0151	
7	2	6	6	1	5	6	5	7453.3991	0.0414							6	5	8377.1038	0.0146		6	3	3	5	2	3	5	4	9095.2121	0.0061
						8	7	7453.3991	-0.0182	12	0	12	11	1	11	13	12	8394.3640	0.0206							7	6	9095.2121	0.0174	
						7	6	7453.8583	0.0065							11	10	8394.3640	0.0082							6	5	9095.2121	0.0437	
4	3	2	3	2	1	4	3	7645.8035	0.0057							12	11	8394.3640	0.0427		13	0	13	12	1	12	14	13	9116.1606	-0.0113
						3	2	7645.9537	-0.0511	5	3	3	4	2	3	5	4	8408.6986	0.0047							13	12	9116.1606	-0.0030	
						5	4	7645.9537	-0.0141							6	5	8408.9394	0.0185							12	11	9116.1606	-0.0210	
4	3	1	3	2	1	4	3	7646.2234	0.0098							4	3	8408.9394	-0.0417		6	3	4	5	2	4	6	5	9167.3095	0.0001
						5	4	7646.3742	-0.0118	5	3	2	4	2	3	5	4	8410.3639	0.0078							7	6	9167.5344	0.0125	
						3	2	7646.3742	-0.0494							4	3	8410.6104	-0.0408							5	4	9167.5344	-0.0371	
4	3	1	3	2	2	4	3	7657.3885	0.0102							6	5	8410.6104	0.0208		6	3	3	5	2	4	6	5	9172.2825	-0.0004
						4	4	7657.3885	0.0100	8	2	6	7	1	6	9	8	8444.9634	0.0037							7	6	9172.5020	-0.0076	
						5	4	7657.6437	0.0218							7	6	8444.9634	0.0006							5	4	9172.5020	-0.0597	
						3	2	7657.6437	-0.0407							8	7	8444.9634	0.0031		9	2	7	8	1	7	8	7	9203.0914	-0.0211
11	0	11	10	1	10	10	9	7661.6013	-0.0036							8	7	8560.2435	0.0602							9	8	9203.0914	0.0649	
						12	11	7661.6013	0.0126							10	9	8560.2435	0.0139							10	9	9203.0914	-0.0096	
						11	10	7661.6013	0.0545							9	8	8560.6692	-0.0022		13	1	13	12	0	12	12	11	9276.3505	0.0084
7	2	5	6	1	5	6	5	7719.7079	0.0167							7	6	8561.0019	-0.0054							13	12	9276.3505	-0.0645	
						8	7	7719.7079	0.0094							8	7	8561.6424	-0.0052							14	13	9276.3505	0.0113	
						7	6	7719.7079	-0.0626							6	5	8561.7837	0.0140		14	1	13	13	2	12	14	13	9521.4838	0.0074
6	2	4	5	1	5	6	5	7811.8049	-0.0126							13	12	8632.8084	0.0265							13	12	9521.6840	0.0054	
						7	6	7812.7570	0.0018							12	11	8633.0313	0.0001							15	14	9521.6840	0.0232	
						5	4	7812.9579	0.0042							14	13	8633.0313	0.0227		11	2	10	10	1	9	12	11	9603.3568	0.0085
11	1	11	10	0	10	10	9	7971.0229	-0.0068							7	6	8826.9133	-0.0128							11	10	9603.7453	-0.0128	
						12	11	7971.0229	-0.0073							8	7	8827.9281	-0.0008		7	3	5	6	2	4	7	6	9783.7215	-0.0526

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res
						6	5	9783.7215	0.0249
						8	7	9783.7215	0.0196
7	3	4	6	2	4	7	6	9796.0879	-0.0587
						6	5	9796.0879	-0.0113
						8	7	9796.0879	-0.0128
14	0	14	13	1	13	13	12	9829.3846	0.0014
						15	14	9829.3846	0.0093
						14	13	9829.3846	0.0085
8	2	6	7	1	7	8	7	9915.6854	0.0006
						9	8	9916.7629	0.0069
						7	6	9916.8949	-0.0187
14	1	14	13	0	13	15	14	9942.3091	0.0023
						13	12	9942.3091	-0.0011
						14	13	9942.3091	-0.0557
7	3	4	6	2	5	7	6	9947.7583	-0.0011
						8	7	9947.9781	-0.0150
12	2	11	11	1	10	13	12	10113.8936	-0.0077
						11	10	10113.8936	0.0211
5	4	2	4	3	1	5	4	10266.8130	0.0047
						6	5	10266.9817	0.0174
						4	3	10266.9817	-0.0012
5	4	1	4	3	2	5	4	10267.2355	-0.0003
						6	5	10267.4059	0.0116
						4	3	10267.4059	-0.0076
7	6	1	7	5	2	7	7	10288.7982	0.0042
						8	8	10289.1366	-0.0296
						6	6	10289.2461	0.0261
6	6	0	6	5	1	6	6	10290.4027	0.0020
						7	7	10290.9468	0.0506
						5	5	10290.9468	-0.0329

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res
9	2	8	8	1	8	9	8	10440.7085	-0.0159
						8	7	10441.3764	-0.0540
						10	9	10441.3764	0.0332
8	3	6	7	2	5	9	8	10449.5572	-0.0089
						7	6	10449.5572	0.0063
						8	7	10449.7195	0.0015
8	3	5	7	2	5	7	6	10476.6073	0.0030
						9	8	10476.6073	-0.0069
						8	7	10476.7276	0.0062
15	0	15	14	1	14	16	15	10536.0036	0.0112
						15	14	10536.0036	0.0046
						14	13	10536.0036	0.0047
15	1	15	14	0	14	16	15	10614.7612	-0.0204
						14	13	10614.7612	-0.0242
						15	14	10614.8370	0.0103
8	3	6	7	2	6	8	7	10715.6325	-0.0042
						7	6	10715.8291	-0.0552
						9	8	10715.8291	-0.0182
8	3	5	7	2	6	8	7	10742.6397	-0.0003
						9	8	10742.8707	-0.0246
6	4	3	5	3	2	6	5	11008.9214	-0.0006
						5	4	11009.0580	-0.0325
						7	6	11009.0580	-0.0075
6	4	2	5	3	3	6	5	11010.6502	0.0070
						7	6	11010.8047	0.0113
						5	4	11010.8047	-0.0151
9	3	7	8	2	6	10	9	11082.8205	-0.0129
						8	7	11082.8205	0.0095
						9	8	11083.0542	-0.0025
9	3	6	8	2	6	10	9	11136.2620	-0.0113

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res	
9	3	6	8	2	6	8	7	11136.2620	0.0033	
						9	8	11136.4239	-0.0023	
14	2	13	13	1	12	15	14	11145.6768	-0.0225	
							12	11145.6768	-0.0038	
							13	11145.9724	-0.0309	
16	0	16	15	1	15	16	15	11237.7103	-0.0065	
							14	11237.7103	-0.0021	
							16	11237.7103	0.0034	
10	2	9	9	1	9	10	9	11418.5007	0.0005	
						11	10	11419.1387	0.0285	
						9	8	11419.1387	-0.0476	
9	3	6	8	2	7	9	8	11564.1284	-0.0013	
						10	9	11564.3981	-0.0217	
7	4	4	6	3	3	7	6	11748.8368	-0.0073	
							6	5	11748.9768	-0.0053
							8	7	11748.9768	0.0157
7	4	3	6	3	4	7	6	11754.0200	-0.0135	
							8	7	11754.1776	0.0124
							6	5	11754.1776	-0.0111
5	5	1	4	4	0	6	5	12138.6670	-0.0125	
							4	3	12138.6670	0.0192
							5	4	12138.6670	0.0632
8	4	5	7	3	4	8	7	12484.8763	0.0783	
							7	6	12484.8763	-0.0234
							9	8	12484.8763	-0.0079
8	4	4	7	3	4	8	7	12485.5285	0.0849	
							7	6	12485.5285	-0.0185
							9	8	12485.5285	-0.0027
8	4	4	7	3	5	8	7	12497.8011	-0.0150	
							7	6	12497.9377	-0.0120

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res
						9	8	12497.9377	0.0075
6	5	2	5	4	1	6	5	12882.0287	0.0001
						7	6	12882.1694	0.0201
						5	4	12882.1694	0.0137
9	4	6	8	3	5	8	7	13214.2707	-0.0021
						9	8	13214.2707	0.0614
						10	9	13214.2707	0.0080
9	4	5	8	3	5	10	9	13215.9521	0.0138
						8	7	13215.9521	0.0032
						9	8	13215.9521	0.0702
9	4	6	8	3	6	10	9	13241.3201	0.0094
						8	7	13241.3201	-0.0062
						9	8	13241.3201	0.1074
9	4	5	8	3	6	9	8	13242.9891	0.1038
						8	7	13242.9891	-0.0132
						10	9	13242.9891	0.0027
7	5	3	6	4	2	7	6	13625.1576	-0.0163
						8	7	13625.2859	-0.0113
						6	5	13625.2859	-0.0261
10	4	7	9	3	6	9	8	13933.5421	-0.0154
						11	10	13933.5421	-0.0100
						10	9	13933.5421	0.0077
10	4	6	9	3	6	10	9	13937.4342	0.0172
						9	8	13937.4342	-0.0122
						11	10	13937.4342	-0.0062
10	4	6	9	3	7	9	8	13990.8426	-0.0516
						11	10	13990.8426	-0.0377
						10	9	13990.8426	0.0562
4	3	2	3	2	2	4	3	7656.9696	0.0071
						5	4	7657.2287	0.0250

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res
						3	3	7657.2287	-0.0370
6	2	5	5	1	5	6	5	7660.1949	-0.0099
12	5	8	12	4	9	11	11	8371.2640	-0.0266
						13	13	8371.2640	-0.0188
						12	12	8371.2640	0.0714
5	3	3	4	2	2	5	4	8375.3286	0.0053
						6	5	8375.4261	0.0056
						4	3	8375.4261	-0.0209
4	4	1	3	3	0	4	3	9523.7176	0.0297
						3	2	9523.7176	-0.0352
						5	4	9523.7176	-0.0792
4	4	0	3	3	1	5	4	9523.8739	0.0158
						3	2	9523.8739	0.0596
						4	3	9523.7176	-0.0308
4	4	1	3	3	1	4	3	9523.7176	-0.0295
						3	2	9523.8739	0.0609
						5	4	9523.8739	0.0171
4	4	0	3	3	0	4	3	9523.7176	0.0284
						3	2	9523.7176	-0.0365
12	1	12	11	0	11	13	12	8618.6531	-0.0061
						11	10	8618.6531	-0.0077

Table S6. Observed frequencies and residuals (MHz) for $+ac/+ac/-sc$ 4 for $J'_{K'_a K'_c} \leftarrow J''_{K''_a K''_c}$ and $F' \leftarrow F''$ transitions.

J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Obs	Res	J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Obs	Res	J'	K'_a	K'_c	J''	K''_a	K''_c	F'	F''	Obs	Res
7	2	6	6	1	5	8	7	7050.2332	-0.0081							4	3	7687.5244	-0.0292	6	3	4	5	2	3	6	5	8344.0585	0.0580
						6	5	7050.2332	0.0058	5	3	2	4	2	3	5	4	7694.6308	0.0058							5	4	8344.0585	-0.0062
						7	6	7050.4079	-0.0011							4	3	7694.9007	-0.0301							7	6	8344.0585	0.0107
10	1	9	9	2	8	10	9	7293.6257	0.0353							6	5	7694.9007	0.0337	6	3	3	5	2	3	5	4	8365.9089	-0.0349
						11	10	7293.6257	-0.0209	18	4	15	17	5	12	17	16	7903.0844	0.0046							7	6	8365.9089	-0.0143
10	0	10	9	1	9	9	8	7500.1466	-0.0108							19	18	7903.0844	-0.0022							6	5	8365.9089	0.0539
						11	10	7500.1466	0.0000	6	2	4	5	1	5	6	5	7904.227	0.0053	6	3	4	5	2	4	6	5	8528.6285	0.0033
						10	9	7500.1466	-0.0108							7	6	7904.86	0.0140							7	6	8528.8434	0.0071
6	2	5	5	1	5	6	5	7552.3151	-0.0048							5	4	7905.0109	0.0273							5	4	8528.8434	-0.0431
						7	6	7552.7333	0.0064	7	6	1	7	5	2	7	7	7961.8129	-0.0163	8	2	6	7	1	6	8	7	8534.1607	0.0034
						5	4	7552.8366	0.0087							6	6	7962.2366	-0.0486							9	8	8534.2795	-0.0083
7	1	6	6	0	6	8	7	7558.6325	0.0355							8	8	7962.2366	0.0088							7	6	8534.2795	-0.0333
						6	5	7558.6325	-0.0497	6	6	0	6	5	1	6	6	7965.9364	-0.0067	6	3	3	5	2	4	6	5	8550.4848	0.0051
5	3	3	4	2	2	5	4	7605.6407	0.0039							7	7	7966.4939	0.0207							5	4	8550.7331	-0.0325
						6	5	7605.7523	-0.0067							5	5	7966.4939	-0.0687							7	6	8550.7331	0.0213
						4	3	7605.7523	-0.0403	9	2	8	8	1	7	10	9	8178.5058	-0.0107	7	2	6	6	1	6	7	6	8572.9708	0.0022
10	1	10	9	0	9	11	10	7609.4834	-0.0225							8	7	8178.5058	0.0006							8	7	8573.3636	0.0122
						10	9	7609.4834	-0.0639							9	8	8178.6817	-0.0023							6	5	8573.3636	-0.0668
						9	8	7609.4834	-0.0301	11	0	11	10	1	10	12	11	8252.0744	0.0041	14	2	12	13	3	10	14	13	8721.2261	-0.0064
5	3	2	4	2	2	5	4	7613.007	0.0050							10	9	8252.0744	-0.0046	10	2	9	9	1	8	11	10	8734.5978	-0.0086
						6	5	7613.1221	-0.0121							11	10	8252.0744	-0.0087							9	8	8734.5978	0.0002
						4	3	7613.1221	-0.0477	4	4	1	3	3	0	3	2	8299.0663	-0.0511							10	9	8734.7622	0.0031
8	2	7	7	1	6	9	8	7621.0254	-0.0100							4	3	8299.0663	0.0185	12	0	12	11	1	11	11	10	8996.5061	-0.0003
						7	6	7621.0254	0.0032							5	4	8299.1995	0.0353							13	12	8996.5061	0.0070
						8	7	7621.206	-0.0026	4	4	0	3	3	1	3	2	8299.3443	-0.0500							12	11	8996.5061	-0.0063
7	2	5	6	1	5	7	6	7643.8373	-0.0076							4	3	8299.3443	0.0209	12	1	12	11	0	11	12	11	9037.9663	-0.0148
						8	7	7643.9586	0.0164							5	4	8299.4756	0.0349							11	10	9037.9663	0.0028
						6	5	7643.9586	-0.0078	11	1	11	10	0	10	12	11	8319.9826	-0.0006							13	12	9037.9663	0.0091
5	3	3	4	2	3	5	4	7687.2702	0.0104							11	10	8319.9826	-0.0317	7	3	5	6	2	4	6	5	9038.2264	0.0057
						4	5	7687.5244	0.0407							10	9	8319.9826	-0.0076							8	7	9038.2264	0.0103

J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res	J	K _a	K _c	J	K _a	K _c	F	F	Obs	Res
						7	6	9038.2264	-0.0090							14	13	9736.0284	0.0216							9	8	10278.0021	0.0073
7	3	4	6	2	4	6	5	9091.9146	-0.0014	13	1	13	12	0	12	14	13	9760.985	0.0183	8	3	5	7	2	6	8	7	10391.0534	0.0029
						7	6	9091.9146	0.0278							12	11	9760.985	0.0126							9	8	10391.2825	-0.0230
						8	7	9091.9146	0.0086							13	12	9760.985	-0.0007							7	6	10391.2825	-0.0659
5	4	2	4	3	1	5	4	9104.5555	0.0081	8	3	5	7	2	5	8	7	9797.6115	-0.0029	14	0	14	13	1	13	13	12	10472.3964	0.0162
						4	3	9104.7365	0.0023							9	8	9797.6115	0.0067							15	14	10472.3964	0.0217
						6	5	9104.7365	0.0225							7	6	9797.6115	0.0021							14	13	10472.3964	0.0094
5	4	1	4	3	2	5	4	9106.5083	0.0146	12	2	11	11	1	10	13	12	9890.1848	-0.0052	14	1	14	13	0	13	14	13	10487.2524	0.0059
						4	3	9106.6757	-0.0096							11	10	9890.1848	-0.0014							15	14	10487.2524	0.0216
						6	5	9106.6757	0.0115							12	11	9890.3108	0.0122							13	12	10487.2524	0.0165
12	1	11	11	2	10	12	11	9111.7313	0.0130	6	4	3	5	3	2	6	5	9906.498	0.0034	9	3	6	8	2	6	10	9	10498.1744	0.0080
						13	12	9111.7313	-0.0094							7	6	9906.6642	0.0168							8	7	10498.1744	0.0053
						11	10	9111.7313	-0.0171							5	4	9906.6642	-0.0100							9	8	10498.1744	-0.0101
11	2	10	10	1	9	10	9	9301.7373	-0.0044	6	4	2	5	3	2	6	5	9906.9728	0.0093	13	2	12	12	1	11	12	11	10505.6573	0.0196
						12	11	9301.7373	-0.0107							7	6	9907.1321	0.0151							14	13	10505.6573	0.0178
						11	10	9301.8775	-0.0023							5	4	9907.1321	-0.0118	5	5	1	4	4	0	5	4	10555.2329	0.0423
7	3	4	6	2	5	7	6	9443.7932	0.0047	6	4	3	5	3	3	6	5	9913.8666	0.0068							6	5	10555.2329	-0.0387
						6	5	9444.021	-0.0508							5	4	9914.0451	-0.0063							4	3	10555.2329	-0.0049
						8	7	9444.021	-0.0039							7	6	9914.0451	0.0225	5	5	0	4	4	1	5	4	10555.2329	0.0314
9	2	7	8	1	7	9	8	9487.6089	0.0030	6	4	2	5	3	3	6	5	9914.332	0.0032							6	5	10555.2329	-0.0496
						8	7	9487.7872	-0.0103							5	4	9914.4966	-0.0245							4	3	10555.2329	-0.0158
						10	9	9487.7872	0.0155							7	6	9914.4966	0.0044	7	4	4	6	3	3	7	6	10700.6791	-0.0037
8	2	7	7	1	7	8	7	9626.8838	-0.0091	13	1	12	12	2	11	14	13	9963.5148	-0.0113							8	7	10700.8185	0.0123
						9	8	9627.3049	0.0473							13	12	9963.5148	-0.0032							6	5	10700.8185	-0.0101
						7	6	9627.3049	-0.0169							12	11	9963.5148	-0.0170	7	4	3	6	3	3	7	6	10702.3992	0.0066
8	3	6	7	2	5	7	6	9682.805	0.0183	8	3	6	7	2	6	8	7	10276.3058	0.0068							8	7	10702.5316	0.0140
						9	8	9682.805	0.0150							7	6	10276.4794	-0.0463							6	5	10702.5316	-0.0086
						8	7	9682.805	-0.0580							9	8	10276.4794	-0.0114	7	4	4	6	3	4	7	6	10722.5339	-0.0034
13	0	13	12	1	12	13	12	9736.0284	0.0086	9	3	7	8	2	6	10	9	10277.8736	-0.0079							6	5	10722.7034	-0.0043
						12	11	9736.0284	0.0153							8	7	10277.8736	0.0000							8	7	10722.7034	0.0216

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res
7	4	3	6	3	4	7	6	10724.2473	0.0002
						8	7	10724.4044	0.0112
						6	5	10724.4044	-0.0149
14	1	13	13	2	12	15	14	10782.2511	-0.0063
						13	12	10782.2511	-0.0107
						14	13	10782.2511	-0.0090
10	3	8	9	2	7	11	10	10827.9218	-0.0058
						9	8	10827.9218	0.0043
						10	9	10828.0682	-0.0001
14	2	13	13	1	12	13	12	11148.7226	0.0231
						15	14	11148.7226	0.0226
						14	13	11148.7226	-0.0445
9	3	7	8	2	7	9	8	11190.9487	0.0053
						8	7	11191.1503	-0.0141
						10	9	11191.1503	0.0162
15	0	15	14	1	14	14	13	11206.8165	0.0279
						15	14	11206.8165	0.0214
						16	15	11206.8165	0.0327
10	3	7	9	2	7	9	8	11214.0339	0.0000
						10	9	11214.0339	-0.0061
						11	10	11214.0339	0.0030
15	1	15	14	0	14	16	15	11215.5159	-0.0256
						14	13	11215.5159	-0.0302
						15	14	11215.5159	-0.0388
11	3	9	10	2	8	12	11	11340.1139	-0.0055
						10	9	11340.1139	0.0053
						11	10	11340.2642	-0.0128
6	5	1	5	4	2	6	5	11361.8119	-0.0886
						7	6	11361.998	-0.0317
6	5	2	5	4	1	6	5	11361.8119	0.0095

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res
						7	6	11361.998	0.0666
9	3	6	8	2	7	9	8	11411.1443	0.0111
						10	9	11411.3986	-0.0201
						8	7	11411.3986	-0.0611
8	4	5	7	3	4	7	6	11480.6672	-0.0020
						8	7	11480.6672	0.1029
						9	8	11480.6672	0.0142
8	4	4	7	3	4	8	7	11485.7468	0.0984
						9	8	11485.7468	0.0059
						7	6	11485.7468	-0.0108
8	4	5	7	3	5	8	7	11534.2107	-0.0048
						7	6	11534.3679	0.0031
						9	8	11534.3679	0.0250
8	4	4	7	3	5	8	7	11539.2988	-0.0007
						7	6	11539.444	-0.0090
						9	8	11539.444	0.0133
7	5	3	6	4	2	7	6	12167.5539	-0.0073
						6	5	12167.7064	-0.0028
						8	7	12167.7064	0.0131
7	5	2	6	4	3	7	6	12168.058	0.0033
						8	7	12168.2088	0.0214
						6	5	12168.2088	0.0052
9	4	6	8	3	5	10	9	12237.013	0.0112
						8	7	12237.013	0.0008
						9	8	12237.013	0.0625
9	4	5	8	3	6	9	8	12364.7403	-0.0109
						8	7	12364.8828	-0.0102
						10	9	12364.8828	0.0090
6	6	1	5	5	0	6	5	12811.2254	0.0551
						7	6	12811.2254	-0.0044

J	K _a	K _c	J''	K _a ''	K _c ''	F'	F''	Obs	Res
						5	4	12811.2254	0.0211
10	4	7	9	3	6	10	9	12958.567	0.0050
						11	10	12958.567	-0.0069
						9	8	12958.567	-0.0120
8	5	4	7	4	3	8	7	12971.4809	-0.0197
						7	6	12971.6259	-0.0120
						7	8	12971.6259	-0.0027
8	5	3	7	4	4	8	7	12973.3001	-0.0163
						7	6	12973.4476	-0.0081
						7	8	12973.4476	0.0013
7	6	2	6	5	1	6	5	13618.0266	-0.0289
						8	7	13618.0266	-0.0278
						7	6	13618.0266	0.0735
11	4	8	10	3	7	11	10	13633.8258	-0.0219
						10	9	13633.8258	0.0051
						12	11	13633.8258	0.0059
9	5	5	8	4	4	9	8	13772.1031	-0.0066
						8	7	13772.2234	-0.0059
						10	9	13772.2234	0.0084
9	5	4	8	4	5	9	8	13777.5442	-0.0187
						10	9	13777.6812	0.0088
						8	7	13777.6812	-0.0060

