Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The axial/equatorial conformational landscape and intramolecular dispersion: new insights from the rotational spectra of monoterpenoids

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Supplementary information

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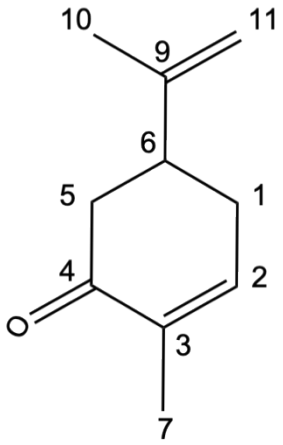
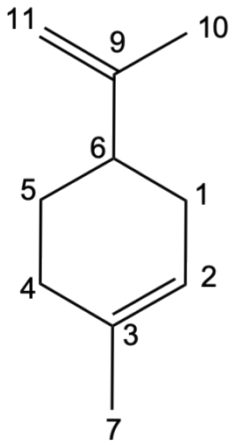
Figure S12-S14. NCI plots for the observed conformers of carvone, limonene and perillaldehyde showing the intramolecular interactions..

Experimental Methods

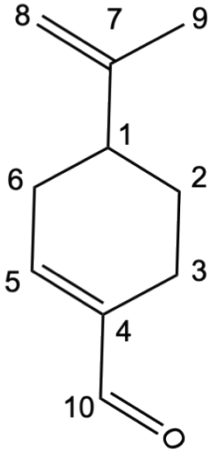
Commercial samples of R-(-)-carvone (98%), R-(+)-limonene (97%) and S-(-)-perillaldehyde (91%) were purchased and used without further purification. The three terpenes have relatively low vapour pressures and so they were placed in a bespoke heated nozzle and were slightly heated to temperatures of 380 K (carvone), 340 K (limonene) and 406 K (perillaldehyde) to increase their concentration in the gas phase. The molecular beam was created by seeding the vaporised molecules into the carrier gas (Ne, He or Ar) at backing pressures of 5 bar, and supersonically expanding the mixture into the vacuum chamber through a pulsed nozzle. Molecular pulses of 1000 μs when using Ne and 600 μs when using He and Ar were found to be optimal. Four 4 μs chirped pulses spaced 30 μs and spanning the 2-8 GHz frequency range were applied to polarise the molecules in each molecular pulse. Free induction decays were collected for 20 μs after each polarisation pulse, and transformed to the frequency domain using a fast Fourier transform algorithm. Final spectra were obtained by coherently adding 1.1 million FIDs for carvone, 1.0 million FIDs and perillaldehyde, and 1.5 M FIDs for limonene.



carvone



limonene



perillaldehyde

Table S1. Theoretical spectroscopic parameters of the six stable conformers of **carvone**.

Carvone	**Eq-A**					**Eq-C**					**Eq-a**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	2226.1	2252.8	2214.5	2239.1	2241.7	2246.7	2276.4	2234.9	2258.8	2262.3	2195.6	2223.0	2191.5	2215.0	2218.1
B (MHz)	658.4	660.3	646.9	653.1	655.1	673.9	679.1	663.4	668.6	671.4	680.8	680.8	673.4	679.6	682.5
C (MHz)	581.3	582.0	571.0	576.8	578.4	556.7	553.4	547.0	551.8	553.0	562.3	562.3	548.2	552.4	553.7
μ_a (D)	1.8	1.9	1.9	1.9	1.8	1.9	2.1	1.9	2.0	2.1	1.6	1.8	1.8	1.8	1.8
μ_b (D)	2.7	2.8	3.0	2.9	2.7	2.8	3.0	3.0	3.2	3.2	2.5	2.5	2.7	2.7	2.7
μ_c (D)	0.7	0.8	0.7	0.8	0.4	0.6	0.5	0.7	0.4	0.6	0.4	0.2	0.4	0.4	0.4
τ C_{10}–C_9–C_6–C_5	127.1	129.7	122.5	110.9	124.9	-10.6	-3.9	-11.2	-10.9	-10.1	-102.2	-123.1	-111.8	-113.2	-113.8
ΔE (cm^{-1})	0	13	0	0	0	163	0	120	111	85	238	62	141	145	143
ΔE_{ZPC} (cm^{-1})	0	32	0	0	0	164	0	136	135	99	235	123	171	176	137
ΔG^{380} (cm^{-1})	0	24	0	0	0	139	0	215	191	175	189	151	217	187	242
	Ax-a					**Ax-C**					**Ax-A**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	1581.7	1612.6	1651.7	1649.5	1638.2	1618.4	1674.1	1722.3	1719.3	1706.3	1779.5	1816.7	1822.6	1812.1	1811.9
B (MHz)	941.1	923.6	858.3	879.8	893.2	921.2	896.2	840.2	855.4	867.9	842.6	834.0	807.6	820.4	825.3
C (MHz)	806.0	792.9	742.4	761.9	771.1	810.0	783.9	733.3	749.6	761.3	774.9	765.5	740.0	753.6	758.2
μ_a (D)	1.1	1.3	1.5	1.8	1.4	2.2	2.3	2.4	2.4	2.4	1.2	1.3	1.4	1.3	1.3
μ_b (D)	2.6	2.7	2.8	2.8	2.8	2.6	2.9	3.1	3.1	3.1	2.9	3.1	3.2	3.2	3.2
μ_c (D)	1.1	1.2	1.4	1.3	1.3	0.6	0.7	0.6	0.6	0.7	0.5	0.5	0.5	0.5	0.5
τ C_{10}–C_9–C_6–C_5	-120.9	-119.7	-112.6	-113.6	-115.5	9.6	4.0	-5.8	-3.3	-1.3	112.6	114.8	116.7	115.3	115.5
ΔE (cm^{-1})	128	293	779	527	370	12	164	726	465	303	261	364	785	433	318
ΔE_{ZPC} (cm^{-1})	196	402	801	569	428	122	343	769	506	355	317	456	833	459	368
ΔG^{380} (cm^{-1})	361	495	807	609	554	364	586	898	610	480	476	526	1031	635	564

Table S2. Theoretical spectroscopic parameters of the six stable conformers of **limonene**.

Limonene	**Eq-A**					**Eq-C**					**Eq-a**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	3054.6	3075.2	3060.3	3060.1	3066.6	3052.1	3072.2	3059.4	3058.8	3062.9	3028.9	3062.3	3046.6	3042.1	3049.5
B (MHz)	719.3	723.3	710.4	713.8	715.9	744.2	749.3	735.2	737.4	741.3	740.5	756.3	734.1	737.1	740.5
C (MHz)	680.8	680.6	673.1	675.8	677.7	648.2	646.4	641.7	643.6	644.8	653.9	638.4	643.4	645.4	646.4
μ_a (D)	0.3	0.4	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.2	0.3	0.5	0.3	0.3
μ_b (D)	0.3	0.4	0.2	0.3	0.3	0.1	0.2	0.2	0.2	0.2	0.5	0.7	0.3	0.6	0.6
μ_c (D)	0.3	0.3	0.4	0.4	0.4	0.3	0.3	0.3	0.3	0.3	0.2	0.1	0.4	0.2	0.2
τ C_{11}–C_9–C_6–C_5	128.7	132.8	120.3	126.6	126.6	-11.4	-6.8	-12.5	-12.5	-12.5	-96	-122.7	-101.2	-101.5	-101.4
ΔE (cm^{-1})	57	4	0	0	0	222	0	100	110	103	328	179	188	234	213
ΔE_{ZPC} (cm^{-1})	9	45	0	0	0	169	0	88	101	88	273	184	157	186	171
ΔG^{340} (cm^{-1})	0	60	0	0	0	122	0	111	53	57	230	220	113	67	74
	Ax-A					**Ax-a**					**Ax-C**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	2194.7	2201.2	2320.7	2264.4	2269.4	2132.2	2133.6	2264.9	2261.2	2229.3	1896.9	1960.8	2058.3	2005.5	1996.4
B (MHz)	943.9	944.5	879.7	907.4	912.4	952.3	954.4	892.2	900.2	915.0	1024.2	999.6	940.8	964.4	974.9
C (MHz)	919.3	920.8	864.9	886.7	891.3	921.5	918.3	860.9	877.3	887.5	960.9	928.4	863.6	890.2	901.7
μ_a (D)	0.4	0.5	0.6	0.6	0.6	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.0	0.1	0.1
μ_b (D)	0.1	0.1	0.1	0.1	0.1	0.5	0.6	0.6	0.6	0.6	0.1	0.2	0.2	0.2	0.2
μ_c (D)	0.0	0.0	0.1	0.1	0.1	0.2	0.3	0.3	0.3	0.3	0.2	0.3	0.3	0.3	0.3
τ C_{11}–C_9–C_6–C_5	90.8	87.8	101.3	96.4	96.4	-112.9	-115.2	-105.9	-102.5	-102.5	23.5	20.0	11.4	15.6	15.6
ΔE (cm^{-1})	551	590	1065	739	625	0	41	565	258	139	932	645	1149	932	782
ΔE_{ZPC} (cm^{-1})	590	643	1123	764	670	0	82	606	289	152	1027	771	1251	1027	876
ΔG^{340} (cm^{-1})	738	719	1258	792	703	80	166	742	346	108	1081	917	1428	1081	931

Table S3. Theoretical spectroscopic parameters of the twelve stable conformers of **perillaldehyde**.

Perillaldehyde	**Eq-A_0**					**Eq-C_0**					**Eq-a_0**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	2888.0	2900.8	2890.0	2891.5	2896.6	2845.0	2858.6	2853.8	2851.9	2857.8	2905.2	2934.2	2923.5	2920.0	2927.1
B (MHz)	536.0	539.8	531.2	533.0	534.6	550.8	555.6	544.6	546.1	548.5	544.1	554.7	540.3	541.7	543.7
C (MHz)	507.9	509.9	503.3	504.9	506.4	489.8	490.2	486.3	487.6	488.7	492.3	484.1	485.6	487.2	488.3
μ_a (D)	2.7	2.9	3.1	3.1	3.1	2.7	2.9	3.1	3.1	3.1	2.8	3.1	3.3	3.3	3.3
μ_b (D)	1.5	1.6	1.5	1.5	1.5	1.2	1.2	1.1	1.1	1.1	1.6	1.8	1.6	1.6	1.6
μ_c (D)	0.2	0.1	0.3	0.2	0.2	0.5	0.6	0.6	0.6	0.6	0.2	0.1	0.1	0.2	0.2
$\tau(C_8–C_7–C_1–C_2$	128.7	131.4	125.7	126.9	126.5	-11.3	-6.7	-14.1	-14.0	-12.8	-95.6	-122.4	-100.8	-100.2	-100.8
ΔE (cm^{-1})	1335	1141	1152	1148	1168	1506	1148	1271	1261	1277	1606	1320	1339	1366	1366
ΔE_{ZPC} (cm^{-1})	1204	1118	1082	1089	1092	1373	1120	1197	1207	1198	1473	1293	1275	1303	1291
ΔG^{406} (cm^{-1})	1035	1093	1012	1019	1003	1178	1111	1128	1140	1125	1269	1306	1169	1180	1147
	Ax-a_0					**Ax-A_0**					**Ax-C_0**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	2051.0	2056.1	2165.1	2157.3	2134.0	2086.4	2110.2	2177.3	2142.5	2148.7	1722.0	1788.5	1892.5	1828.1	1821.6
B (MHz)	690.2	692.3	655.1	662.0	670.3	695.4	693.5	657.9	672.9	675.5	753.4	731.6	1159.4	704.7	711.8
C (MHz)	672.7	672.0	633.1	643.8	651.0	669.3	667.5	636.3	649.0	651.7	709.9	687.3	1369.6	660.7	667.5
μ_a (D)	3.1	3.4	3.6	3.6	3.6	2.5	2.7	2.8	2.8	2.8	2.7	2.9	3.2	3.1	3.1
μ_b (D)	1.6	1.7	1.7	1.7	1.7	1.4	1.5	1.5	1.5	1.5	1.5	1.4	1.2	1.3	1.3
μ_c (D)	0.5	0.6	0.6	0.6	0.6	0.3	0.2	0.2	0.2	0.2	0.8	1.1	1.4	1.3	1.3
τ $C_8–C_7–C_1–C_2$	-112.4	-114.3	-107.2	-104.6	-107.1	90.5	89.0	98.9	94.6	95.2	23.8	18.7	11.5	15.6	15.9
ΔE (cm^{-1})	1168.4	1055.3	1633.5	1302.8	1195.2	1707.1	1712.0	2209.1	1854.5	1761.4	1956.6	1785.2	2313.7	2084.5	1960.3
ΔE_{ZPC} (cm^{-1})	1101.2	1157.5	1600.5	1304.5	1181.4	1748.7	1767.2	2185.6	1873.3	1783.6	1969.1	1920.1	2360.2	2134.1	1998.4
ΔG^{406} (cm^{-1})	1041.6	1213.9	1587.0	1323.2	1203.2	1821.0	1839.2	2172.8	1895.4	1824.7	1949.6	2023.3	2408.5	2180.3	2060.0

Perillaldehyde	**Eq-A**					**Eq-C**					**Eq-a**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	2926.2	2950.4	2942.1	2939.5	2947.4	2950.9	2975.2	2964.4	2961.6	2969.9	2866.0	2904.3	2892.2	2883.5	2893.1
B (MHz)	537.1	540.1	531.7	534.2	535.3	547.5	552.0	541.5	543.3	545.5	551.1	560.7	547.0	549.4	551.0
C (MHz)	510.7	512.3	505.4	507.6	508.7	492.0	491.4	487.5	489.3	489.8	495.3	487.1	487.6	489.7	490.4
μ_a (D)	2.9	3.0	3.3	3.2	3.3	3.0	3.2	3.4	3.4	3.4	2.9	3.0	3.3	3.2	3.2
μ_b (D)	1.5	1.6	1.7	1.7	1.7	1.7	1.9	1.9	1.9	1.9	1.4	1.5	1.5	1.5	1.5
μ_c (D)	0.6	0.7	0.6	0.7	0.7	0.4	0.4	0.4	0.4	0.4	0.4	0.1	0.4	0.4	0.4
τ C_8–C_7–C_1–C_2	128.8	131.4	126.7	128.1	127.7	-11.9	-6.9	-13.8	-13.8	-12.2	-95.8	-123.1	-103.1	-102.6	-103.6
ΔE (cm^{-1})	118.6	1.0	0	0	0	307.1	30.0	139.7	137.9	132.0	376.9	153.6	178.5	212.7	187.7
ΔE_{ZPC} (cm^{-1})	55.6	0	0	0	0	239.7	70.7	128.1	135.5	117.1	310.6	245.4	153.2	182.8	158.0
ΔG^{406} (cm^{-1})	0	0	0	0	4.8	131.9	165.5	102.1	95.3	73.7	215.1	373.1	83.6	100.3	69.4
	Ax-a					**Ax-A**					**Ax-C**				
	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ	MP2	M062X	B3LYP	B3LYP-D3	B3LYP-D3BJ
A (MHz)	1882.3	1910.8	2022.0	2017.0	1986.7	1993.5	2022.2	2135.1	2066.7	2062.4	1754.1	1804.3	1939.2	1878.3	1866.3
B (MHz)	725.5	721.1	673.6	683.1	692.8	705.0	700.9	658.6	679.1	683.9	749.5	736.9	684.8	703.4	710.7
C (MHz)	690.7	686.5	647.1	656.0	664.1	689.7	688.1	647.0	667.4	672.0	718.2	700.8	639.9	661.1	670.1
μ_a (D)	2.8	2.9	3.3	3.2	3.2	2.4	2.5	2.8	2.7	2.7	2.9	3.1	3.4	3.3	3.3
μ_b (D)	2.0	2.2	2.1	2.3	2.2	2.0	2.2	2.2	2.3	2.3	2.1	2.3	2.4	2.4	2.4
μ_c (D)	0.7	0.9	1.1	0.9	1.0	1.0	1.0	0.9	0.9	1.0	0.7	0.8	0.9	0.9	0.9
τ C_8–C_7–C_1–C_2	-114.3	-114.2	-107.5	-104.3	-108.1	91.8	91.7	102.1	102.1	95.1	21.6	18.9	8.6	8.6	13.4
ΔE (cm^{-1})	0	0	522.5	223.0	90.5	612.1	598.5	1077.2	741.4	625.5	760.7	707.1	1185.4	974.2	828.1
ΔE_{ZPC} (cm^{-1})	0	82.2	567.3	256.3	109.4	647.4	740.1	1129.2	812.1	717.7	842.1	864.5	1272.6	1087.2	941.5
ΔG^{406} (cm^{-1})	60.4	193.1	633.2	303.5	0	754.8	948.1	1202.5	931.2	884.0	924.0	1021.7	1325.8	1207.5	1072.8

Table S4. Experimental spectroscopic parameters of the five observed conformers of **carvone**.

	Eq-A	**Eq-C**	**Eq-a**	**Ax-a**	**Ax-C**
A[a] (MHz)	2237.2055(11)[e]	2256.91513(93)	2212.7903(13)	1621.8211(18)	1687.7984(26)
B (MHz)	656.27834(29)	672.90566(26)	684.52333(27)	904.92320(51)	878.27624(98)
C (MHz)	579.64159(29)	554.50351(25)	554.73193(25)	780.45872(54)	771.3069(12)
Δ_J (kHz)	0.0131(35)	0.0118(37)	0.0197(39)	0.200(14)	0.203(27)
Δ_{JK} (kHz)	0.268(16)	0.054(15)	-0.086(28)	-0.56(10)	-0.82(11)
Δ_K (kHz)	-1.77(16)	-0.96(12)	-	-	-
δ_K (kHz)	1.201(56)	-	-	-	-
$a/b/c$[b]	y/y/y	y/y/y	y/y/y	y/y/y	y/y/y
σ[c] (kHz)	8	7	5	5	4
N[d]	78	85	45	23	25

[a] A, B and C are the rotational constants, Δ_J, Δ_{JK}, Δ_K, δ_K are the quartic centrifugal distortion constants.
[b] a, b, and c are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Table S5. Experimental spectroscopic parameters of the five observed conformers of **limonene**.

	Eq-A	**Eq-C**	**Eq-a**	**Ax-a**
A[a] (MHz)	3058.0149(12)[e]	3053.78717(54)	3040.4812 (26)	2163.1282(13)
B (MHz)	717.04957(32)	742.17003(27)	745.64408(39)	935.41576(52)
C (MHz)	679.25501(30)	646.69228(28)	643.75616(36)	903.88486(48)
Δ_J (kHz)	0.0165(48)	0.0222(47)	-	0.208(17)
Δ_{JK} (kHz)	0.088(28)	-	-	-0.940(65)
Δ_K (kHz)	-	-	-	-
$a/b/c$[b]	y/y/y	y/y/y	y/y/n	y/y/y
σ[c] (kHz)	7	6	4	6
N[d]	59	53	18	33

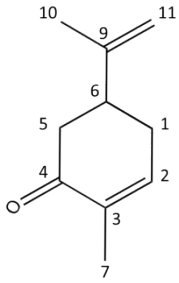
[a] A, B and C are the rotational constants, Δ_J, Δ_K, Δ_{JK} are the quartic centrifugal distortion constants.
[b] a, b, and c are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Table S6. Experimental spectroscopic parameters of the five observed conformers of **perillaldehyde**.

	Eq-A	**Eq-C**	**Eq-a**	**Ax-a**
A[a] (MHz)	2932.68531(72)[e]	2954.62015(52)	2880.66517(99)	1919.41562(92)
B (MHz)	536.55638(16)	547.00873(17)	554.09056(34)	710.46341(44)
C (MHz)	510.20051(19)	491.61401(18)	489.85916(30)	678.65905(46)
Δ_J (kHz)	0.0136(18)	0.0110(20)	0.0145(37)	0.1514(95)
Δ_{JK} (kHz)	0.078(16)	-	0.077(22)	-0.996(38)
Δ_K (kHz)	-	-	-	2.70(13)
δ_J (kHz)	-	-	-0.00228(65)	-
$a/b/c$[b]	y/y/y	y/y/y	y/y/n	y/y/y
σ[c] (kHz)	6	5	7	7
N[d]	76	78	59	53

[a] A, B and C are the rotational constants, Δ_J, Δ_{JK}, Δ_K, δ_J are the quartic centrifugal distortion constants.
[b] a, b, and c are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Table S7.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-A** of **carvone**.



J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2395.1944	-0.0024
2	0	2	1	0	1	2469.1175	-0.0021
2	1	1	1	1	0	2548.4753	-0.0046
3	1	3	2	1	2	3591.1234	0.0003
3	0	3	2	0	2	3696.8987	-0.0029
3	2	1	2	2	0	3718.6275	0.0188
3	1	2	2	1	1	3820.9844	-0.0029
4	1	4	3	1	3	4785.1243	-0.0018
4	0	4	3	0	3	4916.6788	-0.0031
4	2	3	3	2	2	4941.5540	0.0044
4	2	2	3	2	1	4968.5390	-0.0039
4	1	3	3	1	2	5091.3263	-0.0040
5	0	5	4	0	4	6126.2000	-0.0029
5	2	4	4	2	3	6173.5242	-0.0087
5	2	3	4	2	2	6226.9257	0.0115
5	1	4	4	1	3	6358.6399	-0.0035
6	1	6	5	1	5	7165.4505	0.0003
6	0	6	5	0	5	7323.8773	-0.0023
6	2	5	5	2	4	7403.2650	0.0103
6	2	4	5	2	3	7494.8360	-0.0074
6	1	5	5	1	4	7621.9315	-0.0052
2	1	2	1	0	1	3976.1096	-0.0132
3	1	3	2	0	2	5098.1232	-0.0031
4	1	4	3	0	3	6186.3488	-0.0019
5	1	5	4	0	4	7246.3698	0.0004
3	0	3	2	1	2	2189.8956	-0.0028
4	0	4	3	1	3	3515.4607	0.0034
5	0	5	4	1	4	4856.5275	-0.0066
6	0	6	5	1	5	6203.7079	-0.0052
7	0	7	6	1	6	7547.4487	-0.0072
1	1	0	0	0	0	2893.4803	-0.0071
2	1	1	1	0	1	4206.0427	-0.0048
3	1	2	2	0	2	5557.9106	-0.0046
4	1	3	3	0	3	6952.3350	-0.0089
4	0	4	3	1	2	3055.6650	-0.0033
5	0	5	4	1	3	4090.5365	-0.0045
6	0	6	5	1	4	5055.7804	0.0032
7	0	7	6	1	5	5943.0369	0.0035
7	1	6	6	2	5	4804.0912	0.0116
8	1	7	7	2	6	6305.5217	-0.0004
9	1	8	8	2	7	7826.7504	-0.0064
4	1	3	4	0	4	2035.6623	0.0004
5	1	4	5	0	5	2268.0987	-0.0037
6	1	5	6	0	6	2566.1588	-0.0007
7	1	6	7	0	7	2937.0313	-0.0022
8	1	7	8	0	8	3385.8184	0.0044
9	1	8	9	0	9	3914.1060	0.0061
10	1	9	10	0	10	4519.1745	0.0169
2	2	0	2	1	1	4745.5070	-0.0088
3	2	1	3	1	2	4643.1551	0.0179
4	2	2	4	1	3	4520.3675	0.0177
6	2	4	6	1	5	4261.5225	-0.0047
7	2	5	7	1	6	4153.8325	-0.0003
8	2	6	8	1	7	4080.3177	-0.0019

9	2	7	9	1	8	4054.7047	-0.0034
10	2	8	10	1	9	4089.0036	-0.0004
2	2	1	2	1	2	4972.7302	0.0096
3	2	2	3	1	3	5089.3551	0.0056
4	2	3	4	1	4	5245.7837	0.0107
5	2	4	5	1	5	5442.6107	0.0054
6	2	5	6	1	6	5680.3920	-0.0178
7	2	6	7	1	7	5959.5656	-0.0172
8	2	7	8	1	8	6280.2230	-0.0132
9	2	8	9	1	9	6642.0849	-0.0054
10	2	9	10	1	10	7044.3904	-0.0007
2	2	1	1	1	0	7291.2880	0.0121
2	2	0	1	1	0	7293.9908	-0.0050
2	2	0	1	1	1	7370.6493	0.0120
5	3	3	4	3	2	6188.3108	0.0120
5	3	2	4	3	1	6189.5676	0.0038
6	3	4	5	3	3	7428.8055	0.0123
6	3	3	5	3	2	7432.1646	0.0087
6	2	5	6	1	5	4075.9785	-0.0088
7	2	6	7	1	6	3826.1942	-0.0033
8	2	7	8	1	7	3548.6647	0.0086
7	3	4	7	2	5	7870.6640	-0.0098
8	3	5	8	2	6	7740.1137	-0.0051
9	3	6	9	2	7	7572.9936	0.0141

Table S7.II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2390.5329	-0.0043
2	0	2	1	0	1	2465.6499	-0.0089
2	1	1	1	1	0	2546.4816	0.0024
3	1	3	2	1	2	3584.0568	0.0025
3	0	3	2	0	2	3691.3894	0.0029
3	1	2	2	1	1	3817.9036	0.0015
4	1	4	3	1	3	4775.5572	-0.0024
4	0	4	3	0	3	4908.7393	0.0010
4	1	3	3	1	2	5087.0539	0.0013
5	1	5	4	1	4	5964.5233	-0.0055
5	0	5	4	0	4	6115.3787	0.0022
5	1	4	4	1	3	6353.0225	0.0043
6	1	6	5	1	5	7150.5569	0.0020
6	0	6	5	0	5	7309.7064	0.0026
6	1	5	5	1	4	7614.7525	0.0013
2	1	2	1	0	1	3950.6142	-0.0162
3	1	3	2	0	2	5069.0267	0.0008
4	1	4	3	0	3	6153.2015	0.0025
5	1	5	4	0	4	7208.9925	0.0030
3	0	3	2	1	2	2206.4055	-0.0094
5	0	5	4	1	4	4870.9154	-0.0004
6	0	6	5	1	5	6216.0935	0.0027
7	0	7	6	1	6	7556.8175	-0.0029

Table S7.III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2387.0431	-0.0075
2	0	2	1	0	1	2462.2095	-0.0100
2	1	1	1	1	0	2543.0958	-0.0069
3	1	3	2	1	2	3578.8171	-0.0026
3	1	2	2	1	1	3812.8315	-0.0007
4	1	4	3	1	3	4768.5715	-0.0002
4	0	4	3	0	3	4901.7974	-0.0015
4	1	3	3	1	2	5080.2868	0.0037
5	1	5	4	1	4	5955.7812	-0.0001
5	0	5	4	0	4	6106.6506	0.0013
5	1	4	4	1	3	6344.5425	0.0031
6	1	6	5	1	5	7140.0410	0.0000
6	0	6	5	0	5	7299.1608	-0.0016
6	1	5	5	1	4	7604.5540	0.0036
2	1	2	1	0	1	3945.0022	-0.0080
3	1	3	2	0	2	5061.6097	-0.0007
4	1	4	3	0	3	6143.9815	0.0076
5	1	5	4	0	4	7197.9575	0.0011

Table S7.IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2384.2997	-0.0055
2	1	1	1	1	0	2536.5740	0.0150
3	1	3	2	1	2	3574.8088	0.0007
3	0	3	2	0	2	3679.9390	-0.0003
3	1	2	2	1	1	3803.1290	-0.0007
4	1	4	3	1	3	4763.4145	0.0013
4	0	4	3	0	3	4894.2318	-0.0014
4	1	3	3	1	2	5067.5675	0.0014
5	1	5	4	1	4	5949.6255	0.0048
5	0	5	4	0	4	6098.4012	0.0023
5	1	4	4	1	3	6329.0163	0.0003
6	1	6	5	1	5	7133.0335	-0.0044
6	0	6	5	0	5	7290.8583	-0.0010
6	1	5	5	1	4	7586.5074	0.0026
2	1	2	1	0	1	3965.8050	-0.0102
3	1	3	2	0	2	5082.8750	0.0019
4	1	4	3	0	3	6166.3477	0.0008
5	1	5	4	0	4	7221.7362	0.0018
4	0	4	3	1	3	3491.2982	-0.0012
5	0	5	4	1	4	4826.2854	0.0002
6	0	6	5	1	5	6167.5225	-0.0012
7	0	7	6	1	6	7505.5607	-0.0043

Table S7.V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2388.4188	-0.0026
2	0	2	1	0	1	2462.4790	0.0110
2	1	1	1	1	0	2541.9987	0.0069

3	1	3	2	1	2	3580.9489	0.0010
3	0	3	2	0	2	3686.8748	-0.0002
4	1	4	3	1	3	4771.5410	0.0032
4	0	4	3	0	3	4903.2251	0.0014
4	1	3	3	1	2	5078.3144	0.0024
5	0	5	4	0	4	6109.2485	0.0038
5	1	4	4	1	3	6342.3332	0.0052
6	1	6	5	1	5	7144.9787	-0.0070
6	0	6	5	0	5	7303.3451	-0.0073
6	1	5	5	1	4	7602.2930	0.0016
2	1	2	1	0	1	3963.5539	-0.0163
3	1	3	2	0	2	5082.0504	0.0003
4	1	4	3	0	3	6166.7167	0.0038
5	1	5	4	0	4	7223.1780	0.0057
4	0	4	3	1	3	3508.0470	-0.0016
5	0	5	4	1	4	4845.7527	-0.0027
7	0	7	6	1	6	7529.4788	-0.0031

Table S7.VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	3587.9153	-0.0022
3	0	3	2	0	2	3694.4163	-0.0027
3	1	2	2	1	1	3819.6484	-0.0011
4	1	4	3	1	3	4780.7890	0.0051
4	0	4	3	0	3	4913.0860	-0.0016
5	1	5	4	1	4	5971.1667	-0.0033
5	0	5	4	0	4	6121.2761	-0.0018
5	1	4	4	1	3	6356.1866	0.0055
6	0	6	5	0	5	7317.3987	-0.0004
6	1	5	5	1	4	7618.7783	0.0059
2	1	2	1	0	1	3962.9275	-0.0072
3	1	3	2	0	2	5083.2845	0.0008
4	1	4	3	0	3	6169.6498	0.0012
5	1	5	4	0	4	7227.7337	0.0026
4	0	4	3	1	3	3524.2263	0.0034
6	0	6	5	1	5	6210.9461	0.0001
7	0	7	6	1	6	7553.2366	-0.0073

Table S7.VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	3587.5040	0.0034
3	0	3	2	0	2	3692.9477	-0.0147
3	1	2	2	1	1	3816.6204	0.0006
4	1	4	3	1	3	4780.3175	0.0031
4	0	4	3	0	3	4911.5026	-0.0025
4	1	3	3	1	2	5085.5275	-0.0001
5	1	5	4	1	4	5970.7120	-0.0015
5	0	5	4	0	4	6119.8468	-0.0009
5	1	4	4	1	3	6351.4332	0.0083
6	1	6	5	1	5	7158.2987	-0.0048
6	0	6	5	0	5	7316.4080	-0.0011
6	1	5	5	1	4	7613.3305	0.0018

2	1	2	1	0	1	3973.2141	-0.0112
3	1	3	2	0	2	5094.2634	0.0034
4	1	4	3	0	3	6181.6155	0.0035
5	1	5	4	0	4	7240.8250	0.0046

Table S7.VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2361.8640	0.0017
2	0	2	1	0	1	2434.0405	-0.0093
3	1	3	2	1	2	3541.2066	0.0009
3	0	3	2	0	2	3644.6371	-0.0038
3	1	2	2	1	1	3765.4479	-0.0051
4	1	4	3	1	3	4718.7215	0.0007
4	0	4	3	0	3	4847.6290	-0.0009
4	1	3	3	1	2	5017.4581	0.0008
5	1	5	4	1	4	5893.9235	-0.0001
5	0	5	4	0	4	6040.8492	-0.0025
5	1	4	4	1	3	6266.5966	0.0026
6	1	6	5	1	5	7066.4350	0.0038
6	0	6	5	0	5	7222.7515	0.0010
6	1	5	5	1	4	7511.9370	0.0055
2	1	2	1	0	1	3948.2597	0.0005
3	1	3	2	0	2	5055.4154	0.0002
4	1	4	3	0	3	6129.4922	-0.0028
5	1	5	4	0	4	7175.7890	0.0002
4	0	4	3	1	3	3436.8581	0.0024
5	0	5	4	1	4	4758.9842	-0.0024
6	0	6	5	1	5	6087.8124	-0.0011
7	0	7	6	1	6	7414.1270	-0.0011

Table S7.IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2378.8149	0.0178
2	0	2	1	0	1	2451.7230	0.0083
2	1	1	1	1	0	2529.9140	0.0108
3	1	3	2	1	2	3566.5890	0.0148
3	0	3	2	0	2	3671.0095	0.0084
3	1	2	2	1	1	3793.1785	0.0027
4	1	4	3	1	3	4752.5117	0.0266
4	0	4	3	0	3	4882.5377	0.0118
4	1	3	3	1	2	5054.3545	0.0023
5	1	5	4	1	4	5936.0634	0.0262
5	0	5	4	0	4	6084.1055	0.0190
5	1	4	4	1	3	6312.6040	0.0074
6	1	6	5	1	5	7116.8872	0.0451
6	0	6	5	0	5	7274.1370	0.0229
6	1	5	5	1	4	7566.9631	0.0088
3	1	3	2	0	2	5079.2287	0.0172
4	1	4	3	0	3	6160.7250	0.0295
5	1	5	4	0	4	7214.2539	0.0471
4	0	4	3	1	3	3474.3175	0.0019

5	0	5	4	1	4	4805.9169	-0.0001
6	0	6	5	1	5	6143.9815	-0.0123
7	0	7	6	1	6	7479.2179	0.0159

Table S7.X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2369.3369	0.0074
2	0	2	1	0	1	2440.6236	0.0049
3	1	3	2	1	2	3552.4359	0.0016
3	0	3	2	0	2	3654.6049	-0.0024
3	1	2	2	1	1	3773.8530	0.0012
4	1	4	3	1	3	4733.7390	-0.0033
4	0	4	3	0	3	4861.1257	-0.0004
4	1	3	3	1	2	5028.7125	0.0008
5	1	5	4	1	4	5912.7710	-0.0065
5	0	5	4	0	4	6058.0411	-0.0031
5	1	4	4	1	3	6280.7619	0.0060
6	1	6	5	1	5	7089.1654	0.0032
6	0	6	5	0	5	7243.8180	-0.0061
6	1	5	5	1	4	7529.0707	0.0002
2	1	2	1	0	1	3943.8147	-0.0147
3	1	3	2	0	2	5055.6491	0.0041
4	1	4	3	0	3	6134.7848	0.0048
5	1	5	4	0	4	7186.4349	0.0035
4	0	4	3	1	3	3460.0842	-0.0042
5	0	5	4	1	4	4784.3890	-0.0013
7	0	7	6	1	6	7444.1580	0.0032

Table S7.XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{11}$ isotopologue of conformer **Eq-A** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2364.7476	0.0061
2	0	2	1	0	1	2435.7190	-0.0028
3	1	3	2	1	2	3545.5715	0.0040
3	0	3	2	0	2	3647.3220	-0.0025
3	1	2	2	1	1	3765.9835	-0.0006
4	1	4	3	1	3	4724.6150	0.0009
4	0	4	3	0	3	4851.5275	-0.0023
4	1	3	3	1	2	5018.2618	0.0091
5	1	5	4	1	4	5901.4106	0.0016
5	0	5	4	0	4	6046.2215	-0.0025
5	1	4	4	1	3	6267.7380	0.0030
6	1	6	5	1	5	7075.5777	0.0007
6	0	6	5	0	5	7229.8769	0.0016
6	1	5	5	1	4	7513.5272	-0.0005
2	1	2	1	0	1	3940.8563	0.0014
3	1	3	2	0	2	5050.6949	-0.0057
4	1	4	3	0	3	6127.9887	-0.0016
5	1	5	4	0	4	7177.8694	0.0000
4	0	4	3	1	3	3448.1619	0.0082
5	0	5	4	1	4	4769.7488	-0.0147

Table S8.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
2	1	2	1	1	1	2336.4181	0.0025
2	0	2	1	0	1	2448.4244	-0.0012
2	1	1	1	1	0	2573.2180	-0.0019
3	1	3	2	1	2	3500.7306	0.0007
3	0	3	2	0	2	3656.7798	0.0000
3	1	2	2	1	1	3855.7196	-0.0007
4	1	4	3	1	3	4660.6681	0.0001
4	0	4	3	0	3	4846.8028	-0.0004
4	1	3	3	1	2	5132.9820	-0.0006
5	1	5	4	1	4	5815.2460	0.0011
5	0	5	4	0	4	6014.4640	-0.0018
5	1	4	4	1	3	6402.7430	-0.0015
6	1	6	5	1	5	6963.8313	-0.0059
6	0	6	5	0	5	7158.7201	-0.0026
6	1	5	5	1	4	7662.3038	-0.0033
3	2	2	2	2	1	3682.2244	-0.0005
4	2	3	3	2	2	4904.6589	0.0024
4	2	2	3	2	1	4967.4798	-0.0012
5	2	4	4	2	3	6122.8382	0.0020
5	2	3	4	2	2	6245.3574	-0.0045
6	2	5	5	2	4	7335.7409	0.0053
6	2	4	5	2	3	7541.2332	-0.0072
4	3	2	3	3	1	4921.7860	-0.0047
4	3	1	3	3	0	4923.0740	-0.0108
5	3	3	4	3	2	6156.8348	0.0111
5	3	2	4	3	1	6161.3420	0.0073
6	3	4	5	3	3	7393.8431	0.0055
6	3	3	5	3	2	7405.7800	0.0009
3	0	3	2	1	2	2184.7837	0.0043
4	0	4	3	1	3	3530.8525	-0.0002
5	0	5	4	1	4	4884.6502	-0.0003
6	0	6	5	1	5	6228.1255	-0.0028
7	0	7	6	1	6	7546.5576	-0.0072
1	1	1	0	0	0	2811.4277	0.0083
2	1	2	1	0	1	3920.4175	-0.0084
3	1	3	2	0	2	4972.7293	-0.0010
5	1	5	4	0	4	6945.0575	-0.0027
6	1	6	5	0	5	7894.4315	-0.0001
1	1	0	0	0	0	2929.8309	0.0093
2	1	1	1	0	1	4275.6316	-0.0008
3	1	2	2	0	2	5682.9288	0.0017
4	1	3	3	0	3	7159.1297	-0.0002
4	0	4	3	1	2	2820.6540	-0.0018
5	0	5	4	1	3	3702.1322	-0.0068
6	0	6	5	1	4	4458.1149	-0.0023
3	1	2	3	0	3	2026.1487	0.0014
4	1	3	4	0	4	2312.3288	0.0021
5	1	4	5	0	5	2700.6074	0.0019
6	1	5	6	0	6	3204.1925	0.0026
7	1	6	7	0	7	3830.3949	0.0030
8	1	7	8	0	8	4577.2121	0.0007
9	1	8	9	0	9	5432.2950	-0.0027
11	1	10	11	0	11	7377.8196	0.0005
5	1	4	4	2	3	2052.5315	0.0074

6	1	5	5	2	4	3591.9943	-0.0008
7	1	6	6	2	5	5164.7458	0.0106
8	1	7	7	2	6	6759.9744	-0.0007
8	2	7	8	1	7	2981.8939	0.0050
7	2	6	7	1	6	3377.6325	-0.0087
6	2	5	6	1	5	3743.7413	0.0007
5	2	4	5	1	4	4070.3096	-0.0024
4	2	3	4	1	3	4350.1980	-0.0224
2	2	1	2	1	2	5107.2569	0.0087
3	2	2	3	1	3	5288.7476	0.0043
4	2	3	4	1	4	5532.7202	-0.0116
5	2	4	5	1	5	5840.3189	-0.0042
6	2	5	6	1	6	6212.2125	-0.0090
7	2	6	7	1	7	6648.3812	-0.0068
8	2	7	8	1	8	7147.7469	-0.0062
9	2	8	9	1	9	7708.0361	0.0029
7	2	5	7	1	6	4109.1822	-0.0054
6	2	4	6	1	5	4166.4337	-0.0007
5	2	3	5	1	4	4287.5155	0.0144
4	2	2	4	1	3	4444.9091	0.0254
3	2	1	3	1	2	4610.4064	0.0211
5	3	3	4	3	2	6156.8322	0.0085
5	3	2	4	3	1	6161.3363	0.0016
6	3	4	5	3	3	7393.8348	-0.0028
6	3	3	5	3	2	7405.7840	0.0049
6	2	5	6	1	5	3743.7373	-0.0033
7	2	6	7	1	6	3377.6360	-0.0052
8	2	7	8	1	7	2981.8939	0.0050
6	3	3	6	2	4	7924.4962	-0.0006
7	3	4	7	2	5	7732.0749	-0.0002
9	3	6	9	2	7	7204.4885	0.0042

Table S8.II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	*J"*	$K"_{-1}$	$K"_{+1}$	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2445.1372	-0.0080
2	1	1	1	1	0	2571.0075	0.0043
3	1	3	2	1	2	3494.6362	0.0062
3	0	3	2	0	2	3651.4347	-0.0000
3	1	2	2	1	1	3852.2830	0.0015
4	1	4	3	1	3	4652.3563	0.0010
4	0	4	3	0	3	4838.9244	-0.0055
4	1	3	3	1	2	5128.1747	0.0038
5	1	5	4	1	4	5804.5979	0.0040
5	0	5	4	0	4	6003.5751	-0.0008
5	1	4	4	1	3	6396.3387	0.0043
6	1	6	5	1	5	6950.7197	-0.0025
6	0	6	5	0	5	7144.4519	-0.0090
6	1	5	5	1	4	7653.9803	0.0015
2	1	2	1	0	1	3896.7306	-0.0153
3	1	3	2	0	2	4946.2363	0.0057
4	1	4	3	0	3	5947.1556	0.0045
5	1	5	4	0	4	6912.8203	0.0052
4	0	4	3	1	3	3544.1347	0.0006
6	0	6	5	1	5	6235.2240	0.0022

7	0	7	6	1	6	7549.0470	-0.0053

Table S8.III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2329.1298	-0.0145
2	1	1	1	1	0	2568.0237	0.0051
3	0	3	2	0	2	3646.6119	-0.0062
3	1	2	2	1	1	3847.7865	0.0024
4	1	4	3	1	3	4645.7473	-0.0037
4	0	4	3	0	3	4832.3706	-0.0031
4	1	3	3	1	2	5122.1397	0.0063
5	1	5	4	1	4	5796.2908	-0.0011
5	0	5	4	0	4	5995.1930	-0.0008
5	1	4	4	1	3	6388.7169	0.0008
6	1	6	5	1	5	6940.7087	0.0082
6	0	6	5	0	5	7134.1815	-0.0106
6	1	5	5	1	4	7644.7207	-0.0010
2	1	2	1	0	1	3889.6336	-0.0044
3	1	3	2	0	2	4937.3531	-0.0008
4	1	4	3	0	3	5936.4899	0.0030
5	1	5	4	0	4	6900.4155	0.0103
4	0	4	3	1	3	3541.6422	0.0045
5	0	5	4	1	4	4891.0904	0.0098
6	0	6	5	1	5	6228.9780	-0.0028
7	0	7	6	1	6	7540.6605	-0.0063

Table S8.IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2437.2595	-0.0059
2	1	1	1	1	0	2561.1170	0.0081
3	1	3	2	1	2	3485.1969	0.0008
3	0	3	2	0	2	3640.2644	-0.0008
3	1	2	2	1	1	3837.6150	0.0014
4	1	4	3	1	3	4640.0450	-0.0079
4	0	4	3	0	3	4825.1860	0.0005
4	1	3	3	1	2	5108.9569	-0.0015
5	0	5	4	0	4	5988.0260	0.0015
5	1	4	4	1	3	6372.9161	-0.0021
6	1	6	5	1	5	6933.2666	-0.0057
6	0	6	5	0	5	7127.6946	-0.0010
6	1	5	5	1	4	7626.8430	0.0027
2	1	2	1	0	1	3910.2741	-0.0051
3	1	3	2	0	2	4958.2152	0.0052
4	1	4	3	0	3	5958.0023	0.0046
5	1	5	4	0	4	6922.4282	-0.0024
6	1	6	5	0	5	7867.6837	0.0053
4	0	4	3	1	3	3507.2518	0.0111
5	0	5	4	1	4	4855.2163	0.0040
6	0	6	5	1	5	6193.2815	-0.0080
7	0	7	6	1	6	7506.8062	-0.0008

Table S8.V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2441.5600	-0.0098
3	1	3	2	1	2	3490.6795	0.0034
3	0	3	2	0	2	3646.4938	0.0090
3	1	2	2	1	1	3845.2130	-0.0022
4	1	4	3	1	3	4647.2623	0.0037
4	0	4	3	0	3	4833.0640	0.0053
4	1	3	3	1	2	5118.9712	0.0025
5	1	5	4	1	4	5798.4835	0.0056
5	0	5	4	0	4	5997.2682	0.0013
5	1	4	4	1	3	6385.2110	-0.0031
6	1	6	5	1	5	6943.7074	-0.0046
6	0	6	5	0	5	7138.0816	0.0015
6	1	5	5	1	4	7641.2541	0.0060
3	1	3	2	0	2	4957.5019	-0.0111
4	1	4	3	0	3	5958.2775	-0.0092
5	1	5	4	0	4	6923.7056	-0.0004
6	1	6	5	0	5	7870.1544	0.0033
3	0	3	2	1	2	2179.6437	-0.0042
4	0	4	3	1	3	3522.0188	-0.0117
5	0	5	4	1	4	4872.0285	-0.0103
6	0	6	5	1	5	6211.6440	0.0031
7	0	7	6	1	6	7526.1563	0.0073

Table S8.VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2334.2500	-0.0080
2	0	2	1	0	1	2446.8449	0.0010
2	1	1	1	1	0	2572.4595	-0.0018
3	1	3	2	1	2	3497.4238	0.0042
3	0	3	2	0	2	3654.1065	0.0024
3	1	2	2	1	1	3854.5035	0.0022
4	0	4	3	0	3	4842.7015	-0.0001
4	1	3	3	1	2	5131.1989	0.0030
5	1	5	4	1	4	5809.3861	0.0054
5	0	5	4	0	4	6008.5937	0.0077
5	1	4	4	1	3	6400.2290	-0.0009
6	1	6	5	1	5	6956.5615	0.0013
6	0	6	5	0	5	7150.7961	-0.0059
6	1	5	5	1	4	7658.8430	0.0053
2	1	2	1	0	1	3905.8065	-0.0152
3	1	3	2	0	2	4956.3999	0.0026
4	1	4	3	0	3	5958.4250	0.0059
6	1	6	5	0	5	7873.0681	-0.0042
5	0	5	4	1	4	4892.8618	-0.0067
6	0	6	5	1	5	6234.2816	-0.0082
7	0	7	6	1	6	7549.9679	0.0030

Table S8.VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2445.8776	-0.0003
3	1	3	2	1	2	3497.3195	-0.0081
3	0	3	2	0	2	3653.0366	-0.0007
3	1	2	2	1	1	3851.4253	0.0015
4	0	4	3	0	3	4841.9565	0.0028
4	1	3	3	1	2	5127.2980	0.0028
5	1	5	4	1	4	5809.6625	-0.0039
5	0	5	4	0	4	6008.5932	-0.0138
5	1	4	4	1	3	6395.7105	0.0038
6	0	6	5	0	5	7151.9325	-0.0049
6	1	5	5	1	4	7653.9803	0.0048
2	1	2	1	0	1	3918.2612	-0.0064
3	1	3	2	0	2	4969.7116	-0.0057
4	1	4	3	0	3	5972.8495	0.0042
5	1	5	4	0	4	6940.5785	0.0205
6	1	6	5	0	5	7889.1563	-0.0030
4	0	4	3	1	3	3525.2894	0.0156
6	0	6	5	1	5	6219.9837	-0.0027
7	0	7	6	1	6	7537.3776	-0.0068

Table S8.VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	1	0	2535.6416	0.0007
3	1	3	2	1	2	3453.2275	-0.0011
3	0	3	2	0	2	3606.0120	0.0012
3	1	2	2	1	1	3799.5630	0.0036
4	1	4	3	1	3	4597.6693	0.0008
4	0	4	3	0	3	4780.5075	0.0005
4	1	3	3	1	2	5058.5145	0.0026
5	1	5	4	1	4	5736.9905	0.0006
5	0	5	4	0	4	5933.6121	-0.0009
5	1	4	4	1	3	6310.3695	0.0040
6	1	6	5	1	5	6870.5793	-0.0002
6	0	6	5	0	5	7064.1310	-0.0048
6	1	5	5	1	4	7552.5850	0.0032
2	1	2	1	0	1	3892.8486	-0.0160
3	1	3	2	0	2	4932.0388	0.0025
4	1	4	3	0	3	5923.6989	0.0049
5	1	5	4	0	4	6880.1826	0.0056
6	1	6	5	0	5	7817.1422	-0.0013
4	0	4	3	1	3	3454.4851	0.0037
5	0	5	4	1	4	4790.4220	-0.0039
6	0	6	5	1	5	6117.5709	-0.0009
7	0	7	6	1	6	7421.3783	-0.0058

Table S8.IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$

2	0	2	1	0	1	2431.3215	-0.0016
2	1	1	1	1	0	2554.2700	-0.0084
3	1	3	2	1	2	3477.3706	-0.0041
3	0	3	2	0	2	3631.6038	0.0057
3	1	2	2	1	1	3827.4380	0.0048
4	1	4	3	1	3	4629.7248	-0.0046
4	0	4	3	0	3	4814.0669	0.0004
4	1	3	3	1	2	5095.5181	0.0039
5	1	5	4	1	4	5776.8662	-0.0020
5	0	5	4	0	4	5974.7535	0.0005
5	1	4	4	1	3	6356.3431	0.0054
6	0	6	5	0	5	7112.5107	-0.0053
6	1	5	5	1	4	7607.3070	0.0046
1	1	1	0	0	0	2807.6693	0.0007
2	1	2	1	0	1	3909.6556	-0.0196
3	1	3	2	0	2	4955.7219	-0.0049
4	1	4	3	0	3	5953.8611	0.0030
5	1	5	4	0	4	6916.6705	0.0107
6	1	6	5	0	5	7860.0798	0.0001
4	0	4	3	1	3	3489.9222	-0.0156
5	0	5	4	1	4	4834.9647	0.0033
6	0	6	5	1	5	6170.6063	-0.0028
7	0	7	6	1	6	7482.2570	0.0050

Table S8.X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
2	1	1	1	1	0	2535.9555	0.0070
3	1	3	2	1	2	3454.2785	0.0042
3	0	3	2	0	2	3606.7488	0.0001
3	1	2	2	1	1	3800.0190	0.0013
4	1	4	3	1	3	4599.0575	-0.0015
4	0	4	3	0	3	4781.4735	-0.0016
4	1	3	3	1	2	5059.1179	0.0015
5	1	5	4	1	4	5738.7260	0.0021
5	0	5	4	0	4	5934.8095	0.0007
5	1	4	4	1	3	6311.1140	0.0055
6	1	6	5	1	5	6872.6599	0.0030
6	0	6	5	0	5	7065.5700	-0.0040
6	1	5	5	1	4	7553.4522	0.0007
2	1	2	1	0	1	3886.8950	-0.0127
3	1	3	2	0	2	4926.6256	-0.0007
4	1	4	3	0	3	5918.9360	-0.0006
5	1	5	4	0	4	6876.1907	0.0053
6	1	6	5	0	5	7814.0326	-0.0009
4	0	4	3	1	3	3461.5869	-0.0106
5	0	5	4	1	4	4797.3509	0.0037
7	0	7	6	1	6	7427.6477	-0.0045

Table S8.XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{11}$ isotopologue of conformer **Eq-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}

2	0	2	1	0	1	2420.8371	0.0033
2	1	1	1	1	0	2543.5240	0.0069
3	1	3	2	1	2	3462.1097	0.0039
3	0	3	2	0	2	3615.8062	-0.0007
4	1	4	3	1	3	4609.3530	0.0051
4	0	4	3	0	3	4792.9124	-0.0030
4	1	3	3	1	2	5073.9377	0.0000
5	1	5	4	1	4	5751.3581	-0.0021
5	0	5	4	0	4	5948.1931	-0.0011
5	1	4	4	1	3	6329.3084	0.0004
6	1	6	5	1	5	6887.5275	0.0001
6	0	6	5	0	5	7080.5435	-0.0032
6	1	5	5	1	4	7574.7681	-0.0004
2	1	2	1	0	1	3885.0685	-0.0071
3	1	3	2	0	2	4926.3482	0.0006
4	1	4	3	0	3	5919.8938	0.0052
5	1	5	4	0	4	6878.3344	0.0009
6	1	6	5	0	5	7817.6644	-0.0023
4	0	4	3	1	3	3482.3712	-0.0034
5	0	5	4	1	4	4821.2203	-0.0006
6	0	6	5	1	5	6150.4045	-0.0029
7	0	7	6	1	6	7455.3882	0.0043

Table S9.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-a** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2348.7212	0.0024
2	0	2	1	0	1	2470.5875	-0.0019
2	1	1	1	1	0	2608.2962	-0.0054
3	1	3	2	1	2	3518.2694	0.0001
3	0	3	2	0	2	3686.2744	-0.0017
3	1	2	2	1	1	3907.3398	-0.0009
4	1	4	3	1	3	4682.4636	0.0013
4	0	4	3	0	3	4879.5297	0.0011
4	1	3	3	1	2	5199.8141	-0.0015
5	1	5	4	1	4	5840.1770	0.0078
5	0	5	4	0	4	6046.0549	-0.0004
5	1	4	4	1	3	6482.8140	-0.0015
6	1	6	5	1	5	6990.7544	0.0026
6	0	6	5	0	5	7185.8556	-0.0005
6	1	5	5	1	4	7752.8263	-0.0012
3	2	2	2	2	1	3717.7662	0.0005
3	2	1	2	2	0	3749.2462	-0.0071
4	2	3	3	2	2	4950.8535	0.0008
4	2	2	3	2	1	5028.3425	0.0120
5	2	4	4	2	3	6178.6766	0.0022
5	2	3	4	2	2	6328.8014	-0.0075
6	2	5	5	2	4	7399.9696	-0.0001
6	2	4	5	2	3	7649.2744	-0.0097
3	0	3	2	1	2	2279.8787	-0.0007
4	0	4	3	1	3	3641.1379	-0.0008
5	0	5	4	1	4	5004.7346	0.0029
6	0	6	5	1	5	6350.4197	0.0012
7	0	7	6	1	6	7663.4077	0.0009
1	1	1	0	0	0	2767.5143	-0.0081
2	1	2	1	0	1	3876.9769	-0.0091
3	1	3	2	0	2	4924.6643	-0.0016
4	1	4	3	0	3	5920.8519	-0.0003
5	1	5	4	0	4	6881.4938	0.0010
6	1	6	5	0	5	7826.1894	0.0001
1	1	0	0	0	0	2897.3285	0.0147
2	1	1	1	0	1	4266.3538	-0.0064
4	1	3	3	0	3	7216.6567	0.0056
3	1	2	3	0	3	2016.8365	0.0011
4	1	3	4	0	4	2337.1250	0.0025
5	1	4	5	0	5	2773.8863	0.003
6	1	5	6	0	6	3340.8529	-0.0013
4	3	1	3	3	0	4973.8141	0.0081
5	3	3	4	3	2	6220.4511	-0.0049
6	3	4	5	3	3	7471.0759	-0.0024
6	3	3	5	3	2	7487.7525	0.0037

Table S10.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Ax-a** of **carvone**.

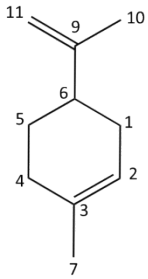
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	3246.2992	0.0040
2	0	2	1	0	1	3355.9144	-0.0016
2	1	1	1	1	0	3495.2259	0.0017
3	0	3	2	0	2	4998.1064	-0.0021
3	1	3	2	1	2	4860.6472	-0.0020
3	1	2	2	1	1	5232.9293	0.0022
4	0	4	3	0	3	6604.2398	-0.0002
4	1	4	3	1	3	6465.9277	0.0017
4	1	3	3	1	2	6957.1491	-0.0044
3	2	2	2	2	1	5056.1469	0.0092
3	2	1	2	2	0	5114.1374	-0.0160
4	2	3	3	2	2	6729.9172	0.0065
4	2	2	3	2	1	6867.0760	-0.0018
1	1	1	0	0	0	2402.2810	0.0008
2	1	2	1	0	1	3963.1924	-0.0019
3	1	3	2	0	2	5467.9268	-0.0007
4	1	4	3	0	3	6935.7436	-0.0015
2	0	2	1	1	1	2639.0200	0.0031
3	0	3	2	1	2	4390.8300	-0.0002
4	0	4	3	1	3	6134.4203	-0.0006
5	0	5	4	1	4	7846.3356	0.0011
2	1	1	1	0	1	4336.5898	0.0021
3	1	2	2	0	2	6213.6018	0.0030

Table S11.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Ax-C** of **carvone**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	1	1	1	0	3406.1321	-0.0002
2	0	2	1	0	1	3289.2443	0.0002
2	1	2	1	1	1	3192.1944	0.0008
3	1	3	2	1	2	4782.3441	0.0001
3	0	3	2	0	2	4909.6180	-0.0011
3	1	2	2	1	1	5102.6735	-0.0013
4	1	4	3	1	3	6366.1364	0.0019
4	0	4	3	0	3	6503.8701	0.0035
4	1	3	3	1	2	6790.5646	-0.0024
5	1	5	4	1	4	7942.6387	0.0036
1	1	1	0	0	0	2459.1069	0.0008
2	1	2	1	0	1	4001.7167	-0.0007
3	1	3	2	0	2	5494.8174	0.0000
4	1	4	3	0	3	6951.3256	-0.0071
2	0	2	1	1	1	2479.7243	0.0041
3	0	3	2	1	2	4197.1473	0.0015
4	0	4	3	1	3	5918.6675	-0.0009
5	0	5	4	1	4	7623.4478	0.0003
2	1	1	1	0	1	4322.6359	0.0103
3	1	2	2	0	2	6136.0526	-0.0037
2	2	0	1	1	0	5844.6307	0.0014
3	2	1	2	2	0	4987.8492	-0.0060
4	2	2	3	2	1	6684.9586	-0.0053

4	3	2	3	3	1	6616.5571	0.0042
4	3	1	3	3	0	6619.9987	0.0009

Table S12.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-A** of **limonene**.



J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	3	0	3	2248.4633	-0.0018
2	1	2	2	0	2	2303.6163	-0.0078
1	1	1	1	0	1	2340.9576	-0.0075
1	1	0	1	0	1	2378.7598	0.0001
2	1	1	2	0	2	2417.0071	-0.0007
3	1	2	3	0	3	2475.2293	0.0002
4	1	3	4	0	4	2554.4370	0.0022
5	1	4	5	0	5	2655.9607	0.0032
2	1	2	1	1	1	2754.8155	0.0018
2	0	2	1	0	1	2792.1536	-0.0011
2	1	1	1	1	0	2830.4014	-0.0014
4	0	4	3	1	3	3332.2172	0.0038
1	1	1	0	0	0	3737.2660	-0.0036
1	1	0	0	0	0	3775.0590	-0.0052
3	1	3	2	1	2	4131.9371	-0.0005
3	2	2	2	2	1	4188.9094	-0.0004
3	2	1	2	2	0	4190.7285	0.0033
3	0	3	2	0	2	4187.0979	0.0013
3	1	2	2	1	1	4245.3195	0.0017
5	0	5	4	1	4	4795.9466	0.0044
2	1	2	1	0	1	5095.7763	-0.0025
2	1	1	1	0	1	5209.1617	-0.0008
4	1	4	3	1	3	5508.7271	0.0006
4	0	4	3	0	3	5580.6766	-0.0019
4	2	3	3	2	2	5584.8654	0.0072
4	3	2	3	3	1	5586.1171	0.0116
4	3	1	3	3	0	5586.1171	-0.0088
4	2	2	3	2	1	5589.3902	-0.0036
4	1	3	3	1	2	5659.8865	0.0022
3	1	3	2	0	2	6435.5591	-0.0026
3	1	2	2	0	2	6662.3263	0.0006
5	1	5	4	1	4	6885.0749	-0.0019
5	0	5	4	0	4	6972.4545	-0.0009
5	2	4	4	2	3	6980.5003	-0.0021
5	2	3	4	2	2	6989.5657	0.0042
5	1	4	4	1	3	7073.9753	-0.0028
4	1	4	3	0	3	7757.1879	-0.0037
6	1	5	6	0	6	2781.4281	-0.0005
7	1	6	7	0	7	2932.7427	0.0004
5	2	4	5	1	5	7364.8167	0.0093
6	2	5	6	1	6	7479.6607	-0.0217
4	0	4	3	1	2	3105.4468	-0.0027
8	1	7	8	0	8	3112.0095	0.0107
7	1	6	6	2	4	3182.2388	-0.0129
7	1	6	6	2	5	3213.9556	0.0243
9	1	8	9	0	9	3321.4221	-0.0031
5	0	5	4	1	3	4418.0186	-0.0019
6	0	6	5	1	4	5706.0326	-0.0068
6	0	6	5	1	5	6272.8702	0.0079
8	2	6	8	1	7	6503.9045	0.0031

7	2	5	7	1	6	6613.5375	0.0081
6	2	4	6	1	5	6717.9636	0.0011
5	2	3	5	1	4	6813.8559	0.0074
4	2	2	4	1	3	6898.2719	0.0068
7	0	7	6	1	5	6967.4669	-0.0050
3	2	1	3	1	2	6968.7748	0.0192
2	2	0	2	1	1	7023.3421	-0.0061
7	2	6	7	1	7	7614.1651	-0.0108
7	0	7	6	1	6	7760.8640	-0.0075

Table S12.II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2750.3909	0.0086
2	0	2	1	0	1	2789.1135	-0.0024
3	1	3	2	1	2	4125.2657	0.0008
3	0	3	2	0	2	4182.4297	-0.0055
3	1	2	2	1	1	4242.9495	0.0029
4	1	4	3	1	3	5499.7763	-0.0062
4	0	4	3	0	3	5574.2767	0.0057
4	1	3	3	1	2	5656.6651	-0.0082
1	1	1	0	0	0	3705.2310	-0.0042
2	1	2	1	0	1	5060.8107	-0.0010
3	1	3	2	0	2	6396.9661	0.0054
1	1	0	0	0	0	3744.4546	-0.0091
3	1	2	2	0	2	6632.3369	0.0089

Table S12.III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2742.9992	-0.0124
3	1	3	2	1	2	4114.2209	0.0054
3	0	3	2	0	2	4170.8411	-0.0008
3	1	2	2	1	1	4230.7287	-0.0071
4	1	4	3	1	3	5485.0653	0.0028
4	0	4	3	0	3	5558.8648	0.0007
4	1	3	3	1	2	5640.4082	0.0030
1	1	1	0	0	0	3707.3299	0.00520
2	1	2	1	0	1	5059.4165	0.0071
3	1	3	2	0	2	6392.2512	-0.0048
1	1	0	0	0	0	3746.1491	-0.0169
2	1	1	1	0	1	5175.9434	0.0099
3	1	2	2	0	2	6625.3000	-0.0004

Table S12.IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2737.7131	-0.0076
2	0	2	1	0	1	2774.5956	-0.0038
3	1	3	2	1	2	4106.3028	-0.0027
3	0	3	2	0	2	4160.7910	-0.0030
3	1	2	2	1	1	4218.2675	0.0046
4	1	4	3	1	3	5474.5670	0.0027
4	0	4	3	0	3	5545.6650	0.0001

4	1	3	3	1	2	5623.8292	0.0036
1	1	1	0	0	0	3733.1113	0.0066
2	1	2	1	0	1	5083.3075	0.0030
3	1	3	2	0	2	6415.0113	0.0007
1	1	0	0	0	0	3770.4166	-0.0083
3	1	2	2	0	2	6638.9266	-0.0021

Table S12.V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2742.6070	0.0023
2	0	2	1	0	1	2781.0999	-0.0018
3	1	3	2	1	2	4113.6025	0.0000
3	0	3	2	0	2	4170.4288	-0.0018
3	1	2	2	1	1	4230.5523	-0.0021
4	1	4	3	1	3	5484.2442	0.0038
4	0	4	3	0	3	5558.3005	0.0042
4	1	3	3	1	2	5640.1557	-0.0027
1	1	1	0	0	0	3704.3034	-0.0024
2	1	2	1	0	1	5056.1186	0.0034
3	1	3	2	0	2	6388.6088	-0.0072
1	1	0	0	0	0	3743.2930	0.0019
2	1	1	1	0	1	5173.0788	0.0079
3	1	2	2	0	2	6622.5200	-0.0036

Table S12.VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2750.7347	-0.0098
2	0	2	1	0	1	2789.3645	0.0012
3	1	3	2	1	2	4125.8170	0.0067
3	0	3	2	0	2	4182.8172	0.0023
3	1	2	2	1	1	4243.1335	-0.0039
4	1	4	3	1	3	5500.5150	0.0013
4	0	4	3	0	3	5574.7958	0.0025
4	1	3	3	1	2	5656.9308	-0.0009
1	1	1	0	0	0	3707.6233	-0.0043
2	1	2	1	0	1	5063.4383	-0.0060
1	1	0	0	0	0	3746.7502	0.0123
3	1	2	2	0	2	6634.5493	0.0000

Table S12.VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2752.9638	0.0073
2	0	2	1	0	1	2790.1235	0.0008
3	1	3	2	1	2	4129.1581	0.0040
3	0	3	2	0	2	4184.0567	-0.0018
3	1	2	2	1	1	4241.9955	-0.0029
4	1	4	3	1	3	5505.0227	0.0029
4	0	4	3	0	3	5576.6369	-0.0092
4	1	3	3	1	2	5655.4655	0.0023
1	1	1	0	0	0	3734.5999	-0.0024
2	1	2	1	0	1	5092.2712	-0.0010
3	1	3	2	0	2	6431.3084	0.0048
4	1	4	3	0	3	7752.2608	-0.0041
3	1	2	2	0	2	6656.9983	0.0027

Table S12.VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2741.9320	-0.0003
2	1	1	1	1	0	2778.7879	-0.0024
3	1	3	2	1	2	4058.6151	0.0073
3	0	3	2	0	2	4111.8518	0.0034
3	1	2	2	1	1	4167.9088	-0.0117
4	1	4	3	1	3	5410.9959	0.0034
4	0	4	3	0	3	5480.5046	-0.0020
4	1	3	3	1	2	5556.7310	0.0023
1	1	1	0	0	0	3725.1709	0.0080
2	1	2	1	0	1	5059.8847	-0.0151
3	1	3	2	0	2	6376.5782	0.0029
4	1	4	3	0	3	7675.7176	-0.0019
1	1	0	0	0	0	3761.6033	0.0018
3	1	2	2	0	2	6595.2080	0.0042

Table S12.IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2736.8055	0.0038
2	0	2	1	0	1	2773.6340	-0.0029
3	1	3	2	1	2	4104.9257	-0.0020
3	0	3	2	0	2	4159.3488	-0.0040
3	1	2	2	1	1	4216.7542	0.0030
4	1	4	3	1	3	5472.7398	0.0114
4	0	4	3	0	3	5543.7400	-0.0081
4	1	3	3	1	2	5621.8068	-0.0044
1	1	1	0	0	0	3732.5282	0.0009
2	1	2	1	0	1	5082.2921	0.0021
3	1	3	2	0	2	6413.5777	-0.0031
1	1	0	0	0	0	3769.7951	-0.0078
3	1	2	2	0	2	6637.2391	0.0080

Table S12.X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2725.5529	0.0101
2	0	2	1	0	1	2760.6720	0.0002
2	1	1	1	1	0	2796.6031	-0.0066
3	1	3	2	1	2	4088.0658	0.0041
3	0	3	2	0	2	4139.9949	-0.0002
3	1	2	2	1	1	4194.6582	-0.0009
4	0	4	3	0	3	5518.0962	-0.0090
4	1	3	3	1	2	5592.4006	0.0027
1	1	1	0	0	0	3701.9932	-0.0099
2	1	2	1	0	1	5047.0088	0.0014
1	1	0	0	0	0	3737.5412	0.0047
3	1	2	2	0	2	6587.5989	0.0039

Table S12.XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{11}$ isotopologue of conformer **Eq-A** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2754.3017	-0.0098
3	1	3	2	1	2	4078.5975	0.0125
3	0	3	2	0	2	4130.4631	0.0043
3	1	2	2	1	1	4185.0443	-0.0076
4	1	4	3	1	3	5437.6470	-0.0008
4	0	4	3	0	3	5505.3987	0.0007
4	1	3	3	1	2	5579.5894	-0.0009
1	1	1	0	0	0	3702.8912	0.0027
1	1	0	0	0	0	3738.3776	-0.0008
3	1	2	2	0	2	6581.9698	0.0044
3	1	3	2	0	2	6369.0225	-0.0063

Table S13.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	2	0	2	2219.0294	-0.00692
1	1	1	1	0	1	2311.6135	-0.00364
1	1	0	1	0	1	2407.0991	0.00420
2	1	1	2	0	2	2505.4773	0.00772
3	1	2	3	0	3	2658.4184	0.00104
2	1	2	1	1	1	2682.2461	-0.00006
2	0	2	1	0	1	2774.8248	-0.00218
4	0	4	3	1	2	2868.2135	-0.00298
4	1	3	4	0	4	2872.2199	-0.00068
2	1	1	1	1	0	2873.2019	0.00023
5	1	4	5	0	5	3154.7998	-0.00143
4	0	4	3	1	3	3441.0290	0.00096
1	1	1	0	0	0	3700.4780	-0.00137
1	1	0	0	0	0	3795.9572	0.00008
3	1	3	2	1	2	4021.5835	-0.00051
3	0	3	2	0	2	4155.0127	-0.00182
3	1	2	2	1	1	4307.9635	0.00120
2	1	2	1	0	1	4993.8600	-0.00330
2	1	1	1	0	1	5280.2990	0.00244
4	1	4	3	1	3	5358.8570	0.00135
4	0	4	3	0	3	5526.6334	-0.00044
4	1	3	3	1	2	5740.4365	-0.00057
5	1	5	4	1	4	6693.4974	0.00068
5	0	5	4	0	4	6887.1578	0.00513
5	1	4	4	1	3	7169.7328	-0.00051
3	1	3	2	0	2	6240.6162	-0.00413
4	1	4	3	0	3	7444.4591	-0.00236
3	1	2	2	0	2	6813.4365	0.00461
5	2	3	4	2	2	6994.9983	-0.00589
6	1	5	6	0	6	3515.0638	0.00312
7	1	6	6	2	4	3716.0325	0.00169
7	1	6	7	0	7	3961.8218	-0.00643
5	0	5	4	1	3	4014.9300	-0.00209
3	2	1	2	2	0	4178.1679	0.01335
9	2	8	9	1	8	5047.3799	0.01779
6	0	6	5	1	4	5079.7812	-0.00294
8	2	7	8	1	7	5432.3088	-0.00803
4	2	3	3	2	2	5553.1910	0.00112
4	2	2	3	2	1	5582.0015	0.00277
7	2	6	7	1	6	5784.5210	-0.00328
7	0	7	6	1	5	6052.7977	0.00165
6	2	5	6	1	5	6099.6367	-0.00191
6	2	4	6	1	5	6298.5900	-0.00348
5	2	4	5	1	4	6374.3546	-0.00189
5	2	3	5	1	4	6474.7725	-0.00066
6	0	6	5	1	5	6510.4150	0.00130
4	2	3	4	1	3	6606.2250	-0.00147
4	2	2	4	1	3	6649.5100	0.00772
3	2	1	3	1	2	6807.9345	-0.00611
5	2	4	4	2	3	6937.8572	-0.00613
3	2	1	3	1	3	7380.7341	-0.01807
4	2	2	4	1	4	7603.9081	0.01286
5	2	3	5	1	5	7905.4120	0.00928

Table S13.II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2678.7261	0.00100
2	0	2	1	0	1	2772.0988	0.01525
3	1	3	2	1	2	4016.2424	-0.00648
3	0	3	2	0	2	4150.6774	-0.00364
3	1	2	2	1	1	4305.2181	-0.00268
4	1	4	3	1	3	5351.6416	-0.00455
4	0	4	3	0	3	5520.4550	-0.00086
5	1	5	4	1	4	6684.3443	0.00551

Table S13.III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2764.5546	0.00462
2	1	1	1	1	0	2863.3623	0.00566
3	1	3	2	1	2	4005.6400	-0.01004
3	0	3	2	0	2	4139.4695	0.00496
3	1	2	2	1	1	4293.1555	-0.00446
4	1	4	3	1	3	5337.5473	-0.00410
4	0	4	3	0	3	5505.6503	-0.00415
4	1	3	3	1	2	5720.6326	-0.00042
5	1	5	4	1	4	6666.7855	0.00854

Table S13.IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2757.3150	-0.00424
2	1	1	1	1	0	2854.4355	0.00702
3	1	3	2	1	2	3997.0400	0.00293
3	0	3	2	0	2	4128.9439	-0.00009
3	1	2	2	1	1	4279.8490	-0.00269
4	1	4	3	1	3	5326.1998	-0.01117
4	0	4	3	0	3	5492.2235	-0.00078
5	1	5	4	1	4	6652.8287	0.00836

Table S13.V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2763.4625	-0.01097
3	1	3	2	1	2	4003.9865	-0.00189
3	0	3	2	0	2	4137.8344	-0.00415
3	1	2	2	1	1	4291.6105	0.01053
4	1	4	3	1	3	5335.3346	0.00365
4	0	4	3	0	3	5503.4682	0.00225
4	1	3	3	1	2	5718.5427	-0.00470
5	1	5	4	1	4	6663.9947	0.00077

Table S13.VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2771.9627	-0.01995
3	1	3	2	1	2	4015.3345	-0.00036
3	0	3	2	0	2	4150.4388	0.00108
3	1	2	2	1	1	4305.8970	0.00021
4	1	4	3	1	3	5350.3897	0.00286
4	0	4	3	0	3	5519.9619	-0.00075
4	1	3	3	1	2	5737.5327	0.00481
5	1	5	4	1	4	6682.7045	0.00189

Table S13.VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Eq-C** of **limonene.**

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2772.8612	-0.00147
3	1	3	2	1	2	4018.9803	0.00893
3	0	3	2	0	2	4152.0958	0.00096
3	1	2	2	1	1	4304.6634	0.00020
4	0	4	3	0	3	5522.7900	-0.00026
4	1	4	3	1	3	5355.3720	-0.01206
5	1	5	4	1	4	6689.1800	0.00442

Table S13.VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	1	3	2	1	2	3951.6575	-0.00089
3	0	3	2	0	2	4080.7423	0.00798
3	1	2	2	1	1	4227.8904	0.00643
4	0	4	3	0	3	5428.5668	-0.00866
4	1	3	3	1	2	5633.9255	-0.00548
5	0	5	4	0	4	6766.1071	0.00319

Table S13.IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2756.5215	-0.01203
2	1	2	1	1	1	2665.1508	0.00496
2	1	1	1	1	0	2853.5460	-0.00613
3	0	3	2	0	2	4127.7737	-0.00335
3	1	2	2	1	1	4278.5486	0.00846
3	1	3	2	1	2	3995.9844	0.00107
4	0	4	3	0	3	5490.6917	0.00196

Table S13.X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2647.3794	-0.00923
2	0	2	1	0	1	2738.2707	0.00270
3	0	3	2	0	2	4100.3912	0.00291
3	1	2	2	1	1	4250.3695	-0.00085
4	0	4	3	0	3	5454.1870	-0.00285
4	1	3	3	1	2	5663.7528	0.00030
5	1	5	4	1	4	6606.7068	0.00342

Table S13.XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{11}$ isotopologue of conformer **Eq-C** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2651.2901	0.00833
2	0	2	1	0	1	2742.4195	0.00080
3	1	3	2	1	2	3975.1725	-0.00601
3	0	3	2	0	2	4106.5722	0.00319
3	1	2	2	1	1	4257.0265	0.00075
4	1	3	3	1	2	5672.6040	0.00016

Table S14.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-a** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	2676.9171	0.00455
2	0	2	1	0	1	2775.4819	-0.00065
2	1	1	1	1	0	2880.6955	0.00711
3	1	3	2	1	2	4013.3324	0.00455
3	1	2	2	1	1	4318.9263	0.00225
4	1	4	3	1	3	5347.3877	0.00026
4	0	4	3	0	3	5524.6340	0.00193
4	1	3	3	1	2	5754.5374	0.00342
5	1	5	4	1	4	6678.4587	0.00017
5	0	5	4	0	4	6881.6762	-0.00657
5	1	4	4	1	3	7186.4888	0.00667
1	1	1	0	0	0	3684.2278	-0.00955
2	1	2	1	0	1	4971.7490	-0.00066
3	1	3	2	0	2	6209.5953	0.00033
4	1	4	3	0	3	7402.0297	-0.00029
4	0	4	3	1	3	3469.9883	-0.00122
5	0	5	4	1	4	5004.2776	-0.00725
6	0	6	5	1	5	6549.7982	-0.00234

Table S15.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Ax-a** of **limonene**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1	3647.0734	0.00595
2	0	2	1	0	1	3677.9947	-0.00032
2	1	1	1	1	0	3710.1237	-0.00555
3	1	3	2	1	2	5470.2174	-0.00006
3	0	3	2	0	2	5515.4861	0.00353
3	1	2	2	1	1	5564.8011	-0.00193
4	1	4	3	1	3	7292.9169	-0.00003
4	0	4	3	0	3	7351.1723	0.00566
4	1	3	3	1	2	7418.9916	-0.00617
1	1	0	0	0	0	3098.5446	-0.00045
2	1	1	1	0	1	4969.3752	0.00070
3	1	2	2	0	2	6856.1822	-0.00031
1	1	1	0	0	0	3067.0114	-0.00275
2	1	2	1	0	1	4874.7812	-0.00061
3	1	3	2	0	2	6667.0064	0.00214
2	0	2	1	1	1	2450.2853	0.00464
3	0	3	2	1	1	4224.0950	-0.00809
4	0	4	3	1	2	6010.4595	-0.00720
4	0	4	3	1	3	6199.6365	-0.00846
3	0	3	2	1	2	4318.6906	-0.00518
2	0	2	1	1	0	2418.7519	0.00214
4	1	4	3	2	1	3464.4906	0.00161
5	1	4	4	2	3	5698.5765	0.00799
2	2	1	1	1	0	7393.3023	0.01870
5	2	4	5	1	5	3969.3051	0.00522
4	2	3	4	1	4	3889.2233	-0.00424
3	2	2	3	1	3	3825.4194	-0.01214
5	2	3	5	1	4	3517.4408	0.00059
4	2	2	4	1	3	3582.9500	0.00263

3	2	1	3	1	2	3639.2473	-0.00239
5	2	4	5	1	4	3496.5385	0.00264
4	2	3	4	1	3	3573.9678	-0.00065
3	2	2	3	1	2	3636.2456	-0.00768

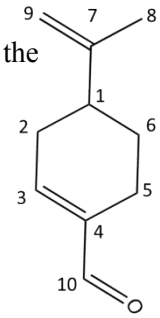


Table S16.I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2093.2959	-0.00121
2	1	1	1	1	0	2119.8626	-0.00630
2	1	2	1	1	1	2067.1554	-0.00175
3	0	3	2	0	2	3139.4044	0.00003
3	1	3	2	1	2	3100.5999	-0.00042
3	1	2	2	1	1	3179.6660	-0.00084
4	0	4	3	0	3	4184.8629	0.00025
4	1	4	3	1	3	4133.8804	-0.00214
4	1	3	3	1	2	4239.2984	-0.00099
5	0	5	4	0	4	5229.4585	0.00106
5	1	5	4	1	4	5166.9528	0.00007
5	1	4	4	1	3	5298.7081	-0.00072
6	0	6	5	0	5	6272.9767	-0.00088
6	1	6	5	1	5	6199.7598	-0.00219
6	1	5	5	1	4	6357.8334	-0.00177
7	0	7	6	0	6	7315.2177	-0.00052
7	1	7	6	1	6	7232.2636	-0.00050
7	1	6	6	1	5	7416.6143	-0.00130
1	1	1	0	0	0	3442.8840	-0.00160
1	1	0	0	0	0	3469.2399	-0.00158
2	1	2	1	0	1	4463.2863	0.00038
2	1	1	1	0	1	4542.3521	-0.00145
3	1	3	2	0	2	5470.5858	-0.00333
3	1	2	2	0	2	5628.7198	-0.00347
4	1	3	3	0	3	6728.6187	0.00041
4	1	4	3	0	3	6465.0650	-0.00229
5	1	5	4	0	4	7447.1546	-0.00277
5	1	4	4	0	4	7842.4700	0.00554
5	0	5	4	1	4	2949.2538	0.00100
6	0	6	5	1	4	3659.9810	0.01044
6	0	6	5	1	5	4055.2784	0.00075
7	0	7	6	1	6	5170.7446	0.01071
8	0	8	7	1	7	6294.4714	0.01656
1	1	1	1	0	1	2396.1254	-0.00337
1	1	0	1	0	1	2422.4872	0.00255
2	1	1	2	0	2	2449.0561	-0.00034
2	1	2	2	0	2	2369.9804	-0.00841
3	1	3	3	0	3	2331.1795	-0.00526
3	1	2	3	0	3	2489.3231	0.00420
4	1	3	4	0	4	2543.7596	0.00396
5	1	4	5	0	5	2613.0116	0.00458
2	2	0	2	1	1	7188.6062	0.00460
2	2	1	2	1	2	7267.4511	-0.00190
3	2	2	3	1	3	7307.1229	0.00290
3	2	1	3	1	3	7308.2046	0.00355
3	2	2	3	1	2	7148.9834	-0.00246
3	2	1	3	1	2	7150.0714	0.00449
5	2	3	5	1	4	7038.6955	0.00788
6	2	4	6	1	5	6967.9615	0.00444
6	2	5	6	1	6	7506.2072	-0.01573

7	2	5	7	1	6	6888.9998	0.00409
7	2	6	7	1	7	7599.5465	-0.00587
8	2	7	8	1	8	7706.5034	-0.01289
8	2	6	8	1	7	6803.4465	0.01419
3	2	2	2	2	1	3140.2614	-0.00592
3	2	1	2	2	0	3141.1407	0.00856
4	2	3	3	2	2	4186.8540	0.00062
4	2	2	3	2	1	4189.0167	0.00191
4	3	2	3	3	1	4187.4529	0.00531
4	3	1	3	3	0	4187.4529	-0.00134
5	2	4	4	2	3	5233.2883	-0.00569
5	2	3	4	2	2	5237.6230	0.00887
6	2	5	5	2	4	6279.5568	0.00399
6	2	4	5	2	3	6287.0991	-0.00550
6	3	4	5	3	3	6281.7035	0.02399
6	3	3	5	3	2	6281.7035	-0.03809
7	2	6	6	2	5	7325.5940	0.00046
7	2	5	6	2	4	7337.6515	-0.00275
7	3	5	6	3	4	7329.0772	0.07944
7	3	4	6	3	3	7329.0772	-0.06019
5	0	5	4	1	3	2685.6966	-0.00520
6	0	6	5	1	4	3659.9672	-0.00336
7	0	7	6	1	5	4617.3481	-0.00552
8	0	8	7	1	6	5556.7153	-0.00777
9	0	9	8	1	7	6476.8334	-0.00582
10	0	10	9	1	8	7376.3750	-0.00258

Table S16.II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
3	0	3	2	0	2	3135.3553	0.00184
3	1	3	2	1	2	3096.7498	-0.00196
3	1	2	2	1	1	3175.3991	0.00112
4	0	4	3	0	3	4179.4707	-0.00150
4	1	4	3	1	3	4128.7556	0.00182
4	1	3	3	1	2	4233.6101	-0.00022
5	0	5	4	0	4	5222.7322	-0.00444
5	1	5	4	1	4	5160.5459	-0.00010
5	1	4	4	1	3	5291.5952	-0.00674
6	1	6	5	1	5	6192.0795	-0.00050
6	1	5	5	1	4	6349.3087	-0.00484
7	0	7	6	0	6	7305.8730	0.00008
7	1	7	6	1	6	7223.3119	0.00189
7	1	6	6	1	5	7406.6932	0.01019

Table S16.III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	ν_{obs}-ν_{calc}
3	0	3	2	0	2	3136.8417	0.00342
3	1	3	2	1	2	3097.1289	0.01127
3	1	2	2	1	1	3178.1040	-0.00018

4	0	4	3	0	3	4181.3941	0.01288
4	1	4	3	1	3	4129.2363	0.01212
4	1	3	3	1	2	4237.2033	0.00272
5	0	5	4	0	4	5225.0265	0.01693
5	1	4	4	1	3	5296.0706	0.01014
6	0	6	5	0	5	6267.5255	0.02551
6	1	6	5	1	5	6192.7149	0.00232
6	1	5	5	1	4	6354.6259	0.00582
7	0	7	6	0	6	7308.6450	0.00868
7	1	7	6	1	6	7224.0068	0.01263
7	1	6	6	1	5	7412.8307	0.01810

Table S16.IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3133.2814	-0.00394
3	1	3	2	1	2	3093.6398	-0.00262
4	0	4	3	0	3	4176.6588	0.00935
4	1	4	3	1	3	4124.5935	0.00159
4	1	3	3	1	2	4232.3465	-0.00405
5	0	5	4	0	4	5219.1043	0.00069
5	1	5	4	1	4	5155.3081	-0.01006
5	1	4	4	1	3	5289.9977	-0.00248
6	0	6	5	0	5	6260.4281	0.00249
6	1	5	5	1	4	6347.3504	-0.00073
7	0	7	6	0	6	7300.3959	-0.00441
7	1	7	6	1	6	7215.9049	0.00647
7	1	6	6	1	5	7404.3407	0.00378

Table S16.V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3129.8939	0.00401
3	1	3	2	1	2	3091.2797	0.00814
3	1	2	2	1	1	3169.9375	-0.01355
4	0	4	3	0	3	4172.1900	0.00258
4	1	4	3	1	3	4121.4505	0.00366
4	1	3	3	1	2	4226.3473	-0.00044
5	0	5	4	0	4	5213.6323	0.00165
5	1	5	4	1	4	5151.4005	-0.01181
5	1	4	4	1	3	5282.5155	-0.00821
6	0	6	5	0	5	6253.9991	-0.01149
6	1	6	5	1	5	6181.1196	0.00004
6	1	5	5	1	4	6338.4256	0.00593
7	0	7	6	0	6	7293.1282	0.00376
7	1	7	6	1	6	7210.5265	0.00369
7	1	6	6	1	5	7393.9812	0.00770

Table S16.VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$

3	0	3	2	0	2	3133.5405	0.00081
3	1	3	2	1	2	3093.4875	0.00165
3	1	2	2	1	1	3175.1786	0.00780
4	0	4	3	0	3	4176.9707	0.00969
4	1	4	3	1	3	4124.3819	0.00553
4	1	3	3	1	2	4233.2887	0.00492
5	0	5	4	0	4	5219.4556	0.00670
5	1	5	4	1	4	5155.0597	0.02173
5	1	4	4	1	3	5291.1689	0.01361
6	0	6	5	0	5	6260.7984	0.02282
6	1	6	5	1	5	6185.4241	0.00603
6	1	5	5	1	4	6348.7199	-0.00032
7	0	7	6	0	6	7300.7347	0.01399
7	1	7	6	1	6	7215.4780	0.01087

Table S16.VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3135.6555	-0.00772
3	1	3	2	1	2	3095.5974	0.01597
3	1	2	2	1	1	3177.3230	0.00117
4	0	4	3	0	3	4179.7925	-0.00018
4	1	4	3	1	3	4127.1692	-0.00135
4	1	3	3	1	2	4236.1462	-0.00570
5	0	5	4	0	4	5222.9852	-0.00377
5	1	5	4	1	4	5158.5256	-0.00521
5	1	4	4	1	3	5294.7487	0.00813
6	1	6	5	1	5	6189.6067	-0.00293
6	1	5	5	1	4	6353.0263	0.00355
7	0	7	6	0	6	7305.6807	0.00219
7	1	7	6	1	6	7220.3596	0.00212
7	1	6	6	1	5	7410.9260	-0.00413

Table S16.VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3117.6118	-0.00886
3	1	3	2	1	2	3079.3654	0.01058
3	1	2	2	1	1	3157.3144	0.01154
4	0	4	3	0	3	4155.8458	-0.00092
4	1	4	3	1	3	4105.5591	-0.00326
4	1	3	3	1	2	4209.4944	0.00627
5	0	5	4	0	4	5193.2355	0.00143
5	1	5	4	1	4	5131.5593	-0.00457
5	1	4	4	1	3	5261.4484	-0.00836
6	0	6	5	0	5	6229.5793	0.00185
6	1	6	5	1	5	6157.3136	0.00184
6	1	5	5	1	4	6313.1487	-0.00187
7	0	7	6	0	6	7264.6774	-0.00017
7	1	7	6	1	6	7182.7610	-0.00003

Table S16.IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_8$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3099.2124	-0.00009
3	1	3	2	1	2	3062.4913	0.00755
3	1	2	2	1	1	3137.2466	-0.00707
4	0	4	3	0	3	4131.3738	-0.00047
4	1	4	3	1	3	4083.0916	0.00629
4	1	3	3	1	2	4182.7680	-0.00611
5	0	5	4	0	4	5162.7688	0.01022
5	1	5	4	1	4	5103.4949	-0.00078
5	1	4	4	1	3	5228.0942	0.00033
6	0	6	5	0	5	6193.1747	-0.00018
6	1	6	5	1	5	6123.6702	-0.00039
7	0	7	6	0	6	7222.4352	-0.00260
7	1	7	6	1	6	7143.5600	-0.00805
7	1	6	6	1	5	7317.9180	0.00417

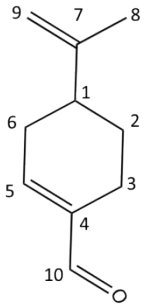
Table S16.X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3105.4790	0.00198
3	1	3	2	1	2	3068.6232	-0.00439
3	1	2	2	1	1	3143.6499	-0.00217
4	0	4	3	0	3	4139.7113	-0.00659
4	1	4	3	1	3	4091.2639	-0.01095
4	1	3	3	1	2	4191.2996	-0.00339
5	0	5	4	0	4	5173.1775	0.00397
5	1	5	4	1	4	5113.7366	0.00754
5	1	4	4	1	3	5238.7520	0.00080
6	0	6	5	0	5	6205.6507	-0.00087
6	1	5	5	1	4	6285.9542	0.01184
7	0	7	6	0	6	7236.9642	-0.00070
7	1	7	6	1	6	7157.8854	0.00352
7	1	6	6	1	5	7332.8126	-0.00707

Table S16. XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Eq-A** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	3106.7478	-0.00906
3	1	3	2	1	2	3068.6238	-0.00581
3	1	2	2	1	1	3146.2987	0.00752
4	1	4	3	1	3	4091.2644	0.00073
4	1	3	3	1	2	4194.8096	0.00207
5	0	5	4	0	4	5175.1433	-0.00275
5	1	4	4	1	3	5243.1112	0.00254
6	0	6	5	0	5	6207.8841	-0.00275
6	1	6	5	1	5	6135.8847	0.01433
6	1	5	5	1	4	6291.1428	0.00601
7	0	7	6	0	6	7239.3968	0.00438
7	1	7	6	1	6	7157.7427	-0.00829
7	1	6	6	1	5	7338.8220	-0.00945

Table S17. I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-C** of **perillaldehyde**.



J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1		-0.01440
						2076.2858	
2	1	1	1	1	0	2132.6525	0.01265
2	1	2	1	1	1	2021.8498	-0.00062
3	0	3	2	0	2	3112.0899	0.00077
3	1	3	2	1	2	3032.1894	0.00006
3	1	2	2	1	1	3198.3630	-0.00041
4	0	4	3	0	3	4145.0546	-0.00077
4	1	4	3	1	3	4041.8389	0.00017
4	1	3	3	1	2	4263.3567	-0.00045
5	0	5	4	0	4	5174.2934	0.00107
5	1	5	4	1	4	5050.5929	0.00100
5	1	4	4	1	3	5327.3549	0.00089
6	0	6	5	0	5	6198.9540	-0.00053
6	1	6	5	1	5	6058.2602	-0.00127
6	1	5	5	1	4	6390.0656	-0.00063
7	0	7	6	0	6	7218.3076	-0.00069
7	1	7	6	1	6	7064.6812	-0.00229
7	1	6	6	1	5	7451.1790	-0.00102
3	2	2	2	2	1	3115.8728	0.00576
3	2	1	2	2	0	3119.6522	0.00725
4	2	3	3	2	2	4153.7557	0.00255
4	2	2	3	2	1	4163.1830	-0.00285
5	2	3	4	2	2	5209.8193	-0.00429
5	2	4	4	2	3	5191.0188	0.01038
6	2	5	5	2	4	6227.4816	0.00597
6	2	4	5	2	3	6260.2403	-0.00457
7	2	6	6	2	5	7262.9985	0.00014
7	2	5	6	2	4	7315.0182	-0.00532
5	3	3	4	3	2	5196.2594	0.00764
5	3	2	4	3	1	5196.4535	-0.00973
6	3	4	5	3	3	6236.6473	0.00164
6	3	3	5	3	2	6237.2048	-0.00439
6	4	3	5	4	2	6234.9441	0.00536
6	4	2	5	4	1	6234.9441	0.00216
7	3	5	6	3	4	7277.5739	-0.00122
7	3	4	6	3	3	7278.8414	-0.00017
7	4	4	6	4	3	7275.0433	-0.00044
7	4	3	6	4	2	7275.0433	-0.01113
1	1	1	0	0	0	3446.2338	-0.00032
2	1	2	1	0	1	4429.4630	0.00116
3	1	3	2	0	2	5385.3504	-0.00058
4	1	4	3	0	3	6315.1007	0.00012
5	1	5	4	0	4	7220.6366	-0.00051
5	0	5	4	1	4	3004.2472	0.00008
6	0	6	5	1	5	4152.6081	-0.00165
7	0	7	6	1	6	5312.6632	0.00663
8	0	8	7	1	7	6479.7706	0.00075
1	1	0	0	0	0	3501.6219	-0.00694
2	1	1	1	0	1	4595.6439	-0.00209
3	1	2	2	0	2	5717.7116	0.00240
4	1	3	3	0	3	6868.9768	-0.00042
1	1	0	1	0	1	2463.0095	0.00336
2	1	1	2	0	2	2519.3496	0.00381

3	1	2	3	0	3	2605.6219	0.00183
4	1	3	4	0	4	2723.9236	0.00175
5	1	4	5	0	5	2876.9852	0.00168
6	1	5	6	0	6	3068.0980	0.00278
7	1	6	7	0	7	3300.9695	0.00255
8	1	7	8	0	8	3579.5194	-0.00105
2	2	0	2	1	1	7223.7860	0.00679
2	2	1	2	1	2	7389.0261	0.00768
3	2	2	3	1	3	7472.7060	0.00988
4	2	2	4	1	3	7044.9008	0.01136
4	2	3	4	1	4	7584.5929	-0.01764
5	2	3	5	1	4	6927.3617	0.00268
6	2	5	6	1	6	7894.2303	-0.01092
6	2	4	6	1	5	6797.5381	0.00044
7	2	5	7	1	6	6661.3745	-0.00666
8	2	6	8	1	7	6525.5768	-0.00885
9	1	8	9	0	9	3907.6162	0.00959
10	1	9	10	0	10	4288.6549	-0.00659
1	1	1	1	0	1	2407.6182	0.00678
2	1	2	2	0	2	2353.1625	0.00086
5	0	5	4	1	3	2450.3696	-0.00089
6	0	6	5	1	4	3321.9690	-0.00201
7	0	7	6	1	5	4150.2132	0.00013
8	0	8	7	1	6	4930.8275	-0.00232
9	0	9	8	1	7	5659.5945	0.00536

Table S17. II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	*J"*	$K"_{-1}$	$K"_{+1}$	ν_{obs}	ν_{obs}-ν_{calc}
3	0	3	2	0	2		0.00456
						3108.1699	
3	1	2	2	1	1	3194.1236	-0.00854
4	0	4	3	0	3	4139.8429	-0.00864
4	1	3	3	1	2	4257.7181	-0.00460
5	0	5	4	0	4	5167.8245	-0.00740
5	1	5	4	1	4	5044.5171	0.00082
5	1	4	4	1	3	5320.3217	-0.00116
6	0	6	5	0	5	6191.2650	-0.00074
6	1	5	5	1	4	6381.6587	0.01186
7	0	7	6	0	6	7209.4251	0.00219
7	1	7	6	1	6	7056.2181	0.00277
7	1	6	6	1	5	7441.3834	0.00031

Table S17. III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	*J"*	$K"_{-1}$	$K"_{+1}$	ν_{obs}	ν_{obs}-ν_{calc}
5	0	5	4	0	4		0.00550
						5169.5064	
5	1	5	4	1	4	5044.5178	-0.00179
5	1	4	4	1	3	5324.9524	0.00385
6	0	6	5	0	5	6192.8364	0.00815
6	1	5	5	1	4	6387.0570	-0.01415

4	1	3	3	1	2	4261.4940	0.00397
3	0	3	2	0	2	3109.4904	-0.00635
3	1	2	2	1	1	3197.0032	0.00765
7	1	6	6	1	5	7447.5327	0.00253
7	0	7	6	0	6	7210.6580	-0.00562

Table S17. IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2		-0.00182
						3105.7977	
3	1	2	2	1	1	3192.6802	0.00017
4	0	4	3	0	3	4136.5689	-0.00332
4	1	4	3	1	3	4032.8008	-0.00819
4	1	3	3	1	2	4255.7526	-0.00136
5	0	5	4	0	4	5163.5345	-0.00012
5	1	5	4	1	4	5039.2656	-0.00239
5	1	4	4	1	3	5317.8068	-0.00131
6	0	6	5	0	5	6185.8102	-0.01541
6	1	6	5	1	5	6044.6327	0.01177
6	1	5	5	1	4	6378.5519	0.00439
7	0	7	6	0	6	7202.7102	0.00852
7	1	6	6	1	5	7437.6518	0.00162

Table S17. V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2		0.00699
						3102.6772	
3	1	3	2	1	2	3023.1796	-0.01353
3	1	2	2	1	1	3188.4491	-0.00142
4	0	4	3	0	3	4132.5309	-0.01492
4	1	4	3	1	3	4029.8637	0.00797
4	1	3	3	1	2	4250.1497	-0.00300
5	1	5	4	1	4	5035.6350	0.00316
5	1	4	4	1	3	5310.8730	0.00358
6	0	6	5	0	5	6180.4013	0.00585
6	1	6	5	1	5	6040.3364	0.00049
6	1	5	5	1	4	6370.3176	0.00116
7	0	7	6	0	6	7196.8023	-0.00234
7	1	6	6	1	5	7428.1841	0.00019

Table S17. VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	0	4	3	0	3		0.00116
						4137.5174	
4	1	4	3	1	3	4033.4030	-0.00550
4	1	3	3	1	2	4257.2086	0.00073
5	0	5	4	0	4	5164.6363	-0.00202
5	1	4	4	1	3	5319.6080	0.00326
6	0	6	5	0	5	6187.0414	0.00046
6	1	6	5	1	5	6045.4716	-0.00091
6	1	5	5	1	4	6380.6720	0.00001
3	0	3	2	0	2	3106.5592	0.01557
3	1	2	2	1	1	3193.7741	-0.00578
5	1	5	4	1	4	5040.0002	0.00108

7	1	6	6	1	5	7440.0802	-0.00341

Table S17. VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2		-0.00160
						3108.5543	
3	1	3	2	1	2	3027.9175	-0.00115
3	1	2	2	1	1	3195.7734	-0.00055
4	0	4	3	0	3	4140.1979	-0.00475
4	1	4	3	1	3	4036.1096	-0.00045
4	1	3	3	1	2	4259.8722	0.00469
5	0	5	4	0	4	5168.0033	0.00161
5	1	5	4	1	4	5043.3800	0.00266
5	1	4	4	1	3	5322.9283	-0.00245
6	0	6	5	0	5	6191.0857	0.00108
6	1	6	5	1	5	6049.5276	-0.00057
6	1	5	5	1	4	6384.6701	0.00466
7	1	6	6	1	5	7444.7418	-0.00403

Table S17. VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2		-0.00634
						3090.7039	
4	0	4	3	0	3	4116.6655	-0.00824
4	1	4	3	1	3	4014.7601	-0.00156
5	0	5	4	0	4	5139.0097	-0.00194
6	1	6	5	1	5	6017.7770	0.00777
6	0	6	5	0	5	6156.9050	0.00546
6	1	5	5	1	4	6345.0416	-0.00213
3	1	2	2	1	1	3175.7474	-0.00896
5	1	5	4	1	4	5016.7819	-0.01078
5	1	4	4	1	3	5289.7814	0.01279
7	0	7	6	0	6	7169.6160	-0.00279
7	1	7	6	1	6	7017.5364	0.00539

Table S17. IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_8$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2		0.00779
						3072.6207	
3	1	2	2	1	1	3156.9422	-0.00903
4	0	4	3	0	3	4092.5809	0.00048
4	1	4	3	1	3	3991.5112	-0.00285
4	1	3	3	1	2	4208.1919	0.00953
5	0	5	4	0	4	5108.9575	0.00424
6	0	6	5	0	5	6120.9114	-0.00263
6	1	6	5	1	5	5982.9328	-0.00225
6	1	5	5	1	4	6307.4843	-0.00440

7	1	7	6	1	6	6976.9197	0.00136

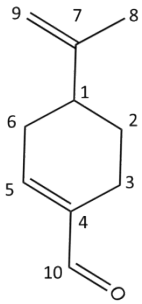
Table S17. X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2		-0.00513
						3077.9018	
3	1	3	2	1	2	2999.0595	-0.00726
3	1	2	2	1	1	3163.0065	-0.00369
4	0	4	3	0	3	4099.5522	-0.00362
4	1	4	3	1	3	3997.6952	0.00113
4	1	3	3	1	2	4216.2409	0.00159
5	0	5	4	0	4	5117.5418	0.00161
5	1	5	4	1	4	4995.4473	0.00670
5	1	4	4	1	3	5268.4844	-0.00476
6	0	6	5	0	5	6131.0277	-0.00083
6	1	6	5	1	5	5992.1246	0.00255
6	1	5	5	1	4	6319.4842	0.00698
7	1	7	6	1	6	6987.5745	-0.00257

Table S17. XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Eq-C** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2		0.00335
						3079.9457	
3	1	3	2	1	2	3001.4800	-0.00300
3	1	2	2	1	1	3164.5350	-0.00126
4	0	4	3	0	3	4102.3539	-0.00413
4	1	4	3	1	3	4000.9353	-0.00187
4	1	3	3	1	2	4218.2944	-0.00274
5	0	5	4	0	4	5121.1861	0.00315
5	1	5	4	1	4	4999.5213	-0.00661
5	1	4	4	1	3	5271.1026	0.00301
6	1	6	5	1	5	5997.0670	-0.00701
6	1	5	5	1	4	6322.6664	-0.00125
6	0	6	5	0	5	6135.5950	-0.00493
7	1	7	6	1	6	6993.4267	0.01027

Table S18. I Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Eq-a** of **perillaldehyde**.



J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	1	2	1	1	1		0.00672
						2023.6739	
2	0	2	1	0	1	2086.5884	0.00111
2	1	1	1	1	0	2152.1351	0.00497
3	0	3	2	0	2	3126.6031	-0.00141
3	1	3	2	1	2	3034.6869	-0.00128
3	2	2	2	2	1	3131.8440	-0.00173
3	2	1	2	2	0	3137.0947	0.00591
3	1	2	2	1	1	3227.3650	-0.00112
4	1	4	3	1	3	4044.7551	-0.00222
4	0	4	3	0	3	4162.7083	-0.00294
4	1	3	3	1	2	4301.5827	-0.00094
5	1	5	4	1	4	5053.5932	-0.00243
5	0	5	4	0	4	5193.6691	-0.00271
5	1	4	4	1	3	5374.4028	-0.00074
6	1	6	5	1	5	6060.9538	-0.00210
6	0	6	5	0	5	6218.3669	-0.00320
6	1	5	5	1	4	6445.4124	0.00019
7	1	7	6	1	6	7066.6270	-0.00220
7	0	7	6	0	6	7235.9023	-0.00232
7	1	6	6	1	5	7514.1489	-0.00378
4	2	3	3	2	2	4174.7794	0.00701
4	2	2	3	2	1	4187.8600	0.00390
5	2	4	4	2	3	5216.8464	0.02290
5	2	3	4	2	2	5242.8785	-0.01307
6	2	5	5	2	4	6257.7975	0.01631
7	2	6	6	2	5	7297.4387	0.00962
7	2	5	6	2	4	7369.1225	-0.00878
1	1	1	0	0	0	3370.5118	-0.01230
2	1	2	1	0	1	4350.2338	-0.00783
3	1	3	2	0	2	5298.3357	-0.00682
4	1	4	3	0	3	6216.4887	-0.00663
5	1	5	4	0	4	7107.3740	-0.00572
6	1	6	5	0	5	7974.6623	-0.00150
5	0	5	4	1	4	3139.8910	0.00328
6	0	6	5	1	5	4304.6670	0.00481
7	0	7	6	1	6	5479.6075	-0.00341
8	0	8	7	1	7	6658.6854	0.00130
1	1	0	1	0	1	2390.8107	0.00484
2	1	1	2	0	2	2456.3511	0.00240
3	1	2	3	0	3	2557.1141	0.00378
4	1	3	4	0	4	2695.9860	0.00328
8	1	7	8	0	8	3716.4125	-0.00590
9	1	8	9	0	9	4111.5241	-0.00445
10	1	9	10	0	10	4570.8790	-0.00019
11	1	10	11	0	11	5096.4959	0.00379
9	2	7	9	1	8	6096.3635	-0.00454
8	2	6	8	1	7	6219.4177	-0.00072
7	2	5	7	1	6	6358.1757	0.00164
6	2	4	6	1	5	6503.2011	0.00565
5	2	3	5	1	4	6645.5118	-0.00541
4	2	2	4	1	3	6777.0419	0.01272
3	2	1	3	1	2	6890.7619	0.00519
2	2	0	2	1	1	6981.0208	-0.01324

2	2	1	2	1	2	7172.4217	0.00497
3	2	2	3	1	3	7269.5766	0.00231
4	2	3	4	1	4	7399.6052	0.01585
5	2	4	5	1	5	7562.8138	-0.00342
6	2	5	6	1	6	7759.6423	-0.00022
7	2	6	7	1	7	7990.4343	-0.00810

Table S18. II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	0	4	3	0	3		0.00572
						4157.5257	
4	1	4	3	1	3	4039.9126	-0.00790
4	1	3	3	1	2	4295.9060	-0.00321
5	0	5	4	0	4	5187.2423	0.00031
5	1	4	4	1	3	5367.3271	0.00037
6	1	6	5	1	5	6053.7437	0.00603
6	0	6	5	0	5	6210.7370	-0.00167
3	1	3	2	1	2	3031.0541	0.00036
3	0	3	2	0	2	3122.6744	-0.00858
3	1	2	2	1	1	3223.1085	0.00555

Table S18. III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		0.00628
						4041.1250	
4	0	4	3	0	3	4159.2496	0.00622
4	1	3	3	1	2	4298.5717	-0.00678
5	1	5	4	1	4	5049.0130	-0.00271
5	0	5	4	0	4	5189.2126	0.00905
6	1	6	5	1	5	6055.4146	-0.00123
6	0	6	5	0	5	6212.8244	0.00403
7	1	7	6	1	6	7060.1041	-0.00440
7	0	7	6	0	6	7229.1828	-0.00580

Table S18. IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		0.00361
						4036.3431	
4	0	4	3	0	3	4154.8310	-0.00249
4	1	3	3	1	2	4294.6800	0.00643
5	1	5	4	1	4	5043.0325	0.00575
5	0	5	4	0	4	5183.6325	0.00372
5	1	4	4	1	3	5365.7110	-0.00038
6	1	6	5	1	5	6048.2070	-0.00104
7	1	7	6	1	6	7051.6675	-0.00430
3	0	3	2	0	2	3120.7820	-0.00741
3	1	2	2	1	1	3222.2025	-0.00569

Table S18. V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		0.00141
						4032.6596	
4	0	4	3	0	3	4150.0042	-0.00218
4	1	3	3	1	2	4288.0317	-0.00026
5	1	5	4	1	4	5038.4966	-0.00162
5	1	4	4	1	3	5357.4983	0.00392
5	0	5	4	0	4	5177.8987	-0.00293
6	1	6	5	1	5	6042.8765	0.00016
6	1	5	5	1	4	6425.1752	0.00770
7	0	7	6	0	6	7214.2172	0.00042
7	1	7	6	1	6	7045.5859	0.00052
3	1	3	2	1	2	3025.6069	0.00584
3	0	3	2	0	2	3117.0170	-0.00627
3	1	2	2	1	1	3217.1735	-0.01508

Table S18. VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		-0.00051
						4035.2945	
4	0	4	3	0	3	4154.3203	-0.00242
4	1	3	3	1	2	4295.0067	-0.00366
5	1	5	4	1	4	5041.6808	-0.00607
5	0	5	4	0	4	5182.8385	-0.00791
5	1	4	4	1	3	5366.1002	0.00778
6	1	6	5	1	5	6046.5595	0.00738
6	0	6	5	0	5	6204.8975	-0.00197
6	1	5	5	1	4	6435.2942	-0.00033
3	1	3	2	1	2	3027.6342	0.00364
3	0	3	2	0	2	3120.4706	-0.00417
3	1	2	2	1	1	3222.4791	0.00027
7	0	7	6	0	6	7219.5713	0.00397

Table S18. VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
5	1	5	4	1	4		0.00150
						5045.1754	
5	0	5	4	0	4	5186.6574	-0.00406
6	1	5	5	1	4	6440.5646	0.00308
6	0	6	5	0	5	6209.3759	-0.01119
4	0	4	3	0	3	4157.4161	-0.00970
3	1	3	2	1	2	3029.7445	0.00524
3	0	3	2	0	2	3122.8405	0.00812
7	0	7	6	0	6	7224.6945	0.00935

4	1	4	3	1	3	4038.0955	-0.00131

Table S18. VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		0.00243
						4017.6479	
4	0	4	3	0	3	4134.0977	-0.00257
4	1	3	3	1	2	4270.8589	-0.00285
5	1	5	4	1	4	5019.7731	0.00005
5	1	4	4	1	3	5336.0825	0.00407
6	1	6	5	1	5	6020.4608	-0.00272
6	0	6	5	0	5	6176.1934	0.00188
6	1	5	5	1	4	6399.5354	-0.00418
3	1	3	2	1	2	3014.3244	0.00251
3	0	3	2	0	2	3105.0117	-0.00112
3	1	2	2	1	1	3204.2955	0.00579
7	0	7	6	0	6	7187.2168	-0.00316

Table S18. IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_8$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		-0.00387
						3998.0038	
4	0	4	3	0	3	4113.9422	-0.00036
5	1	5	4	1	4	4995.2325	0.00217
5	1	4	4	1	3	5310.1893	0.00140
6	1	6	5	1	5	5991.0204	0.00149
6	0	6	5	0	5	6146.0022	-0.00187
6	1	5	5	1	4	6368.4831	0.00574
3	0	3	2	0	2	3089.8836	-0.00254
7	0	7	6	0	6	7152.0417	0.00164
7	1	6	6	1	5	7424.5678	-0.00527

Table S18. X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		0.00568
						3996.5733	
5	1	4	4	1	3	5309.9728	-0.00086
6	1	6	5	1	5	5988.7650	-0.00079
6	0	6	5	0	5	6144.1808	-0.00138
6	1	5	5	1	4	6368.1558	-0.00089
7	0	7	6	0	6	7149.6386	-0.00013
7	1	6	6	1	5	7424.1139	0.00672
3	0	3	2	0	2	3089.2341	-0.00885
3	1	2	2	1	1	3188.6594	-0.00655

Table S18. XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Eq-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		0.00013
						4003.6653	
4	0	4	3	0	3	4119.4654	-0.00159
4	1	3	3	1	2	4255.3346	0.00526
5	1	5	4	1	4	5002.3295	0.00472
5	0	5	4	0	4	5140.0164	0.00517
5	1	4	4	1	3	5316.7021	0.00817
6	1	6	5	1	5	5999.5583	-0.00550
6	0	6	5	0	5	6154.5451	0.00614
7	0	7	6	0	6	7162.1674	-0.00296
7	1	6	6	1	5	7433.7753	-0.01262
3	1	3	2	1	2	3003.8177	-0.00593
3	0	3	2	0	2	3093.9900	0.00584

Table S19. I. Measured frequencies and residuals (in MHz) for the rotational transitions of the conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
2	0	2	1	0	1	2777.6176	-0.00318
2	1	1	1	1	0	2810.0460	-0.00242
2	1	2	1	1	1	2746.4422	0.00250
3	0	3	2	0	2	4164.8783	0.00287
3	1	3	2	1	2	4119.2667	-0.00040
3	1	2	2	1	1	4214.6702	-0.00244
3	2	2	2	2	1	4167.3788	0.00387
3	2	1	2	2	0	4169.8494	-0.00113
4	0	4	3	0	3	5550.2715	-0.00086
4	1	4	3	1	3	5491.6354	0.00134
4	1	3	3	1	2	5618.8038	-0.00248
4	2	3	3	2	2	5555.9913	-0.00992
4	2	2	3	2	1	5562.1800	0.00013
4	3	2	3	3	1	5557.7565	0.01744
4	3	1	3	3	0	5557.7565	-0.02778
5	0	5	4	0	4	6933.2220	0.00041
5	1	5	4	1	4	6863.4088	0.00443
5	1	4	4	1	3	7022.2668	-0.00118
5	2	4	4	2	3	6944.2031	0.00284
5	3	3	4	3	2	6947.7508	0.07399
5	3	2	4	3	1	6947.7508	-0.08420
1	1	1	0	0	0	2598.0696	-0.00375
1	1	0	0	0	0	2629.8836	0.00589
2	1	2	1	0	1	3955.3860	-0.00520
2	1	1	1	0	1	4050.7959	-0.00838
3	1	3	2	0	2	5297.0321	-0.00542
3	1	2	2	0	2	5487.8527	-0.00344
4	1	4	3	0	3	6623.7976	0.00146
5	1	5	4	0	4	7936.9262	-0.00195
3	0	3	2	1	2	2987.1071	0.00208
4	0	4	3	1	3	4418.1157	0.00542
5	0	5	4	1	4	5859.6986	0.00079
6	0	6	5	1	5	7309.4800	0.00178
2	2	1	1	1	0	6436.8786	-0.00386
2	2	0	1	1	0	6437.5116	0.00985
2	2	1	1	1	1	6468.6981	0.01128
2	2	0	1	1	1	6469.3063	0.00019
3	2	2	2	1	1	7794.2190	0.01003
3	2	1	2	1	2	7892.7192	0.00226
2	2	0	2	1	1	3627.4594	0.00607
3	2	1	3	1	2	3582.6307	-0.00052
5	2	3	5	1	4	3460.2629	0.01142
6	2	4	6	1	5	3388.6805	0.00783
2	2	1	2	0	2	4899.9963	-0.02124
3	2	2	3	1	3	3770.3607	0.00575
4	3	1	4	2	2	6117.0550	-0.00157
4	3	2	4	2	3	6126.2753	-0.00205
5	3	3	5	2	4	6129.7555	0.00160
5	3	2	5	2	3	6108.3863	0.00938
6	3	3	6	2	4	6093.4132	-0.01260
2	2	1	2	1	2	3722.2384	-0.00872
3	2	2	3	1	2	3579.5196	-0.01673
4	2	3	4	1	4	3834.7348	0.01268

Table S19. II. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_1$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		-0.00218
						5464.1020	
4	0	4	3	0	3	5517.1513	-0.00577
4	1	3	3	1	2	5578.3078	-0.00664
5	1	5	4	1	4	6829.1971	0.00682
5	0	5	4	0	4	6892.6554	0.00091
5	1	4	4	1	3	6971.8834	0.00611
2	0	2	1	0	1	2760.6206	0.00529
3	1	3	2	1	2	4098.5174	-0.00714
3	1	2	2	1	1	4184.2131	0.01119

Table S19. III. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_2$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	1	4	3	1	3		0.00633
						5461.1200	
4	0	4	3	0	3	5518.8194	0.00036
4	1	3	3	1	2	5586.0650	0.00328
5	0	5	4	0	4	6894.0688	-0.00123
5	1	5	4	1	4	6825.2920	-0.00137
5	1	4	4	1	3	6981.3870	0.00465
3	1	3	2	1	2	4096.3545	-0.00331
3	1	2	2	1	1	4190.0845	-0.00928
2	0	2	1	0	1	2761.7984	-0.00613

Table S19. IV. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_3$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
3	0	3	2	0	2	4151.8443	-0.00206
3	1	2	2	1	1	4200.9201	0.00116
4	0	4	3	0	3	5532.9653	-0.00540
4	1	4	3	1	3	5475.1018	-0.00681
4	1	3	3	1	2	5600.4872	0.00083
5	0	5	4	0	4	6911.7083	0.00210
5	1	5	4	1	4	6842.7815	0.00717
5	1	4	4	1	3	6999.3988	0.00038

Table S19. V. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_4$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
5	0	5	4	0	4		0.00234
						6913.3970	
5	1	5	4	1	4	6838.8391	-0.00899
5	1	4	4	1	3	7010.8227	-0.00230
4	0	4	3	0	3	5535.1038	-0.00215
4	1	4	3	1	3	5472.1619	0.00687

4	1	3	3	1	2	5609.8445	0.00122
3	1	3	2	1	2	4104.7615	0.00362
2	0	2	1	0	1	2770.5154	0.00506

Table S19. VI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_5$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
5	0	5	4	0	4		-0.00074
						6915.7022	
5	1	5	4	1	4	6842.5956	0.00024
5	1	4	4	1	3	7010.5273	0.00753
4	0	4	3	0	3	5536.7314	0.00208
4	1	4	3	1	3	5475.1014	0.00184
4	1	3	3	1	2	5609.5287	-0.00867
3	0	3	2	0	2	4154.9907	-0.00724
3	1	2	2	1	1	4207.7962	0.00184
2	0	2	1	0	1	2771.1700	0.00003

Table S19. VII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_6$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	0	4	3	0	3	5535.5198	-0.00275
4	1	4	3	1	3	5477.0922	-0.00012
4	1	3	3	1	2	5603.7553	-0.00593
5	1	5	4	1	4	6845.2380	0.00121
5	1	4	4	1	3	7003.4800	0.00734
3	1	3	2	1	2	4108.3548	-0.00138
3	1	2	2	1	1	4203.3800	-0.00388
2	0	2	1	0	1	2770.2282	0.00412

Table S19. VIII. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_7$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	0	4	3	0	3	5541.6708	0.02662
4	1	3	3	1	2	5611.0210	0.00128
5	0	5	4	0	4	6922.3045	0.00058
5	1	5	4	1	4	6851.8994	0.00374
5	1	4	4	1	3	7012.4951	-0.00322
3	1	3	2	1	2	4112.3892	-0.00688
3	0	3	2	0	2	4158.4638	-0.00334
3	1	2	2	1	1	4208.8541	0.00487
2	1	2	1	1	1	2741.8692	0.00275

Table S19. IX. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_8$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
5	0	5	4	0	4		0.00425
						6920.2647	
5	1	5	4	1	4	6854.4265	0.00669
5	1	4	4	1	3	7003.1837	-0.01170
4	0	4	3	0	3	5539.4938	-0.00273

4	1	4	3	1	3	5484.3561	0.00724
4	1	3	3	1	2	5603.4443	0.00644
3	0	3	2	0	2	4156.5410	-0.01205
3	1	3	2	1	2	4113.7335	-0.01117
3	1	2	2	1	1	4203.0967	0.01306
2	0	2	1	0	1	2771.9466	-0.01075
2	1	2	1	1	1	2742.7270	-0.00262
2	1	1	1	1	0	2802.3018	0.00863

Table S19. X. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_9$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	0	4	3	0	3		-0.00289
						5492.2868	
4	1	3	3	1	2	5558.8262	0.00328
5	0	5	4	0	4	6861.0071	0.00060
5	1	5	4	1	4	6792.7806	0.00503
5	1	4	4	1	3	6947.3605	-0.00019
3	0	3	2	0	2	4121.2594	-0.00435
3	1	3	2	1	2	4076.8138	-0.00796
3	1	2	2	1	1	4169.6571	0.00458
2	0	2	1	0	1	2748.4961	0.00952
2	1	1	1	1	0	2780.0075	-0.01231

Table S19. XI. Measured frequencies and residuals (in MHz) for the rotational transitions of the $^{13}C_{10}$ isotopologue of conformer **Ax-a** of **perillaldehyde**.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs}-\nu_{calc}$
4	0	4	3	0	3	5475.9874	0.00127
4	1	4	3	1	3	5416.4561	-0.00372
4	1	3	3	1	2	5545.7615	-0.01372
5	1	5	4	1	4	6769.3981	0.00193
5	1	4	4	1	3	6930.9367	0.00384
3	0	3	2	0	2	4109.2388	-0.00206
3	1	3	2	1	2	4062.9097	0.00383
3	1	2	2	1	1	4159.9343	0.01397
2	0	2	1	0	1	2740.5638	-0.00567

Table S20. Experimental and theoretical vibrationally-corrected rotational constants (A_0, B_0, C_0) of the observed axial conformers of carvone, and their percentage changes.

		Eq-A		
	Exp.	MP2	B3LYP	B3LYP-D3BJ
A[a] (MHz)	2237.2055(11)[b]	2208.1 (-1.3%)[c]	2217.2 (-0.9%)	2222.2 (-0.7%)
B (MHz)	656.27834(29)	653.1 (-0.5%)	645.9 (-1.6%)	650.3 (-0.9%)
C (MHz)	579.64159(29)	576.7 (-0.5%)	570.6 (-1.6%)	573.9 (-1.0%)
		Eq-C		
	Exp.	MP2	B3LYP	B3LYP-D3BJ
A (MHz)	2256.91513(93)	2225.1 (-1.4%)	2238.7 (-0.8%)	2244.1 (-0.6%)
B (MHz)	672.90566(26)	666.3 (-1.0%)	660.0 (-1.9%)	665.7 (-1.1%)
C (MHz)	554.50351(25)	554.7 (0.0%)	547.0 (-1.4%)	549.0 (-1.0%)
		Eq-a		
	Exp.	MP2	B3LYP	B3LYP-D3BJ
A (MHz)	2212.7903(13)	2177.3 (-1.6%)	2194.5 (-0.8%)	2200.2 (-0.6%)
B (MHz)	684.52333(27)	676.3 (-1.2%)	670.3 (-2.1%)	678.1 (-0.9%)
C (MHz)	554.73193(25)	557.5 (0.5%)	548.5 (-2.1%)	549.0 (-1.0%)
		Ax-a		
	Exp.	MP2	B3LYP	B3LYP-D3BJ
A (MHz)	1621.8211(18)	1572.2 (-3.1%)	1662.7 (2.5%)	1626.7 (0.3%)
B (MHz)	904.92320(51)	928.1 (2.6%)	845.6 (-6.6%)	881.9 (-2.5%)
C (MHz)	780.45872(54)	799.5 (2.4%)	736.7 (-5.6%)	765.3 (-1.9%)
		Ax-C		
	Exp.	MP2	B3LYP	B3LYP-D3BJ
A (MHz)	1687.7984(26)	1596.3 (-5.4%)	1731.8 (2.6%)	1686.4 (-0.1%)
B (MHz)	878.27624(98)	907.6 (3.3%)	820.8 (-6.5%)	853.0 (-2.9%)
C (MHz)	771.3069(12)	803.5 (4.2%)	723.6 (-6.2%)	753.7 (-2.3%)

[a] A, B and C are the rotational constants. [b] Standard error in parentheses in units of the last digit. [c] Deviation from the experiment; calculated as $(A_{calc} - A_{exp})/A_{exp}$ x 100%

Table S21. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Eq-A** of **carvone**.

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	2216.2049(29)[e]	2213.2408(15)	2234.6806(27)	2229.8422(36)	2226.0685(25)
B (MHz)	656.11051(37)	655.28014(17)	653.16945(33)	654.69223(46)	656.21796(32)
C (MHz)	578.14434(29)	577.25893(13)	577.04735(27)	577.91183(37)	578.95787(26)
Δ_J (kHz)	[0.0131]	[0.0131]	[0.0131]	[0.0131]	[0.0131]
Δ_K (kHz)	[-1.77]	[-1.77]	[-1.77]	[-1.77]	[-1.77]
Δ_{JK} (kHz)	[0.268]	[0.268]	[0.268]	[0.268]	[0.268]
δ_K (kHz)	[-1.201]	[-1.201]	[-1.201]	[-1.201]	[-1.201]
a/b/c[b]	y/y/n	y/y/n	y/y/n	y/y/n	y/y/n
σ[c] (kHz)	5	5	5	6	4
N[d]	23	18	22	20	17
	$^{13}C_6$	$^{13}C_7$	$^{13}C_9$	$^{13}C_{10}$	$^{13}C_{11}$
A[a] (MHz)	2235.9379(40)	2232.9374(19)	2236.9185(40)	2222.1994(31)	2222.4155(31)
B (MHz)	655.48650(46)	646.53932(23)	651.36113(46)	647.69837(38)	646.30090(40)
C (MHz)	579.09831(36)	571.77644(19)	575.81765(36)	573.87914(30)	572.81563(30)
Δ_J (kHz)	[0.0131]	[0.0131]	[0.0131]	[0.0131]	[0.0131]
Δ_K (kHz)	[-1.77]	[-1.77]	[-1.77]	[-1.77]	[-1.77]
Δ_{JK} (kHz)	[0.268]	[0.268]	[0.268]	[0.268]	[0.268]
δ_K (kHz)	[-1.201]	[-1.201]	[-1.201]	[-1.201]	[-1.201]
a/b/c[b]	y/y/n	y/y/n	y/y/n	y/y/n	y/y/n
σ[c] (kHz)	6	3	6	5	5
N[d]	16	22	22	21	20

[a] A, B and C are the rotational constants, Δ_J, Δ_K, Δ_{JK}, δ_J are the quartic centrifugal distortion constants.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Table S22. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Eq-C** of **carvone**.

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	2236.9011(32)[e]	2232.3569(35)	2253.9185(28)	2249.8089(38)	2244.4538(34)
B (MHz)	672.57409(45)	671.86407(51)	669.66312(37)	671.11781(51)	672.89089(44)
C (MHz)	553.281489(31)	552.42694(35)	552.12016(25)	552.86588(31)	553.78923(30)
Δ_J (kHz)	[0.0118]	[0.0118]	[0.0118]	[0.0118]	[0.0118]
Δ_K (kHz)	[-0.96]	[-0.96]	[-0.96]	[-0.96]	[-0.96]
Δ_{JK} (kHz)	[0.054]	[0.054]	[0.054]	[0.054]	[0.054]
$a/b/c$[b]	y/y/n	y/y/n	y/y/n	y/y/n	y/y/n
σ[c] (kHz)	6	6	5	6	6
N[d]	21	21	22	22	21
	$^{13}C_6$	$^{13}C_7$	$^{13}C_9$	$^{13}C_{10}$	$^{13}C_{11}$
A[a] (MHz)	2256.2437(47)	2251.0313(26)	2256.6642(35)	2244.4036(27)	2239.4705(19)
B (MHz)	672.11144(62)	662.78793(35)	667.75847(49)	662.81593(36)	664.99424(27)
C (MHz)	554.00790(42)	547.27768(22)	551.00358(34)	547.50127(23)	548.53497(17)
Δ_J (kHz)	[0.0118]	[0.0118]	[0.0118]	[0.0118]	[0.0118]
Δ_K (kHz)	[-0.96]	[-0.96]	[-0.96]	[-0.96]	[-0.96]
Δ_{JK} (kHz)	[0.054]	[0.054]	[0.054]	[0.054]	[0.054]
$a/b/c$[b]	y/y/n	y/y/n	y/y/n	y/y/n	y/y/n
σ[c] (kHz)	8	5	7	5	3
N[d]	19	22	23	21	22

[a] A, B and C are the rotational constants, Δ_J, Δ_K, Δ_{JK}, are the quartic centrifugal distortion constants.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Table S23. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Eq-A** of **limonene**.

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	3027.4468(29)[e]	3031.2822(33)	3058.0046(21)	3028.4010(17)	3029.7191(26)
B (MHz)	717.01722(63)	714.88413(77)	712.42056(46)	714.89032(39)	717.01909(45)
C (MHz)	677.78867(59)	676.04278(72)	675.10033(44)	675.90507(37)	677.90878(54)
Δ_J (kHz)	[0.0165]	[0.0165]	[0.0165]	[0.0165]	[0.0165]
Δ_{JK} (kHz)	[0.088]	[0.088]	[0.088]	[0.088]	[0.088]
$a/b/c$[b]	y/y/y	y/y/y	y/y/y	y/y/y	y/y/y
σ[c] (kHz)	6	8	4	4	6
N[d]	13	13	13	14	12
	$^{13}C_6$	$^{13}C_7$	$^{13}C_9$	$^{13}C_{10}$	$^{13}C_{11}$
A[a] (MHz)	3055.7672(22)	3057.7943(30)	3057.6458(27)	3029.5008(30)	3031.9549(32)
B (MHz)	716.45126(41)	703.80743(58)	712.15734(58)	708.03600(64)	706.42374(64)
C (MHz)	678.83536(36)	667.36886(52)	674.88175(55)	672.50257(79)	670.93383(62)
Δ_J (kHz)	[0.0165]	[0.0165]	[0.0165]	[0.0165]	[0.0165]
Δ_{JK} (kHz)	[0.088]	[0.088]	[0.088]	[0.088]	[0.088]
$a/b/c$[b]	y/y/y	y/y/y	y/y/y	y/y/y	y/y/y
σ[c] (kHz)	4	6	6	6	6
N[d]	13	14	13	12	11

[a] A, B and C are the rotational constants, Δ_J, Δ_{JK}, are the quartic centrifugal distortion constants.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit
[d] N is the number of the fitted transitions
[e] Standard error in parentheses in units of last digit

Table S24. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Eq-C** of **limonene**.

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	3025.34(70)[e]	3026.29(61)	3053.71(66)	3024.11(64)	3022.21(77)
B (MHz)	741.9389(16)	739.80323(85)	737.1796(12)	739.55220(96)	742.1881(12)
C (MHz)	645.59564(87)	643.94765(75)	642.89046(79)	643.66269(78)	645.31447(95)
Δ_J (kHz)	[0.0222]	[0.0222]	[0.0222]	[0.0222]	[0.0222]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	7	6	6	6	7
N[d]	8	9	8	8	8
	$^{13}C_6$	$^{13}C_7$	$^{13}C_9$	$^{13}C_{10}$	$^{13}C_{11}$
A[a] (MHz)	3050.75(68)	3052.60(46)	3053.11(74)	3026.05(50)	3026.1(12)
B (MHz)	741.5618(14)	727.9542(11)	736.9390(14)	732.11563(67)	733.29576(87)
C (MHz)	646.31297(82)	635.8627(15)	642.7359(14)	638.42457(70)	639.32891(93)
Δ_J (kHz)	[0.0222]	[0.0222]	[0.0222]	[0.0222]	[0.0222]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	6	6	6	4	4
N[d]	7	6	7	7	6

[a] A, B and C are the rotational constants, Δ_J is the quartic centrifugal distortion constants.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit
[d] N is the number of the fitted transitions
[e] Standard error in parentheses in units of last digit

Table S25. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Eq-A** of **perillaldehyde**.

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	2932.21(98)[e]	2909.8(14)	2910.7(11)	2933.3(16)	2901.5(12)
B (MHz)	535.80964(28)	536.45813(44)	535.83714(37)	534.90459(51)	536.02758(50)
C (MHz)	509.59387(28)	509.46228(48)	508.89567(40)	508.67773(50)	508.79936(43)
Δ_J (kHz)	[0.0136]	[0.0136]	[0.0136]	[0.0136]	[0.0136]
Δ_{JK} (kHz)	[0.078]	[0.078]	[0.078]	[0.078]	[0.078]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	4	6	5	7	6
N[d]	14	14	13	15	14
	$^{13}C_6$	$^{13}C_7$	$^{13}C_8$	$^{13}C_9$	$^{13}C_{10}$
A[a] (MHz)	2904.5(14)	2930.8 (14)	2910.7(13)	2904.2(15)	2927.1(17)
B (MHz)	536.39022(43)	532.73519(50)	529.12719(43)	530.21501(43)	530.87589(50)
C (MHz)	509.14301(43)	506.75216(43)	504.20357(37)	505.20653(47)	504.98835(54)
Δ_J (kHz)	[0.0136]	[0.0136]	[0.0136]	[0.0136]	[0.0136]
Δ_{JK} (kHz)	[0.078]	[0.078]	[0.078]	[0.078]	[0.078]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	6	6	5	6	7
N[d]	14	14	14	14	13

[a] A, B and C are the rotational constants, Δ_J, Δ_{JK}, are the quartic centrifugal distortion constants.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit

Table S26. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Eq-C** of **perillaldehyde**.

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	2952.65(36)[e]	2927.97(49)	2931.58(38)	2953.49(40)	2924.38(47)
B (MHz)	546.25501(43)	546.96855(55)	546.15302(49)	545.27906(50)	546.39089(42)
C (MHz)	491.05179(54)	490.83779(99)	490.40109(58)	490.18996(57)	490.42508(48)
Δ_J (kHz)	[0.0110]	[0.0110]	[0.0110]	[0.0110]	[0.0110]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	6	7	7	7	5
N[d]	12	10	13	13	12
	$^{13}C_6$	$^{13}C_7$	$^{13}C_8$	$^{13}C_9$	$^{13}C_{10}$
A[a] (MHz)	2925.61(25)	2953.51(42)	2930.76(54)	2926.14(39)	2950.36(44)
B (MHz)	546.72054(22)	543.04832(67)	539.79974(56)	540.92888(38)	541.10696(41)
C (MHz)	490.76523(24)	488.41263(54)	485.61832(48)	486.27779(33)	486.75266(35)
Δ_J (kHz)	[0.0110]	[0.0110]	[0.0110]	[0.0110]	[0.0110]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	3	7	5	4	5
N[d]	13	12	10	13	13

[a] A, B and C are the rotational constants, Δ_J is the quartic centrifugal distortion constant.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Table S27. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Eq-a** of **perillaldehyde.**

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	2879.19(34)[e]	2859.14(24)	2859.51(54)	2879.71(24)	2850.19(19)
B (MHz)	533.32676(56)	553.75943(97)	553.32821(51)	552.30180(47)	553.46190(41)
C (MHz)	489.30499(53)	489.36902(48)	488.71899(42)	488.43398(40)	488.50673(41)
Δ_J (kHz)	[0.0145]	[0.0145]	[0.0145]	[0.0145]	[0.0145]
Δ_{JK} (kHz)	[0.077]	[0.077]	[0.077]	[0.077]	[0.077]
δ_J (kHz)	[-0.00228]	[-0.00228]	[-0.00228]	[-0.00228]	[-0.00228]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	5	6	5	6	5
N[d]	10	9	10	13	13
	$^{13}C_6$	$^{13}C_7$	$^{13}C_8$	$^{13}C_9$	$^{13}C_{10}$
A[a] (MHz)	2848.93(30)	2880.364(13)	2862.27(14)	2848.65(22)	2878.44(27)
B (MHz)	553.95349(94)	550.01454(27)	547.35704(14)	547.42664(38)	547.97186(55)
C (MHz)	488.81266(78)	486.68676(27)	484.29879(28)	484.04224(51)	485.03255(52)
Δ_J (kHz)	[0.0145]	[0.0145]	[0.0145]	[0.0145]	[0.0145]
Δ_{JK} (kHz)	[0.077]	[0.077]	[0.077]	[0.077]	[0.077]
δ_J (kHz)	[-0.00228]	[-0.00228]	[-0.00228]	[-0.00228]	[-0.00228]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	7	3	3	5	6
N[d]	9	12	10	9	12

[a] A, B and C are the rotational constants, Δ_J is the quartic centrifugal distortion constant.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Table S28. Experimental rotational constants of all the singly-substituted ^{13}C isotopologues of conformer **Ax-a** of **perillaldehyde**.

	$^{13}C_1$	$^{13}C_2$	$^{13}C_3$	$^{13}C_4$	$^{13}C_5$
A[a] (MHz)	1897.08(94) [e]	1917.59(63)	1912.87(56)	1897.37(51)	1904.08(54)
B (MHz)	704.562(73)	706.22539(57)	708.05727(49)	710.03181(63)	709.78026(55)
C (MHz)	676.00112(72)	674.97769(56)	676.70192(54)	675.59491(56)	676.15715(60)
Δ_J (kHz)	[0.1514]	[0.1514]	[0.1514]	[0.1514]	[0.1514]
Δ_K (kHz)	[2.70]	[2.70]	[2.70]	[2.70]	[2.70]
Δ_{JK} (kHz)	[-0.996]	[-0.996]	[-0.996]	[-0.996]	[-0.996]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	6	5	4	5	5
N[d]	9	9	8	8	9
	$^{13}C_6$	$^{13}C_7$	$^{13}C_8$	$^{13}C_9$	$^{13}C_{10}$
A[a] (MHz)	1918.7(11)	1909.80(47)	1902.4(12)	1918.31(88)	1906.3(18)
B (MHz)	708.54987(52)	709.58209(43)	708.01895(99)	702.74164(71)	701.47458(92)
C (MHz)	676.87150(50)	677.42841(47)	678.23718(98)	671.79576(86)	669.13377(89)
Δ_J (kHz)	[0.1514]	[0.1514]	[0.1514]	[0.1514]	[0.1514]
Δ_K (kHz)	[2.70]	[2.70]	[2.70]	[2.70]	[2.70]
Δ_{JK} (kHz)	[-0.996]	[-0.996]	[-0.996]	[-0.996]	[-0.996]
$a/b/c$[b]	y/n/n	y/n/n	y/n/n	y/n/n	y/n/n
σ[c] (kHz)	4	4	9	6	7
N[d]	8	9	12	10	9

[a] A, B and C are the rotational constants, Δ_J Δ_K Δ_{JK}, are the quartic centrifugal distortion constants.
[b] *a*, *b*, and *c* are the type of transitions observed.
[c] σ is the rms deviation of the fit.
[d] N is the number of the fitted transitions.
[e] Standard error in parentheses in units of last digit.

Structural Determination

The observed spectrum of all three terpenoids was quite intense, and therefore it was possible to measure the transitions arising from the ^{13}C isotopologues of the two most stable equatorial conformers of carvone and limonene (Eq-A and Eq-C), and of all the observed conformers of perillaldehyde. Their rotational constants were obtained from the fits of the observed transitions to the same Hamiltonian used for the parent species (see Tables S7-S19). The substitution coordinates of the Eq-A and Eq-C conformers of carvone and limonene, and all conformers of perillaldehyde (see Tables S29-S36) were determined from applying the Kraitchmann equations (J. Kraitchman, *Am. J. Phys.*, 1953, **21**, 17–24; C. C. Costain, *J. Chem. Phys.*, 1958, **29**, 864–874) and the program KRA (Z. Kisiel, PROSPE-Programs for Rotational Spectroscopy. *Spectrosc. from Sp.* **2001**, 91–106) using the experimental moments of inertia. All terpenoids have several carbon atoms placed extremely close to the inertial axes, which returned imaginary numbers when applying the Kaitchmann equations, preventing determination of their coordinates (which were fixed to zero) and introduced large uncertainties. Limonene and perillaldehyde also display a substantial number of atomic coordinates affected by large errors. The obtained absolute values of the r_s coordinates (the Kraitchmann equations do not return their signs) are compared to the theoretical ones predicted by the best performing methods, B3LYP-D3BJ and MP2.

The effective (r_0) structures for the above conformers have been determined from least-squares fit of the experimental moments of inertia of the observed isotopologues using the program STRFIT (Z. Kisiel, PROSPE-Programs for Rotational Spectroscopy. *Spectrosc. from Sp.* **2001**, 91–106), and are presented in Tables S37-S40. Non fitted parameters were fixed to the B3LYP-D3BJ/6-311++G(d,p) values.

Table S29. Substitution coordinates of the carbon atoms of **carvone Eq-A** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	0.3963(38)	1.4517(10)	0.2019(75)	0.411442	-1.451698	-0.213513	0.416149	-1.456650	-0.227355
C_2	1.0777(14)	1.56482(97)	0.102(15)	-1.081728	-1.560432	-0.112550	-1.080673	-1.569796	-0.130703
C_3	1.91703(79)	0.5073(30)	0.020(76)	-1.920423	-0.516143	-0.001514	-1.918313	-0.511968	-0.009269
C_4	1.3668(11)	0.8660(18)	0.031(49)	-1.380137	0.869712	-0.027991	-1.368083	0.871633	-0.030250
C_5	0.000(12)	1.0232(15)	0.2947(51)	0.110333	1.030215	-0.271825	0.113174	1.010912	-0.326843
C_6	0.9014(17)	0.089(17)	0.3475(44)	0.927670	-0.114702	0.345760	0.915310	-0.117632	0.332912
C_7	3.40718(44)	0.6502(23)	0.140(11)	-3.409586	-0.658871	0.131070	-3.408118	-0.648543	0.134032
C_9	2.40949(63)	0.054(28)	0.1626(94)	2.421846	0.056635	0.169511	2.407669	0.055449	0.176050
C_{10}	2.95340(51)	0.1995(76)	1.2294(12)	2.953251	0.229104	-1.230090	2.955144	0.270365	-1.212972
C_{11}	3.22438(47)	0.050(30)	1.2369(12)	3.232926	0.053849	1.229131	3.211799	0.021215	1.255090

Table S30. Substitution coordinates of the carbon atoms of **carvone Eq-C** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	0.4357(35)	1.3519(11)	0.4279(35)	0.448225	-1.354799	-0.427455	0.394168	-1.312563	-0.468398
C_2	1.0305(15)	1.54066(99)	0.3207(47)	-1.037590	-1.536667	-0.321694	-1.096255	-1.485197	-0.363672
C_3	1.90960(79)	0.5484(28)	0.00(57)	-1.914235	-0.553054	-0.060488	-1.960275	-0.485934	-0.066339
C_4	1.4144(11)	0.8415(18)	0.065(23)	-1.426290	0.845501	0.076609	-1.446603	0.901068	0.102751
C_5	0.0000(95)	1.0976(14)	0.2063(74)	0.045411	1.098666	-0.196344	0.017446	1.130664	-0.219738
C_6	0.9059(17)	0.000(29)	0.2640(58)	0.932379	-0.061965	0.257773	0.877636	-0.041717	0.249515
C_7	3.38848(45)	0.7690(20)	0.092(16)	-3.392577	-0.772762	0.082919	-3.441324	-0.688017	0.087387
C_9	2.40741(63)	0.112(14)	0.112(14)	2.420100	0.156646	0.062871	2.367600	0.154737	0.076195
C_{10}	3.30653(46)	0.8668(17)	0.7243(21)	3.314904	-0.861694	0.723684	3.243965	-0.883212	0.734264
C_{11}	2.92494(52)	1.1775(13)	0.6249(24)	2.927157	1.174218	-0.635022	2.896703	1.170411	-0.630688

Table S31. Substitution coordinates of the carbon atoms of **limonene Eq-A** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	0.000(13)	1.2758(12)	0.2179(70)	-0.044344	-1.277564	0.212245	-0.051237	-1.272046	0.272935
C_2	1.4523(10)	1.1996(13)	0.1727(89)	1.458773	-1.196348	0.177112	1.453679	-1.194504	0.230965
C_3	2.14410(71)	0.00(18)	0.025(60)	2.151110	-0.070339	-0.016776	2.145007	-0.064622	-0.019743
C_4	1.4499(10)	1.2644(12)	0.1733(87)	1.458832	1.261303	-0.194610	1.447173	1.256900	-0.242715
C_5	0.000(11)	1.2246(12)	0.2236(68)	-0.014483	1.230047	0.220284	-0.013806	1.222459	0.206887
C_6	0.6821(22)	0.000(25)	0.3545(43)	-0.712987	-0.011867	-0.358175	-0.703515	-0.028563	-0.351544
C_7	3.64730(42)	0.035(43)	0.105(14)	3.653054	-0.047435	-0.083515	3.647998	-0.045282	-0.099363
C_9	2.20014(69)	0.000(97)	0.143(11)	-2.212620	-0.009950	-0.150198	-2.200723	-0.016341	-0.153941
C_{10}	2.73009(53)	0.1619(94)	1.2472(12)	-2.726555	0.179363	1.254224	-2.726944	0.266286	1.231690
C_{11}	3.03618(50)	0.151(10)	1.1941(13)	-3.046393	-0.169347	-1.180241	-3.031593	-0.243266	-1.188645

Table S32. Substitution coordinates of the carbon atoms of **limonene Eq-C** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	0.00(11)	1.1568(85)	0.473(21)	-0.075820	-1.160729	0.471948	-0.086763	-1.156074	0.481497
C_2	1.4160(60)	1.1559(74)	0.423(21)	1.428249	-1.148877	0.401715	1.418864	-1.150310	0.417441
C_3	2.1522(42)	0.09(10)	0.00(15)	2.158719	-0.106650	-0.003809	2.152745	-0.103405	-0.008220
C_4	1.4947(60)	1.2064(75)	0.427(21)	1.509831	1.198989	-0.399681	1.502603	1.197506	-0.415335
C_5	0.000(55)	1.3090(82)	0.150(73)	0.049391	1.301970	0.046112	0.054102	1.297262	0.064107
C_6	0.654(14)	0.180(52)	0.365(26)	-0.715414	0.019524	-0.291625	-0.707533	0.021431	-0.293086
C_7	3.6501(18)	0.198(33)	0.164(40)	3.657994	-0.158156	-0.100243	3.653477	-0.160661	-0.106005
C_9	2.1960(46)	0.08(12)	0.174(59)	-2.211540	0.077367	-0.054822	-2.201891	0.077952	-0.066716
C_{10}	2.9980(24)	1.0784(67)	0.621(12)	-3.003455	-1.077140	-0.615778	-2.994497	-1.077753	-0.627570
C_{11}	2.80595(81)	1.0743(21)	0.6223(37)	-2.812323	1.067224	0.608867	-2.805394	1.069846	0.614426

Table S33. Substitution coordinates of the carbon atoms of **perillaldehyde Eq-A** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	1.112(13)	0.000(63)	0.285(51)	1.115882	0.002205	-0.367205	1.103534	0.014497	-0.354886
C_2	0.356(55)	1.146(17)	0.218(92)	0.342434	-1.172864	0.257219	0.344436	-1.154058	0.290038
C_3	1.119(15)	1.138(15)	0.12(15)	-1.131857	-1.134689	-0.154622	-1.123089	-1.134944	-0.140666
C_4	1.722(14)	0.10(23)	0.00(11)	-1.719176	0.241671	0.012451	-1.713315	0.239740	0.024564
C_5	0.950(19)	1.354(13)	0.17(11)	-0.962828	1.341235	0.163458	-0.958206	1.350031	0.191555
C_6	0.582(36)	1.314(16)	0.000(99)	0.534576	1.333278	0.153675	0.543319	1.339591	0.189511
C_7	2.5912(80)	0.220(95)	0.253(83)	2.613324	-0.076018	-0.154616	2.599877	-0.075549	-0.168248
C_8	3.4457(56)	0.000(73)	1.181(17)	3.454710	0.022417	-1.185615	3.429354	0.033550	-1.222763
C_9	3.1137(72)	0.326(68)	1.268(18)	3.111328	-0.267171	1.255028	3.122636	-0.301295	1.228935
C_{10}	3.1647(80)	0.490(52)	0.306(84)	-3.182636	0.395612	0.013344	-3.181858	0.393868	0.002397

Table S34. Substitution coordinates of the carbon atoms of **perillaldehyde Eq-C** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	1.0828(50)	0.091(60)	0.326(17)	1.117387	-0.024998	-0.293192	1.105364	-0.025959	-0.288906
C_2	0.262(28)	1.2501(59)	0.00(33)	0.290024	-1.255496	0.096032	0.287526	-1.248561	0.132029
C_3	1.1511(50)	1.1065(53)	0.356(17)	-1.170930	-1.097098	-0.333617	-1.165909	-1.100987	-0.321214
C_4	1.7133(35)	0.247(4)	0.070(87)	-1.725724	0.244841	0.061678	-1.718868	0.241515	0.072471
C_5	0.9407(76)	1.2700(56)	0.405(18)	-0.940919	1.274178	0.418200	-0.930760	1.276360	0.442756
C_6	0.5336(75)	1.2232(33)	0.4541(89)	0.555330	1.220100	0.430825	0.569154	1.214980	0.451571
C_7	2.5938(24)	0.181(35)	0.180(35)	2.611883	-0.148739	-0.068289	2.600105	-0.149194	-0.090464
C_8	3.4406(24)	0.9409(87)	0.730(11)	3.454750	0.929414	-0.701474	3.437975	0.934422	-0.724430
C_9	3.1641(12)	1.1390(53)	0.6282(97)	3.165808	-1.133350	0.641444	3.164585	-1.139421	0.625303
C_{10}	3.1747(21)	0.471(14)	0.170(39)	-3.183877	0.442798	0.067158	-3.181067	0.447655	0.058588

Table S35. Substitution coordinates of the carbon atoms of **perillaldehyde Eq-a** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	1.0828(50)	0.00(29)	0.301(18)	-1.113880	-0.009768	-0.272139	-1.103741	-0.008179	-0.267053
C_2	0.359(11)	0.9510(42)	0.6489(63)	-0.366018	0.960357	0.667765	-0.365932	0.916538	0.718755
C_3	1.0884(78)	1.1088(77)	0.274(31)	1.102098	1.102729	0.256315	1.094908	1.092040	0.299894
C_4	1.7212(23)	0.240(17)	0.03(14)	1.732268	-0.232837	-0.036938	1.723432	-0.232586	-0.039462
C_5	1.0044(32)	1.3625(24)	0.169(20)	1.012094	-1.353640	-0.209142	1.003348	-1.360789	-0.238548
C_6	0.490(10)	1.4058(36)	0.000(42)	-0.484085	-1.403009	-0.150215	-0.496104	-1.410003	-0.171882
C_7	2.59906(96)	0.000(28)	0.162(15)	-2.613671	0.034712	-0.055049	-2.601118	0.048547	-0.060676
C_8	3.2821(12)	1.2877(30)	0.5902(66)	-3.304093	1.239688	-0.641980	-3.292523	1.202768	-0.742267
C_9	3.31495(79)	0.9436(28)	0.5075(53)	-3.300101	-0.901650	0.602647	-3.284824	-0.834941	0.689814
C_{10}	3.1921(14)	0.333(13)	0.165(27)	3.197110	-0.320473	-0.141593	3.192622	-0.313397	-0.162796

Table S36. Substitution coordinates of the carbon atoms of **perillaldehyde Ax-a** in Å.

	r_s			B3LYP-D3BJ			MP2		
	$\|a\|$	$\|b\|$	$\|c\|$	a	b	c	a	b	c
C_1	1.698(19)	0.18(17)	1.760(19)	1.705136	-0.127430	-1.744821	1.662840	-0.099204	-1.769905
C_2	2.013(11)	0.15(15)	0.481(46)	2.049248	0.145263	-0.485255	1.977018	0.190105	-0.493470
C_3	1.356(14)	0.562(34)	0.769(26)	1.384465	-0.482298	0.729307	1.403930	-0.543136	0.703815
C_4	0.612(29)	1.735(10)	0.250(79)	0.545955	-1.735980	0.425206	0.583014	-1.789699	0.352710
C_5	0.812(23)	1.451(13)	0.16(12)	-0.850944	-1.435180	-0.024663	-0.807653	-1.452659	-0.105371
C_6	1.379(27)	0.27(14)	0.16(24)	-1.420804	-0.221782	0.055245	-1.372678	-0.233324	0.053745
C_7	0.675(24)	0.943(17)	0.665(25)	-0.698949	0.971769	0.617129	-0.658533	0.911017	0.717264
C_8	0.527(79)	0.416(95)	1.483(29)	0.496626	0.545936	1.471737	0.520554	0.401241	1.546015
C_9	2.768(11)	0.00(18)	0.428(72)	-2.798478	-0.063352	-0.434060	-2.743044	-0.029356	-0.454819
C_{11}	2.991(21)	1.296(50)	0.42(16)	3.147237	1.130328	-0.173321	2.941225	1.305179	-0.167087

Table S37. Effective r_0 bond lengths (in Å), bond angles and dihedral angles (in degrees) of the **Eq-A** and **Eq-C** conformers of **carvone.**

Bond length	**Eq-A**	**Eq-C**
$r(C_1–C_2)$	1.511(8)	1.505(10)
$r(C_2–C_3)$	1.350(6)	1.351(8)
$r(C_3–C_4)$	1.486(7)	1.481(9)
$r(C_4–C_5)$	1.514(10)	1.526(14)
$r(C_6–C_9)$	1.522(7)	1.526(5)
$r(C_6–C_1)$	1.531(19)	1.543(10)
$r(C_9–C_{11})$	1.343(12)	1.345(5)
$r(C_9–C_{10})$	1.509(15)	1.509(7)
$r(C_3–C_7)$	1.502(3)	1.502(4)
Angle		
$\angle C_1C_2C_3$	124.3(2)	124.3(3)
$\angle C_2C_3C_4$	119.7(2)	119.4(2)
$\angle C_6C_1C_2$	111.3(6)	111.6(5)
$\angle C_2C_3C_7$	123.2(5)	123.4(6)
$\angle C_5C_6C_9$	112.9(11)	113.9(6)
$\angle C_6C_9C_{10}$	118.4(9)	115.7(2)
$\angle C_6C_9C_{11}$	120.5(13)	-
Dihedral angle		
$\tau(C_1C_2C_3C_4)$	-3.4(15)	-3.6(8)
$\tau(C_6C_1C_2C_3)$	-20.8(21)	-20.2(11)
$\tau(C_1C_2C_3C_7)$	177.7(27)	177.2(18)
$\tau(C_4C_5C_6C_9)$	177.2(6)	-
$\tau(C_5C_6C_9C_{10})$	-	189.0(10)
$\tau(C_1C_6C_9C_{11})$	113.2(2)	-
σ^a	0.0088	0.0105

[a] Deviation of the fit

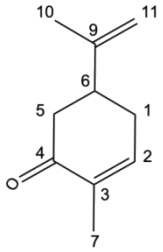


Table S38. Effective r_0 bond lengths (in Å), bond angles and dihedral angles (in degrees) of the **Eq-A** and **Eq-C** conformers of **limonene**.

Bond length	**Eq-A**	**Eq-C**
$r(C_1–C_2)$	1.506(15)	1.472(20)
$r(C_2–C_3)$	-	1.347(10)
$r(C_3–C_4)$	1.508(21)	1.516(9)
$r(C_5–C_6)$	-	1.530(18)
$r(C_6–C_9)$	1.507(15)	1.528(10)
$r(C_6–C_1)$	1.571(18)	1.545(19)
$r(C_9–C_{11})$	1.351(14)	1.353(6)
$r(C_9–C_{10})$	1.522(14)	1.495(7)
$r(C_3–C_7)$	1.498(11)	1.503(4)
Angle		
$\angle C_1C_2C_3$	-	123.7(4)
$\angle C_2C_3C_4$	119.0(7)	121.5(3)
$\angle C_5C_6C_1$	-	107.9(10)
$\angle C_6C_1C_2$	-	113.6(5)
$\angle C_2C_3C_7$	127.8(20)	-
$\angle C_6C_9C_{10}$	117.6(7)	116.2(4)
Dihedral angle		
$\tau(C_6C_1C_2C_3)$	-	-13.9(2)
$\tau(C_1C_2C_3C_7)$	174.7(32)	177.7(16)
$\tau(C_5C_6C_1C_2)$	-	48.5(15)
$\tau(C_{10}C_9C_6C_1)$	-63.0(27)	-
$\tau(C_{11}C_9C_6C_1)$	100.7(24)	-
σ^a	0.057	0.019

[a] Deviation of the fit

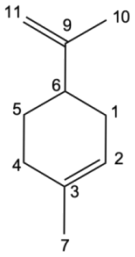
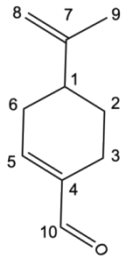


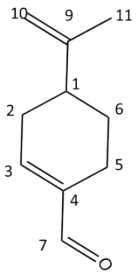
Table S39. Effective r_0 bond lengths (in Å), bond angles and dihedral angles (in degrees) of the **Eq-A**, **Eq-C, Eq-a** conformers of **perillaldehyde**.



Bond length	**Eq-A**	**Eq-C**	**Eq-a**
$r(C_1–C_2)$	1.537(48)	1.506(16)	1.525(21)
$r(C_3–C_2)$	1.490(58)	1.534(17)	1.537(20)
$r(C_4–C_3)$	1.513(31)	1.519(9)	1.507(14)
$r(C_5–C_4)$	1.359(30)	1.332(9)	1.349(19)
$r(C_6–C_1)$	1.490(58)	1.542(14)	1.506(20)
$r(C_7–C_1)$	1.521(23)	1.518(6)	1.531(9)
$r(C_7–C_8)$	1.337(20)	1.339(8)	1.328(11)
$r(C_7–C_9)$	1.536(17)	1.527(10)	1.539(10)
$r(C_4–C_{10})$	1.475(16)	1.475(4)	1.476(5)
Angle			
$\angle C_3C_2C_1$	111.8(23)	111.0(7)	111.0(9)
$\angle C_3C_4C_5$	122.7(12)	-	123.1(5)
$\angle C_6C_1C_2$	111.6(26)	110.3(6)	110.6(8)
$\angle C_9C_7C_1$	117.6(9)	115.4(3)	114.0(4)
$\angle C_4C_3C_2$	-	110.8(3)	110.9(6)
$\angle C_6C_1C_7$	-	-	115.6(8)
$\angle C_{10}C_4C_3$	-	-	118.9(10)
Dihedral angle			
$\tau(C_4C_3C_2C_1)$	-	-	-45.3(12)
$\tau(C_3C_4C_5C_6)$	19.0(33)	-	-
$\tau(C_6C_1C_2C_3)$	61.0(28)	62.9(7)	-
$\tau(C_7C_1C_6C_5)$	-	187.5(7)	189.8(24)
$\tau(C_9C_7C_1C_2)$	-	166.5(3)	-
$\tau(C_8C_7C_1C_6)$	-	-	12.2(19)
σ^a	0.066	0.019	0.021

[a] Deviation of the fit

Table S40. Effective r_0 bond lengths (in Å), bond angles and dihedral angles (in degrees) of the **Ax-a** conformer of **perillaldehyde**.



Bond length	**Ax-a**
$r(C_1–C_2)$	1.367(44)
$r(C_2–C_3)$	1.594(41)
$r(C_3–C_4)$	1.377(36)
$r(C_7–C_4)$	1.468(20)
$r(C_9–C_1)$	1.546(71)
$r(C_{10}–C_9)$	1.547(82)
$r(C_{11}–C_9)$	1.420(25)
Angle	
$\angle C_1C_2C_3$	113.9(13)
$\angle C_2C_3C_4$	120.6(17)
$\angle C_6C_1C_2$	114.2(24)
$\angle C_7C_4C_3$	116.6(26)
$\angle C_9C_1C_2$	117.3(29)
$\angle C_{10}C_9C_1$	114.3(25)
$\angle C_{11}C_9C_1$	132.9(71)
Dihedral angle	
$\tau(C_1C_2C_3C_4)$	-8.0(21)
$\tau(C_6C_1C_2C_3)$	36.1(31)
$\tau(C_{10}C_9C_1C_2)$	8.3(19)
σ^a	0.075

[a] Deviation of the fit

Table S41. Theoretical spectroscopic parameters of the six stable conformers of **carvone** calculated at the M062X-GD3 level of theory.

	Eq-A	**Eq-C**	**Eq-a**	**Ax-a**	**Ax-C**	**Ax-A**
A (MHz)	2252.6	2276.2	2231.9	1612.3	1673.2	1816.3
B (MHz)	660.3	679.1	692.1	923.6	896.6	834.0
C (MHz)	582.0	553.4	552.8	793.0	784.3	765.6
μ_a (D)	1.9	2.1	1.8	1.3	2.3	1.3
μ_b (D)	2.8	3.0	2.5	2.7	2.9	3.1
μ_c (D)	0.8	0.5	0.2	1.2	0.7	0.5
ΔE (cm^{-1})	11	0	61	272	145	346
ΔE_{ZPC} (cm^{-1})	32	0	120	383	325	436
ΔG (cm^{-1})	24	0	146	478	568	506

Table S42. Theoretical spectroscopic parameters of the six stable conformers of **limonene** calculated at the M062X-GD3 level of theory.

	Eq-A	**Eq-C**	**Eq-a**	**Ax-A**	**Ax-a**	**Ax-C**
A (MHz)	3075.1	3072.0	3061.8	2206.9	2131.9	1957.3
B (MHz)	723.4	749.6	756.4	942.5	954.9	1000.9
C (MHz)	680.6	646.2	638.4	918.6	918.9	930.2
μ_a (D)	0.4	0.3	0.3	0.5	0.1	0.1
μ_b (D)	0.4	0.2	0.7	0.1	0.6	0.2
μ_c (D)	0.3	0.3	0.1	0.0	0.3	0.3
ΔE (cm^{-1})	2	0	179	573	24	626
ΔE_{ZPC} (cm^{-1})	45	0	184	659	82	771
ΔG (cm^{-1})	57	0	220	743	151	888

Table S43. Theoretical spectroscopic parameters of the six stable conformers of **limonene** calculated at the M062X-GD3 level of theory.

	Eq-A_0	**Eq-C_0**	**Eq-a_0**	**Ax-a_0**	**Ax-A_0**	**Ax-C_0**
A (MHz)	2900.5	2858.5	2934.2	2049.9	2110.0	1788.8
B (MHz)	539.8	555.5	554.6	694.0	693.3	731.4
C (MHz)	509.9	490.2	484.1	674.0	667.4	687.2
μ_a (D)	2.9	2.9	3.1	3.4	2.7	2.9
μ_b (D)	1.6	1.2	1.8	1.7	1.5	1.4
μ_c (D)	0.1	0.6	0.1	0.5	0.2	1.1
ΔE (cm^{-1})	1152	1162	1333	1054	1707	1782
ΔE_{ZPC} (cm^{-1})	1118	1116	1297	1147	1749	1904
ΔG (cm^{-1})	1099	1093	1305	1222	1821	2005

	Eq-A	**Eq-C**	**Eq-a**	**Ax-a**	**Ax-A**	**Ax-C**
A (MHz)	2949.3	2974.6	2904.5	1910.9	2017.3	1805.2
B (MHz)	540.1	552.0	560.7	721.0	701.9	736.6
C (MHz)	512.3	491.4	487.1	686.5	688.9	700.4
μ_a (D)	3.0	3.2	3.0	2.9	2.5	3.1
μ_b (D)	1.6	1.9	1.5	2.2	2.3	2.3
μ_c (D)	0.7	0.4	0.1	0.9	1.0	0.8
ΔE (cm^{-1})	14	45	168	0	595	704
ΔE_{ZPC} (cm^{-1})	0	73	247	68	723	843
ΔG (cm^{-1})	0	165	370	173	940	993

Figure S1. Geometries of the six conformers of **carvone** calculated at the MP2/6-311++G(d,p) level of theory.

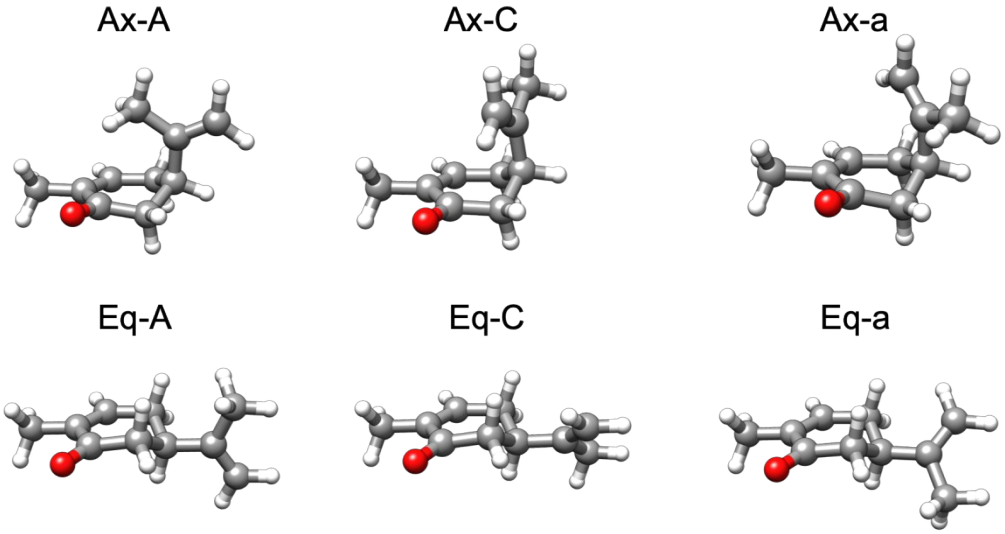


Figure S2. Geometries of the six conformers of **limonene** calculated at the MP2/6-311++G(d,p) level of theory.

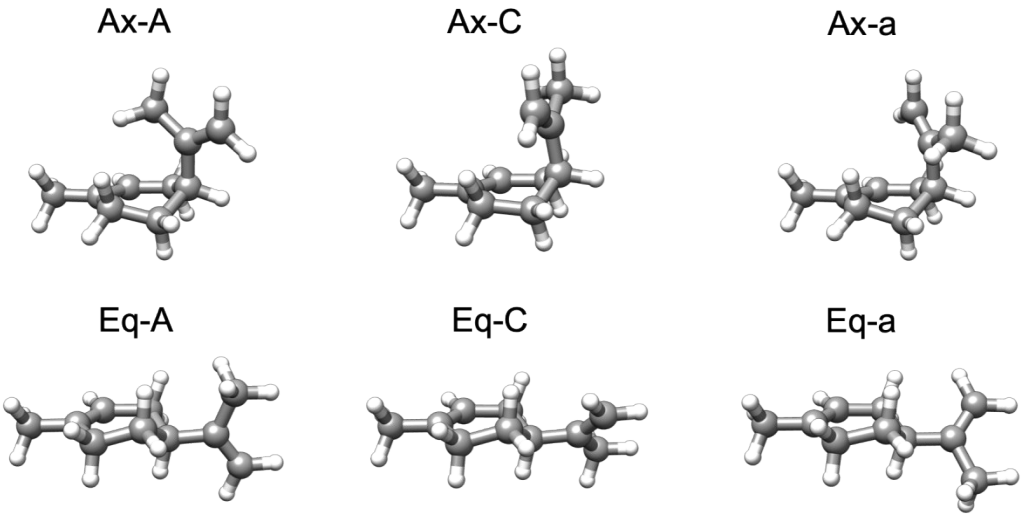


Figure S3. Geometries of the twelve conformers of **perillaldehyde** calculated at the MP2/6-311++G(d,p) level of theory.

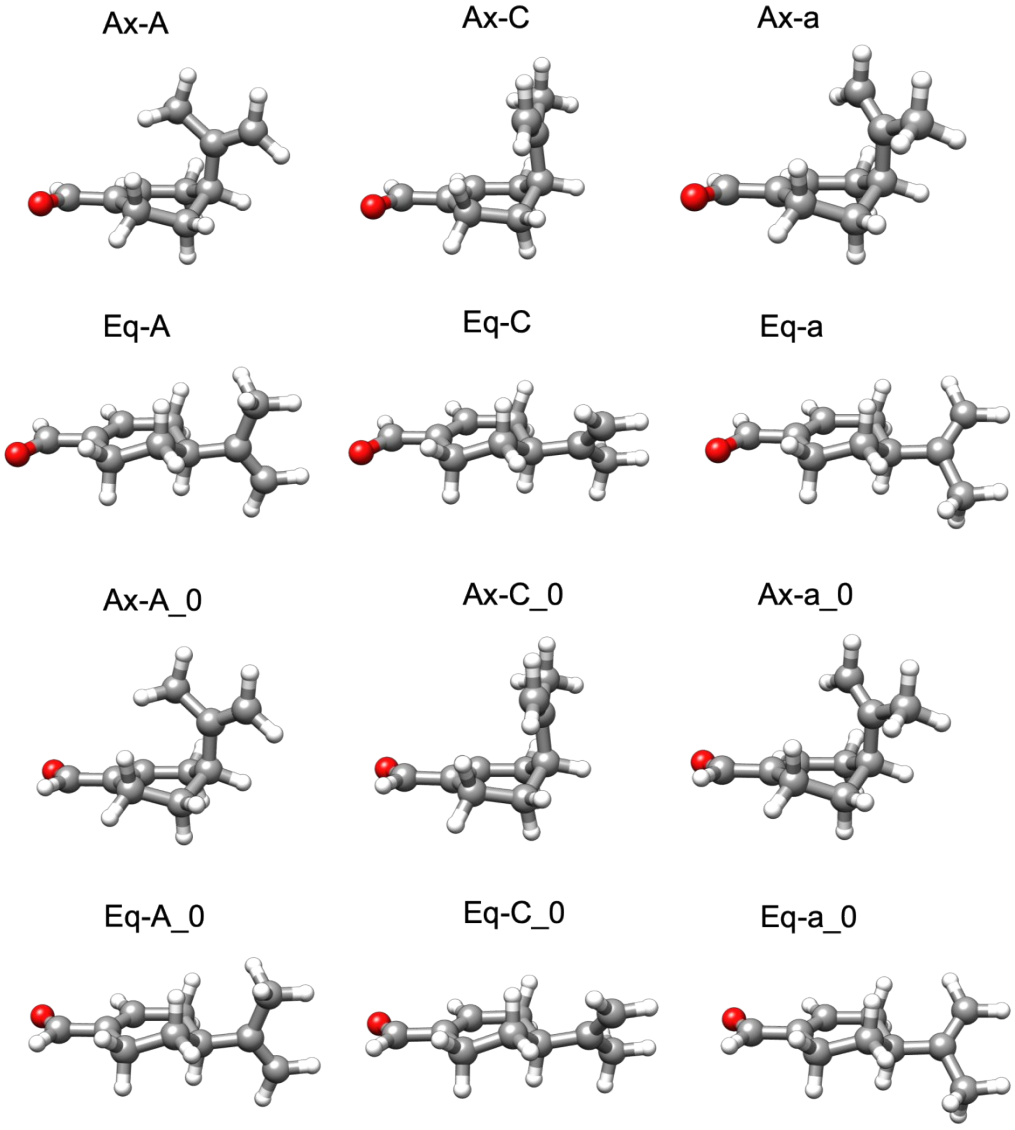
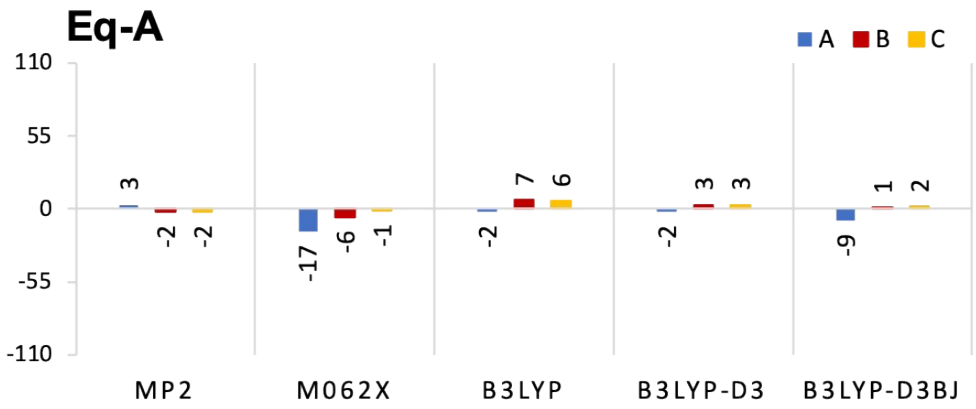
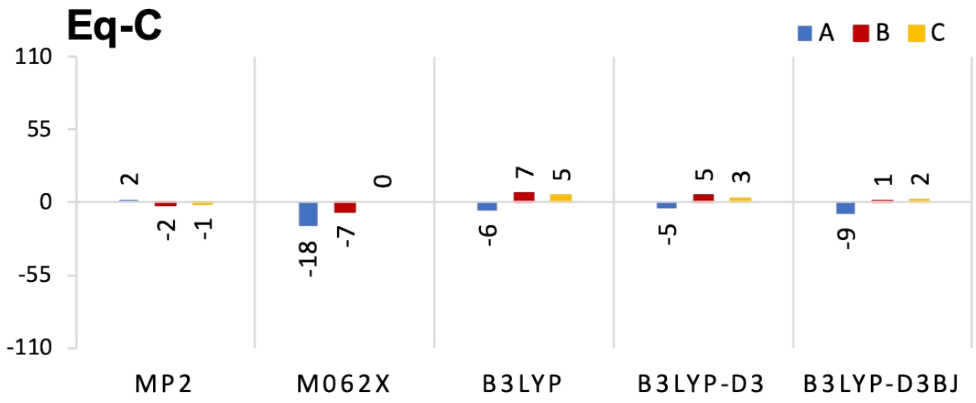
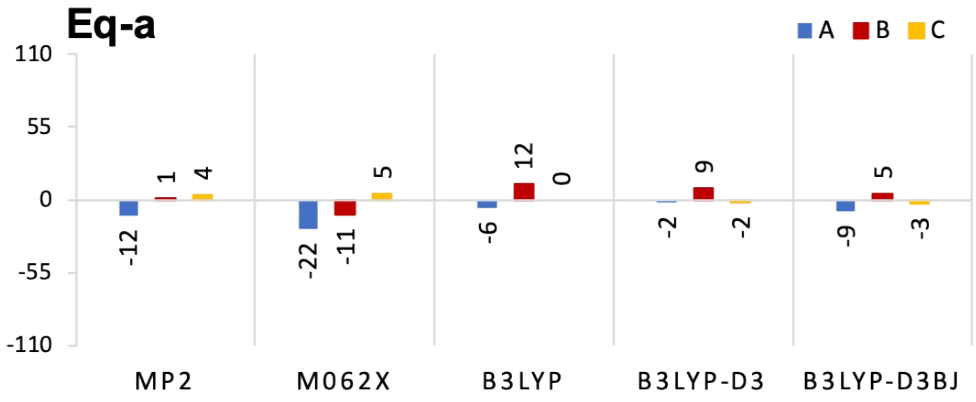


Figure S4. Calculated differences between experimental and theoretical rotational constants (in MHz) for the four observed conformers of **limonene**.







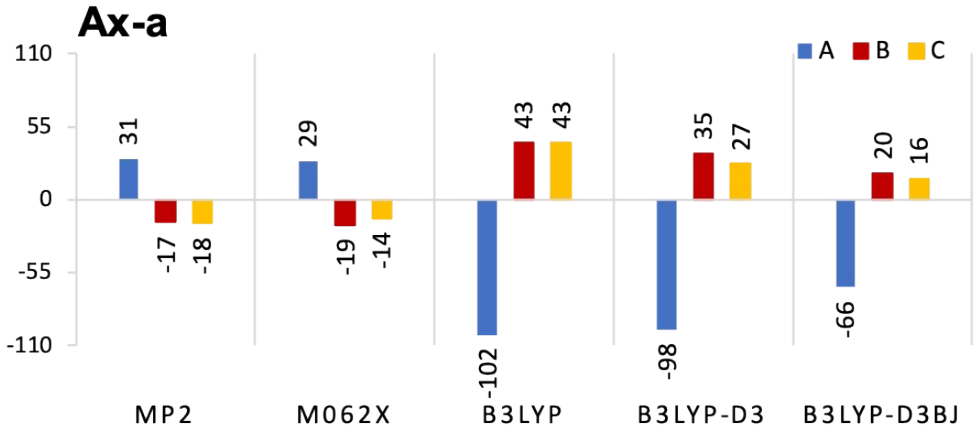


Figure S5. Calculated differences between experimental and theoretical rotational constants (in MHz) for the four observed conformers of **perillaldehyde**.

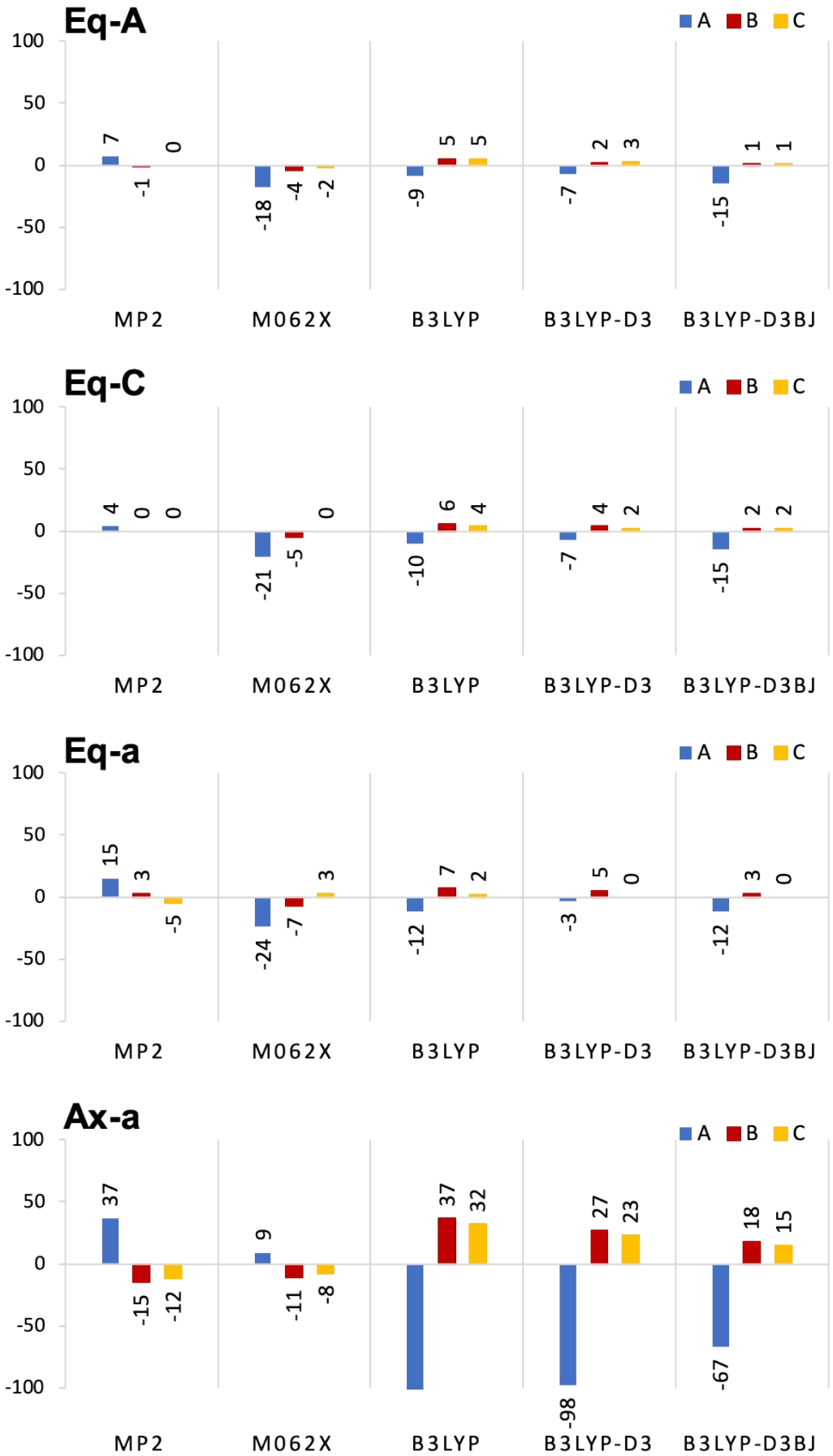


Figure S6. Calculated differences between experimental and theoretical vibrationally-corrected rotational constants A_0, B_0, C_0 (in MHz) for the five observed conformers of **carvone.**

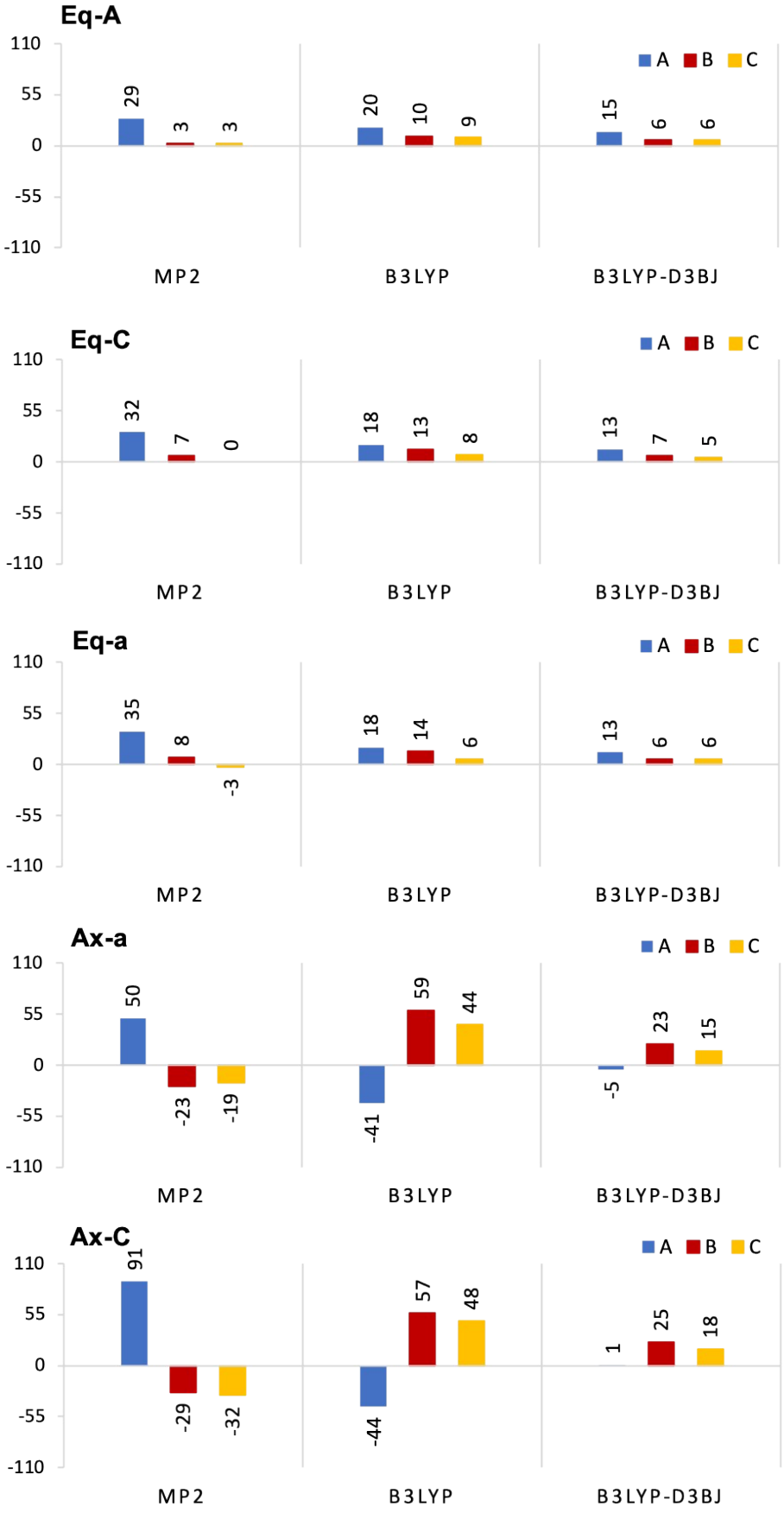
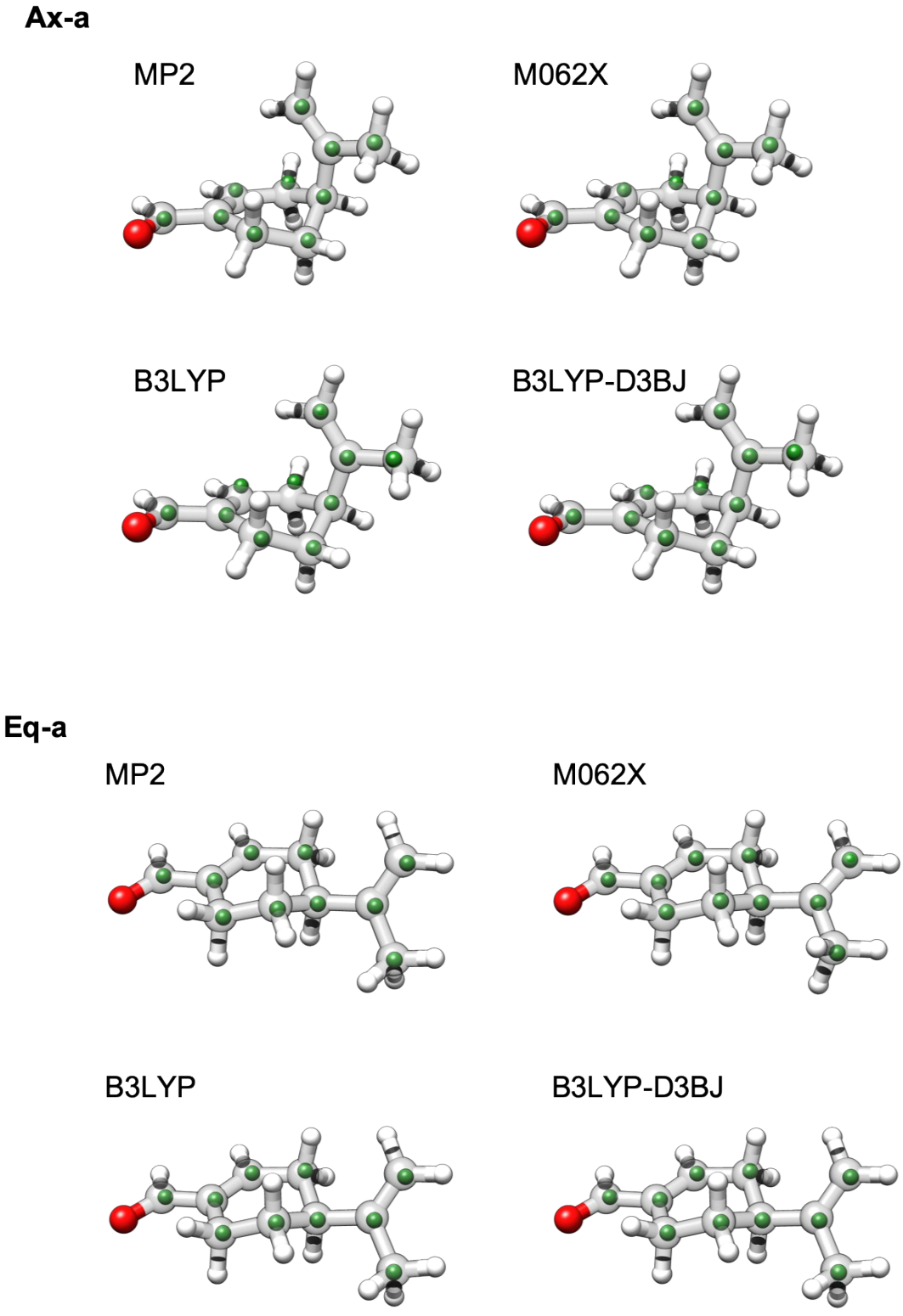
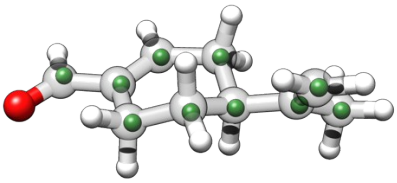


Figure S7. Comparison of the theoretical structures of **perillaldehyde** (full molecular drawing) with the r_s atom coordinates of the C atoms (green spheres).

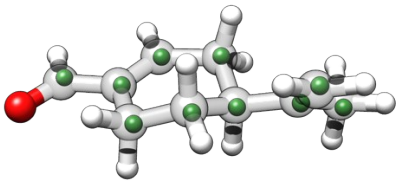


Eq-C

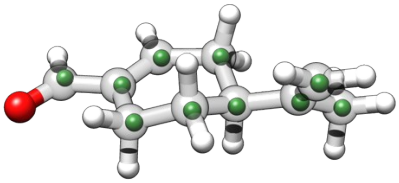
MP2



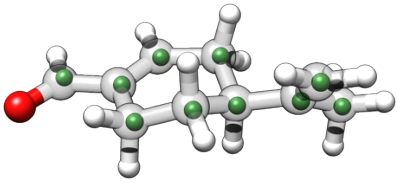
M062X



B3LYP

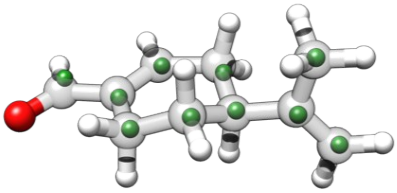


B3LYP-D3BJ

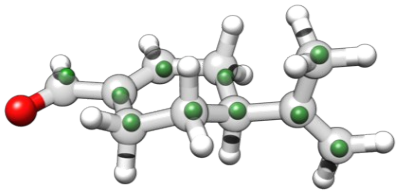


Eq-A

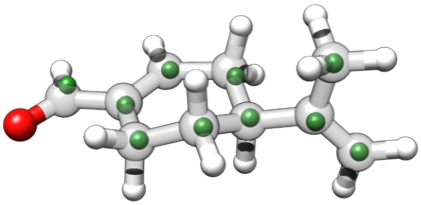
MP2



M062X



B3LYP



B3LYP-D3BJ

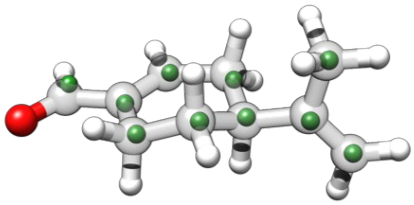
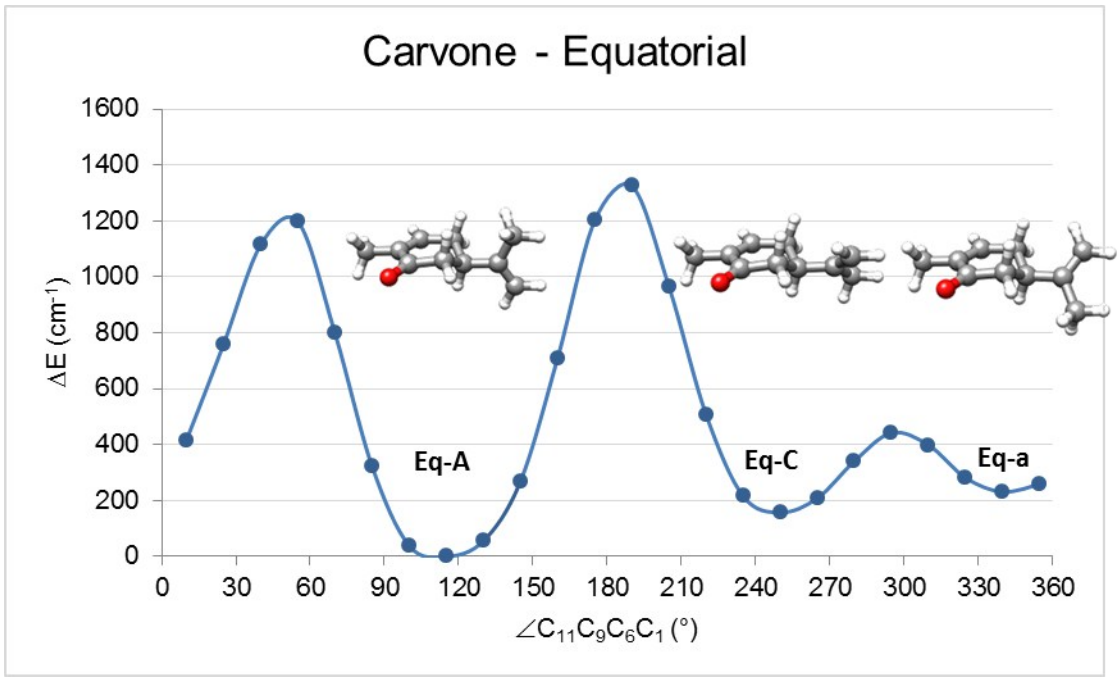


Figure S8. Interconversion barriers between the conformers of **carvone** calculated at the MP2/6-311++G(d,p) level of theory.



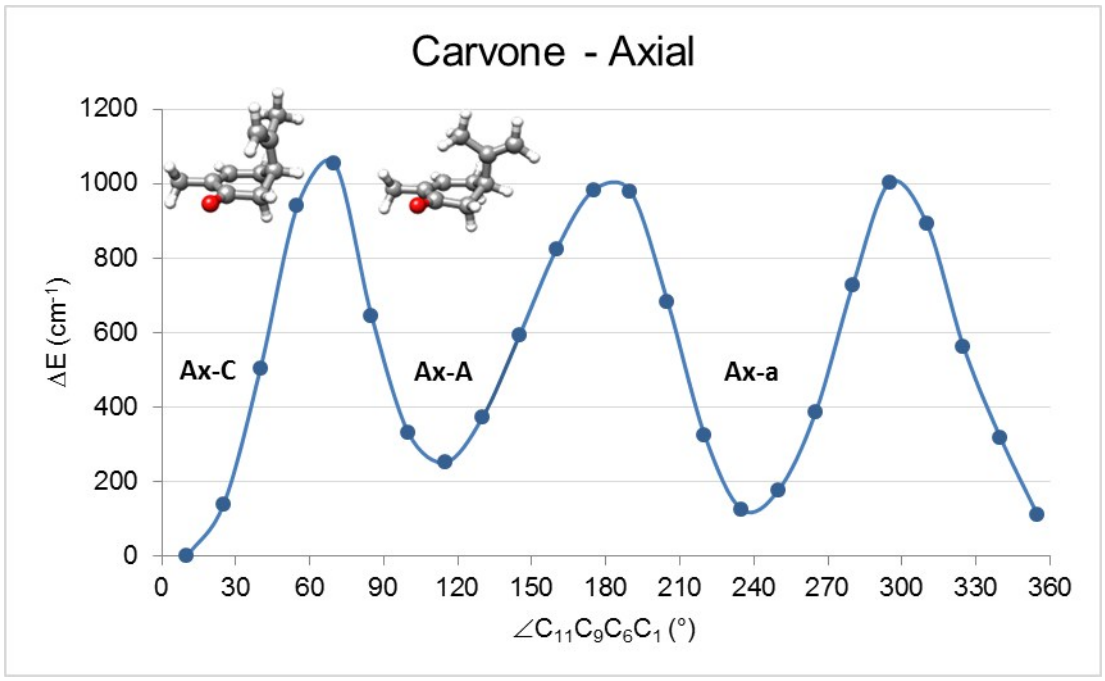
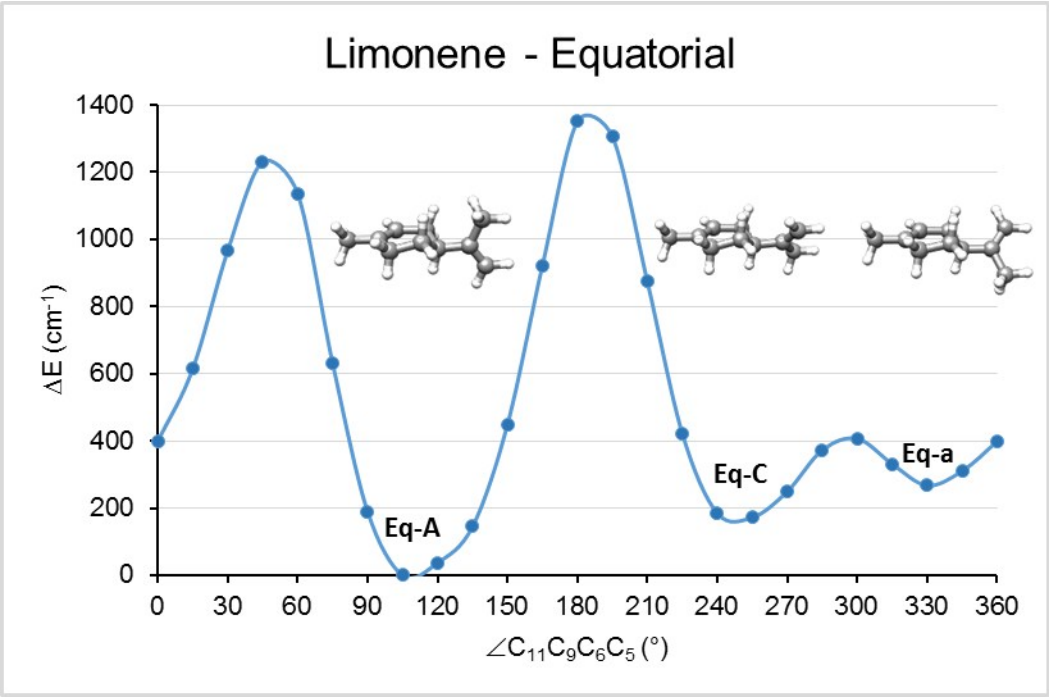


Figure S9. Interconversion barriers between the conformers of **limonene** calculated at the MP2/6-311++G(d,p) level of theory.



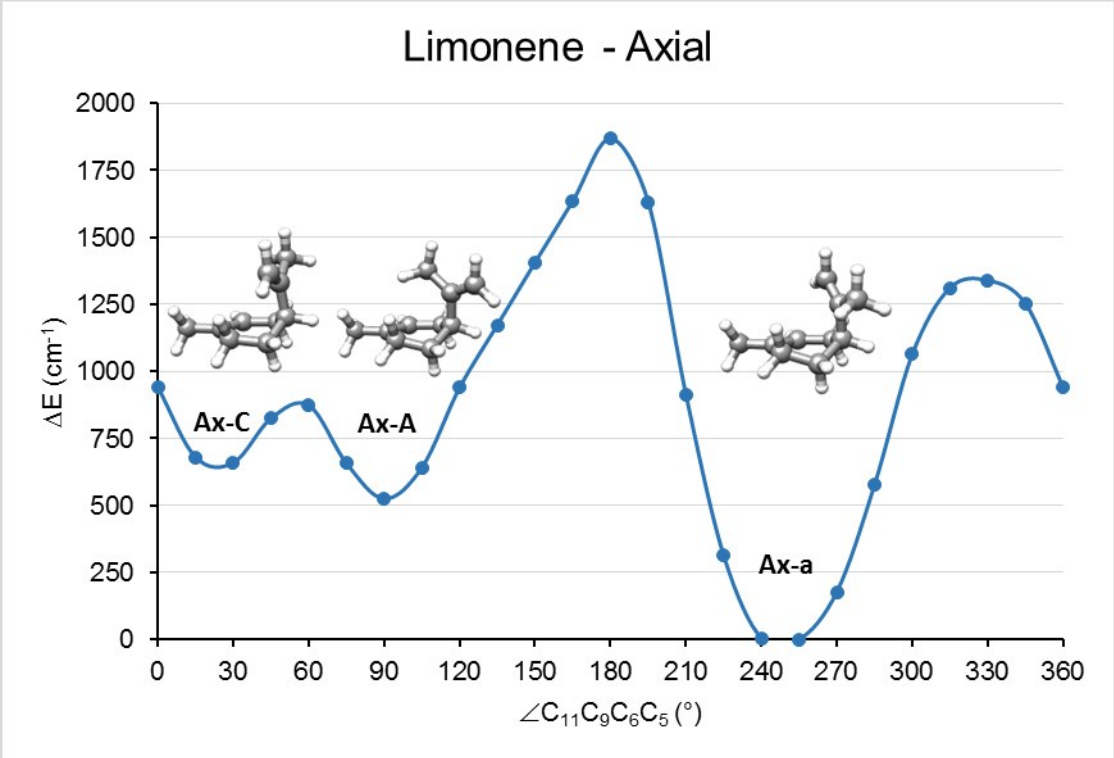
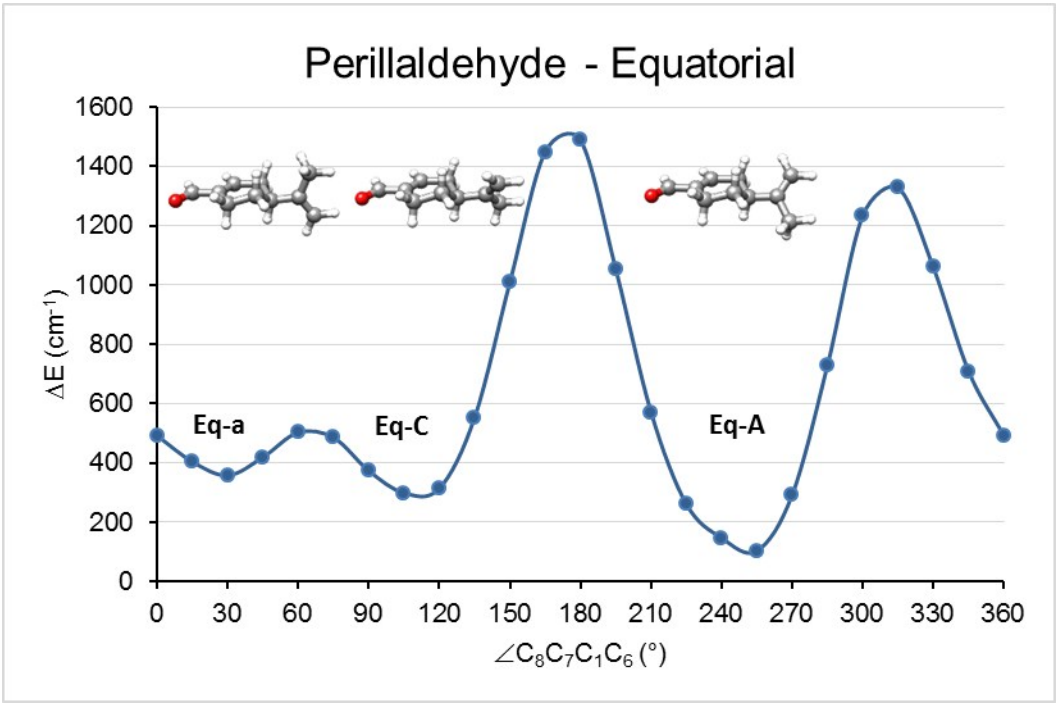


Figure S10. Interconversion barriers between the conformers of **perillaldehyde** calculated at the MP2/6-311++G(d,p) level of theory.



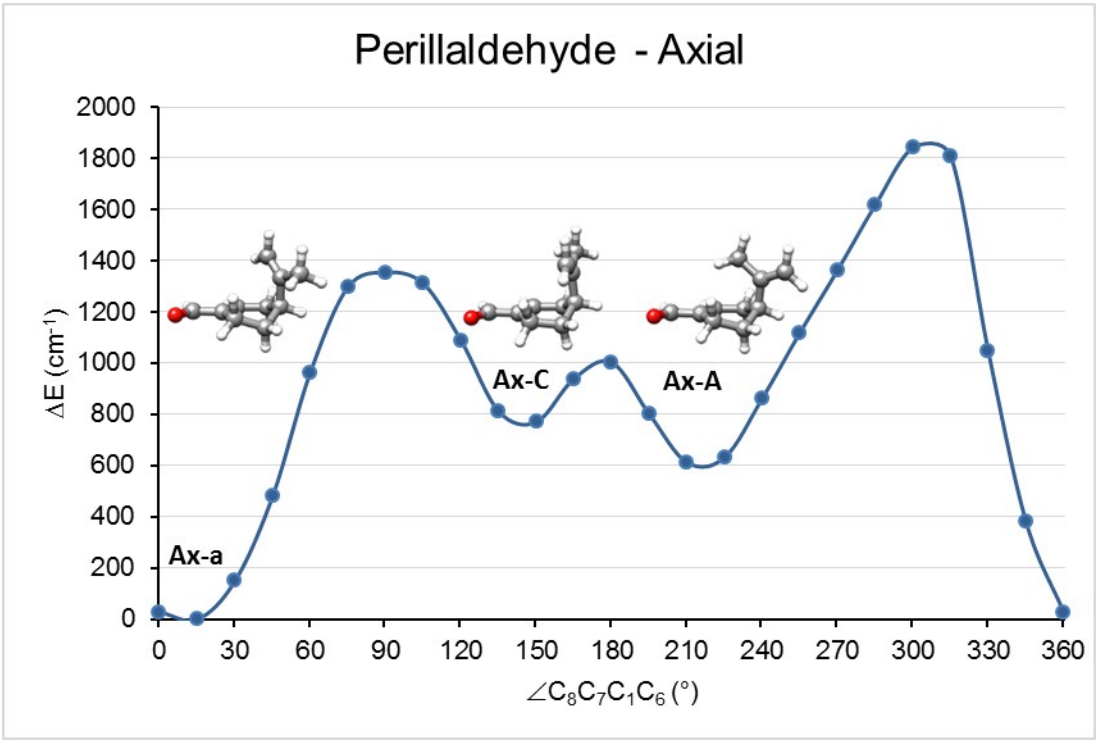
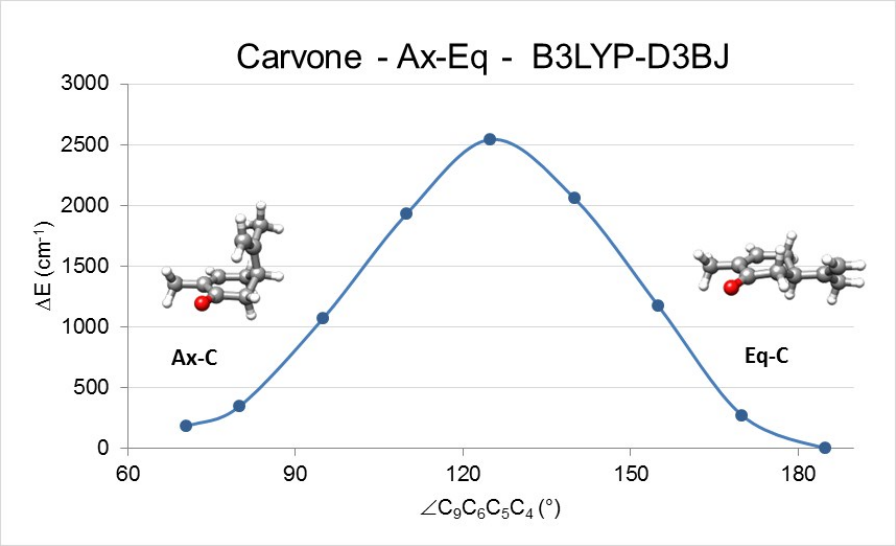


Figure S11. Interconversion barriers between conformers Ax-C and Eq-C of carvone at the B3LYP-D3BJ/6-311++G(d,p) (top) and axial and MP2/6-311++G(d,p) (bottom) levels of theory.



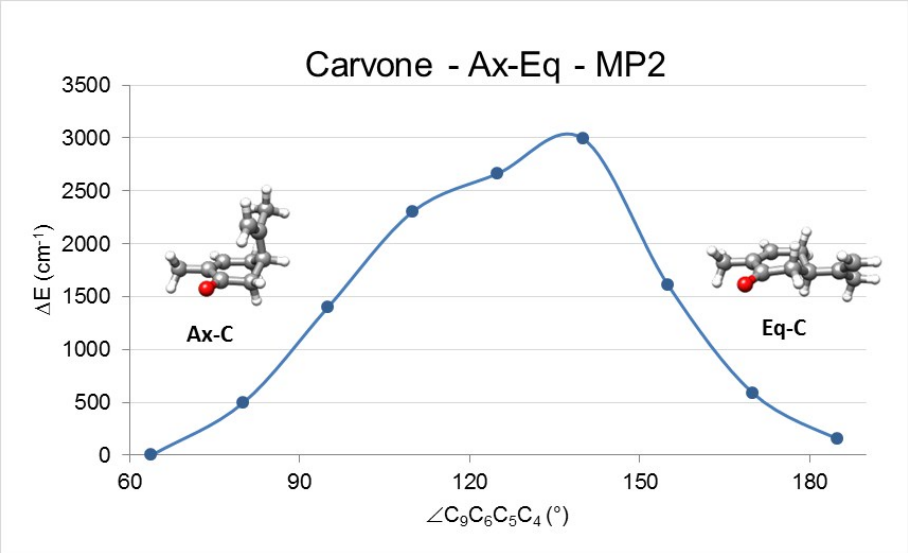


Figure S12. NCI plots for the five observed conformers of **carvone** showing the intramolecular interactions. Red indicates repulsive interactions, blue and green indicates strong and weak attractive interactions, respectively.

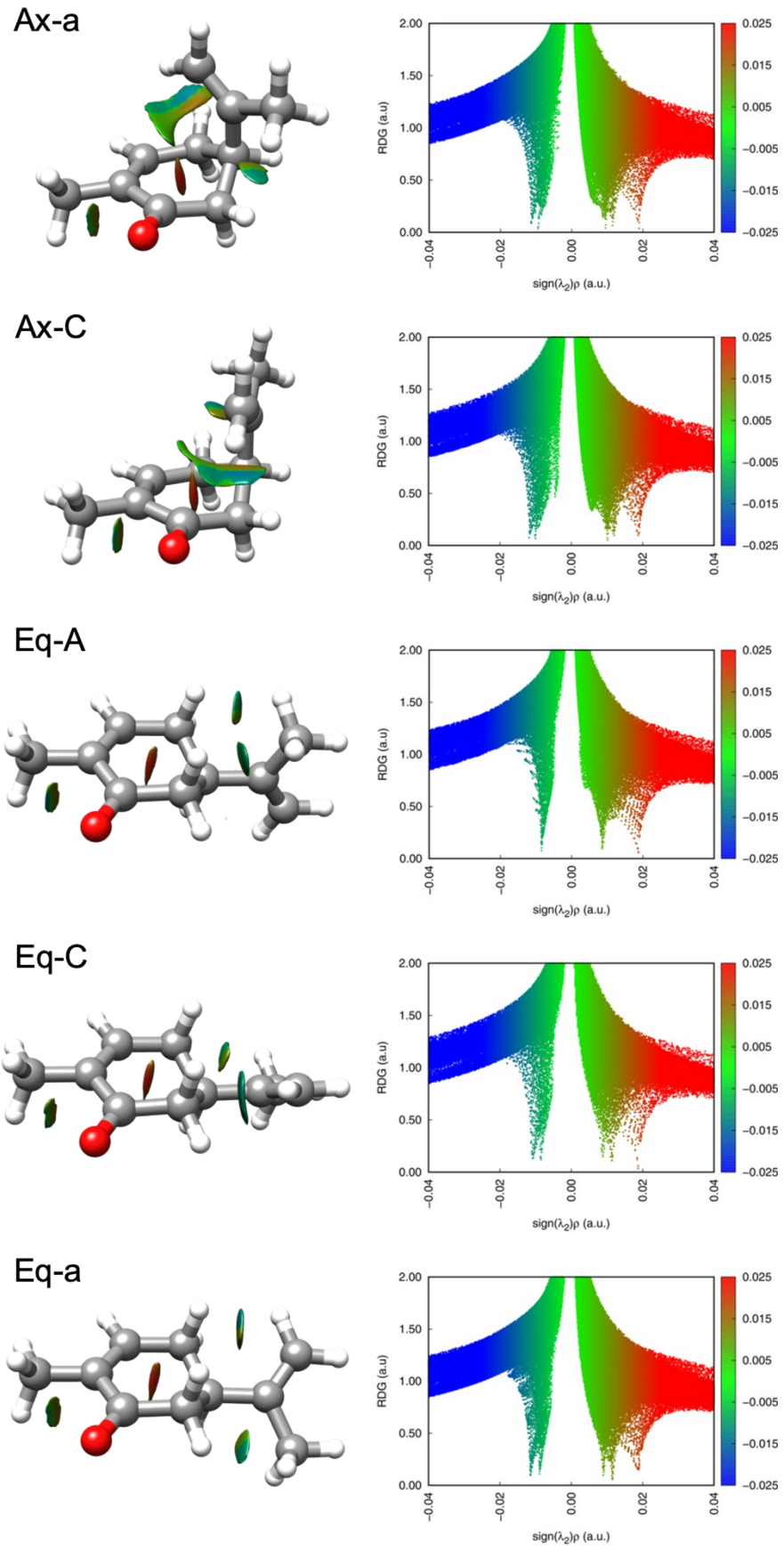


Figure S13. NCI plots for the four observed conformers of **limonene** showing the intramolecular interactions. Red indicates repulsive interactions, blue and green indicates strong and weak attractive interactions, respectively.

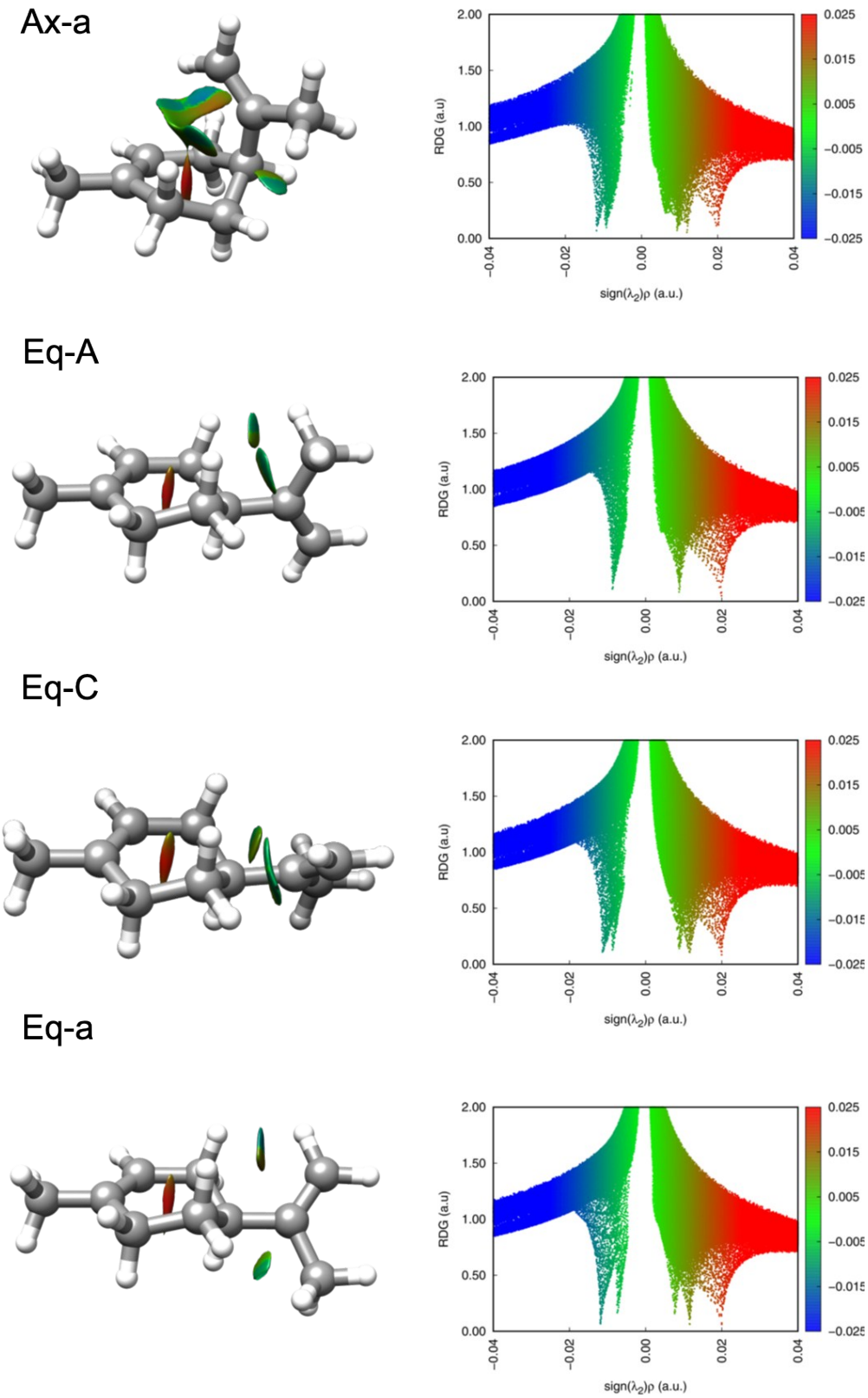


Figure S14. NCI plots for the four observed conformers of **perillaldehyde** showing the intramolecular interactions. Red indicates repulsive interactions, blue and green indicates strong and weak attractive interactions, respectively.