



Supplementary Materials

Essential oil composition and enantioselective profile of *Juniperus communis* var. *depressa* (Cupressaceae) from Utah

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MRR Supplemental Material

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Figure S2. Optimized geometries of low energy isomers of 3-carene / TFIP homochiral isomers. Isomer geometries were optimized at B3LYP GD3BJ def2-TZVP level of theory.

1. δ -3-carene

1.1 Quantum Chemistry

Table S1. Spectroscopic constants for low energy isomers of 3-carene / TFIP heterochiral isomers. Isomer geometries were optimized at B3LYP GD3BJ def2-TZVP level of theory.

Isomer	ΔE (cm ⁻¹)	A (MHz)	B (MHz)	C (MHz)	μ_a (D)	μ_b (D)	μ_c (D)
1	0.0	668.38	276.05	243.72	-2.8	-0.2	-1
2	82.6	808.58	245.86	229.91	-2.5	-1.1	0.3
3	294.8	763.59	258.82	239.62	-1.9	0.7	1.4
4	315.1	908.47	215.95	197.89	-2	-0.7	0.9
5	533.2	688.64	265.47	243.94	1.7	-0.7	0.9
6	552.9	682.75	269.12	231.72	-1.8	1.8	-0.6

*-883.190367 hartree

Table S2. Spectroscopic constants for low energy isomers of 3-carene / TFIP homochiral isomers. Isomer geometries were optimized at B3LYP GD3BJ def2-TZVP level of theory.

Isomer	ΔE (cm ⁻¹)	A (MHz)	B (MHz)	C (MHz)	μ_a (D)	μ_b (D)	μ_c (D)
1	0.0	696.53	274.77	250.21	-2.7	0.7	-0.1
2	186.3	760.04	248.04	222.15	-2.6	0.4	1.3
3	309.4	853.28	216.97	205.33	1.4	-2	0.3
4	329.8	689.26	270.89	235.01	-2.1	-1.6	-0.3
5	375.8	973.68	215.82	202.67	1.7	1.2	0.8
6	393.6	686.75	287.86	244.28	-1	-1.7	1.4

*-883.190527 hartree

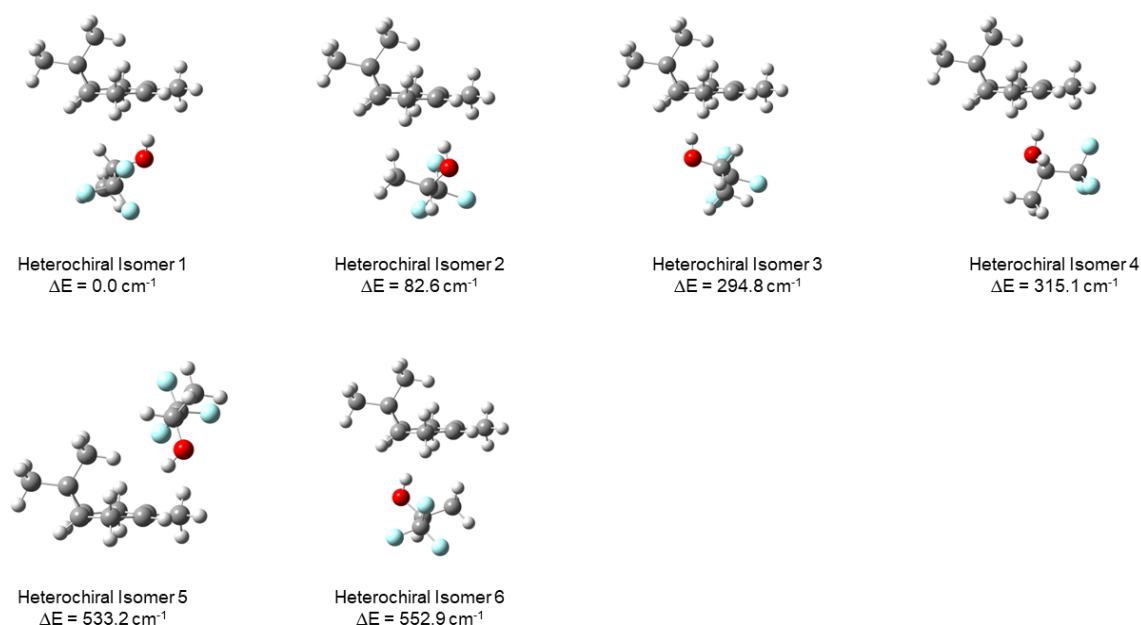


Figure S1. Optimized geometries of low energy isomers of 3-carene / TFIP heterochiral isomers. Isomer geometries were optimized at B3LYP GD3BJ def2-TZVP level of theory.

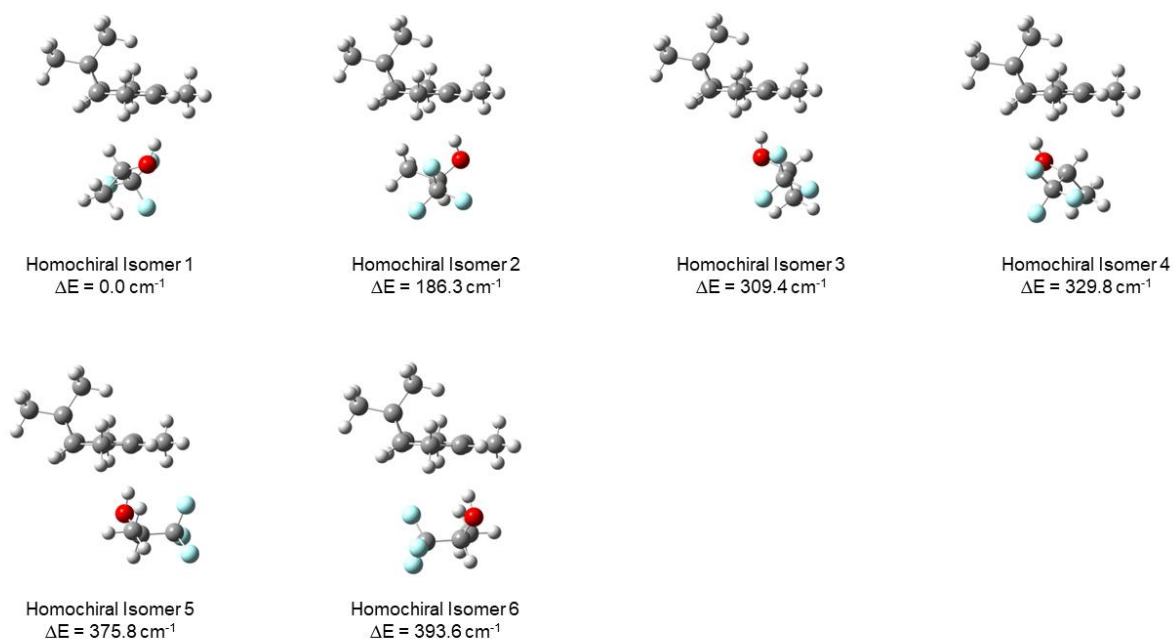


Figure S2. Optimized geometries of low energy isomers of 3-carene / TFIP homochiral isomers. Isomer geometries were optimized at B3LYP GD3BJ def2-TZVP level of theory.

1.2 Experimental Fits

Table S3. Experimental fit 3-carene_TFIP_asn1.

Spectroscopic Constant	Experimental
A / MHz	699.5400(58)
B / MHz	273.54368(15)
C / MHz	249.52309(15)
Δ_J / kHz	0.03875(15)
Δ_{JK} / kHz	0.0138(13)
δ_J / kHz	0.00398(21)
N	115
rms	3.8

Table S4. Experimental fit 3-carene_TFIP_asn2.

Spectroscopic Constant	Experimental
A / MHz	671.7360(37)
B / MHz	273.54053(13)
C / MHz	242.17006(12)
Δ_J / kHz	0.03905(14)
Δ_{JK} / kHz	0.0682(11)
δ_J / kHz	0.00813(16)
N	121
rms	3.7

1.3 Agreement with Theory

Table S5. Comparison of experimental assignment 3-carene_TFIP_asn1 with structure match from theory.

Spectroscopic Constant	3-carene_TFIP_asn1	Homochiral Isomer1	%Error
A / MHz	699.5400(58)	696.53	+0.43
B / MHz	273.54368(15)	274.77	-0.45
C / MHz	249.52309(15)	250.21	-0.28

Table S6. Comparison of experimental assignment 3-carene_TFIP_asn2 with structure match from theory.

Spectroscopic Constant	3-carene_TFIP_asn2	Heterochiral Isomer1	%Error
A / MHz	671.7360(37)	668.38	+0.50
B / MHz	273.54053(13)	276.05	-0.92
C / MHz	242.17006(12)	243.72	-0.64

2. α -Pinene

Enantiopure references standard of (-)- α -pinene was available and used to assign the relative stereochemistry (heterochiral or homochiral) of the non-covalent complexes of α -pinene and propylene oxide (PO).

2.1 Experimental Fits

Table S7. Experimental fit a-pinene_PO_heterochiral.

Spectroscopic Constant	Experimental
A / MHz	1224.38(39)
B / MHz	379.62248(21)
C / MHz	373.95835(21)
Δ_J / kHz	0.07018(58)
Δ_{JK} / kHz	-0.071(26)
δ_J / kHz	-0.00108(79)
N	28
rms	1.6

Table S8. Experimental fit a-pinene_PO_homochiral.

Spectroscopic Constant	Experimental
A / MHz	1192.827(24)
B / MHz	383.51605(28)
C / MHz	358.36245(26)
Δ_J / kHz	0.08284(50)
Δ_{JK} / kHz	0.1778(40)
δ_J / kHz	0.01162(85)
N	47
rms	2.6