Electronic structure, reactivity and Hirshfeld surface analysis of carvone

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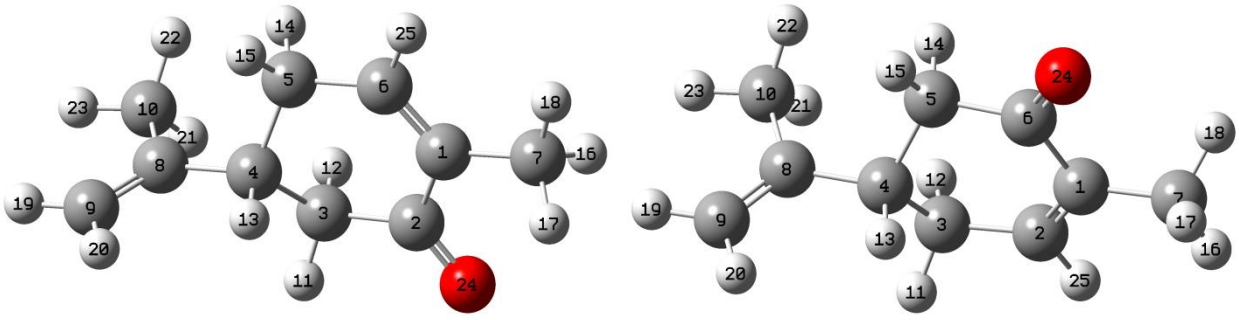

A B

Figure S1. Optimized molecular structures and atom numbering of R-(–)-carvone (A) and S-(+)-carvone (B): O-atoms are in red, C-atoms are in grey and H-atoms are in white.

Table S1. Optimized geometrical parameters of R-(–)-carvone and S-(+)-carvone

Parameters	B3LYP/6-311++G(2d,2p) R-(–)-carvone	XRD data [1] R-(–)-carvone	B3LYP/6-311++G(2d,2p) S-(+)-carvone
Bond lengths (Å)			
C^1–C^2	1.487	1.461	1.342
C^2–C^3	1.520	1.515	1.501
C^3–C^4	1.538	1.550	1.539
C^4–C^5	1.539	1.536	1.538
C^5–C^6	1.501	1.504	1.520
C^6– C^1	1.342	1.322	1.487
C^1–C^7	1.502	1.525	1.502
C^2–O^{24} (H^{25})	1.218	1.290	1.086
C^6–H^{25} (O^{24})	1.086	0.930	1.218
C^4–C^8	1.517	1.512	1.517
C^8–C^9	1.332	1.330	1.332
C^8–C^{10}	1.507	1.429	1.507
Bond angles (degree)			
C^1–C^2–C^3	117.5	118.7	125.0
C^2–C^3–C^4	112.6	109.6	112.3
C^3–C^4–C^5	109.1	108.9	109.1

$C^4–C^5–C^6$	112.3	111.1	112.6
$C^5–C^6–C^1$	125.0	124.6	117.5
$C^6–C^1–C^2$	119.6	120.1	119.6
$C^2–C^1–C^7$	116.9	118.0	123.5
$C^1–C^2–O^{24}(H^{25})$	121.3	117.9	118.6
$C^1–C^6–H^{25}(O^{24})$	118.6	117.5	121.3
$C^3–C^4–C^8$	113.3	113.1	113.1
$C^5–C^4–C^8$	113.1	111.0	113.3
$C^4–C^8–C^9$	120.4	119.7	120.4
$C^4–C^8–C^{10}$	118.4	117.9	118.4
$C^9–C^8–C^{10}$	121.3	122.2	121.3
Dihedral angles (degree)			
$C^1–C^2–C^3–C^4$	–33.6	–35.7	–20.8
$C^1–C^6–C^5–C^4$	20.8	22.1	33.6
$C^2–C^3–C^4–C^8$	–178.0	–178.5	175.2
$C^6–C^5–C^4–C^8$	–175.2	–176.0	178.0
$C^3–C^4–C^8–C^9$	121.7	130.9	113.5
$C^5–C^4–C^8–C^9$	–113.5	–106.4	–121.7
$C^3–C^4–C^8–C^{10}$	–58.2	–53.5	–66.7
$C^5–C^4–C^8–C^{10}$	66.7	69.2	58.2
$C^7–C^1–C^4–C^8$	–173.6	177.3	173.7

[1] J.Sane, J.Rius, T.Calvet, M.A.Cuevas-Diarte, Chiral Molecular Alloys: Patterson-Search Structure Determination of l-Carvone and dl-Carvone from X-ray Powder Diffraction Data at 218 K, Acta Crystallographica,Section B: Structural Science, 53 (1997) 702–707.

Table S2. Energy, Dipole moment, Polarizability and Hyperpolarizability of R-(–)-carvone and S-(+)-carvone calculated with B3LYP/6-311++G(2d,2p)

Parameters	**R-(–)-carvone**	**S-(+)-carvone**
Energy	–464.84305 a.u.	–464.84305 a.u.
Dipole moment	3.5609349 D	3.5610063 D
Polarizability	123.13367 a.u.	123.13433 a.u.
Hyperpolarizability	84.277767 a.u.	84.281854 a.u.