Supplementary Material

Bond	Bond length (Å)	Bond angle (°)	Dihedral angle (°)
2–3	1.500		
3=4	1.347	124.5	
4–5	1.458	126.8	-180.0
5=6	1.366	118.4	-180.0
6–7	1.437	128.2	-180.0
7=8	1.364	123.2	-179.4
8–9	1.445	126.5	179.6
9=10	1.372	118.7	-179.4
10–11	1.432	127.6	179.2
11=12	1.365	123.9	176.2
12–13	1.442	128.8	-178.2
13=14	1.370	119.1	173.3
14–15	1.432	126.8	-175.1
15=15’	1.370	125.9	174.6
15’–14’	1.430	125.1	0.0
14’=13’	1.368	128.3	-168.9
13’–12’	1.446	117.0	180.0
12’=11’	1.356	127.5	-177.0
11’–10’	1.445	122.4	179.4
10’=9’	1.352	127.4	-177.7
9’–8’	1.506	121.0	180.0
5–Me	1.509	118.0	0.0
9–Me	1.511	118.3	1.0
13–Me	1.505	118.6	-4.7
13’–Me	1.509	123.4	1.7
9’–Me	1.503	123.7	0.3

Table 2: This table lists bond lengths, bond angles and dihedral angles for the optimized non-planar 15,15’-cis spheroidene structure used for our frequency calculations reported in Table 1. The Cartesian coordinates in the X-ray structure (11, 20) of the five methyl groups were fixed. For this particular optimization the 14–15=15’–14’ dihedral angle was also fixed at 0.0 °. The value for this dihedral was not found to significantly influence the calculated frequencies or compositions. The angles are defined from top to bottom in the table. The bond angle listed by the 3=4 bond therefore refers to the 2–3=4 bond angle. The dihedral angle listed by the 4–5 bond refers to the 2–3=4–5 dihedral angle, etc.