

Peculiarities of molecular interactions in the L-menthol–thymol system

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S1. Parameters of the $O_{\text{Thymol}} - O_{\text{Thymol}}$ radial distribution functions for the L-menthol thymol mixture at 343 K: molar fractions – x_{thymol} , distance of the first maximum – $r_{\text{max1}}(\text{\AA})$, intensity of the first maximum – I_1 (Probability density), first coordination number – CN_1 .

x_{thymol}	$r_{\text{max1}}, \text{\AA}$	I_1	CN_1
0.01	-	-	-
0.10	3.65	3.09	3.7
0.20	3.25	0.64	0.7
0.33	3.65	1.26	2.0
0.40	3.55	1.45	2.2
0.45	3.55	1.38	2.0
0.50	3.45	1.52	1.8
0.60	3.65	1.27	1.7
0.70	3.45	1.19	1.9
0.80	3.55	1.37	2.0
0.90	3.45	1.32	2.0
0.99	3.45	1.29	2.0

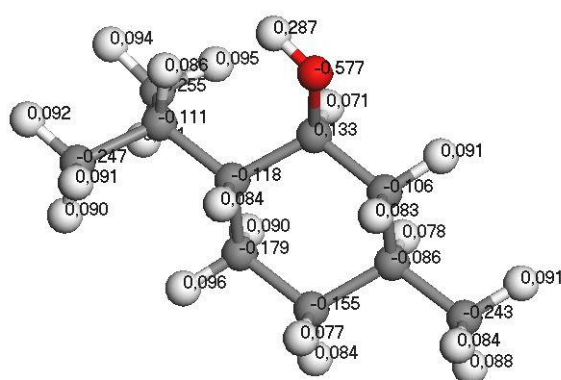
S2. Parameters of the $O_{\text{Thymol}} - O_{\text{L-Menthol}}$ radial distribution functions for the L-menthol thymol mixture at 343 K: molar fractions – x_{thymol} , distance of the first maximum – $r_{\text{max1}}(\text{\AA})$, intensity of the first maximum – I_1 (Probability density), first coordination number – CN_1 .

x_{thymol}	$r_{\text{max1}}, \text{\AA}$	I_1	CN_1
0.01	3.45	1.37	1.1
0.10	3.45	1.47	1.9
0.20	3.55	1.70	2.2
0.33	3.45	1.61	2.0
0.40	3.55	1.53	2.1
0.45	3.45	1.42	2.0
0.50	3.45	1.36	1.8
0.60	3.55	1.60	2.0
0.70	3.55	1.62	2.3
0.80	3.65	1.63	2.0
0.90	3.55	1.54	1.9
0.99	3.55	1.43	2.7

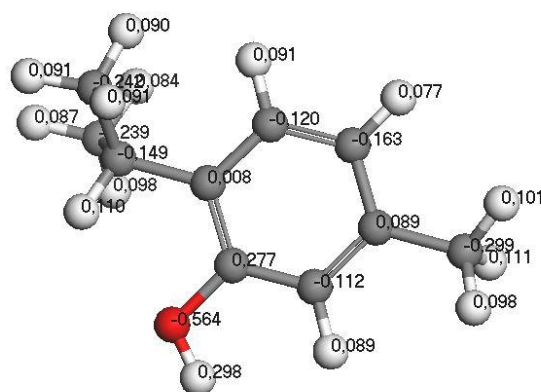
S3. Parameters of the O_L-Menthol – O_L-Menthol radial distribution functions for the L-menthol thymol mixture at 343 K: molar fractions – x_{thymol} , distance of the first maximum – $r_{\text{max1}}(\text{\AA})$, intensity of the first maximum – I_1 (Probability density), first coordination number – CN_1 ..

x_{thymol}	$r_{\text{max1}}, \text{\AA}$	I_1	CN_1
0.01	3.65	1.06	1.7
0.10	3.65	1.05	1.6
0.20	3.65	1.16	1.4
0.33	3.75	0.93	1.5
0.40	3.55	1.09	1.3
0.45	3.75	0.96	1.5
0.50	3.65	0.94	1.5
0.60	3.65	0.94	1.1
0.70	3.45	1.20	1.7
0.80	3.55	1.09	1.3
0.90	3.65	1.26	1.9
0.99	-	-	-

S4. Calculated charges of the atoms in (a) L-menthol and (b) thymol molecules.



a)



b)

S5. Cell created with 50 L-menthol and 50 thymol molecules.

