

Multifaceted Analysis of Intermolecular Interactions in α -Terpineol-Halobenzenes Binary Mixtures: Insights from Thermophysical, Acoustical, and Spectral Techniques, Supported by Quantum Computational Approaches.

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Supplementary Data File:

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Table S1 - List of Chemicals with Details of Supplier, CAS Number, Purity, Purification Method and Applied Method for Final Purity Analysis.

Compound/ Grade	Supplier	CAS number	Initial mass- fraction purity	Purification method	Final mass- fraction purity	Analysis method
α -terpineol	Sigma-Aldrich Chemical, USA	98-55-5	90%	None	-	-
Fluorobenzene	S.D. Fine Chemicals Ltd.	462-06- 6	99%	Fractional distillation	99.9%	GC ^a
Chlorobenzene	S.D. Fine Chemicals Ltd.	108-90- 7	99.5%	Fractional distillation	99.9%	GC ^a
Bromobenzene	S.D. Fine Chemicals Ltd.	108-86- 1	98%	Fractional distillation	99.8%	GC ^a

^aGC = Gas-liquid chromatography

Table S2 - Experimental and Literature Values of Density (ρ) and Speed of Sound (u) of Pure Components at 303.15, 308.15 and 313.15K.

Pure compound	T/K	$\rho/(g\cdot cm^3)$		$u/(m\cdot s^{-1})$	
		Exp.	Lit.	Exp.	Lit.
α -terpineol	303.15	0.928076	----	1407.52	----
	308.15	0.924122	----	1389.73	----
	313.15	0.846075	----	1372.18	----
Fluorobenzene	303.15	1.013116	1.01316 ¹ 1.01314 ^{2,3}	1145.40	1171 ¹ 1172 ^{12,13}
	308.15	1.007072	----	1125.22	----
	313.15	1.000994	----	1105.00	----
Chlorobenzene	303.15	1.095818	1.09547 ⁴	1249.35	1249 ⁴
			1.0950 ⁵		1252 ¹⁴
			1.09510 ⁶		
	308.15	1.090400	1.09006 ⁴	1231.14	1235 ⁴
			1.0900 ⁵		1224 ¹⁰
	313.15	1.084974	1.08366 ⁷	1212.92	1212.63 ⁶
1.08480 ⁸			1212 ¹⁵ 1206 ¹⁶		
Bromobenzene	303.15	1.481122	1.48148 ⁴	1138.18	1131 ¹⁷
			1.48147 ⁷		1146 ¹⁶
			1.4810 ⁵		1137 ⁰⁹
	308.15	1.474362	1.47481 ⁴	1123.11	1122 ¹⁰
			1.4730 ⁵		1120 ¹⁸
	313.15	1.467595	1.4670 ⁹	1107.87	1109 ¹⁶
1.46708 ¹⁰ 1.4680 ¹¹			1118 ⁰⁹		

Standard uncertainties U, in case of ρ and u $U(T) = \pm 0.001$ K, $U(\rho) = \pm 0.000001$ g \cdot cm³ and $U(u) = \pm 0.1$ m \cdot s⁻¹. All physical quantities are measured at atmospheric pressure.

Table S3 - Densities (ρ) and Excess Molar Volume (V_m^E) vs Mole Fraction (x_1) for α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at Different Temperatures.

x_1	ρ (gm·cm ³)			V_m^E (cm ³ ·mol ⁻¹)		
	303.15 K	308.15 K	313.15 K	303.15 K	308.15 K	313.15 K
α-terpineol (1) + Fluorobenzene (2)						
0.0000	1.013116	1.007072	1.000994	0.0000	0.0000	0.0000
0.0596	1.006055	0.999855	0.993664	-0.1422	5.9210	-0.0739
0.1249	0.998914	0.992796	0.986637	-0.2915	-0.2408	-0.1887
0.1965	0.991656	0.985705	0.979794	-0.4449	-0.3874	-0.3376
0.2756	0.984141	0.978455	0.972829	-0.5866	-0.5329	-0.4901
0.3634	0.976201	0.970807	0.965404	-0.6935	-0.6471	-0.6041
0.4612	0.967658	0.962508	0.957356	-0.7349	-0.6899	-0.6499
0.5711	0.958394	0.953452	0.948504	-0.6800	-0.6310	-0.5868
0.6954	0.948565	0.943854	0.939161	-0.5302	-0.4797	-0.4384
0.8370	0.938435	0.933975	0.929525	-0.3056	-0.2569	-0.2172
1.0000	0.928076	0.924122	0.920118	0.0000	0.0000	0.0000
α-terpineol (1) + Chlorobenzene (2)						
0.0000	1.095818	1.090400	1.084974	0.0000	0.0000	0.0000
0.0643	1.079612	1.074084	1.068638	-0.0562	-0.0301	-0.0131
0.1338	1.063566	1.058136	1.052739	-0.1356	-0.1028	-0.0748
0.2094	1.047658	1.042358	1.037075	-0.2395	-0.2032	-0.1707
0.2918	1.031678	1.026558	1.021396	-0.3475	-0.3135	-0.2770
0.3820	1.015394	1.010451	1.005467	-0.4310	-0.3991	-0.3653
0.4811	0.998638	0.993872	0.989082	-0.4624	-0.4325	-0.4037
0.5905	0.981288	0.976645	0.972028	-0.4128	-0.3772	-0.3503
0.7120	0.963474	0.958985	0.954527	-0.2840	-0.2462	-0.2193
0.8476	0.945556	0.941245	0.936981	-0.1168	-0.0810	-0.0603
1.0000	0.928076	0.924122	0.920118	0.0000	0.0000	0.0000
α-terpineol (1) + Bromobenzene (2)						
0.0000	1.481122	1.474362	1.467595	0.0000	0.0000	0.0000
0.0662	1.426185	1.419591	1.412962	-0.0283	-0.0185	-0.0068
0.1375	1.371437	1.365051	1.358683	-0.0770	-0.0597	-0.0453
0.2147	1.316845	1.310745	1.304612	-0.1478	-0.1294	-0.1100
0.2983	1.262222	1.256374	1.250557	-0.2277	-0.2049	-0.1879
0.3894	1.207252	1.201708	1.196213	-0.2845	-0.2623	-0.2489
0.4889	1.151892	1.146655	1.141432	-0.3054	-0.2843	-0.2693
0.5981	1.096012	1.091062	1.086124	-0.2620	-0.2396	-0.2240
0.7184	1.039883	1.035257	1.030608	-0.1719	-0.1535	-0.1381
0.8516	0.983782	0.979472	0.975123	-0.0642	-0.0501	-0.0373
1.0000	0.928076	0.924122	0.920118	0.0000	0.0000	0.0000

Standard uncertainties U, in case of density (ρ), $U(T) = \pm 0.001$ K, $U(\rho) = \pm 0.000001$ g cm⁻³, $U(x_1) = \pm 0.0001$. All physical quantities are measured at atmospheric pressure.

Table S4 - Fitting Coefficients (A_0, A_1, A_2, A_3, A_4) with Standard Deviation (σ) for Least Square Representation of V_m^E for α -terpineol + Fluoro- + Chloro- + and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

T (K)	A_0	A_1	A_2	A_3	A_4	σ
α-terpineol (1) + Fluorobenzene (2)						
303.15	-2.907940	0.710499	1.275060	-0.730129	-0.812287	0.00092
308.15	-2.724070	0.729726	1.619280	-0.853046	-0.613573	0.00204
313.15	-2.566360	0.752075	1.950610	-1.043420	-0.503388	0.00380
α-terpineol (1) + Chlorobenzene (2)						
303.15	-1.842940	0.388738	1.909700	-0.292002	-0.676246	0.00126
308.15	-1.711710	0.428837	2.085980	-0.368352	-0.422092	0.00129
313.15	-1.593730	0.377797	2.261310	-0.368283	-0.447195	0.00155
α-terpineol (1) + Bromobenzene (2)						
303.15	-1.215380	0.290205	1.574790	-0.324692	-0.674607	0.00202
308.15	-1.127610	0.277994	1.637530	-0.334214	-0.658298	0.00250
313.15	-1.068120	0.280916	1.731110	-0.383120	-0.614683	0.00230

Table S5 - Experimental excess molar volume, V_m^E , infinite dilution partial molar volume, $\bar{V}_{m,i}^o$, excess partial molar volume, $\bar{V}_{m,i}^{o,E}$, apparent molar volume, $V_{m,\phi,i}$, apparent molar volume, $V'_{m,\phi,i}$ of α -terpineol (1) + Fluoro-, Chloro- and Bromo benzene (2) at 303.15, 308.15 and 313.15K.

x_1	Molality m_1 (mol·kg ⁻¹)	Molality m_2 (mol·kg ⁻¹)	V_m^E (cm ³ ·mol ⁻¹)	$\bar{V}_{m,1}^o$ (cm ³ ·mol ⁻¹)	$\bar{V}_{m,2}^o$ (cm ³ ·mol ⁻¹)	$\bar{V}_{m,1}^{o,E}$ (cm ³ ·mol ⁻¹)	$\bar{V}_{m,2}^{o,E}$ (cm ³ ·mol ⁻¹)	$V_{m,\phi,1}$ (cm ³ ·mol ⁻¹)	$V_{m,\phi,2}$ (cm ³ ·mol ⁻¹)	$V'_{m,\phi,1}$ (cm ³ ·mol ⁻¹)	$V'_{m,\phi,2}$ (cm ³ ·mol ⁻¹)
α-terpineol (1) + Fluorobenzene (2) at 303.15K											
0.0000	-	-	0.0000	163.778	94.858	-	-	-	-	-	-
0.0596	0.6599	102.2314	-0.1422	164.007	94.864	-2.1966	0.0062	163.8194	95.5917	161.6228	94.7131
0.1249	1.4847	45.4362	-0.2915	164.217	94.891	-1.9865	0.0331	163.8690	96.5156	161.8824	94.5582
0.1965	2.5452	26.5044	-0.4449	164.423	94.958	-1.7800	0.0994	163.9396	97.7168	162.1596	94.4039
0.2756	3.9592	17.0386	-0.5866	164.644	95.088	-1.5598	0.2302	164.0750	99.3565	162.5152	94.2786
0.3634	5.9388	11.3590	-0.6935	164.893	95.308	-1.3100	0.4501	164.2948	101.7312	162.9848	94.2190
0.4612	8.9082	7.5727	-0.7349	165.183	95.626	-1.0205	0.7679	164.6100	105.4375	163.5895	94.2620
0.5711	13.8573	4.8682	-0.6800	165.508	96.011	-0.6957	1.1527	165.0127	111.8513	164.3169	94.4252
0.6954	23.7553	2.8398	-0.5302	165.836	96.375	-0.3671	1.5170	165.4409	124.9668	165.0738	94.6346
0.8370	53.4495	1.2621	-0.3056	166.100	96.654	-0.1035	1.7961	165.8383	164.6438	165.7348	94.7791
1.0000	-	-	0.0000	166.203	97.323	-	-	-	-	-	-
α-terpineol (1) + Fluorobenzene (2) at 308.15K											
0.0000	-	-	0.0000	165.319	95.427	-	-	-	-	-	-
0.0596	0.6610	102.0563	-0.1062	165.336	95.428	-1.5786	0.0005	165.1149	96.1865	163.5549	95.3150
0.1249	1.4873	45.3584	-0.2408	165.369	95.442	-1.5454	0.0149	164.9692	97.1144	163.4403	95.1672
0.1965	2.5496	26.4590	-0.3874	165.434	95.496	-1.4809	0.0684	164.9287	98.3095	163.4623	95.0137
0.2756	3.9660	17.0094	-0.5329	165.545	95.618	-1.3699	0.1906	164.9685	99.9258	163.6111	94.8824
0.3634	5.9490	11.3396	-0.6471	165.715	95.835	-1.1998	0.4078	165.1229	102.2633	163.9338	94.8189
0.4612	8.9235	7.5597	-0.6899	165.950	96.154	-0.9647	0.7268	165.4098	105.9273	164.4539	94.8736
0.5711	13.8810	4.8598	-0.6310	166.240	96.536	-0.6741	1.1082	165.8028	112.2848	165.1356	95.0644
0.6954	23.7961	2.8349	-0.4797	166.551	96.871	-0.3637	1.4436	166.2199	125.2796	165.8610	95.2963
0.8370	53.5412	1.2600	-0.2569	166.809	97.032	-0.1054	1.6047	166.6051	164.5767	166.5022	95.4558
1.0000	-	-	0.0000	166.914	97.269	-	-	-	-	-	-
α-terpineol (1) + Fluorobenzene (2) at 313.15K											
0.0000	-	-	0.0000	166.8130	96.0069	-	-	-	-	-	-
0.0596	0.6621	101.8818	-0.0739	166.6371	96.0019	-1.0037	-0.0049	166.3627	96.7874	165.3972	95.9233
0.1249	1.4898	45.2808	-0.1887	166.5072	96.0045	-1.1336	-0.0023	166.0961	97.7250	164.9960	95.7889
0.1965	2.5539	26.4138	-0.3376	166.4383	96.0458	-1.2025	0.0390	165.8940	98.9025	164.7206	95.6257
0.2756	3.9728	16.9803	-0.4901	166.4452	96.1603	-1.1956	0.1535	165.8377	100.4897	164.6671	95.4838
0.3634	5.9592	11.3202	-0.6041	166.5393	96.3766	-1.1015	0.3697	165.9571	102.7996	164.8768	95.4278
0.4612	8.9388	7.5468	-0.6499	166.7232	96.6990	-0.9176	0.6921	166.2144	106.4169	165.3143	95.4928
0.5711	13.9048	4.8515	-0.5868	166.9836	97.0790	-0.6572	1.0721	166.5997	112.7152	165.9561	95.7108
0.6954	23.8368	2.8301	-0.4384	167.2797	97.3878	-0.3611	1.3810	167.0009	125.5688	166.6493	95.9487

0.8370	53.6329	1.2578	-0.2172	167.5345	97.4540	-0.1064	1.4471	167.3764	164.4566	167.2750	96.1212
1.0000	-	-	0.0000	167.6408	97.4174	-	-	-	-	-	-
α-terpineol (1) + Chlorobenzene (2) at 303.15K											
0.0000	-	-	0.0000	165.4971	102.7150	-	-	-	-	-	-
0.0643	0.6101	94.4116	-0.0562	165.5088	102.7107	-0.6946	-0.0043	165.3286	104.4019	164.6340	102.6506
0.1338	1.3727	41.9607	-0.1356	165.4965	102.7082	-0.7068	-0.0068	165.1904	106.4892	164.4836	102.5517
0.2094	2.3531	24.4771	-0.2395	165.4808	102.7306	-0.7225	0.0157	165.0597	109.1505	164.3372	102.4277
0.2918	3.6604	15.7353	-0.3475	165.4838	102.8081	-0.7196	0.0932	165.0125	112.7064	164.2929	102.3175
0.3820	5.4906	10.4902	-0.4310	165.5259	102.9689	-0.6774	0.2539	165.0749	117.7406	164.3975	102.2715
0.4811	8.2359	6.9935	-0.4624	165.6219	103.2201	-0.5814	0.5052	165.2421	125.4085	164.6607	102.3291
0.5905	12.8115	4.4958	-0.4128	165.7734	103.5179	-0.4299	0.8030	165.5042	138.3940	165.0743	102.5098
0.7120	21.9625	2.6225	-0.2840	165.9597	103.7335	-0.2437	1.0186	165.8045	164.6213	165.5608	102.7476
0.8476	49.4156	1.1656	-0.1168	166.1292	103.6609	-0.0741	0.9459	166.0655	243.4558	165.9914	102.8942
1.0000	-	-	0.0000	166.2033	103.2277	-	-	-	-	-	-
α-terpineol (1) + Chlorobenzene (2) at 308.15K											
0.0000	-	-	0.0000	166.8061	103.2253	-	-	-	-	-	-
0.0643	0.6105	94.3467	-0.0301	166.6323	103.2167	-0.2822	-0.0087	166.4299	104.9410	166.1634	103.1845
0.1338	1.3736	41.9319	-0.1028	166.4785	103.2061	-0.4360	-0.0193	166.1324	107.0397	165.7104	103.0874
0.2094	2.3547	24.4603	-0.2032	166.3603	103.2222	-0.5542	-0.0032	165.9316	109.7110	165.3897	102.9651
0.2918	3.6629	15.7245	-0.3135	166.2933	103.2972	-0.6212	0.0719	165.8295	113.2721	165.2190	102.8546
0.3820	5.4944	10.4830	-0.3991	166.2906	103.4582	-0.6238	0.2328	165.8606	118.3147	165.2458	102.8125
0.4811	8.2416	6.9886	-0.4325	166.3594	103.7084	-0.5550	0.4831	166.0079	125.9960	165.4603	102.8749
0.5905	12.8203	4.4927	-0.3772	166.4946	103.9983	-0.4198	0.7730	166.2700	139.0246	165.8559	103.0773
0.7120	21.9776	2.6207	-0.2462	166.6717	104.1867	-0.2428	0.9613	166.5647	165.3246	166.3259	103.3319
0.8476	49.4496	1.1648	-0.0810	166.8385	104.0177	-0.0760	0.7924	166.8169	244.3522	166.7429	103.4863
1.0000	-	-	0.0000	166.9145	103.2127	-	-	-	-	-	-
α-terpineol (1) + Chlorobenzene (2) at 313.15K											
0.0000	-	-	0.0000	167.8517	103.7416	-	-	-	-	-	-
0.0643	0.6109	94.2858	-0.0131	167.6258	103.7303	-0.0150	-0.0113	167.4061	105.4769	167.4219	103.7163
0.1338	1.3745	41.9048	-0.0748	167.4205	103.7127	-0.2203	-0.0288	167.0546	107.5916	166.8618	103.6264
0.2094	2.3563	24.4445	-0.1707	167.2529	103.7192	-0.3879	-0.0224	166.8014	110.2745	166.4376	103.5032
0.2918	3.6653	15.7143	-0.2770	167.1401	103.7843	-0.5007	0.0428	166.6706	113.8500	166.1908	103.3932
0.3820	5.4980	10.4762	-0.3653	167.0972	103.9374	-0.5436	0.1958	166.6668	118.9018	166.1409	103.3464
0.4811	8.2469	6.9841	-0.4037	167.1331	104.1830	-0.5077	0.4414	166.7872	126.5937	166.2940	103.4051
0.5905	12.8286	4.4898	-0.3503	167.2440	104.4691	-0.3968	0.7276	167.0364	139.6491	166.6508	103.6136
0.7120	21.9918	2.6190	-0.2193	167.4060	104.6448	-0.2348	0.9032	167.3252	166.0121	167.0980	103.8834
0.8476	49.4816	1.1640	-0.0603	167.5661	104.4317	-0.0747	0.6901	167.5658	245.1905	167.4950	104.0362
1.0000	-	-	0.0000	167.6408	103.5117	-	-	-	-	-	-
α-terpineol (1) + Bromobenzene (2) at 303.15K											
0.0000	-	-	0.0000	165.9226	106.0061	-	-	-	-	-	-

0.0662	0.4514	91.4805	-0.0283	165.9108	106.0008	-0.2925	-0.0052	165.7749	110.3737	165.4824	105.9705
0.1375	1.0156	40.6580	-0.0770	165.8684	105.9936	-0.3350	-0.0125	165.6433	115.8123	165.3083	105.9043
0.2147	1.7410	23.7172	-0.1478	165.8169	106.0040	-0.3864	-0.0021	165.5147	122.7817	165.1283	105.8157
0.2983	2.7082	15.2467	-0.2277	165.7790	106.0574	-0.4243	0.0513	165.4401	132.0697	165.0158	105.7329
0.3894	4.0623	10.1645	-0.2845	165.7751	106.1758	-0.4283	0.1697	165.4728	145.1225	165.0446	105.7099
0.4889	6.0934	6.7763	-0.3054	165.8192	106.3603	-0.3841	0.3543	165.5787	164.7819	165.1946	105.7627
0.5981	9.4786	4.3562	-0.2620	165.9131	106.5672	-0.2902	0.5612	165.7653	197.7128	165.4750	105.9153
0.7184	16.2491	2.5411	-0.1719	166.0388	106.6894	-0.1646	0.6834	165.9640	263.7248	165.7995	106.0789
0.8516	36.5605	1.1294	-0.0642	166.1545	106.5920	-0.0488	0.5859	166.1280	461.8143	166.0792	106.1594
1.0000	-	-	0.0000	166.2033	106.3557	-	-	-	-	-	-

α -terpineol (1) + Bromobenzene (2) at 308.15K

0.0000	-	-	0.0000	166.8223	106.4921	-	-	-	-	-	-
0.0662	0.4515	91.4526	-0.0185	166.7721	106.4855	-0.1423	-0.0066	166.6170	110.8869	166.4924	106.4657
0.1375	1.0159	40.6456	-0.0597	166.6960	106.4748	-0.2184	-0.0173	166.4639	116.3561	166.2617	106.4055
0.2147	1.7415	23.7099	-0.1294	166.6156	106.4806	-0.2989	-0.0115	166.2968	123.3561	166.0128	106.3158
0.2983	2.7090	15.2421	-0.2049	166.5531	106.5292	-0.3614	0.0371	166.2143	132.6899	165.8662	106.2371
0.3894	4.0635	10.1614	-0.2623	166.5289	106.6427	-0.3856	0.1506	166.2294	145.7985	165.8554	106.2131
0.4889	6.0953	6.7743	-0.2843	166.5568	106.8220	-0.3576	0.3299	166.3232	165.5414	165.9753	106.2656
0.5981	9.4815	4.3549	-0.2396	166.6384	107.0219	-0.2760	0.5298	166.5062	198.6190	166.2378	106.4257
0.7184	16.2541	2.5403	-0.1535	166.7557	107.1311	-0.1588	0.6390	166.6954	264.9068	166.5420	106.5860
0.8516	36.5716	1.1290	-0.0501	166.8668	107.0046	-0.0476	0.5126	166.8527	463.8286	166.8080	106.6667
1.0000	-	-	0.0000	166.9145	106.6967	-	-	-	-	-	-

α -terpineol (1) + Bromobenzene (2) at 313.15K

0.0000	-	-	0.0000	167.7913	106.9831	-	-	-	-	-	-
0.0662	0.4516	91.4289	-0.0068	167.7753	106.9745	0.1345	-0.0086	167.5047	111.4079	167.6721	106.9672
0.1375	1.0161	40.6351	-0.0453	167.6604	106.9597	0.0196	-0.0234	167.2809	116.9030	167.3308	106.9072
0.2147	1.7420	23.7038	-0.1100	167.5078	106.9615	-0.1330	-0.0216	167.1011	123.9395	166.9956	106.8215
0.2983	2.7097	15.2382	-0.1879	167.3724	107.0076	-0.2684	0.0244	166.9864	133.3109	166.7426	106.7397
0.3894	4.0646	10.1588	-0.2489	167.2958	107.1202	-0.3450	0.1371	166.9803	146.4710	166.6567	106.7126
0.4889	6.0968	6.7725	-0.2693	167.2986	107.2990	-0.3422	0.3159	167.0721	166.3028	166.7479	106.7721
0.5981	9.4840	4.3538	-0.2240	167.3749	107.4959	-0.2659	0.5128	167.2521	199.5262	167.0004	106.9386
0.7184	16.2583	2.5397	-0.1381	167.4913	107.5939	-0.1495	0.6108	167.4386	266.1044	167.2990	107.1035
0.8516	36.5811	1.1288	-0.0373	167.5966	107.4349	-0.0442	0.4518	167.5917	465.8852	167.5527	107.1832
1.0000	-	-	0.0000	167.6408	107.0370	-	-	-	-	-	-

Table S6 - Speed of Sound (u) and Deviation in Speed of Sound (Δu) vs Mole Fraction (x_1) for α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

x_1	u (m·s ⁻¹)			Δu (m·s ⁻¹)		
	303.15 K	308.15 K	313.15 K	303.15 K	308.15 K	313.15 K
α-terpineol (1) + Fluorobenzene (2)						
0.0000	1145.40	1125.22	1105.00	0.00	0.00	0.00
0.0596	1164.12	1143.55	1122.98	3.09	2.56	2.05
0.1249	1183.95	1163.05	1142.45	5.82	4.80	4.09
0.1965	1205.12	1184.35	1163.65	8.21	7.15	6.14
0.2756	1227.74	1207.35	1186.61	10.09	9.23	7.97
0.3634	1252.28	1231.91	1211.49	11.64	10.58	9.41
0.4612	1278.79	1258.54	1238.54	12.49	11.32	10.31
0.5711	1307.02	1287.05	1267.39	11.92	10.76	9.80
0.6954	1337.78	1318.12	1298.98	10.10	8.96	8.18
0.8370	1371.72	1352.56	1333.75	6.91	5.93	5.11
1.0000	1407.52	1389.73	1372.18	0.00	0.00	0.00
α-terpineol (1) + Chlorobenzene (2)						
0.0000	1249.35	1231.14	1212.92	0.00	0.00	0.00
0.0643	1259.24	1240.82	1222.42	-0.27	-0.51	-0.73
0.1338	1270.04	1251.57	1233.10	-0.48	-0.79	-1.13
0.2094	1282.06	1263.61	1245.20	-0.41	-0.74	-1.07
0.2918	1295.40	1277.00	1258.63	-0.10	-0.41	-0.76
0.3820	1310.14	1291.79	1273.45	0.38	0.08	-0.30
0.4811	1326.40	1308.08	1289.85	0.96	0.65	0.32
0.5905	1344.31	1326.09	1307.94	1.56	1.30	0.98
0.7120	1363.98	1345.86	1327.85	2.02	1.81	1.54
0.8476	1385.20	1367.25	1349.45	1.78	1.69	1.54
1.0000	1407.52	1389.73	1372.18	0.00	0.00	0.00
α-terpineol (1) + Bromobenzene (2)						
0.0000	1138.18	1123.11	1107.87	0.00	0.00	0.00
0.0662	1154.52	1139.02	1123.39	-1.48	-1.73	-1.97
0.1375	1172.27	1156.48	1140.59	-2.95	-3.30	-3.63
0.2147	1191.96	1175.96	1159.81	-4.04	-4.38	-4.80
0.2983	1213.75	1197.45	1181.18	-4.79	-5.21	-5.55
0.3894	1237.99	1221.51	1205.01	-5.08	-5.43	-5.79
0.4889	1264.98	1248.27	1231.62	-4.89	-5.20	-5.48
0.5981	1295.21	1278.14	1261.25	-4.06	-4.44	-4.71
0.7184	1328.85	1311.58	1294.41	-2.83	-3.07	-3.34
0.8516	1366.35	1348.75	1331.32	-1.21	-1.42	-1.65
1.0000	1407.52	1389.73	1372.18	0.00	0.00	0.00

Standard uncertainties U, $U(T) = \pm 0.001$ K, $U(x) = \pm 0.0001$, $U(u) = \pm 0.1$ m·s⁻¹. All physical quantities are measured at atmospheric pressure.

Table S7 - Fitting Coefficients (A_0 , A_1 , A_2 , A_3 , A_4) with Standard Deviation (σ) for Least Square Representation of Δu for α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

T (K)	A_0	A_1	A_2	A_3	A_4	σ
α-terpineol (1) + Fluorobenzene (2)						
303.15	49.42930	-5.22113	-2.94521	8.89648	16.01420	0.06837
308.15	45.17000	-6.69077	-10.58620	12.60780	18.42820	0.07100
313.15	40.91910	-3.25459	-10.97110	6.06365	9.03726	0.05382
α-terpineol (1) + Chlorobenzene (2)						
303.15	4.42479	12.16710	-0.61336	0.70013	4.30219	0.03188
308.15	3.22196	12.38690	-0.42563	2.93121	2.16985	0.02789
313.15	1.84959	12.59020	-1.02372	4.65247	1.21011	0.03079
α-terpineol (1) + Bromobenzene (2)						
303.15	-19.11620	10.58760	1.31513	0.10534	5.83227	0.03468
308.15	-20.54000	11.05440	1.15293	0.79926	2.93536	0.03455
313.15	-21.71600	11.62210	-0.77618	1.12471	2.06793	0.02010

Table S8 - Isentropic Compressibility (k_s) and Deviation in Isentropic Compressibility (Δk_s) vs Mole Fraction (x_1) for α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

x_1	k_s (TPa ⁻¹)			Δk_s (TPa ⁻¹)		
	303.15 K	308.15 K	313.15 K	303.15 K	308.15 K	313.15 K
α-terpineol (1) + Fluorobenzene (2)						
0.0000	752.36	784.27	818.17	0.00	0.00	0.00
0.0596	733.47	764.81	798.02	-6.46	-6.10	-5.78
0.1249	714.18	744.63	776.55	-12.15	-11.67	-11.53
0.1965	694.35	723.26	753.74	-17.04	-16.99	-17.08
0.2756	674.11	701.12	730.04	-20.79	-21.41	-21.72
0.3634	653.22	678.75	705.75	-23.39	-24.13	-24.87
0.4612	631.95	655.94	680.94	-24.26	-25.02	-26.09
0.5711	610.79	633.16	656.36	-22.50	-23.19	-24.19
0.6954	589.07	609.80	631.04	-18.32	-18.72	-19.57
0.8370	566.32	585.26	604.77	-11.53	-11.52	-11.71
1.0000	543.89	560.29	577.21	0.00	0.00	0.00
α-terpineol (1) + Chlorobenzene (2)						
0.0000	584.65	605.06	626.49	0.00	0.00	0.00
0.0643	584.14	604.71	626.22	2.11	2.52	2.90
0.1338	582.91	603.32	624.72	3.72	4.25	4.82
0.2094	580.72	600.84	621.89	4.60	5.15	5.71
0.2918	577.63	597.36	618.03	4.87	5.36	5.92
0.3820	573.76	593.06	613.29	4.68	5.10	5.62
0.4811	569.17	588.03	607.70	4.13	4.51	4.91
0.5905	563.90	582.26	601.38	3.33	3.64	3.98
0.7120	557.88	575.69	594.17	2.26	2.51	2.77
0.8476	551.17	568.33	586.08	1.08	1.22	1.36
1.0000	543.89	560.29	577.21	0.00	0.00	0.00
α-terpineol (1) + Bromobenzene (2)						
0.0000	521.18	537.71	555.16	0.00	0.00	0.00
0.0662	526.04	542.97	560.80	3.36	3.76	4.18
0.1375	530.60	547.74	565.75	6.30	6.92	7.56
0.2147	534.49	551.69	569.83	8.44	9.13	9.94
0.2983	537.78	555.09	573.14	9.83	10.65	11.41
0.3894	540.47	557.71	575.72	10.44	11.20	11.97
0.4889	542.53	559.69	577.56	10.25	10.94	11.62
0.5981	543.88	561.04	578.79	9.12	9.83	10.44
0.7184	544.58	561.52	579.11	7.09	7.59	8.11
0.8516	544.47	561.24	578.60	3.96	4.30	4.66
1.0000	543.89	560.29	577.21	0.00	0.00	0.00

Table S9 - Fitting Coefficients (A_0, A_1, A_2, A_3, A_4) with Standard Deviation (σ) for Least Square Representation of Δk_s and $k_{s,m}^E$ for α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

T (K)	A_0	A_1	A_2	A_3	A_4	σ
Fitting Coefficients (A_0, A_1, A_2, A_3, A_4) for Δk_s						
α-terpineol (1) + Fluorobenzene (2)						
303.15	-95.4072	23.4319	5.5011	-11.3778	-18.8628	4.72888
308.15	-98.8818	25.9522	15.0411	-19.5000	-19.3462	5.05781
313.15	-102.8890	23.7131	17.7918	-17.4971	-8.2314	5.39728
α-terpineol (1) + Chlorobenzene (2)						
303.15	15.8658	-14.3568	10.8176	-3.7339	-6.6356	0.87874
308.15	17.3522	-15.2378	11.7494	-6.6553	-3.4019	0.93935
313.15	18.9828	-16.5853	13.3929	-8.8511	-1.9408	1.02530
α-terpineol (1) + Bromobenzene (2)						
303.15	40.4911	-14.1148	6.5236	-1.8043	-7.6118	1.69037
308.15	43.4317	-15.2897	7.2325	-2.8208	-5.3005	1.78932
313.15	46.1534	-16.6838	9.8299	-3.6831	-4.7800	1.88005
Fitting Coefficients (A_0, A_1, A_2, A_3, A_4) for $k_{s,m}^E$						
α-terpineol (1) + Fluorobenzene (2)						
303.15	0.00061	0.00043	0.00202	-0.00224	-0.00289	0.000009
308.15	0.00129	0.00067	0.00357	-0.00310	-0.00305	0.000009
313.15	0.00198	0.00025	0.00422	-0.00271	-0.00162	0.000011
α-terpineol (1) + Chlorobenzene (2)						
303.15	0.00368	-0.00116	0.00200	-0.00048	-0.00125	0.000005
308.15	0.00419	-0.00121	0.00229	-0.00085	-0.00084	0.000004
313.15	0.00476	-0.00137	0.00263	-0.00107	-0.00079	0.000004
α-terpineol (1) + Bromobenzene (2)						
303.15	0.00349	-0.00054	0.00126	-0.00036	-0.00133	0.000004
308.15	0.00395	-0.00063	0.00139	-0.00044	-0.00107	0.000006
313.15	0.00439	-0.00072	0.00178	-0.00053	-0.00100	0.000005

Table S10 - Experimental excess molar isentropic compressibility, $K_{s,m}^E$, infinite dilution partial molar isentropic compressibility, $\bar{K}_{s,m,i}^o$, excess partial molar isentropic compressibility, $\bar{K}_{s,m,i}^{o,E}$, apparent molar isentropic compressibility, $K_{s,m,\phi,i}$, apparent molar volume, $K'_{s,m,\phi,i}$ of α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

x_1	Molality m_1 (mol·kg ⁻¹)	Molality m_2 (mol·kg ⁻¹)	$K_{s,m}^E$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$\bar{K}_{s,m,1}^o$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$\bar{K}_{s,m,2}^o$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$\bar{K}_{s,m,1}^{o,E}$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$\bar{K}_{s,m,2}^{o,E}$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$K_{s,m,\phi,1}$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$K_{s,m,\phi,2}$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$K'_{s,m,\phi,1}$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)	$K'_{s,m,\phi,2}$ (TPa) ⁻¹ ·m ⁻³ ·mol ⁻¹)
α-terpineol (1) + Fluorobenzene (2) at 303.15K											
0.0000	-	-	0.000000	0.0919	0.0714	-	-	-	-	-	-
0.0596	0.6599	102.2314	0.000090	0.0919	0.0714	0.0015	0.0000	0.0919	0.0715	0.0934	0.0714
0.1249	1.4847	45.4362	0.000156	0.0917	0.0713	0.0013	-0.0001	0.0916	0.0715	0.0930	0.0715
0.1965	2.5452	26.5044	0.000184	0.0914	0.0713	0.0010	-0.0001	0.0913	0.0716	0.0924	0.0715
0.2756	3.9592	17.0386	0.000193	0.0911	0.0712	0.0007	-0.0001	0.0911	0.0716	0.0918	0.0715
0.3634	5.9388	11.3590	0.000162	0.0907	0.0712	0.0003	-0.0001	0.0908	0.0716	0.0912	0.0715
0.4612	8.9082	7.5727	0.000132	0.0905	0.0713	0.0001	-0.0001	0.0907	0.0716	0.0908	0.0715
0.5711	13.8573	4.8682	0.000176	0.0904	0.0713	0.0000	0.0000	0.0907	0.0718	0.0907	0.0717
0.6954	23.7553	2.8398	0.000191	0.0904	0.0711	0.0000	-0.0002	0.0907	0.0720	0.0907	0.0718
0.8370	53.4495	1.2621	0.000073	0.0904	0.0710	0.0000	-0.0004	0.0905	0.0718	0.0905	0.0714
1.0000	-	-	0.000000	0.0904	0.0734	-	-	-	-	-	-
α-terpineol (1) + Fluorobenzene (2) at 308.15K											
0.0000	-	-	0.000000	0.0978	0.0748	-	-	-	-	-	-
0.0596	0.6610	102.0563	0.000208	0.0971	0.0748	0.0036	0.0000	0.0970	0.0751	0.1006	0.0750
0.1249	1.4873	45.3584	0.000353	0.0964	0.0747	0.0029	-0.0001	0.0964	0.0752	0.0992	0.0751
0.1965	2.5496	26.4590	0.000388	0.0956	0.0746	0.0021	-0.0002	0.0955	0.0753	0.0976	0.0751
0.2756	3.9660	17.0094	0.000358	0.0949	0.0746	0.0013	-0.0003	0.0948	0.0753	0.0962	0.0751
0.3634	5.9490	11.3396	0.000335	0.0942	0.0746	0.0007	-0.0003	0.0945	0.0754	0.0952	0.0751
0.4612	8.9235	7.5597	0.000313	0.0938	0.0747	0.0003	-0.0002	0.0942	0.0754	0.0945	0.0752
0.5711	13.8810	4.8598	0.000363	0.0936	0.0747	0.0000	-0.0002	0.0942	0.0757	0.0942	0.0755
0.6954	23.7961	2.8349	0.000383	0.0935	0.0744	0.0000	-0.0005	0.0941	0.0761	0.0941	0.0756
0.8370	53.5412	1.2600	0.000245	0.0935	0.0738	0.0000	-0.0011	0.0938	0.0764	0.0938	0.0753
1.0000	-	-	0.000000	0.0935	0.0755	-	-	-	-	-	-
α-terpineol (1) + Fluorobenzene (2) at 313.15K											

0.0000	-	-	0.000000	0.1038	0.0786	-	-	-	-	-	-
0.0596	0.6621	101.8818	0.000330	0.1025	0.0785	0.0057	-0.0001	0.1024	0.0789	0.1080	0.0788
0.1249	1.4898	45.2808	0.000529	0.1012	0.0784	0.0044	-0.0002	0.1011	0.0792	0.1054	0.0790
0.1965	2.5539	26.4138	0.000591	0.0999	0.0782	0.0032	-0.0003	0.0998	0.0793	0.1030	0.0790
0.2756	3.9728	16.9803	0.000575	0.0989	0.0781	0.0021	-0.0004	0.0989	0.0794	0.1010	0.0789
0.3634	5.9592	11.3202	0.000532	0.0980	0.0781	0.0012	-0.0005	0.0983	0.0794	0.0995	0.0789
0.4612	8.9388	7.5468	0.000479	0.0974	0.0781	0.0006	-0.0004	0.0978	0.0795	0.0984	0.0790
0.5711	13.9048	4.8515	0.000530	0.0970	0.0781	0.0002	-0.0005	0.0977	0.0798	0.0979	0.0793
0.6954	23.8368	2.8301	0.000526	0.0968	0.0777	0.0001	-0.0008	0.0975	0.0803	0.0976	0.0795
0.8370	53.6329	1.2578	0.000397	0.0968	0.0768	0.0000	-0.0017	0.0972	0.0811	0.0973	0.0793
1.0000	-	-	0.000000	0.0968	0.0764	-	-	-	-	-	-

α -terpineol (1) + Chlorobenzene (2) at 303.15K

0.0000	-	-	0.000000	0.0965	0.0601	-	-	-	-	-	-
0.0643	0.6101	94.4116	0.000348	0.0958	0.0600	0.0054	0.0000	0.0958	0.0604	0.1012	0.0604
0.1338	1.3727	41.9607	0.000634	0.0949	0.0599	0.0046	-0.0002	0.0951	0.0608	0.0997	0.0606
0.2094	2.3531	24.4771	0.000824	0.0941	0.0597	0.0037	-0.0004	0.0943	0.0611	0.0980	0.0607
0.2918	3.6604	15.7353	0.000925	0.0932	0.0594	0.0028	-0.0006	0.0936	0.0614	0.0964	0.0607
0.3820	5.4906	10.4902	0.000958	0.0924	0.0592	0.0020	-0.0009	0.0929	0.0616	0.0949	0.0607
0.4811	8.2359	6.9935	0.000934	0.0917	0.0589	0.0013	-0.0012	0.0923	0.0619	0.0937	0.0607
0.5905	12.8115	4.4958	0.000859	0.0912	0.0586	0.0008	-0.0015	0.0919	0.0622	0.0926	0.0607
0.7120	21.9625	2.6225	0.000706	0.0907	0.0581	0.0003	-0.0019	0.0914	0.0625	0.0917	0.0606
0.8476	49.4156	1.1656	0.000438	0.0905	0.0575	0.0001	-0.0025	0.0909	0.0629	0.0910	0.0604
1.0000	-	-	0.000000	0.0904	0.0573	-	-	-	-	-	-

α -terpineol (1) + Chlorobenzene (2) at 308.15K

0.0000	-	-	0.000000	0.1012	0.0625	-	-	-	-	-	-
0.0643	0.6105	94.3467	0.000424	0.1001	0.0624	0.0066	-0.0001	0.1001	0.0629	0.1067	0.0629
0.1338	1.3736	41.9319	0.000744	0.0989	0.0622	0.0054	-0.0002	0.0991	0.0633	0.1045	0.0631
0.2094	2.3547	24.4603	0.000951	0.0978	0.0620	0.0043	-0.0004	0.0981	0.0637	0.1023	0.0632
0.2918	3.6629	15.7245	0.001055	0.0968	0.0617	0.0032	-0.0007	0.0971	0.0639	0.1004	0.0632
0.3820	5.4944	10.4830	0.001088	0.0958	0.0615	0.0023	-0.0010	0.0964	0.0642	0.0987	0.0632
0.4811	8.2416	6.9886	0.001061	0.0950	0.0612	0.0015	-0.0013	0.0957	0.0645	0.0972	0.0632
0.5905	12.8203	4.4927	0.000982	0.0944	0.0608	0.0008	-0.0016	0.0952	0.0649	0.0960	0.0632
0.7120	21.9776	2.6207	0.000816	0.0939	0.0603	0.0004	-0.0022	0.0947	0.0653	0.0951	0.0631

0.8476	49.4496	1.1648	0.000514	0.0936	0.0595	0.0001	-0.0029	0.0941	0.0658	0.0942	0.0629
1.0000	-	-	0.000000	0.0935	0.0589	-	-	-	-	-	-

α -terpineol (1) + Chlorobenzene (2) at 313.15K

0.0000	-	-	0.000000	0.1058	0.0650	-	-	-	-	-	-
0.0643	0.6109	94.2858	0.000493	0.1044	0.0649	0.0076	-0.0001	0.1044	0.0655	0.1121	0.0655
0.1338	1.3745	41.9048	0.000859	0.1030	0.0648	0.0062	-0.0002	0.1032	0.0660	0.1094	0.0657
0.2094	2.3563	24.4445	0.001084	0.1017	0.0645	0.0049	-0.0005	0.1019	0.0664	0.1069	0.0659
0.2918	3.6653	15.7143	0.001204	0.1005	0.0642	0.0037	-0.0008	0.1009	0.0667	0.1046	0.0659
0.3820	5.4980	10.4762	0.001240	0.0994	0.0639	0.0026	-0.0011	0.1000	0.0670	0.1026	0.0659
0.4811	8.2469	6.9841	0.001202	0.0984	0.0635	0.0017	-0.0015	0.0993	0.0673	0.1009	0.0658
0.5905	12.8286	4.4898	0.001114	0.0977	0.0631	0.0010	-0.0019	0.0986	0.0677	0.0996	0.0658
0.7120	21.9918	2.6190	0.000929	0.0972	0.0625	0.0004	-0.0025	0.0981	0.0682	0.0985	0.0658
0.8476	49.4816	1.1640	0.000586	0.0969	0.0617	0.0001	-0.0033	0.0975	0.0688	0.0976	0.0655
1.0000	-	-	0.000000	0.0968	0.0608	-	-	-	-	-	-

α -terpineol (1) + Bromobenzene (2) at 303.15K

0.0000	-	-	0.000000	0.0947	0.0552	-	-	-	-	-	-
0.0662	0.4514	91.4805	0.000270	0.0943	0.0552	0.0039	0.0000	0.0945	0.0555	0.0984	0.0555
0.1375	1.0156	40.6580	0.000517	0.0938	0.0551	0.0034	-0.0001	0.0942	0.0558	0.0976	0.0557
0.2147	1.7410	23.7172	0.000694	0.0932	0.0550	0.0028	-0.0003	0.0936	0.0561	0.0965	0.0559
0.2983	2.7082	15.2467	0.000810	0.0926	0.0548	0.0022	-0.0005	0.0931	0.0564	0.0953	0.0559
0.3894	4.0623	10.1645	0.000873	0.0920	0.0545	0.0016	-0.0007	0.0926	0.0567	0.0942	0.0560
0.4889	6.0934	6.7763	0.000880	0.0915	0.0543	0.0011	-0.0010	0.0922	0.0570	0.0933	0.0560
0.5981	9.4786	4.3562	0.000824	0.0910	0.0539	0.0006	-0.0013	0.0918	0.0573	0.0924	0.0560
0.7184	16.2491	2.5411	0.000688	0.0907	0.0534	0.0003	-0.0018	0.0914	0.0577	0.0916	0.0559
0.8516	36.5605	1.1294	0.000415	0.0905	0.0528	0.0001	-0.0024	0.0909	0.0580	0.0910	0.0556
1.0000	-	-	0.000000	0.0904	0.0527	-	-	-	-	-	-

α -terpineol (1) + Bromobenzene (2) at 308.15K

0.0000	-	-	0.000000	0.0988	0.0573	-	-	-	-	-	-
0.0662	0.4515	91.4526	0.000321	0.0982	0.0572	0.0047	0.0000	0.0984	0.0576	0.1031	0.0576
0.1375	1.0159	40.6456	0.000600	0.0975	0.0571	0.0040	-0.0001	0.0979	0.0580	0.1019	0.0578
0.2147	1.7415	23.7099	0.000790	0.0968	0.0569	0.0033	-0.0003	0.0972	0.0583	0.1005	0.0580
0.2983	2.7090	15.2421	0.000926	0.0960	0.0567	0.0025	-0.0005	0.0966	0.0586	0.0992	0.0580
0.3894	4.0635	10.1614	0.000986	0.0953	0.0565	0.0018	-0.0008	0.0960	0.0589	0.0979	0.0581

0.4889	6.0953	6.7743	0.000989	0.0947	0.0562	0.0012	-0.0011	0.0955	0.0592	0.0967	0.0581
0.5981	9.4815	4.3549	0.000939	0.0942	0.0558	0.0007	-0.0015	0.0951	0.0596	0.0958	0.0581
0.7184	16.2541	2.5403	0.000775	0.0938	0.0552	0.0003	-0.0020	0.0946	0.0600	0.0949	0.0580
0.8516	36.5716	1.1290	0.000478	0.0936	0.0545	0.0001	-0.0028	0.0941	0.0605	0.0942	0.0577
1.0000	-	-	0.000000	0.0935	0.0541	-	-	-	-	-	-

α -terpineol (1) + Bromobenzene (2) at 313.15K

0.0000	-	-	0.000000	0.1032	0.0594	-	-	-	-	-	-
0.0662	0.4516	91.4289	0.000378	0.1023	0.0593	0.0056	0.0000	0.1025	0.0598	0.1080	0.0598
0.1375	1.0161	40.6351	0.000687	0.1014	0.0592	0.0047	-0.0002	0.1017	0.0602	0.1064	0.0600
0.2147	1.7420	23.7038	0.000904	0.1005	0.0590	0.0038	-0.0004	0.1010	0.0605	0.1047	0.0602
0.2983	2.7097	15.2382	0.001039	0.0996	0.0588	0.0029	-0.0006	0.1002	0.0609	0.1031	0.0602
0.3894	4.0646	10.1588	0.001102	0.0988	0.0585	0.0021	-0.0009	0.0996	0.0612	0.1017	0.0603
0.4889	6.0968	6.7725	0.001098	0.0981	0.0582	0.0013	-0.0012	0.0990	0.0615	0.1004	0.0603
0.5981	9.4840	4.3538	0.001044	0.0975	0.0577	0.0008	-0.0017	0.0985	0.0620	0.0993	0.0603
0.7184	16.2583	2.5397	0.000871	0.0971	0.0571	0.0004	-0.0023	0.0980	0.0625	0.0983	0.0602
0.8516	36.5811	1.1288	0.000548	0.0969	0.0562	0.0001	-0.0032	0.0974	0.0631	0.0975	0.0599
1.0000	-	-	0.000000	0.0968	0.0555	-	-	-	-	-	-

Table S11 - Acoustical Impedances (z) and Deviation in Acoustical impedances (Δz) vs Mole Fraction (x_1) for α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

x_1	z ($\text{g}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$) $\times 10^{-3}$			Δz ($\text{g}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$) $\times 10^{-3}$		
	303.15 K	308.15 K	313.15 K	303.15 K	308.15 K	313.15 K
α-terpineol (1) + Fluorobenzene (2)						
0.0000	1.1604	1.1332	1.1061	0.0000	0.0000	0.0000
0.0596	1.1712	1.1434	1.1159	0.0020	0.0012	0.0004
0.1249	1.1827	1.1547	1.1272	0.0040	0.0026	0.0015
0.1965	1.1951	1.1674	1.1401	0.0060	0.0045	0.0033
0.2756	1.2083	1.1813	1.1544	0.0076	0.0065	0.0051
0.3634	1.2225	1.1959	1.1696	0.0091	0.0079	0.0066
0.4612	1.2374	1.2114	1.1857	0.0097	0.0085	0.0075
0.5711	1.2526	1.2271	1.2021	0.0089	0.0077	0.0067
0.6954	1.2690	1.2441	1.2200	0.0071	0.0059	0.0050
0.8370	1.2873	1.2633	1.2398	0.0048	0.0036	0.0027
1.0000	1.3063	1.2843	1.2626	0.0000	0.0000	0.0000
α-terpineol (1) + Chlorobenzene (2)						
0.0000	1.3691	1.3424	1.3160	0.0000	0.0000	0.0000
0.0643	1.3595	1.3327	1.3063	-0.0055	-0.0060	-0.0062
0.1338	1.3508	1.3243	1.2981	-0.0099	-0.0103	-0.0107
0.2094	1.3432	1.3171	1.2914	-0.0128	-0.0131	-0.0134
0.2918	1.3364	1.3109	1.2856	-0.0143	-0.0146	-0.0148
0.3820	1.3303	1.3053	1.2804	-0.0148	-0.0149	-0.0152
0.4811	1.3246	1.3001	1.2758	-0.0143	-0.0144	-0.0145
0.5905	1.3192	1.2951	1.2714	-0.0128	-0.0130	-0.0131
0.7120	1.3142	1.2907	1.2675	-0.0102	-0.0104	-0.0105
0.8476	1.3098	1.2869	1.2644	-0.0061	-0.0062	-0.0063
1.0000	1.3063	1.2843	1.2626	0.0000	0.0000	0.0000
α-terpineol (1) + Bromobenzene (2)						
0.0000	1.6858	1.6559	1.6259	0.0000	0.0000	0.0000
0.0662	1.6466	1.6169	1.5873	-0.0141	-0.0143	-0.0146
0.1375	1.6077	1.5787	1.5497	-0.0259	-0.0261	-0.0262
0.2147	1.5696	1.5414	1.5131	-0.0347	-0.0347	-0.0348
0.2983	1.5320	1.5044	1.4771	-0.0405	-0.0406	-0.0404
0.3894	1.4946	1.4679	1.4414	-0.0434	-0.0433	-0.0430
0.4889	1.4571	1.4313	1.4058	-0.0431	-0.0429	-0.0424
0.5981	1.4196	1.3945	1.3699	-0.0392	-0.0391	-0.0387
0.7184	1.3818	1.3578	1.3340	-0.0313	-0.0311	-0.0309
0.8516	1.3442	1.3211	1.2982	-0.0184	-0.0183	-0.0183
1.0000	1.3063	1.2843	1.2626	0.0000	0.0000	0.0000

Table S12 - Fitting Coefficients (A_0, A_1, A_2, A_3, A_4) with Standard Deviation (σ) for Least Square Representation of Δz for α -terpineol + Fluoro-, Chloro- and Bromo benzene Mixtures at 303.15, 308.15 and 313.15K.

T (K)	A_0	A_1	A_2	A_3	A_4	σ
α-terpineol (1) + Fluorobenzene (2)						
303.15	0.037970	-0.009791	-0.013628	0.018538	0.020762	0.00008
308.15	0.033690	-0.010360	-0.026255	0.022510	0.023243	0.00009
313.15	0.029285	-0.007551	-0.028326	0.020097	0.011296	0.00008
α-terpineol (1) + Chlorobenzene (2)						
303.15	-0.056061	0.022382	-0.024468	0.006957	0.012200	0.00007
308.15	-0.056846	0.021323	-0.022527	0.012964	0.002442	0.00003
313.15	-0.057280	0.022159	-0.025944	0.014073	0.004067	0.00004
α-terpineol (1) + Bromobenzene (2)						
303.15	-0.171049	0.045651	-0.026915	0.008988	0.014765	0.00007
308.15	-0.170552	0.046396	-0.026262	0.010573	0.010273	0.00008
313.15	-0.168934	0.046462	-0.028014	0.012435	0.004056	0.00004

Table S13 - Optimized geometric parameters with Mulliken Charge values for pure components (α -terpineol and fluorobenzene) and their binary mixtures using DFT/B3LYP with 6-31+G (d,p) at 298.15K.

α -terpineol				Fluorobenzene				α -terpineol + Fluorobenzene (First Possible Interaction Site)				α -terpineol + Fluorobenzene (Second Possible Interaction Site)			
Bond	Bond length (Å)	Atom	Charge (e)	Bond	Bond length (Å)	Atom	Charge (e)	Bond	Bond length (Å)	Atom	Charge (e)	Bond	Bond length (Å)	Atom	Charge (e)
R(1,2)	1.5145	1C	0.370060	R(1,2)	1.3898	1C	0.090434	R(1,2)	1.5144	1C	0.377024	R(1,2)	1.5142	1C	0.374173
R(1,6)	1.3412	2C	-0.456772	R(1,3)	1.3981	2C	-0.053442	R(1,6)	1.3410	2C	-0.528327	R(1,6)	1.3410	2C	-0.632056
R(1,7)	1.5044	3C	-0.248354	R(1,8)	1.0847	3C	-0.167268	R(1,7)	1.5044	3C	-0.132930	R(1,7)	1.5042	3C	-0.041761
R(2,3)	1.5419	4C	-0.074308	R(2,6)	1.3898	4C	-0.119144	R(2,3)	1.5423	4C	0.079823	R(2,3)	1.5428	4C	0.095774
R(2,12)	1.0968	5C	-0.459706	R(2,7)	1.3612	5C	-0.167267	R(2,12)	1.0968	5C	-0.464591	R(2,12)	1.0966	5C	-0.515487
R(2,13)	1.1013	6C	-0.078299	R(3,4)	1.3985	6C	0.090435	R(2,13)	1.1011	6C	-0.090703	R(2,13)	1.1013	6C	-0.081946
R(3,4)	1.5569	7C	-0.682109	R(3,9)	1.0859	7F	-0.349146	R(3,4)	1.5571	7C	-0.681727	R(3,4)	1.5579	7C	-0.682486
R(3,14)	1.0936	8C	0.255856	R(4,5)	1.3985	8H	0.141577	R(3,14)	1.0935	8C	-0.095636	R(3,14)	1.0937	8C	0.006656
R(3,15)	1.0954	9C	-0.472869	R(4,10)	1.0854	9H	0.132347	R(3,15)	1.0956	9C	-0.446877	R(3,15)	1.0951	9C	-0.409385
R(4,5)	1.5578	10C	-0.435955	R(5,6)	1.3981	10H	0.127551	R(4,5)	1.5573	10C	-0.438119	R(4,5)	1.5571	10C	-0.488899
R(4,8)	1.5546	11O	-0.503554	R(5,11)	1.0858	11H	0.132346	R(4,8)	1.5550	11O	-0.402112	R(4,8)	1.5543	11O	-0.443398
R(4,16)	1.0964	12H	0.132484	R(6,12)	1.0847	12H	0.141577	R(4,16)	1.0966	12H	0.132447	R(4,16)	1.0966	12H	0.134879
R(5,6)	1.5099	13H	0.152320					R(5,6)	1.5100	13H	0.153838	R(5,6)	1.5097	13H	0.153879
R(5,17)	1.1008	14H	0.156202					R(5,17)	1.1008	14H	0.154848	R(5,17)	1.1009	14H	0.148567
R(5,18)	1.0945	15H	0.140987					R(5,18)	1.0945	15H	0.138040	R(5,18)	1.0943	15H	0.144998
R(6,19)	1.0889	16H	0.141591					R(6,19)	1.0890	16H	0.140084	R(6,19)	1.0888	16H	0.142239
R(7,20)	1.0987	17H	0.146502					R(7,20)	1.0986	17H	0.147501	R(7,20)	1.0986	17H	0.147691
R(7,21)	1.0985	18H	0.139225					R(7,21)	1.0985	18H	0.139349	R(7,21)	1.0984	18H	0.139023
R(7,22)	1.0945	19H	0.109056					R(7,22)	1.0946	19H	0.108429	R(7,22)	1.0944	19H	0.109965
R(8,9)	1.5376	20H	0.152578					R(8,9)	1.5376	20H	0.152564	R(8,9)	1.5369	20H	0.153363
R(8,10)	1.5379	21H	0.152319					R(8,10)	1.5382	21H	0.151751	R(8,10)	1.5374	21H	0.153640
R(8,11)	1.4466	22H	0.146333					R(8,11)	1.4456	22H	0.146029	R(8,11)	1.4504	22H	0.146681
R(9,23)	1.0944	23H	0.153403					R(9,23)	1.0944	23H	0.151596	R(9,23)	1.0942	23H	0.154675
R(9,24)	1.0948	24H	0.158246					R(9,24)	1.0948	24H	0.156085	R(9,24)	1.0947	24H	0.157987
R(9,25)	1.0971	25H	0.134496					R(9,25)	1.0965	25H	0.141193	R(9,25)	1.0969	25H	0.136291
R(10,26)	1.0945	26H	0.146567					R(10,26)	1.0946	26H	0.145034	R(10,26)	1.0943	26H	0.148479

R(10,27)	1.0972	27H	0.134384		R(10,27)	1.0968	27H	0.139600	R(10,27)	1.0970	27H	0.135684
R(10,28)	1.0930	28H	0.156223		R(10,28)	1.0933	28H	0.153531	R(10,28)	1.0931	28H	0.156119
R(11,29)	0.9668	29H	0.333091		R(11,29)	0.9684	29H	0.357034	R(11,29)	0.9671	29H	0.342396
					R(25,36)	3.8141	30C	0.467792	R(11,38)	2.4080	30C	-0.046864
					R(27,36)	4.0080	31C	0.006514	R(11,39)	4.3252	31C	-0.003482
					R(29,36)	2.1950	32C	-0.734599	R(30,31)	1.3895	32C	-0.024075
					R(30,31)	1.3886	33C	-0.000614	R(30,32)	1.3989	33C	-0.266252
					R(30,32)	1.3986	34C	-0.243582	R(30,37)	1.0848	34C	-0.139928
					R(30,37)	1.0853	35C	0.167138	R(31,35)	1.3896	35C	0.135345
					R(31,35)	1.3885	36F	-0.360355	R(31,36)	1.3633	36F	-0.346448
					R(31,36)	1.3718	37H	0.180611	R(32,33)	1.3993	37H	0.137290
					R(32,33)	1.3985	38H	0.134219	R(32,38)	1.0864	38H	0.175479
					R(32,38)	1.0859	39H	0.126705	R(33,34)	1.3984	39H	0.124454
					R(33,34)	1.3983	40H	0.131320	R(33,39)	1.0858	40H	0.128590
					R(33,39)	1.0856	41H	0.140075	R(34,35)	1.3984	41H	0.138149
					R(34,35)	1.3983			R(34,40)	1.0862		
					R(34,40)	1.0859			R(35,41)	1.0847		
					R(35,41)	1.0847						

Table S14 - Optimized geometric parameters with Mulliken Charge values for pure component (α -terpineol) and in solvation condition with halobenzenes using DFT/B3LYP with 6-31+G (d,p) at 298.15K.

α -terpineol				α -terpineol + Fluorobenzene (Theoretical- Solvation)				α -terpineol + Chlorobenzene (Theoretical- Solvation)				α -terpineol + Bromobenzene (Theoretical- Solvation)			
Bond	Bond length (Å°)	Atom	Charge (e)	Bond	Bond length (Å°)	Atom	Charge (e)	Bond	Bond length (Å°)	Atom	Charge (e)	Bond	Bond length (Å°)	Atom	Charge (e)
R(1,2)	1.5145	1C	0.370060	R(1,2)	1.5144	1C	0.361865	R(1,2)	1.5144	1C	0.361628	R(1,2)	1.5144	1C	0.361887
R(1,6)	1.3412	2C	-0.456772	R(1,6)	1.3420	2C	-0.461158	R(1,6)	1.3420	2C	-0.461041	R(1,6)	1.3420	2C	-0.461168
R(1,7)	1.5044	3C	-0.248354	R(1,7)	1.5047	3C	-0.238441	R(1,7)	1.5047	3C	-0.238401	R(1,7)	1.5047	3C	-0.238445
R(2,3)	1.5419	4C	-0.074308	R(2,3)	1.5429	4C	-0.133057	R(2,3)	1.5429	4C	-0.133803	R(2,3)	1.5429	4C	-0.132987
R(2,12)	1.0968	5C	-0.459706	R(2,12)	1.0964	5C	-0.456821	R(2,12)	1.0964	5C	-0.456578	R(2,12)	1.0964	5C	-0.456843
R(2,13)	1.1013	6C	-0.078299	R(2,13)	1.1011	6C	-0.088872	R(2,13)	1.1011	6C	-0.089377	R(2,13)	1.1011	6C	-0.088826
R(3,4)	1.5569	7C	-0.682109	R(3,4)	1.5583	7C	-0.677551	R(3,4)	1.5584	7C	-0.677478	R(3,4)	1.5583	7C	-0.677557
R(3,14)	1.0936	8C	0.255856	R(3,14)	1.0935	8C	0.338610	R(3,14)	1.0935	8C	0.339858	R(3,14)	1.0935	8C	0.338493
R(3,15)	1.0954	9C	-0.472869	R(3,15)	1.0956	9C	-0.498054	R(3,15)	1.0956	9C	-0.498446	R(3,15)	1.0956	9C	-0.498017
R(4,5)	1.5578	10C	-0.435955	R(4,5)	1.5567	10C	-0.453092	R(4,5)	1.5567	10C	-0.453393	R(4,5)	1.5567	10C	-0.453064
R(4,8)	1.5546	11O	-0.503554	R(4,8)	1.5543	11O	-0.552232	R(4,8)	1.5543	11O	-0.553140	R(4,8)	1.5543	11O	-0.552148
R(4,16)	1.0964	12H	0.132484	R(4,16)	1.0968	12H	0.136445	R(4,16)	1.0968	12H	0.136521	R(4,16)	1.0968	12H	0.136437
R(5,6)	1.5099	13H	0.152320	R(5,6)	1.5101	13H	0.156976	R(5,6)	1.5101	13H	0.157076	R(5,6)	1.5101	13H	0.156967
R(5,17)	1.1008	14H	0.156202	R(5,17)	1.1006	14H	0.149482	R(5,17)	1.1006	14H	0.149384	R(5,17)	1.1006	14H	0.149491
R(5,18)	1.0945	15H	0.140987	R(5,18)	1.0940	15H	0.141731	R(5,18)	1.0940	15H	0.141719	R(5,18)	1.0940	15H	0.141732
R(6,19)	1.0889	16H	0.141591	R(6,19)	1.0891	16H	0.139692	R(6,19)	1.0891	16H	0.139618	R(6,19)	1.0891	16H	0.139699
R(7,20)	1.0987	17H	0.146502	R(7,20)	1.0986	17H	0.150976	R(7,20)	1.0986	17H	0.151076	R(7,20)	1.0986	17H	0.150966
R(7,21)	1.0985	18H	0.139225	R(7,21)	1.0984	18H	0.143782	R(7,21)	1.0984	18H	0.143881	R(7,21)	1.0984	18H	0.143773
R(7,22)	1.0945	19H	0.109056	R(7,22)	1.0946	19H	0.116192	R(7,22)	1.0946	19H	0.116329	R(7,22)	1.0946	19H	0.116179
R(8,9)	1.5376	20H	0.152578	R(8,9)	1.5372	20H	0.156561	R(8,9)	1.5372	20H	0.156640	R(8,9)	1.5372	20H	0.156554
R(8,10)	1.5379	21H	0.152319	R(8,10)	1.5373	21H	0.156173	R(8,10)	1.5373	21H	0.156235	R(8,10)	1.5373	21H	0.156167
R(8,11)	1.4466	22H	0.146333	R(8,11)	1.4517	22H	0.149507	R(8,11)	1.4518	22H	0.149564	R(8,11)	1.4517	22H	0.149502
R(9,23)	1.0944	23H	0.153403	R(9,23)	1.0942	23H	0.157772	R(9,23)	1.0942	23H	0.157872	R(9,23)	1.0942	23H	0.157762
R(9,24)	1.0948	24H	0.158246	R(9,24)	1.0950	24H	0.156509	R(9,24)	1.0950	24H	0.156447	R(9,24)	1.0950	24H	0.156515
R(9,25)	1.0971	25H	0.134496	R(9,25)	1.0966	25H	0.144244	R(9,25)	1.0966	25H	0.144435	R(9,25)	1.0966	25H	0.144227
R(10,26)	1.0945	26H	0.146567	R(10,26)	1.0942	26H	0.151683	R(10,26)	1.0942	26H	0.151788	R(10,26)	1.0942	26H	0.151673
R(10,27)	1.0972	27H	0.134384	R(10,27)	1.0967	27H	0.144304	R(10,27)	1.0967	27H	0.144497	R(10,27)	1.0967	27H	0.144286
R(10,28)	1.0930	28H	0.156223	R(10,28)	1.0932	28H	0.153705	R(10,28)	1.0932	28H	0.153665	R(10,28)	1.0932	28H	0.153709
R(11,29)	0.9668	29H	0.333091	R(11,29)	0.9676	29H	0.353070	R(11,29)	0.9676	29H	0.353426	R(11,29)	0.9676	29H	0.353036

Table S15 - Experimental FT-IR and theoretical IR Frequencies with wavenumbers (cm^{-1}) and Shifting of bands of α -terpineol (1) + Fluoro-, Chloro- and Bromo benzene (2) binary mixtures at 298.15K.

Component/ Mixture	Intermolecular H-Bonded			Free Phenolic -OH Symmetrical Stretching			Aliphatic C-H Symmetrical Stretching			Aromatic C-H Symmetrical Stretching			Aromatic ring C-X stretching			
	$\nu_{O...H}$			ν_{O-H}			ν_{C-H}			ν_{C-H}			ν_{C-X}			
	Exp.	Theoretical		Exp.	Theoretical		Exp.	Theoretical		Exp.	Theoretical		Exp.	Theoretical		
		Scaled	Un-scaled		Scaled	Un-scaled		Scaled	Un-scaled		Scaled	Un-scaled		Scaled	Un-scaled	
α -terpineol	3383.81	-	-	3605.62	3673.28	3810.46	2923.89/ 2965.70	2905.07 (T-7) / 2928.43 (T-9,10)	3013.56 (T-7) / 3037.79 (T-9,10)	3047.81/3008.93	3043.28 (T-6)/ 2969.24 (T-5)/ 2992.39 (T-3)/ 2956.57 (T-2,3,4,5)	3156.93 (T-6)/ 3080.12 (T-5)/ 3104.14 (T-3)/ 3066.98 (T-2,3,4,5)	-	-	-	
Fluorobenzene	-	-	-	-	-	-	-	-	-	3050.03	3093.80	3209.34	1219.59	1196.62	1241.31	
Chlorobenzene	-	-	-	-	-	-	-	-	-	3069.17	3092.06	3207.53	1082.82	1061.17	1100.80	
Bromobenzene	-	-	-	-	-	-	-	-	-	3065.62	3092.58 (X-all)	3208.07 (X-all)	1068.65	1052.27	1091.57	
α -terpineol + Fluorobenzene Experimental	4:1	3385.93	-	-	3606.32	-	-	2924.60/ 2965.70	-	-	3049.93 / 3008.93	-	-	1221.01	-	-
	1:1	3394.44	-	-	3607.74	-	-	2924.60 / 2966.41	-	-	3049.33 / 3008.93	-	-	1220.30	-	-
	1:4	3436.25	-	-	3608.45	-	-	2926.02 / 2967.12	-	-	3050.03	-	-	1219.59	-	-
α -terpineol + Chlorobenzene Experimental	4:1	3395.15	-	-	Not Seen	-	-	2924.60 / 2965.70	-	-	3054.29 / 3008.93	-	-	1083.53	-	-
	1:1	3402.94	-	-	3599.24	-	-	2924.60 / 2965.70	-	-	3068.46	-	-	1083.53	-	-

	1:4	3436.25	-	-	3599.95	-	-	2925.31 / 3966.41	-	-	3069.17	-	-	1083.53	-	-
α-terpineol + Bromobenzene Experimental	4:1	3395.86	-	-	Not Seen	-	-	2923.89 / 2965.70	-	-	3054.29 / 3008.93	-	-	1069.35	-	-
	1:1	3406.49	-	-	3592.86	-	-	2323.89 / 2965.70	-	-	3065.62	-	-	1069.35	-	-
	1:4	3459.63	-	-	3597.11	-	-	2924.60 / 2965.00	-	-	3065.62	-	-	1068.65	-	-
α-terpineol + Fluorobenzene (First possible interaction site)	-	-	-	-	3655.84	3792.36	-	2905.31 (T-7) / 2925.68 (T-9,10)	3013.81 (T-7) / 3034.94 (T-9,10)	-	3041.69 (T-6) / 2971.64 (T-5) / 2991.20 (T-3) / 2955.32 (T-2,3,4,5) / 3092.49 (X-all)	3155.28 (T-6) / 3082.61 (T-5) / 3102.91 (T-3) / 3065.69 (T- 2,3,4,5) / 3207.98 (X-all)	-	1178.90	1222.93	
α-terpineol + Fluorobenzene (Second possible interaction site)	-	-	-	-	3670.18	3807.24	-	2906.18 (T-7) / 2923.35 (T-9,10)	3014.71 (T-7) / 3032.52 (T-9,10)	-	3044.16 (T-6) / 2971.51 (T-5) / 2992.40 (T-3) / 2958.56 (T-2,3,4,5) / 3090.02 (X-all)	3157.84 (T-6) / 3082.48 (T-5) / 3104.15 (T-3) / 3069.05 (T- 2,3,4,5) / 3205.42 (X-all)	-	1195.28	1239.92	
α-terpineol + Fluorobenzene (Theoretical- Solvation)	-	-	-	-	3665.77	3802.67	-	2904.96 (T-7) / 2931.96 (T-9,10)	3013.45 (T-7) / 3041.45 (T-9,10)	-	3041.26 (T-6) / 2973.95 (T-5) /	3154.83 (T-6) / 3085.01 (T-5) /	-	-	-	

											2991.08 (T-3)/ 2956.88 (T-2,3,4,5)	3102.78 (T-3)/ 3067.30 (T- 2,3,4,5)			
α -terpineol + Chlorobenzene (Theoretical- Solvation)	-	-	-	-	3665.61	3802.50	-	2904.96 (T-7) / 2932.00 (T-9,10)	3013.45 (T-7) / 3041.50 (T-9,10)	-	3041.22 (T-6)/ 2974.04 (T-5)/ 2991.00 (T-3)/ 2956.88 (T-2,3,4,5)	3154.79 (T-6)/ 3085.10 (T-5)/ 3102.70 (T-3)/ 3067.30 (T- 2,3,4,5)	-	-	-
α -terpineol + Bromobenzene (Theoretical- Solvation)	-	-	-	-	3665.79	3802.69	-	2904.96 (T-7) / 2931.96 (T-9,10)	3013.45 (T-7) / 3041.45 (T-9,10)		3041.26 (T-6)/ 2973.95 (T-5)/ 2991.09 (T-3)/ 2956.88 (T-2,3,4,5)	3154.84 (T-6)/ 3085.01 (T-5)/ 3102.79 (T-3)/ 3067.30 (T- 2,3,4,5)	-	-	-

Shift in wavenumber with respect to pure α -terpineol values

α -terpineol + Fluorobenzene Experimental	4:1	2.12	-	-	0.7	-	-	0.71 / 0	-	-	2.12 / 0	-	-	-	-	-
	1:1	10.63	-	-	2.12	-	-	0.71 / 0.71	-	-	1.52 / 0	-	-	-	-	-
	1:4	52.44	-	-	2.83	-	-	2.13 / 1.42	-	-	2.22	-	-	-	-	-
α -terpineol + Chlorobenzene Experimental	4:1	11.34	-	-	Not Seen	-	-	0.71	-	-	2.48 / 0	-	-	-	-	-
	1:1	19.13	-	-	-6.38	-	-	0.71 / 0	-	-	20.65	-	-	-	-	-
	1:4	52.44	-	-	5.67	-	-	1.42 / 0.71	-	-	21.36	-	-	-	-	-
α -terpineol + Bromobenzene Experimental	4:1	12.05	-	-	Not Seen	-	-	0 / 0	-	-	6.48 / 0	-	-	-	-	-
	1:1	22.68	-	-	-12.76	-	-	0 / 0	-	-	17.81	-	-	-	-	-
	1:4	75.82	-	-	-8.51	-	-	0.71 /	-	-	17.81	-	-	-	-	-

								-0.70								
α -terpineol + Fluorobenzene (First possible interaction site)	-	-	-	-	-17.45	-18.10	-	0.24 (T-7) / -2.75 (T-9,10)	0.25 (T-7) / -2.85 (T-9,10)	-		-2.1 (T-6) / 4.89 (T-5) / -1.36 (T-3) / 0.32 (T-2,3,4,5)	-	-	-	
α -terpineol + Fluorobenzene (Second possible interaction site)	-	-	-	-	-3.10	-3.22	-	1.11 (T-7) / 5.08 (T-9,10)	1.15 (T-7) / -5.27 (T-9,10)	-	0.88 (T-6) / 2.28 (T-5) / 0.01 (T-3) / 2.00 (T-2,3,4,5)	0.91 (T-6) / 2.36 (T-5) / 0.01 (T-3) / 2.07 (T-2,3,4,5)	-	-	-	
α -terpineol + Fluorobenzene (Theoretical-Solvation)	-	-	-	-	-7.51	7.79	-	-0.11 (T-7) / 3.53 (T-9,10)	-0.11 (T-7) / 3.66 (T-9,10)	-	-2.06 (T-6) / 4.71 (T-5) / -1.31 (T-3) / 0.31 (T-2,3,4,5)	-2.1 (T-6) / 4.89 (T-5) / -1.36 (T-3) / 0.32 (T-2,3,4,5)	-	-	-	
α -terpineol + Chlorobenzene (Theoretical-Solvation)	-	-	-	-	-7.67	-7.96	-	-0.11 (T-7) / 3.58 (T-9,10)	-0.11 (T-7) / 3.71 (T-9,10)	-	-2.06 (T-6) / 4.80 (T-5) / -1.39 (T-3) / 0.31 (T-2,3,4,5)	-2.14 (T-6) / 4.98 (T-5) / -1.44 (T-3) / 0.32 (T-2,3,4,5)	-	-	-	
α -terpineol + Bromobenzene (Theoretical-Solvation)	-	-	-	-	-7.49	-7.77	-	-0.11 (T-7) / 3.53 (T-9,10)	-0.11 (T-7) / 3.66 (T-9,10)	-	-1.93 (T-6) / 4.71 (T-5) / -1.30 (T-3) / 0.31 (T-2,3,4,5)	-2.09 (T-6) / 4.89 (T-5) / -1.35 (T-3) / 0.32 (T-2,3,4,5)	-	-	-	
Shift in wavenumbers with respect to Halobenzene values																
4:1	-	-	-	-	-	-	-	-	-	-0.1	-	-	1.42	-	-	

α -terpineol + Fluorobenzene Experimental	1:1	-	-	-	-	-	-	-	-	-	-0.7	-	-	0.71	-	-
	1:4	-	-	-	-	-	-	-	-	-	0	-	-	0	-	-
α -terpineol + Chlorobenzene Experimental	4:1	-	-	-	-	-	-	-	-	-	-14.88	-	-	0.71	-	-
	1:1	-	-	-	-	-	-	-	-	-	-0.71	-	-	0.71	-	-
	1:4	-	-	-	-	-	-	-	-	-	0	-	-	0.71	-	-
α -terpineol + Bromobenzene Experimental	4:1	-	-	-	-	-	-	-	-	-	-11.33	-	-	0.70	-	-
	1:1	-	-	-	-	-	-	-	-	-	0	-	-	0.70	-	-
	1:4	-	-	-	-	-	-	-	-	-	0	-	-	0	-	-
α -terpineol + Fluorobenzene (First possible interaction site)		-	-	-	-	-	-	-	-	-	-	-1.31 (X-all)	-1.36 (X-all)	-	-17.72	-18.38
α -terpineol + Fluorobenzene (Second possible interaction site)		-	-	-	-	-	-	-	-	-	-	-3.78 (X-all)	-3.92 (X-all)	-	-1.34	-1.39
α -terpineol + Fluorobenzene (Theoretical- Solvation)		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
α -terpineol + Chlorobenzene (Theoretical- Solvation)		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
α -terpineol + Bromobenzene (Theoretical- Solvation)		-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

The Standard Uncertainty U is $U(T) = 0.1K$. All spectra are taken at atmospheric pressure and composition of binary mixture is 4:1, 1:1, and 1:4. Theoretical spectra are calculated using B3LYP/6-31+G(d,p).

(T-2,3,4,5) = this frequency is contributed from α -terpineol molecule's hydrogen atom/s attached with C2, C3, C4 and C5 atoms.

(T-3) = this frequency is contributed from α -terpineol molecule's hydrogen atom/s attached with C3 atom.

(T-5) = this frequency is contributed from α -terpineol molecule's hydrogen atom/s attached with C5 atom.

(T-6) = this frequency is contributed from α -terpineol molecule's hydrogen atom/s attached with C6 atom.

(T-7) = this frequency is contributed from α -terpineol molecule's hydrogen atom/s attached with C7 atom.

(T-9,10) = this frequency is contributed from α -terpineol molecule's hydrogen atom/s attached with C9-C10 atoms.

(X-all) = this frequency is contributed from Halobenzene molecule's hydrogen atoms attached with Carbon atoms of aromatic ring.

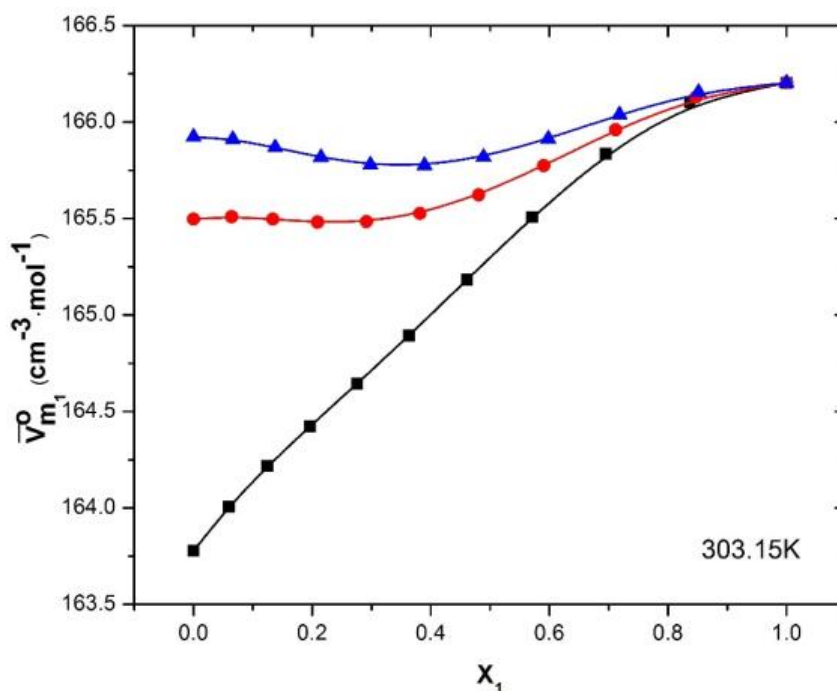


Fig. S1 - Infinite Dilution Partial Molar Volume ($\bar{V}_{m_1}^0$) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of mole fraction at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

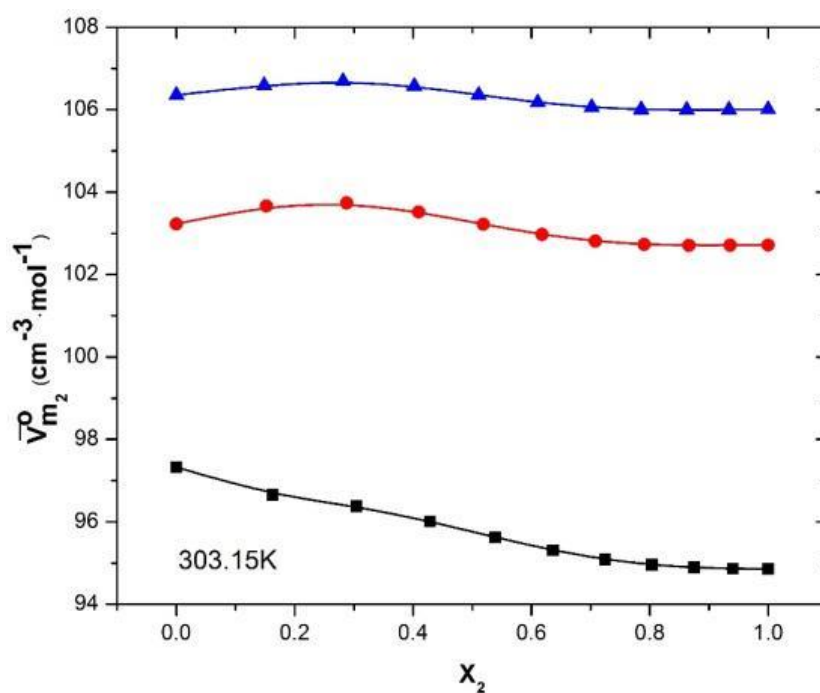


Fig. S2 - Infinite Dilution Partial Molar Volume ($\bar{V}_{m_2}^0$) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of mole fraction at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

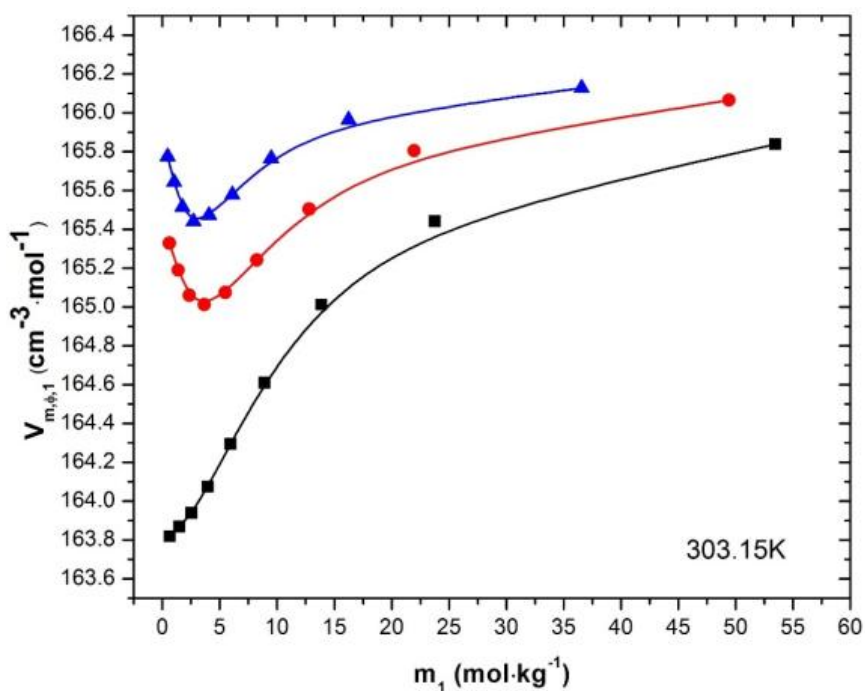


Fig. S3 - Apparent Molar Volume (V_{m,ϕ_1}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of molality (m_1) at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

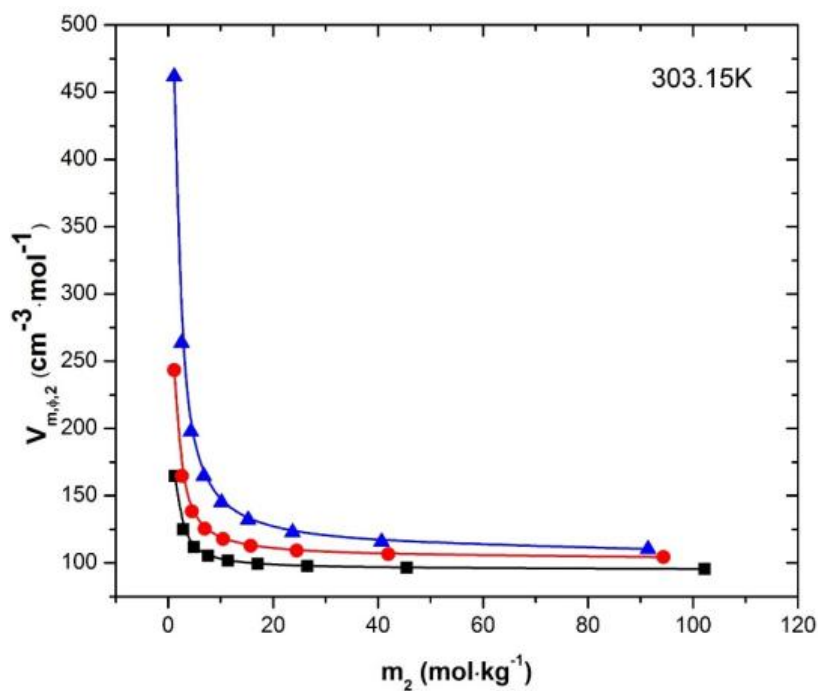


Fig. S4 - Apparent Molar Volume (V_{m,ϕ_2}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of molality (m_2) at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

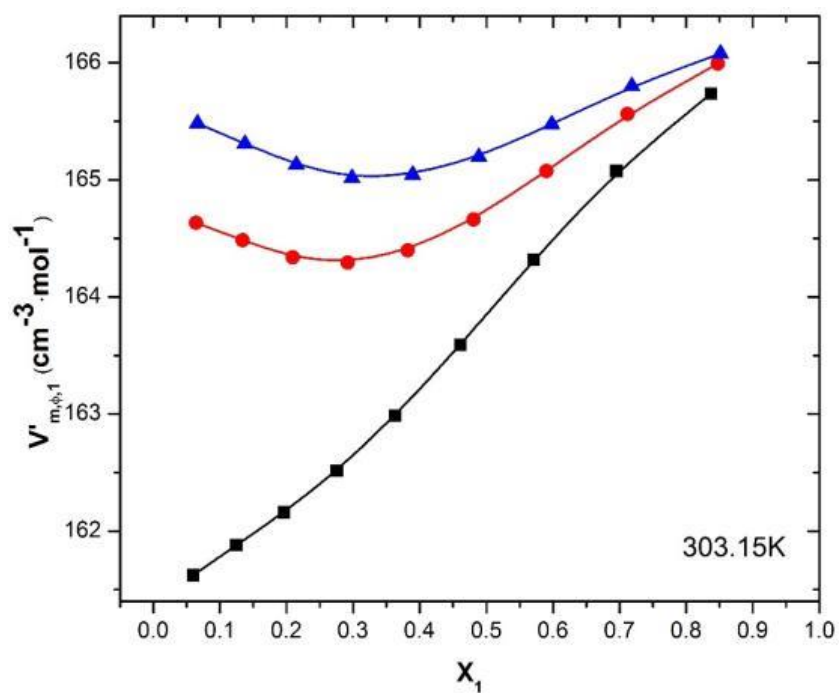


Fig. S5 - Apparent Molar Volume (V'_{m,ϕ_1}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromobenzene (2) as a function of mole fraction at $T = 303.15\text{K}$: \blacksquare , α -terpineol (1) + Fluorobenzene (2); \bullet , α -terpineol (1) + Chlorobenzene (2); \blacktriangle , α -terpineol (1) + Bromobenzene (2).

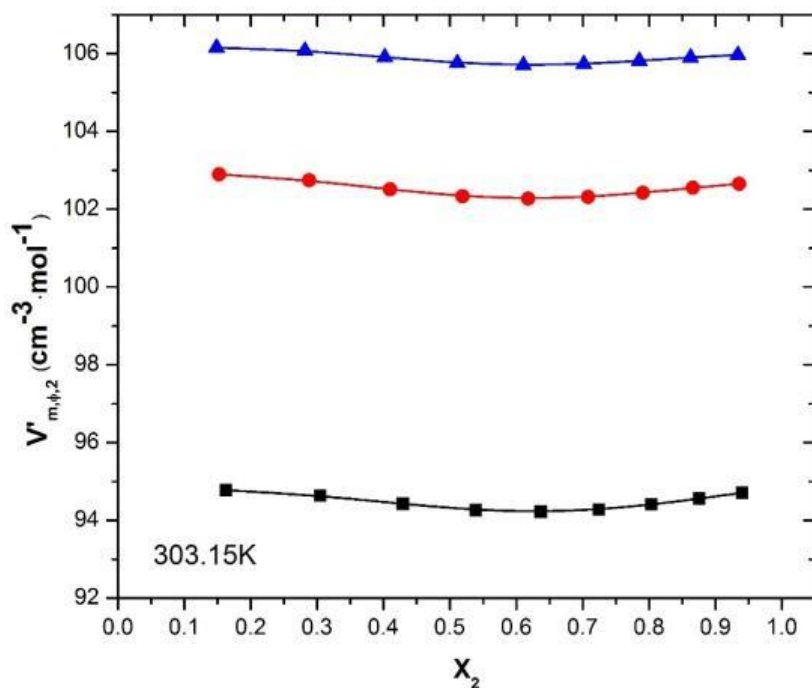


Fig. S6 - Apparent Molar Volume (V'_{m,ϕ_2}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromobenzene (2) as a function of mole fraction at $T = 303.15\text{K}$: \blacksquare , α -terpineol (1) + Fluorobenzene (2); \bullet , α -terpineol (1) + Chlorobenzene (2); \blacktriangle , α -terpineol (1) + Bromobenzene (2).

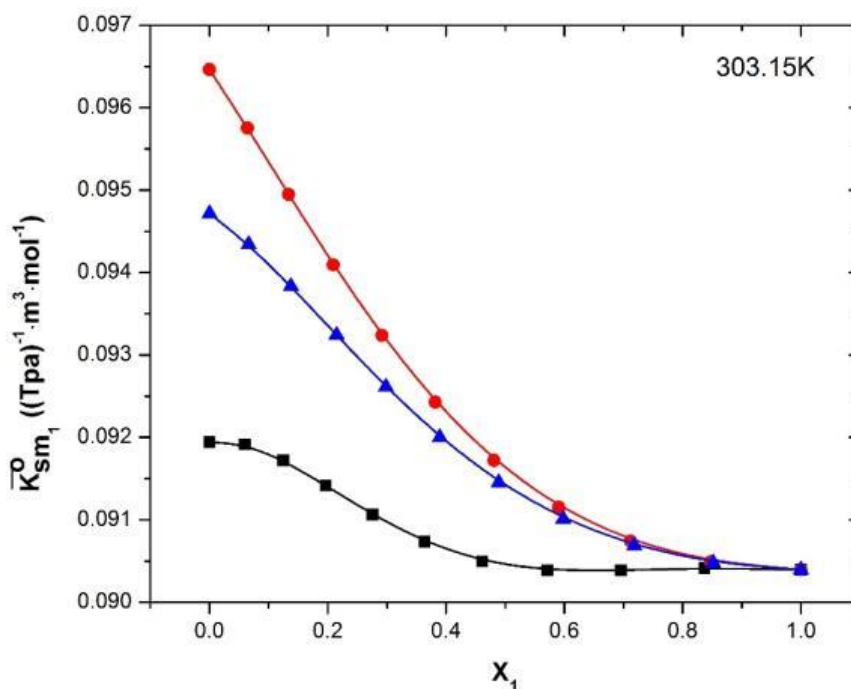


Fig. S7 - Infinite Dilution Partial Molar Isentropic Compressibility (\bar{K}_{s,m_1}^0) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of mole fraction at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

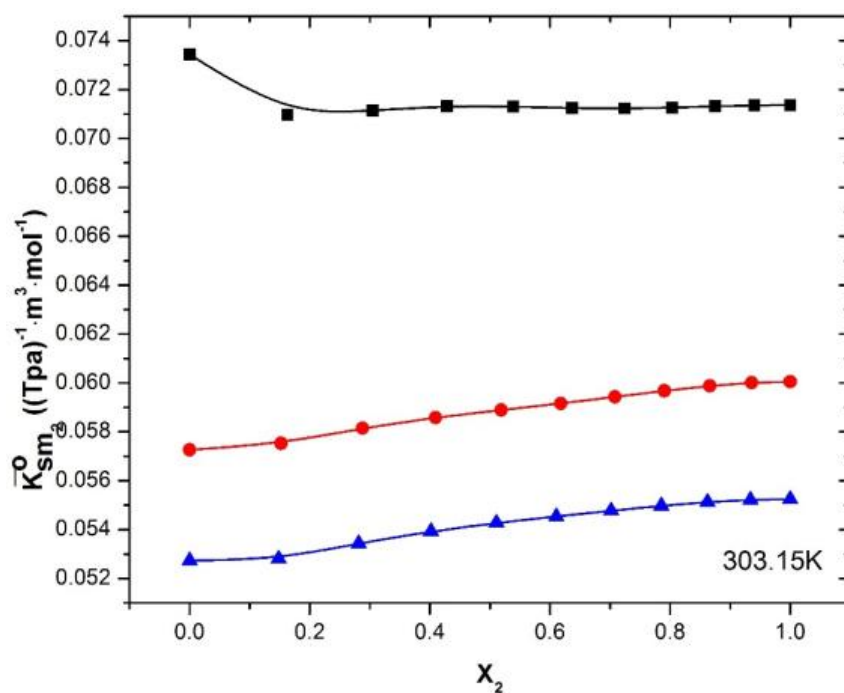


Fig. S8 - Infinite Dilution Partial Molar Isentropic Compressibility (\bar{K}_{s,m_2}^0) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of mole fraction at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

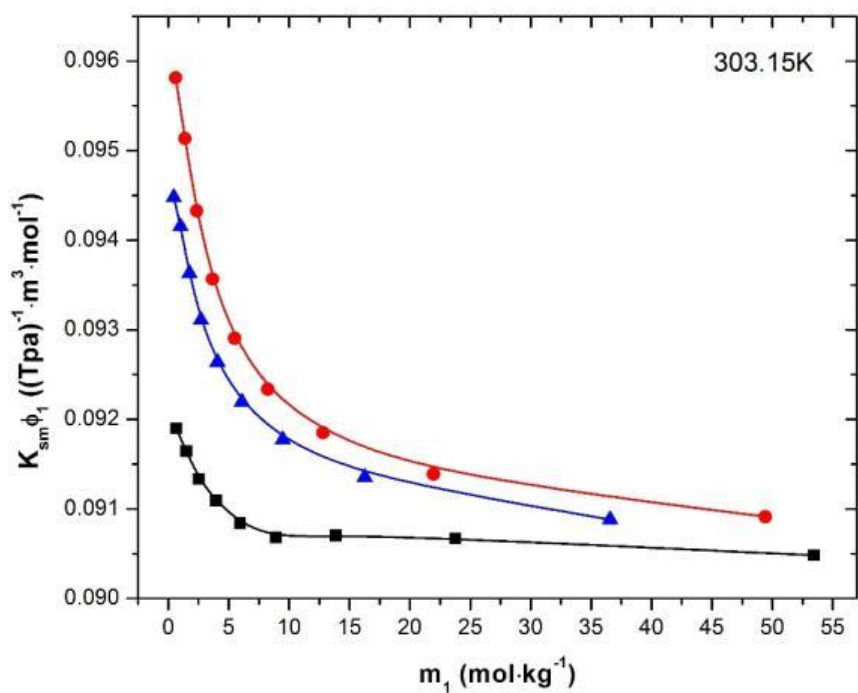


Fig. S9 - Apparent Molar Isentropic Compressibility (K_{s,m,ϕ_1}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of molality (m_1) at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

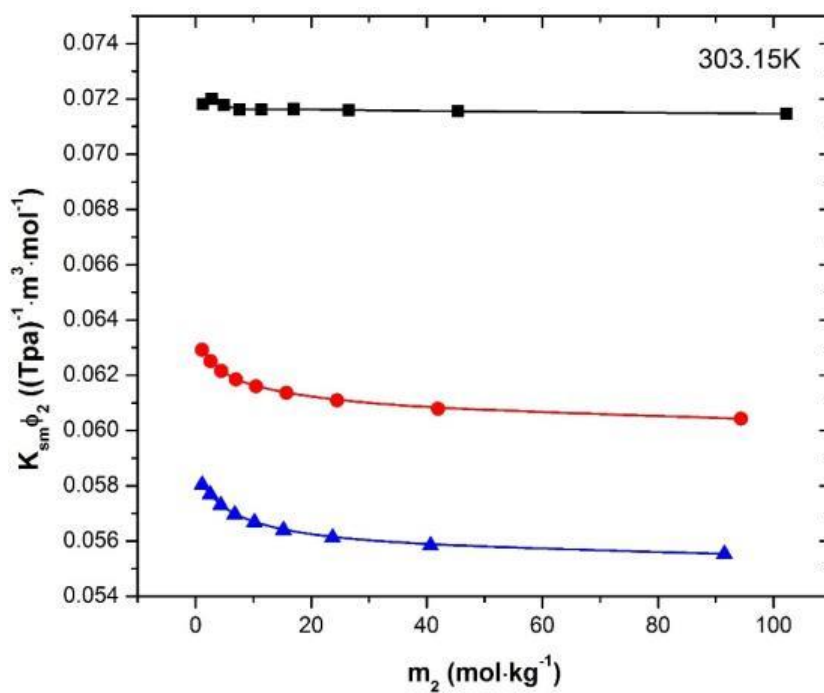


Fig. S10 - Apparent Molar Isentropic Compressibility (K_{s,m,ϕ_2}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of molality (m_2) at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

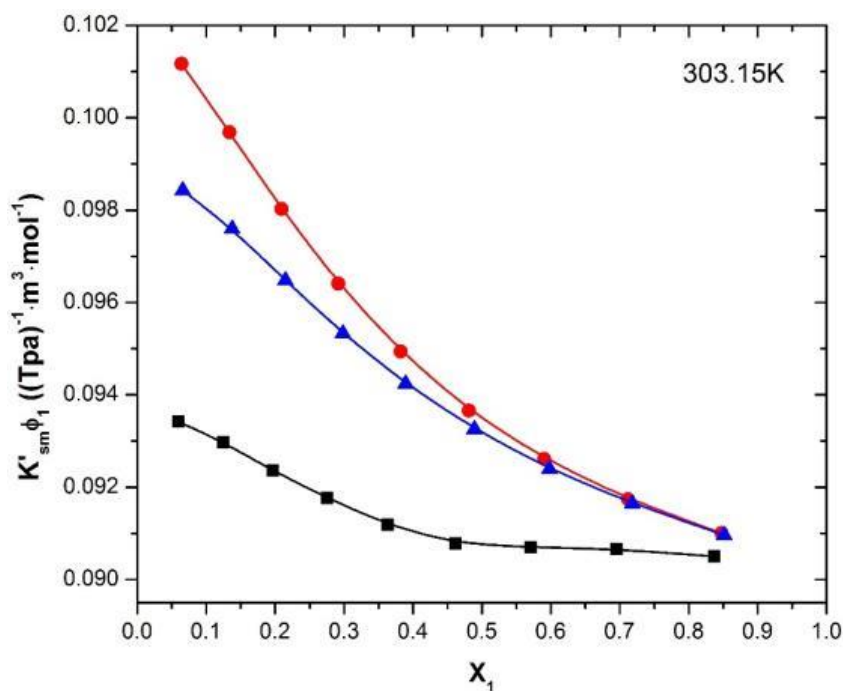


Fig. S11 - Apparent Molar Isentropic Compressibility (K'_{s,m,ϕ_1}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of mole fraction at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

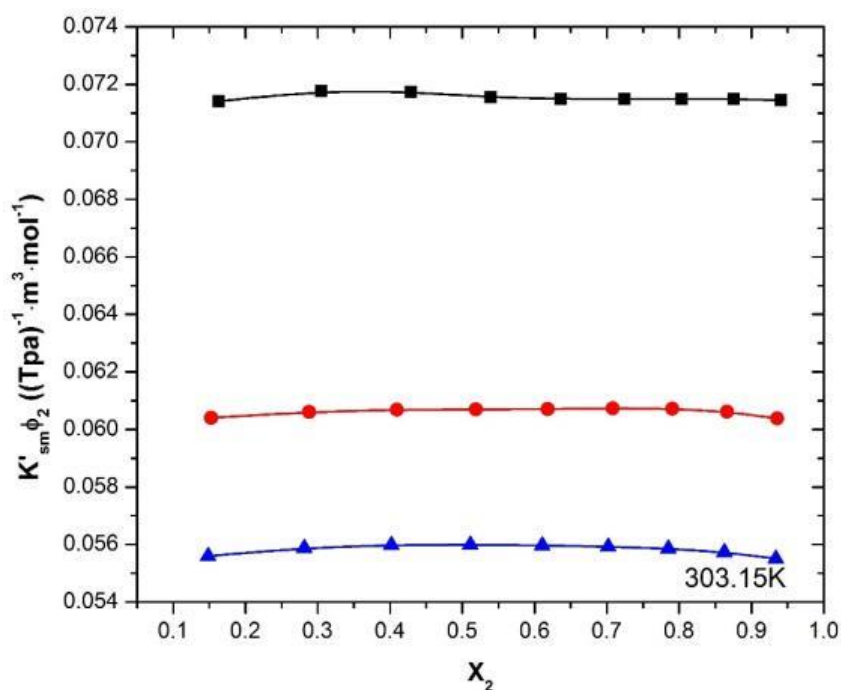


Fig. S12 - Apparent Molar Isentropic Compressibility (K'_{s,m,ϕ_2}) for the system α -terpineol (1) + Fluoro-, Chloro-, and Bromo-benzene (2) as a function of mole fraction at $T = 303.15\text{K}$: ■, α -terpineol (1) + Fluorobenzene (2); ●, α -terpineol (1) + Chlorobenzene (2); ▲, α -terpineol (1) + Bromobenzene (2).

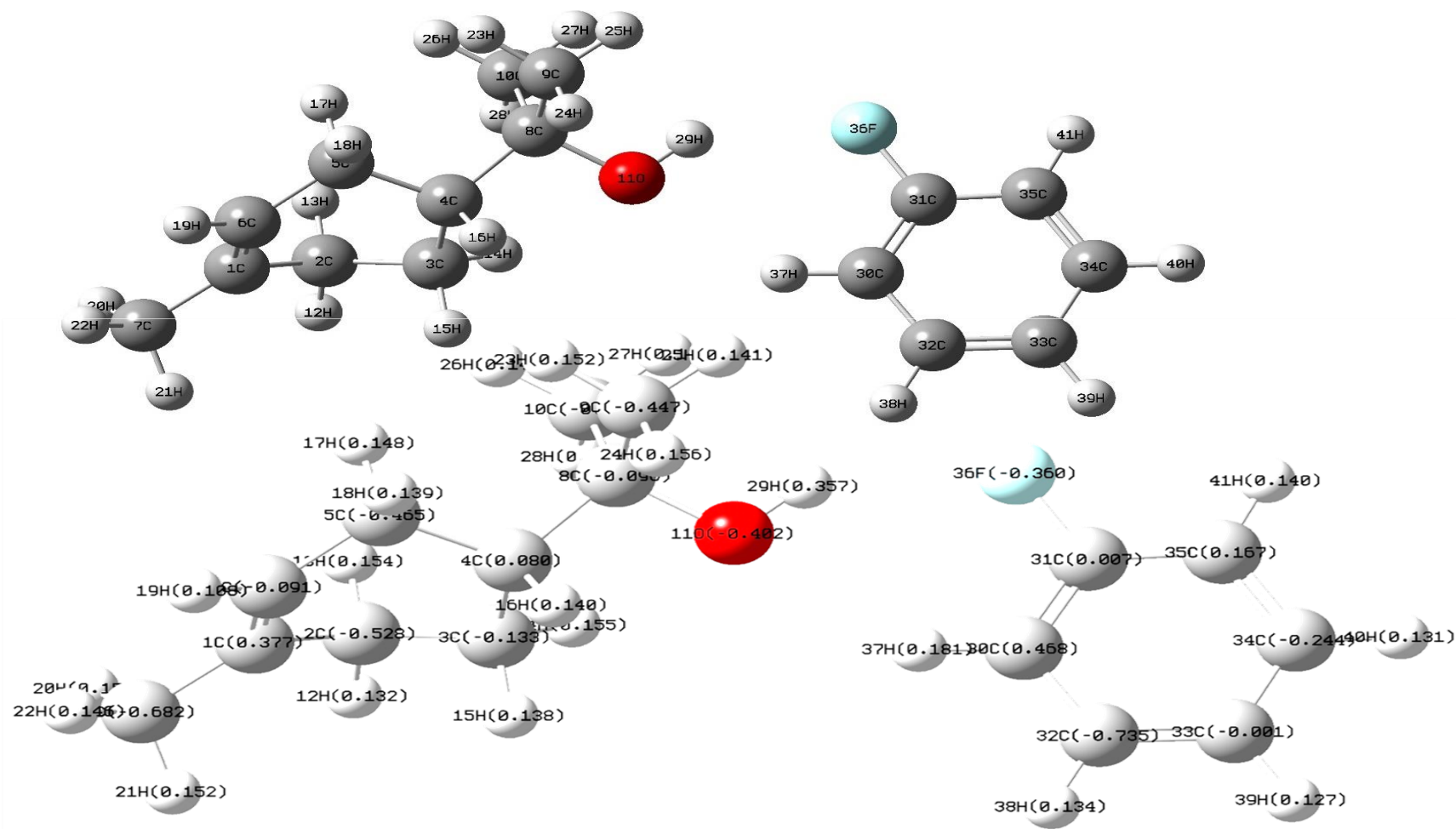


Fig. S13 - Optimized geometric structure of α -terpineol + Fluorobenzene (First Possible Interaction site) with Mulliken charge distribution based on B3LYP/6-31+G(d,p) at 298.15K.

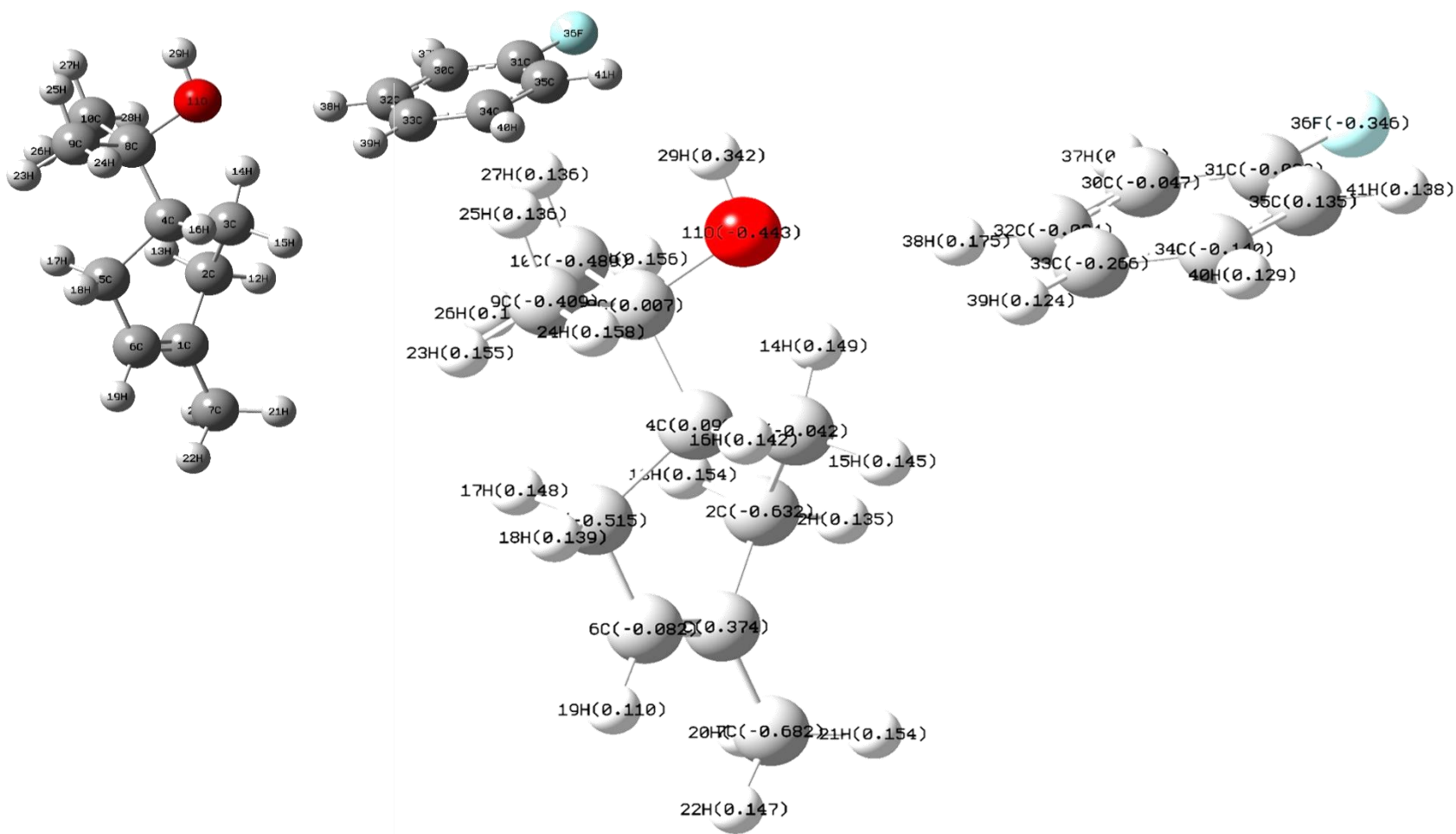


Fig. S14 - Optimized geometric structure of α -terpineol + Fluorobenzene (Second Possible Interaction site) with Mulliken charge distribution based on B3LYP/6-31+G(d,p) at 298.15K.

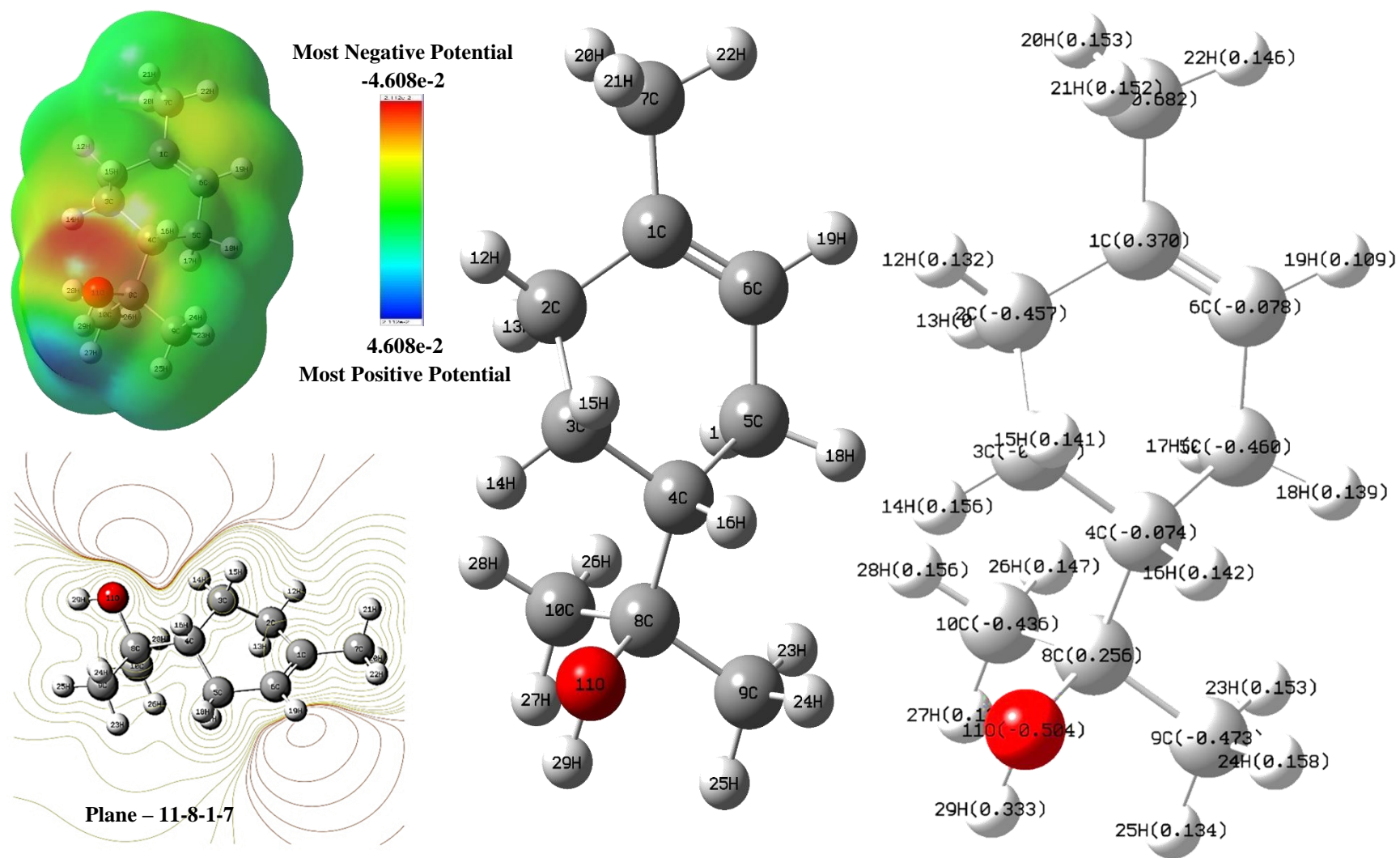
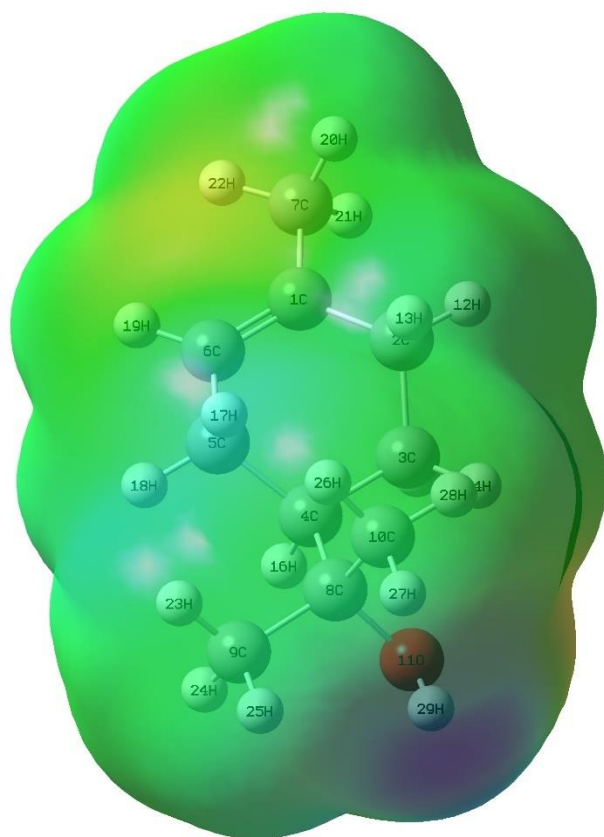


Fig. S15 - Optimized geometric structure of α -terpineol with Mulliken charge distribution, 3D MESP, and 2D electrostatic potential contour map based on B3LYP/6-31+G(d,p) at 298.15K.



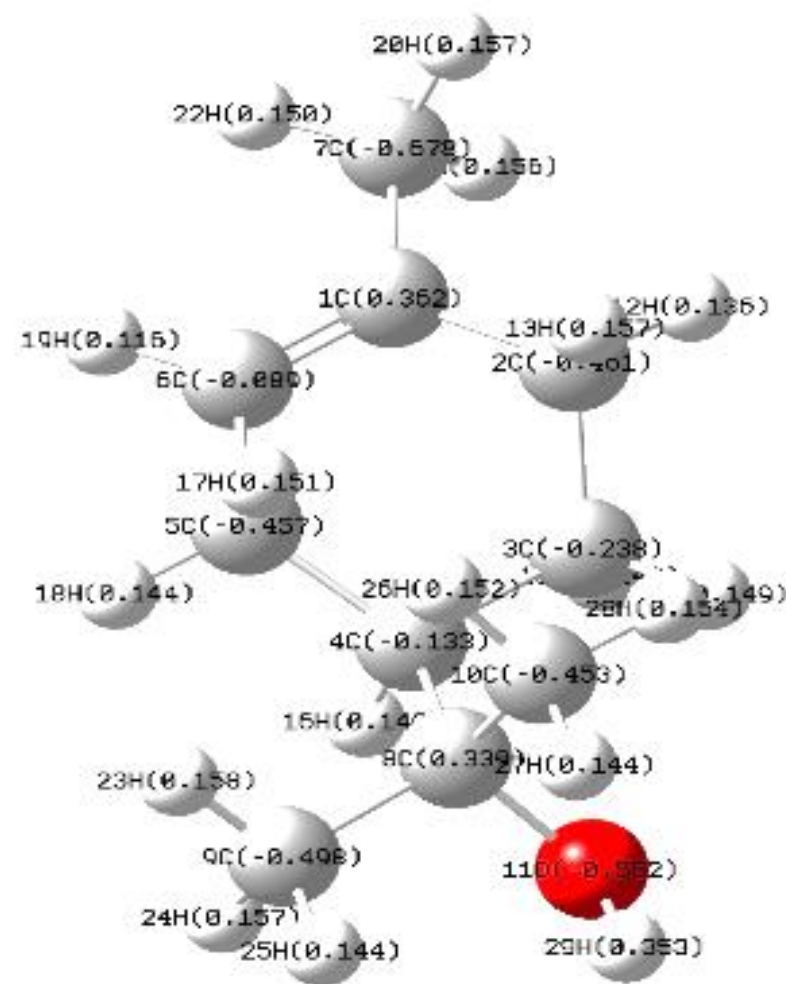
Most Negative Potential

$-5.121e-2$



$5.121e-2$

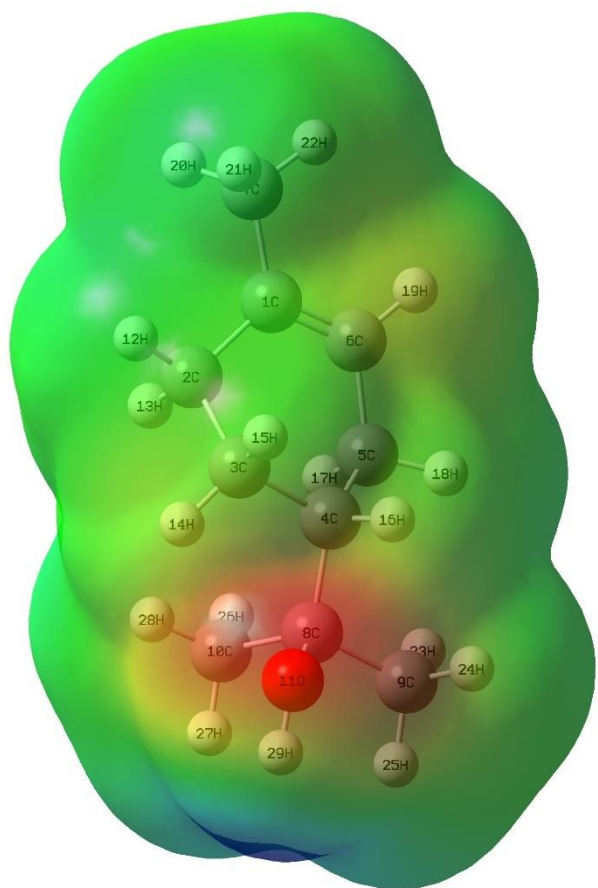
Most Positive Potential



Atomic radii: UFF (Universal Force Field).

Cavity type: Scaled VdW (van der Waals Surface)

Fig. S16 - Optimized geometric structure of α -terpineol in Fluorobenzene solvent environment using Polarizable Continuum (PCM) model with Mulliken charge distribution and 3D MESP based on B3LYP/6-31+G(d,p) at 298.15K.



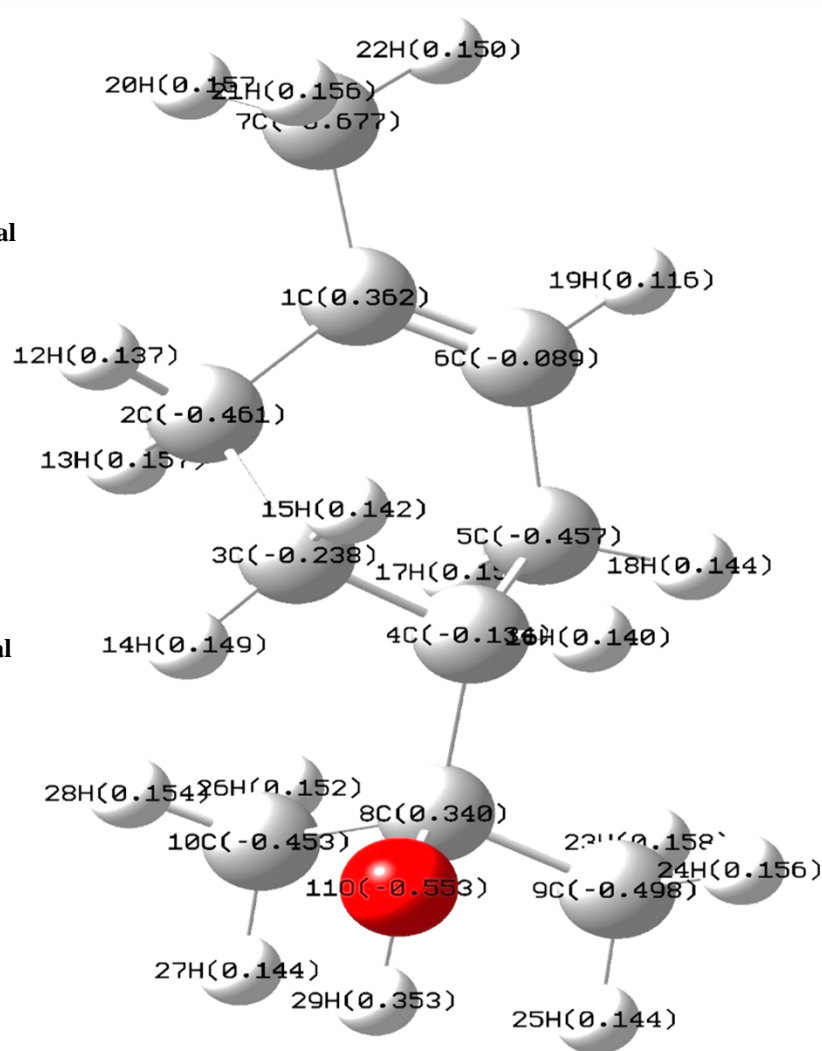
Most Negative Potential

$-5.132e-2$



$5.132e-2$

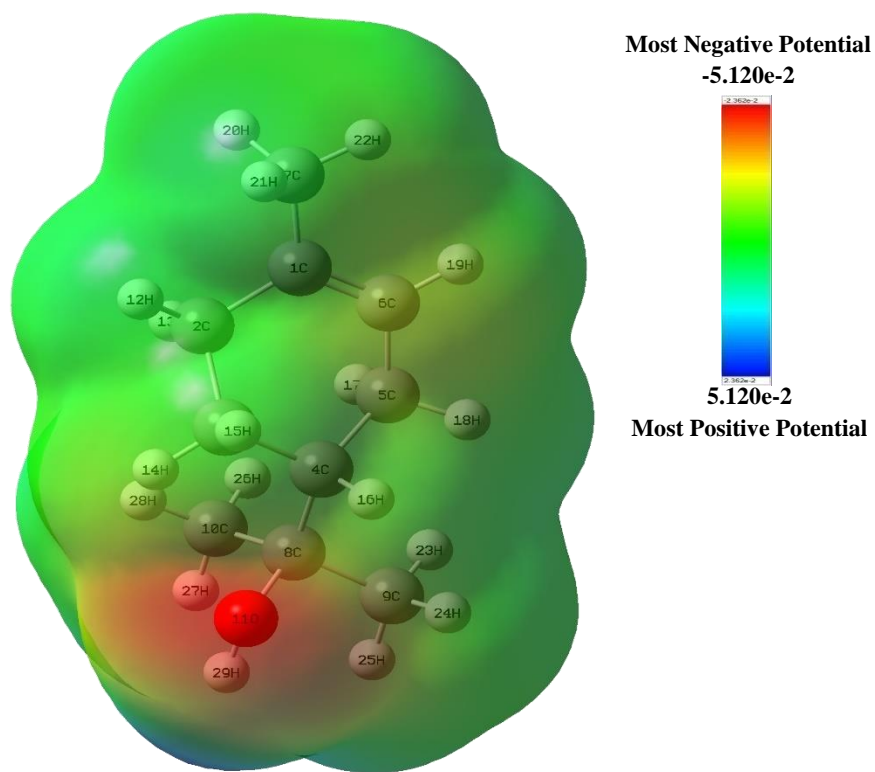
Most Positive Potential



Atomic radii: UFF (Universal Force Field).

Cavity type: Scaled VdW (van der Waals Surface)

Fig. S17 - Optimized geometric structure of α -terpineol in Chlorobenzene solvent environment using Polarizable Continuum (PCM) model with Mulliken charge distribution and 3D MESP based on B3LYP/6-31+G(d,p) at 298.15K.



Atomic radii: UFF (Universal Force Field).

Cavity type: Scaled VdW (van der Waals Surface)

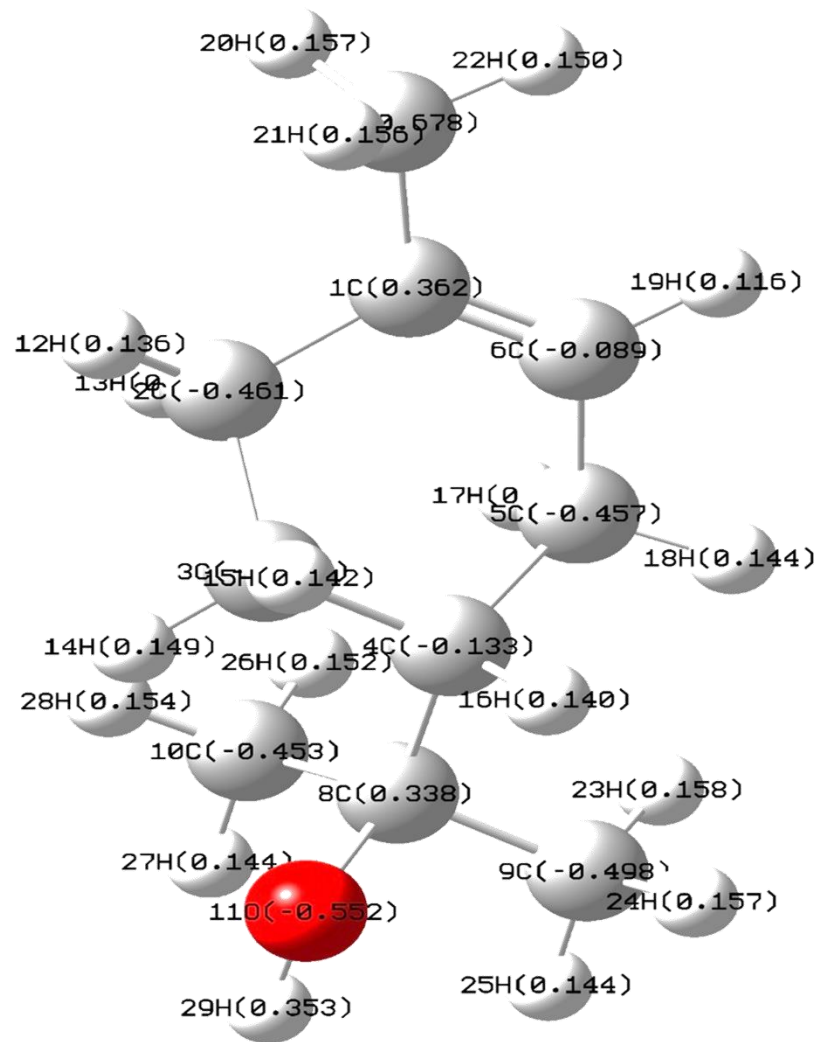
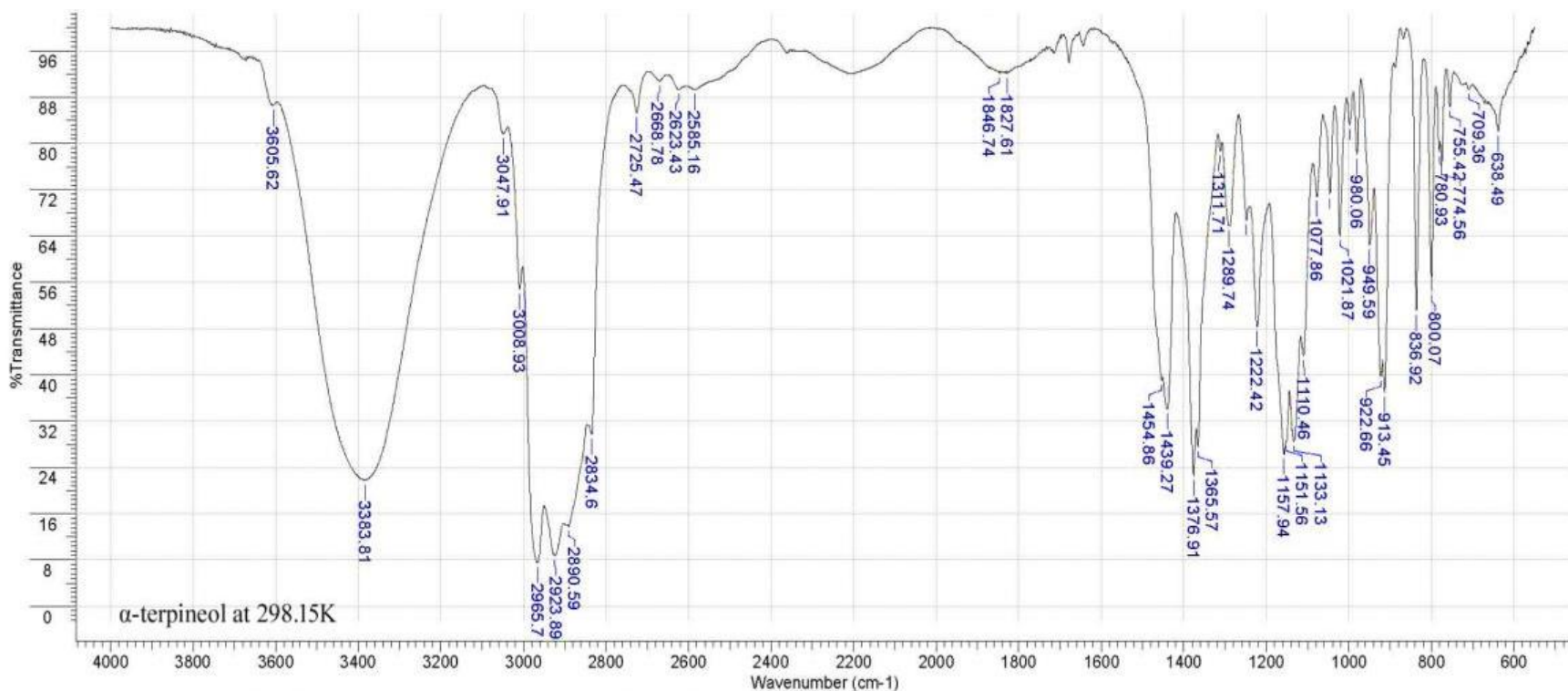
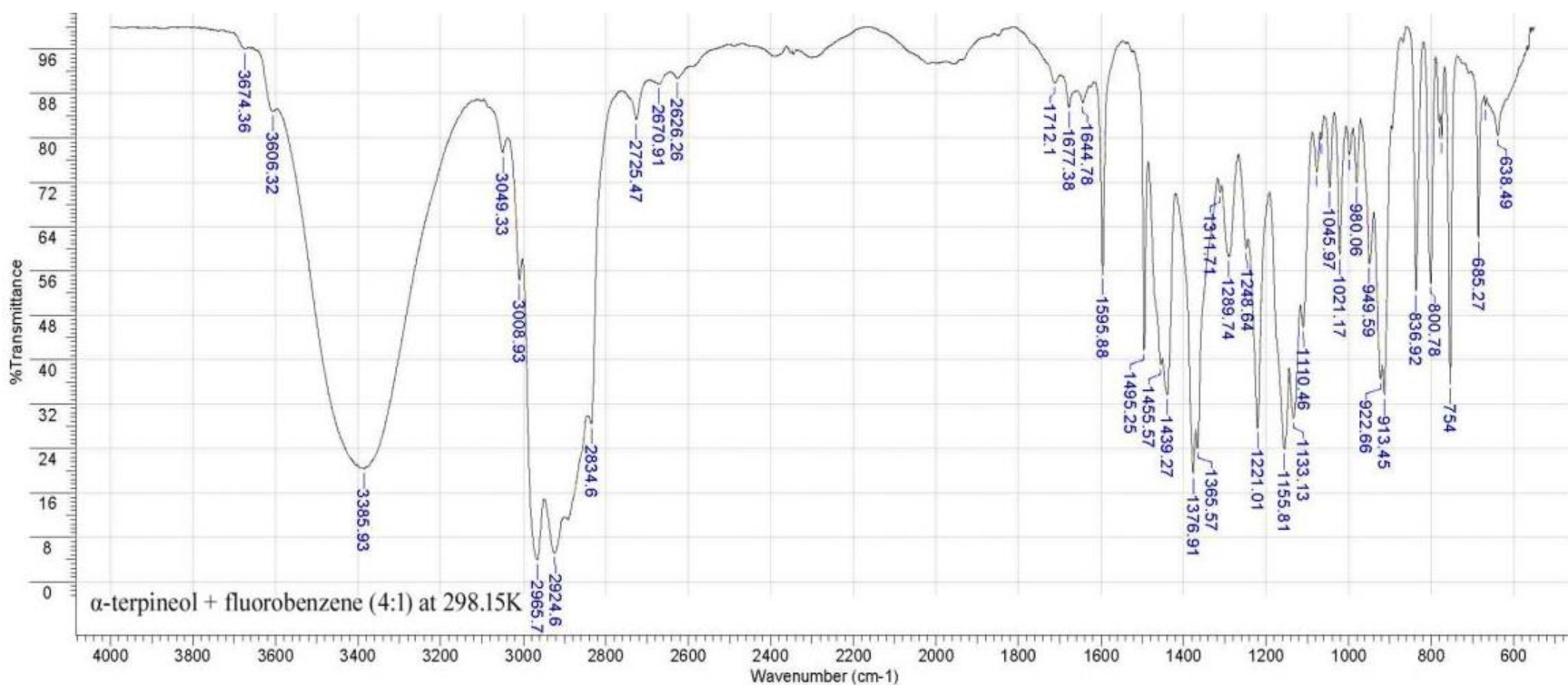


Fig. S18 - Optimized geometric structure of α -terpineol in Bromobenzene solvent environment using Polarizable Continuum (PCM) model with Mulliken charge distribution and 3D MESP based on B3LYP/6-31+G(d,p) at 298.15K.



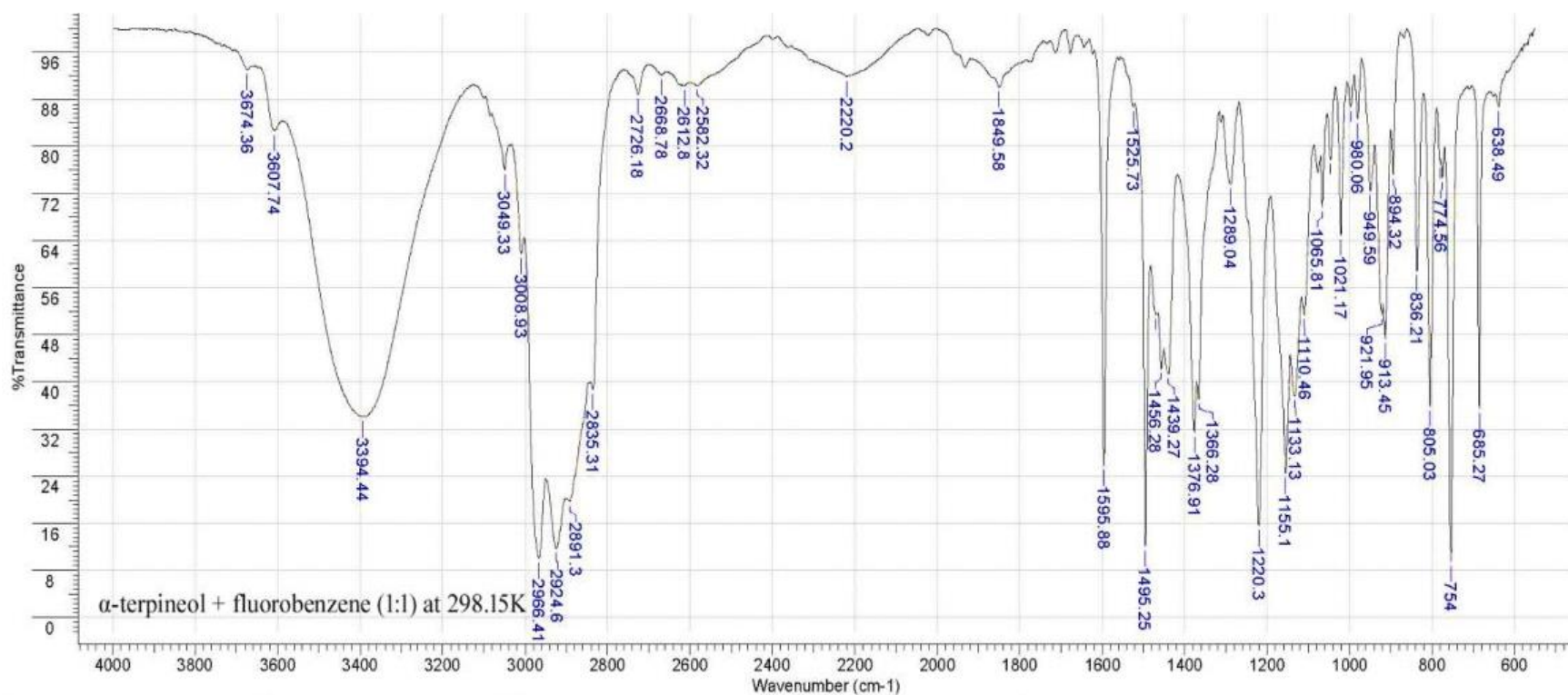
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	638.49	82.124	W	12	997.78	83.236	W	23	1311.71	78.706	W	34	2834.60	29.659	S
2	709.36	89.351	W	13	1021.87	63.998	M	24	1365.57	27.525	S	35	2890.59	13.885	VS
3	755.42	86.390	W	14	1045.97	71.331	M	25	1376.91	22.659	S	36	2923.89	8.718	VS
4	774.56	76.291	W	15	1077.86	70.857	M	26	1439.27	34.042	S	37	2965.70	7.525	VS
5	780.93	78.512	W	16	1110.46	43.282	S	27	1454.86	39.031	S	38	3008.93	54.852	M
6	800.07	54.523	M	17	1133.13	28.544	S	28	1827.61	92.147	VW	39	3047.91	81.685	W
7	836.92	51.143	M	18	1151.56	28.497	S	29	1846.74	92.190	VW	40	3383.81	21.813	S
8	913.45	36.991	S	19	1157.94	26.268	S	30	2585.16	89.291	W	41	3605.62	86.626	W
9	922.66	39.701	S	20	1222.42	48.383	M	31	2623.43	89.371	W				
10	949.59	62.536	M	21	1248.64	66.726	M	32	2668.78	90.806	VW				
11	980.06	78.213	W	22	1289.74	65.713	M	33	2725.47	85.345	W				

Fig. S19 - Experimental FT-IR transmittances spectra of α-terpineol at 298.15K.



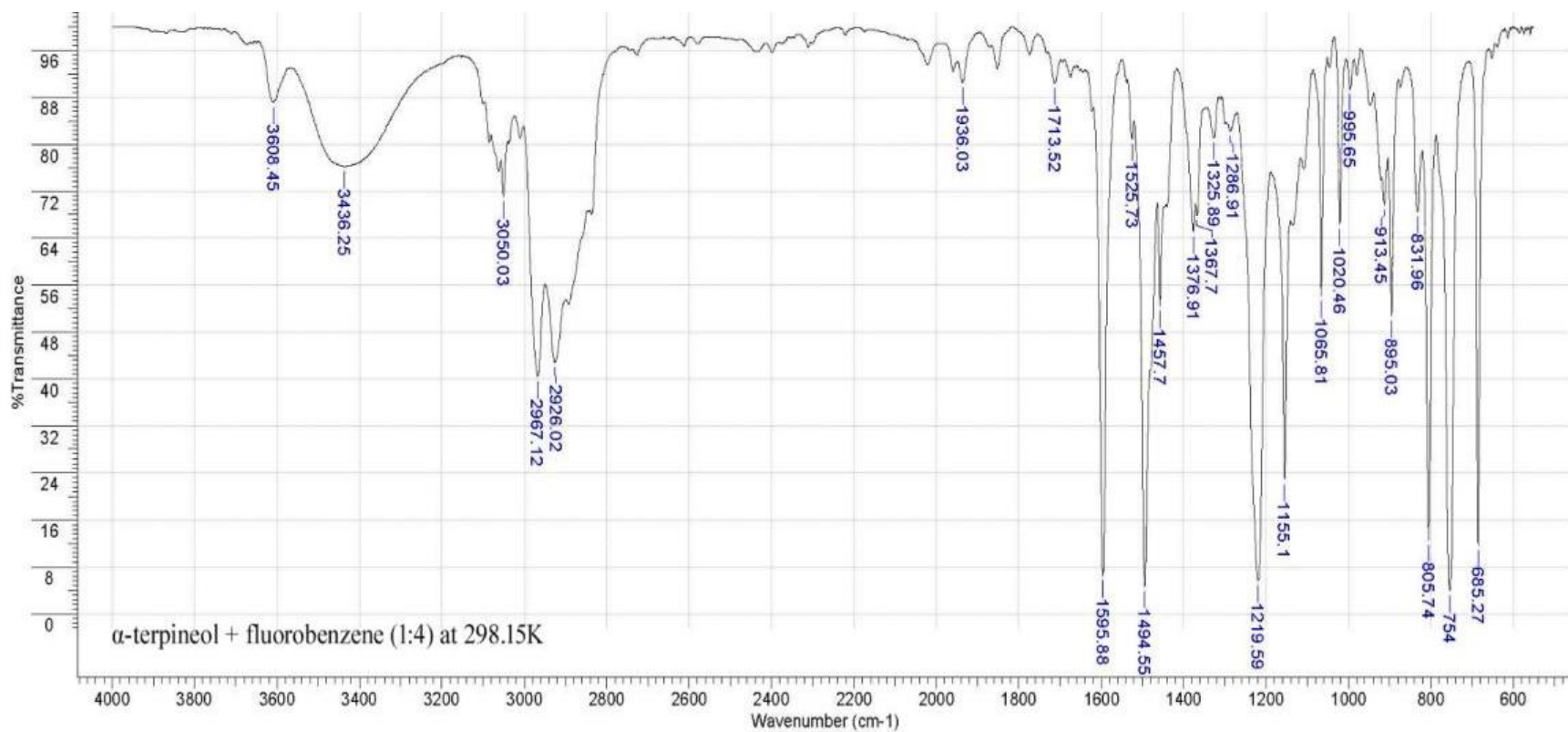
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	638.49	80.379	W	12	980.06	71.902	W	23	1289.74	58.600	M	34	2626.26	90.771	VW
2	668.26	85.908	W	13	997.78	76.887	W	24	1311.71	70.160	M	35	2670.91	89.721	W
3	685.27	62.048	M	14	1021.17	58.931	M	25	1365.57	24.095	S	36	2725.47	83.292	W
4	754.00	35.696	S	15	1045.97	71.137	M	26	1376.91	19.440	S	37	2834.60	28.382	S
5	774.56	79.895	W	16	1065.81	79.685	W	27	1439.27	33.736	S	38	2924.60	5.127	VS
6	780.93	82.642	W	17	1077.15	73.881	W	28	1455.57	39.128	S	39	2965.70	3.966	VS
7	800.78	53.845	M	18	1110.46	45.894	M	29	1495.25	41.703	S	40	3008.93	54.435	M
8	836.92	52.279	M	19	1133.13	29.474	S	30	1595.88	55.308	M	41	3049.33	77.365	W
9	913.45	33.591	S	20	1155.81	23.844	S	31	1644.78	86.464	W	42	3385.93	20.396	S
10	922.66	36.435	S	21	1221.01	27.696	S	32	1677.38	85.500	W	43	3606.32	84.780	W
11	949.59	57.311	M	22	1248.64	60.105	M	33	1712.10	89.928	W	44	3674.36	95.950	VW

Fig. S20 - Experimental FT-IR transmittances spectra of α -terpineol + Fluorobenzene at 4:1 composition ratio at 298.15K.



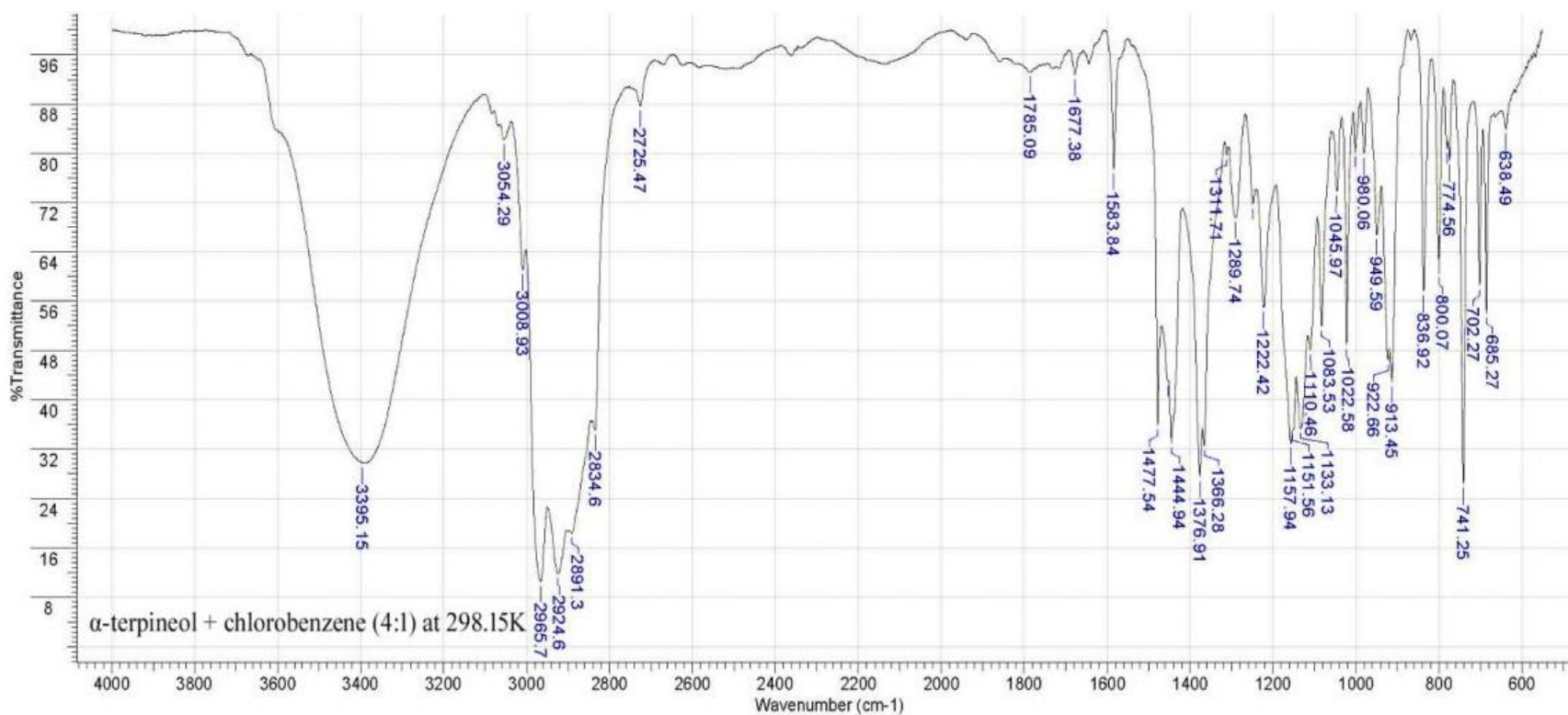
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	638.49	86.694	W	12	980.06	84.673	W	23	1376.91	31.420	S	34	2668.78	92.161	VW
2	685.27	35.478	S	13	997.07	86.715	W	24	1439.27	41.313	S	35	2726.18	88.877	W
3	754.00	9.503	VS	14	1021.17	64.944	M	25	1456.28	42.218	S	36	2835.31	38.720	S
4	774.56	74.596	W	15	1045.97	77.800	W	26	1470.45	51.438	M	37	2891.30	19.730	S
5	780.93	77.123	W	16	1065.81	69.655	M	27	1495.25	12.139	VS	38	2924.60	11.784	VS
6	805.03	35.858	S	17	1110.46	51.344	M	28	1525.73	86.714	W	39	2966.41	10.064	VS
7	836.21	58.869	M	18	1133.13	37.660	S	29	1595.88	25.898	S	40	3008.93	61.781	M
8	894.32	75.289	W	19	1155.10	24.504	S	30	1849.58	90.121	W	41	3049.33	75.987	W
9	913.45	47.372	M	20	1220.30	15.586	VS	31	2220.20	91.859	VW	42	3394.44	34.073	S
10	921.95	51.448	M	21	1289.04	73.571	W	32	2582.32	90.376	W	43	3607.74	82.661	W
11	949.59	72.449	M	22	1366.28	37.084	S	33	2612.80	90.366	W	44	3674.36	93.096	VW

Fig. S21 - Experimental FT-IR transmittances spectra of α-terpineol + Fluorobenzene at 1:1 composition ratio at 298.15K.



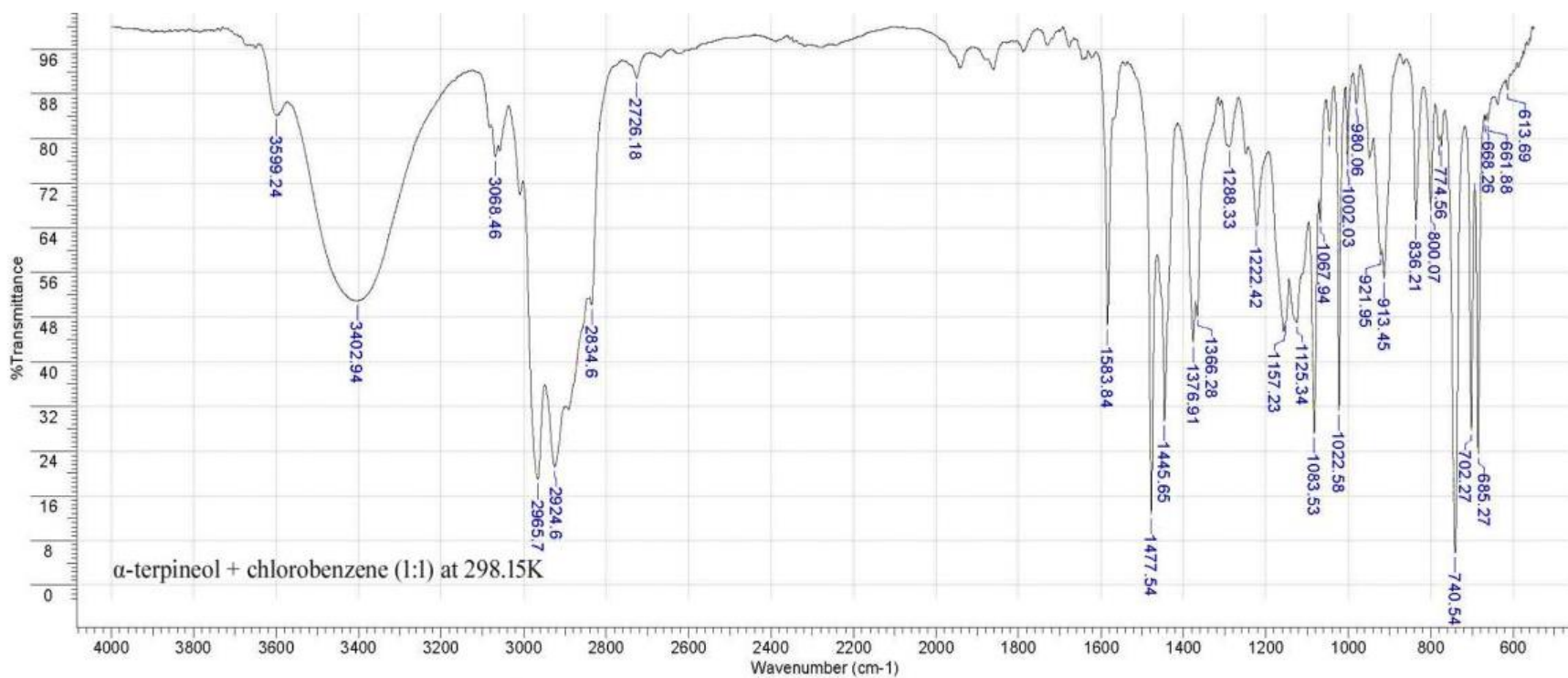
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	685.27	11.724	VS	10	1155.10	22.848	S	19	1595.88	6.493	VS
2	754.00	3.922	VS	11	1219.59	5.739	VS	20	1713.52	90.336	W
3	805.74	12.546	VS	12	1286.91	82.247	W	21	1936.03	90.487	VW
4	831.96	68.482	M	13	1325.89	81.132	W	22	2926.02	42.804	M
5	895.03	50.633	M	14	1367.70	67.840	M	23	2967.12	40.363	S
6	913.45	69.683	M	15	1376.91	65.112	M	24	3050.03	71.000	M
7	995.65	89.390	W	16	1457.70	52.383	M	25	3436.25	76.165	W
8	1020.46	66.357	M	17	1494.55	4.633	VS	26	3608.45	87.113	W
9	1065.81	54.077	M	18	1525.73	80.870	W				

Fig. S22 - Experimental FT-IR transmittances spectra of α -terpineol + Fluorobenzene at 1:4 composition ratio at 298.15K.



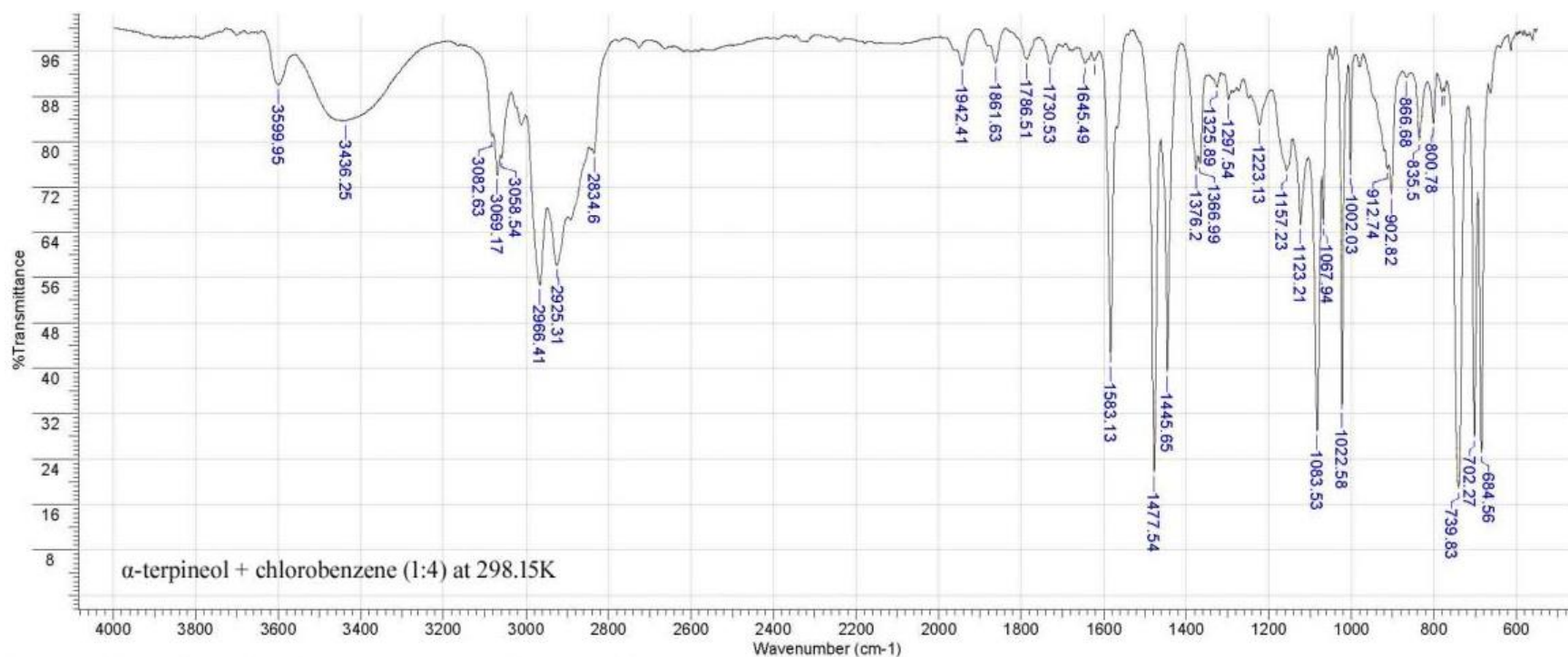
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	638.49	83.869	W	11	949.59	66.828	M	21	1222.42	54.997	M	31	1677.38	92.750	VW
2	685.27	54.050	M	12	980.06	79.946	W	22	1248.64	71.665	M	32	1785.09	93.201	VW
3	702.27	58.629	M	13	1001.32	80.287	W	23	1289.74	69.678	M	33	2725.47	87.667	W
4	741.25	26.489	S	14	1022.58	48.880	M	24	1311.71	79.757	W	34	2834.60	35.092	S
5	774.56	78.825	W	15	1045.97	73.798	W	25	1366.28	32.602	S	35	2891.30	18.363	VS
6	780.93	80.682	W	16	1083.53	51.928	M	26	1376.91	27.616	S	36	2924.60	11.833	VS
7	800.07	60.566	M	17	1110.46	48.162	M	27	1444.94	33.023	S	37	2965.70	10.570	VS
8	836.92	57.634	M	18	1133.13	35.362	S	28	1454.15	43.019	S	38	3008.93	61.167	M
9	913.45	42.924	S	19	1151.56	35.020	S	29	1477.54	35.870	S	39	3054.29	82.207	W
10	922.66	46.360	M	20	1157.94	32.918	S	30	1583.84	77.435	W	40	3395.15	29.756	S

Fig. S23 - Experimental FT-IR transmittances spectra of α-terpineol + Chlorobenzene at 4:1 composition ratio at 298.15K.



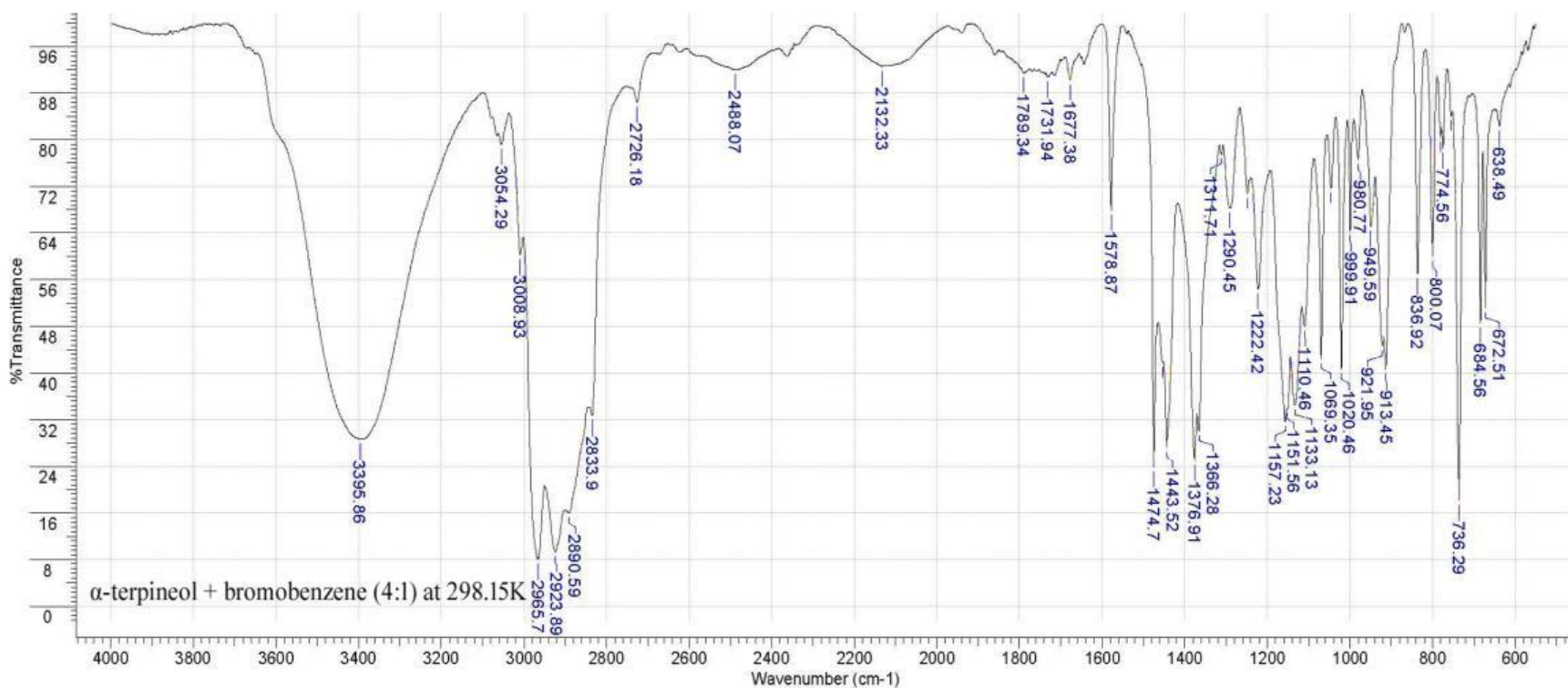
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	613.69	88.805	W	13	980.06	86.310	W	25	1376.91	43.411	S
2	661.88	83.120	W	14	1002.03	75.236	W	26	1445.65	29.401	S
3	668.26	83.249	W	15	1022.58	31.266	S	27	1477.54	12.727	VS
4	685.27	23.588	S	16	1045.97	81.291	W	28	1583.84	46.446	M
5	702.27	27.732	S	17	1067.94	65.043	M	29	2726.18	90.908	VW
6	740.54	5.733	VS	18	1083.53	27.205	S	30	2834.60	50.151	M
7	774.56	78.615	W	19	1125.34	47.039	M	31	2924.60	21.221	S
8	780.93	79.548	W	20	1151.56	47.307	M	32	2965.70	18.967	S
9	800.07	67.090	M	21	1157.23	45.581	M	33	3068.46	76.781	W
10	836.21	65.376	M	22	1222.42	64.348	M	34	3402.94	50.901	M
11	913.45	55.047	M	23	1288.33	78.601	W	35	3599.24	84.176	W
12	921.95	59.216	M	24	1366.28	48.200	M				

Fig. S24 - Experimental FT-IR transmittances spectra of α -terpineol + Chlorobenzene at 1:1 composition ratio at 298.15K.



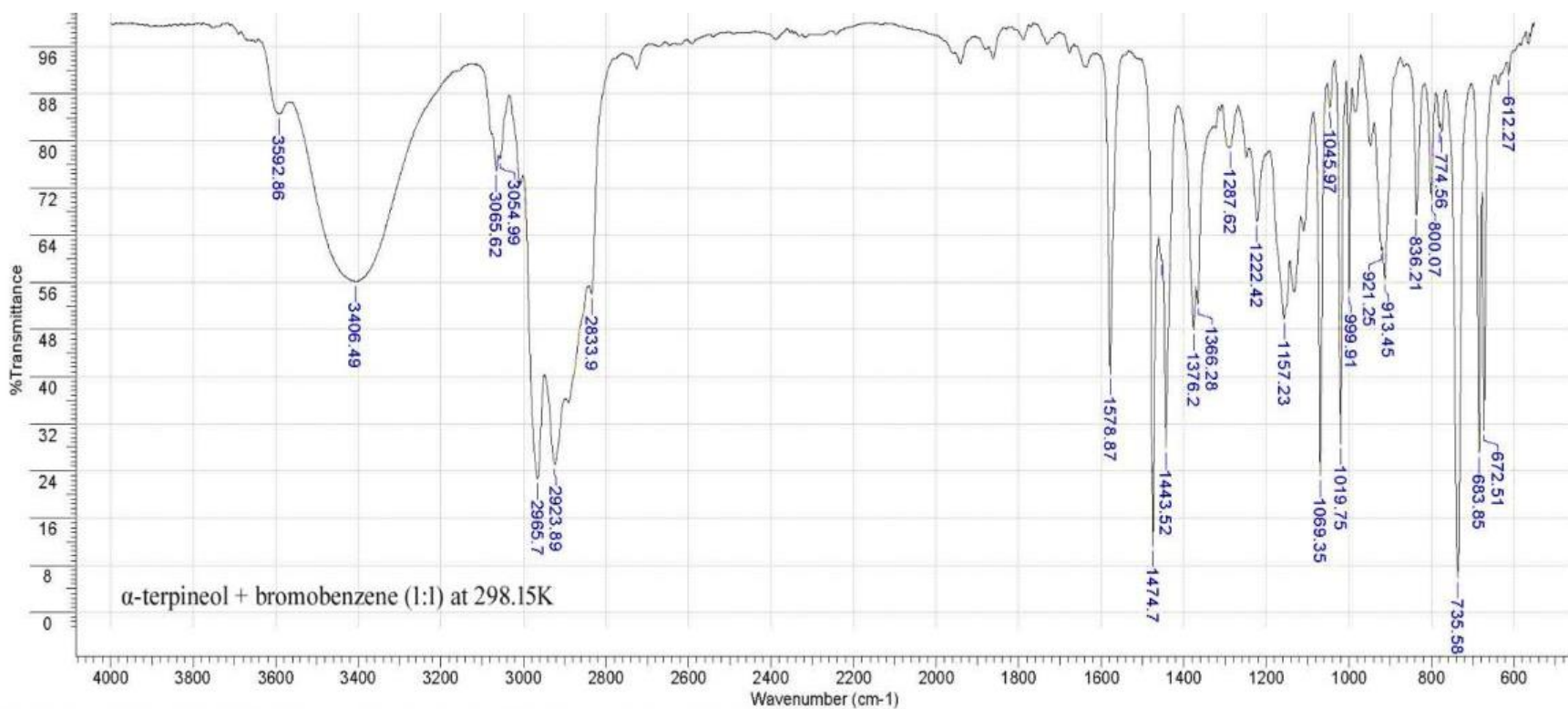
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	684.56	25.078	VS	14	1083.53	29.032	S	27	1730.53	93.729	VW
2	702.27	27.940	S	15	1123.21	65.364	M	28	1786.51	94.568	VW
3	739.83	18.747	VS	16	1157.23	74.898	M	29	1861.63	93.939	VW
4	774.56	88.905	W	17	1223.13	83.017	W	30	1942.41	93.449	VW
5	780.93	88.733	W	18	1297.54	87.465	W	31	2834.60	77.933	W
6	800.78	83.256	W	19	1325.89	89.685	W	32	2925.31	58.178	M
7	835.50	80.291	W	20	1366.99	76.100	W	33	2966.41	54.717	M
8	866.68	91.317	W	21	1376.20	74.970	M	34	3058.54	77.111	W
9	902.82	70.644	M	22	1445.65	39.284	S	35	3069.17	74.197	M
10	912.74	75.168	M	23	1477.54	21.700	VS	36	3082.63	80.847	W
11	1002.03	74.236	M	24	1583.13	41.084	S	37	3436.25	83.723	W
12	1022.58	32.858	S	25	1622.10	94.224	VW	38	3599.95	90.009	W
13	1067.94	65.381	M	26	1645.49	93.776	VW				

Fig. S25 - Experimental FT-IR transmittances spectra of α -terpineol + Chlorobenzene at 1:4 composition ratio at 298.15K.



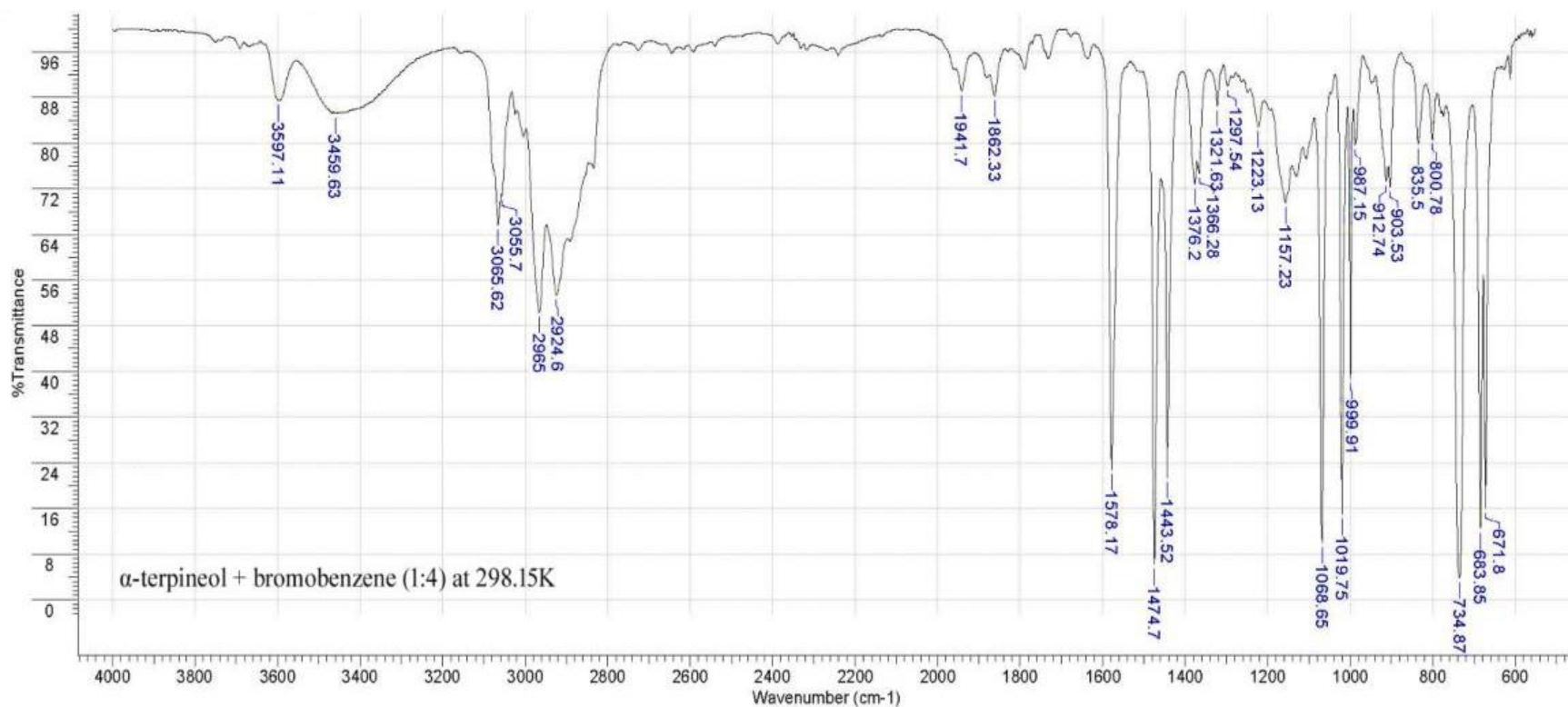
No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	638.49	82.363	W	12	949.59	65.154	M	23	1248.64	70.804	M	34	1789.34	91.486	VW
2	672.51	51.170	M	13	980.77	76.727	W	24	1290.45	68.320	M	35	2132.33	92.623	VW
3	684.56	48.596	M	14	999.91	64.312	M	25	1311.71	77.549	W	36	2488.07	92.019	VW
4	736.29	18.145	S	15	1020.46	40.618	S	26	1366.28	30.056	S	37	2726.18	86.462	W
5	754.71	84.098	W	16	1045.97	71.759	M	27	1376.91	25.088	S	38	2833.90	32.654	S
6	774.56	78.615	W	17	1069.35	42.406	S	28	1443.52	27.210	S	39	2890.59	15.910	VS
7	780.93	80.500	W	18	1110.46	48.011	M	29	1454.15	41.774	S	40	2923.89	9.350	VS
8	800.07	59.960	M	19	1133.13	34.511	S	30	1474.70	23.982	S	41	2965.70	8.081	VS
9	836.92	56.978	M	20	1151.56	33.897	S	31	1578.87	67.932	M	42	3008.93	60.334	M
10	913.45	40.577	S	21	1157.23	31.669	S	32	1677.38	90.326	W	43	3054.29	79.201	W
11	921.95	44.569	S	22	1222.42	54.392	M	33	1731.94	90.744	W	44	3395.86	28.547	S

Fig. S26 - Experimental FT-IR transmittances spectra of α-terpineol + Bromobenzene at 4:1 composition ratio at 298.15K.



No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	612.27	91.216	VW	11	999.91	54.300	M	21	1454.15	59.696	M
2	672.51	30.826	S	12	1019.75	28.671	S	22	1474.70	11.325	VS
3	683.85	27.076	S	13	1045.97	85.750	W	23	1578.87	40.422	S
4	735.58	5.848	VS	14	1069.35	23.153	S	24	2833.90	54.064	M
5	774.56	81.581	W	15	1157.23	49.854	M	25	2923.89	25.132	S
6	780.93	82.236	W	16	1222.42	66.407	M	26	2965.70	22.702	S
7	800.07	70.016	M	17	1287.62	78.957	W	27	3054.99	76.975	W
8	836.21	67.423	M	18	1366.28	52.370	M	28	3065.62	74.973	W
9	913.45	56.340	M	19	1376.20	47.910	M	29	3406.49	56.198	M
10	921.25	61.569	M	20	1443.52	27.897	S	30	3592.86	84.649	W

Fig. S27 - Experimental FT-IR transmittances spectra of α-terpineol + Bromobenzene at 1:1 composition ratio at 298.15K.



No	cm-1	%T	Intensity	No	cm-1	%T	Intensity	No	cm-1	%T	Intensity
1	671.80	16.031	S	11	1068.65	10.015	VS	21	1862.33	88.271	W
2	683.85	12.460	VS	12	1157.23	69.599	M	22	1941.70	89.157	W
3	734.87	3.823	VS	13	1223.13	82.907	W	23	2924.60	53.373	M
4	800.78	80.685	W	14	1297.54	90.125	W	24	2965.00	50.415	M
5	835.50	79.800	W	15	1321.63	86.547	W	25	3055.70	70.836	M
6	903.53	72.302	W	16	1366.28	74.739	W	26	3065.62	65.699	M
7	912.74	73.243	W	17	1376.20	72.756	W	27	3459.63	85.269	W
8	987.15	79.723	W	18	1443.52	21.390	S	28	3597.11	87.456	W
9	999.91	38.735	S	19	1474.70	6.239	VS				
10	1019.75	14.996	S	20	1578.17	22.852	S				

Fig. S28 - Experimental FT-IR transmittances spectra of α -terpineol + Bromobenzene at 1:4 composition ratio at 298.15K.

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