Supplementary Information for:

Composition-dependent Association Behavior in the Mixture of Isopropanol and Trichloromethane: A Volumetric, Vibration Spectroscopic and Quantum Chemical Study

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Table S1

Comparison of densities (ρ / g·cm^{-3}) and refractive indices, n_D of pure liquids with their literature values at T= 298.15 K.

Liquids	ρ		n_D	
	Expt.	Lit.	Expt.	Lit.
isopropanol	0.7814	0.78124[22]	1.3749	1.3753[22]
		0.781588[23]		1.3751[24]
trichloromethane	1.4781	1.4785[25]	1.4428	1.4430[26]
		1.4760[27]		1.4432[28]

Table S2

Experimental density(ρ / g·cm^{-3}) and excess molar volume(V^E / cm^3·mol^{-1}) of isopropanol(1) + trichloromethane(2) mixture at T = (283.15 to 323.15) K

x_1	ρ	V^E	ρ	V^E	ρ	V^E	ρ	V^E
	283.15 K		293.15 K		298.15 K		303.15 K	
0.0000	1.5068	0.0000	1.4877	0.0000	1.4781	0.0000	1.4686	0.0000
0.1000	1.4362	0.1205	1.4179	0.1437	1.4086	0.1618	1.3994	0.1785
0.1971	1.3678	0.2058	1.3503	0.2500	1.3414	0.2797	1.3327	0.3005
0.2836	1.3074	0.2270	1.2907	0.2838	1.2823	0.3144	1.2739	0.3469
0.3964	1.2290	0.1895	1.2133	0.2642	1.2054	0.3046	1.1976	0.3386
0.4944	1.1607	0.1215	1.1462	0.1888	1.1388	0.2326	1.1315	0.2684
0.5908	1.0929	0.0476	1.0793	0.1258	1.0725	0.1652	1.0657	0.2018
0.7134	1.0057	-0.0530	0.9936	0.0115	0.9874	0.0560	0.9813	0.0880
0.8023	0.9417	-0.1256	0.9307	-0.0746	0.9251	-0.0404	0.9196	-0.0208
0.8977	0.8716	-0.1429	0.8618	-0.1103	0.8568	-0.0847	0.8518	-0.0669
1.0000	0.7940	0.0000	0.7856	0.0000	0.7814	0.0000	0.7771	0.0000
x_1	308.15 K		313.15 K		318.15 K		323.15 K	
0.0000	1.4590	0.0000	1.4495	0.0000	1.4398	0.0000	1.4306	0.0000
0.1000	1.3901	0.1955	1.3809	0.2131	1.3716	0.2247	1.3627	0.2405
0.1971	1.3237	0.3337	1.3150	0.3556	1.3060	0.3836	1.2973	0.4208
0.2836	1.2654	0.3796	1.2570	0.4137	1.2484	0.4476	1.2402	0.4826
0.3964	1.1897	0.3728	1.1818	0.4153	1.1738	0.4507	1.1660	0.4987
0.4944	1.1240	0.3114	1.1166	0.3561	1.1091	0.3933	1.1018	0.4416
0.5908	1.0588	0.2386	1.0519	0.2847	1.0448	0.3304	1.0380	0.3780
0.7134	0.9750	0.1281	0.9688	0.1699	0.9625	0.2030	0.9564	0.2433
0.8023	0.9138	0.0158	0.9082	0.0452	0.9024	0.0741	0.8968	0.1083
0.8977	0.8467	-0.0491	0.8417	-0.0305	0.8365	-0.0122	0.8315	0.0090
1.0000	0.7727	0.0000	0.7684	0.0000	0.7639	0.0000	0.7596	0.0000

Table S3

Coefficients (A_i / $cm^3 \cdot mol^{-1}$)of the fitting equation (2) and standard deviations (SD / $cm^3 \cdot mol^{-1}$) of isopropanol(1) + trichloromethane(2) mixture at T = (283.15 to 323.15) K

T/K	A_0	A_1	A_2	A_3	A_4	A_5	SD
283.15	0.4769	1.4850	-0.0816	0.7949	-1.3525	-0.4058	0.0022
293.15	0.7746	1.4412	-0.0484	0.8698	-1.3953	-0.5644	0.0057
298.15	0.9433	1.4054	0.0126	0.8171	-1.3147	-0.4936	0.0064
303.13	1.0929	1.3799	-0.0537	0.9990	-1.1460	-0.7328	0.0079
308.15	1.2440	1.3398	0.1767	1.0230	-1.3779	-0.6739	0.0058
313.15	1.4298	1.3106	0.1070	0.9096	-1.2620	-0.4355	0.0072
318.15	1.5884	1.2135	0.1903	1.4952	-1.3692	-1.2372	0.0063
323.15	1.7815	1.1809	0.2271	1.7019	-1.3689	-1.5546	0.0066

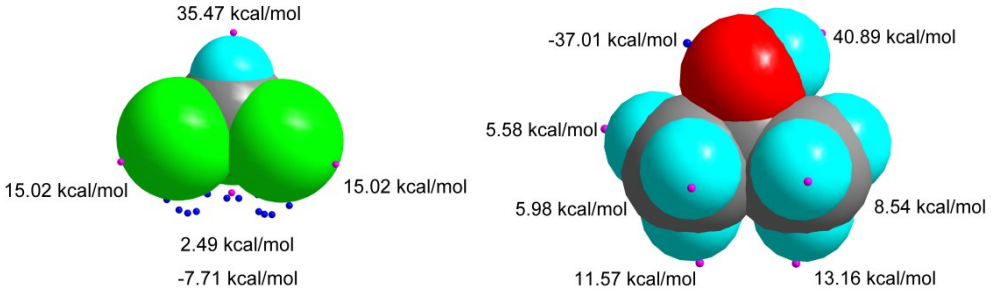

Figure S1. Plots of molecular electrostatic surface potential of isopropanol and trichloromethane at the ωB97X-D/6-311++G (d, P) level.

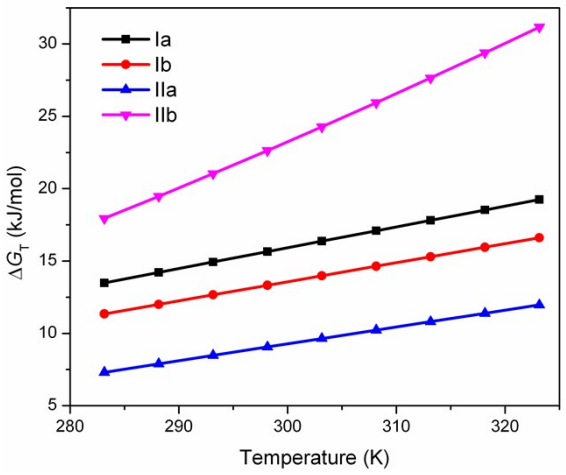

Figure S2. Gibbs free energy changes, ΔG_T of **Ia**, **Ib**, **IIa** and **IIb** with temperature varying from T = (283.15 to 323.15) K at the ωB97X-D/6-311++G (d, P) level.

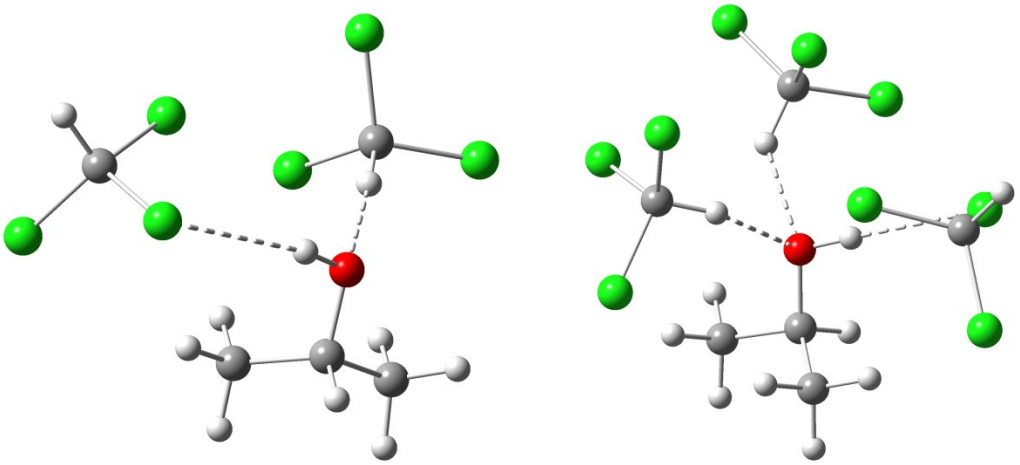

Figure S3 Optimized structures of trimer and tetramer of isopropanol and trichloromethane at the ωB97X-D/6-311++G (d, P) level

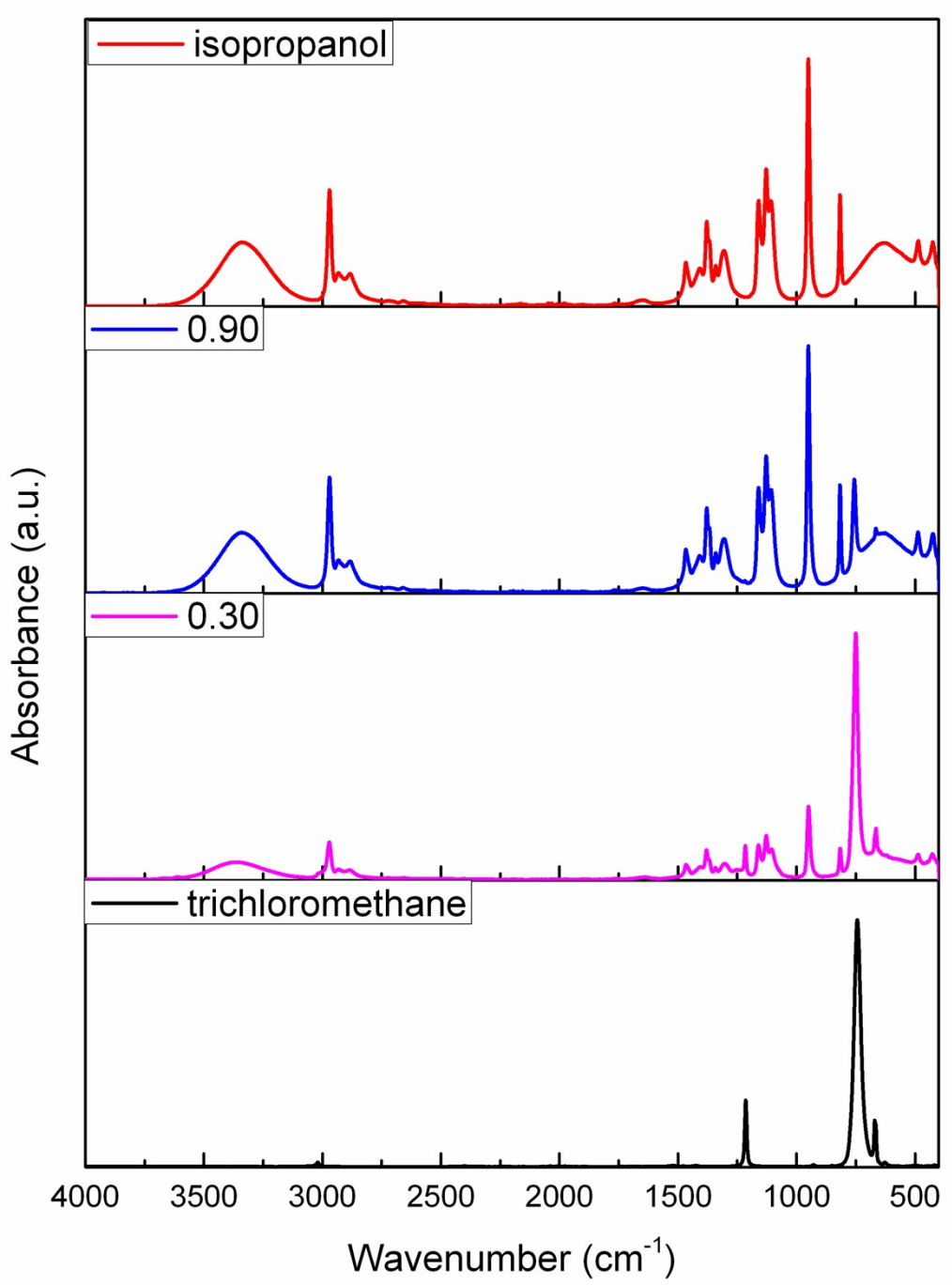

Figure S4. FT-IR spectra for isopropanol, trichloromethane and the mixtures studied at x_1 = 0.30 and 0.90.

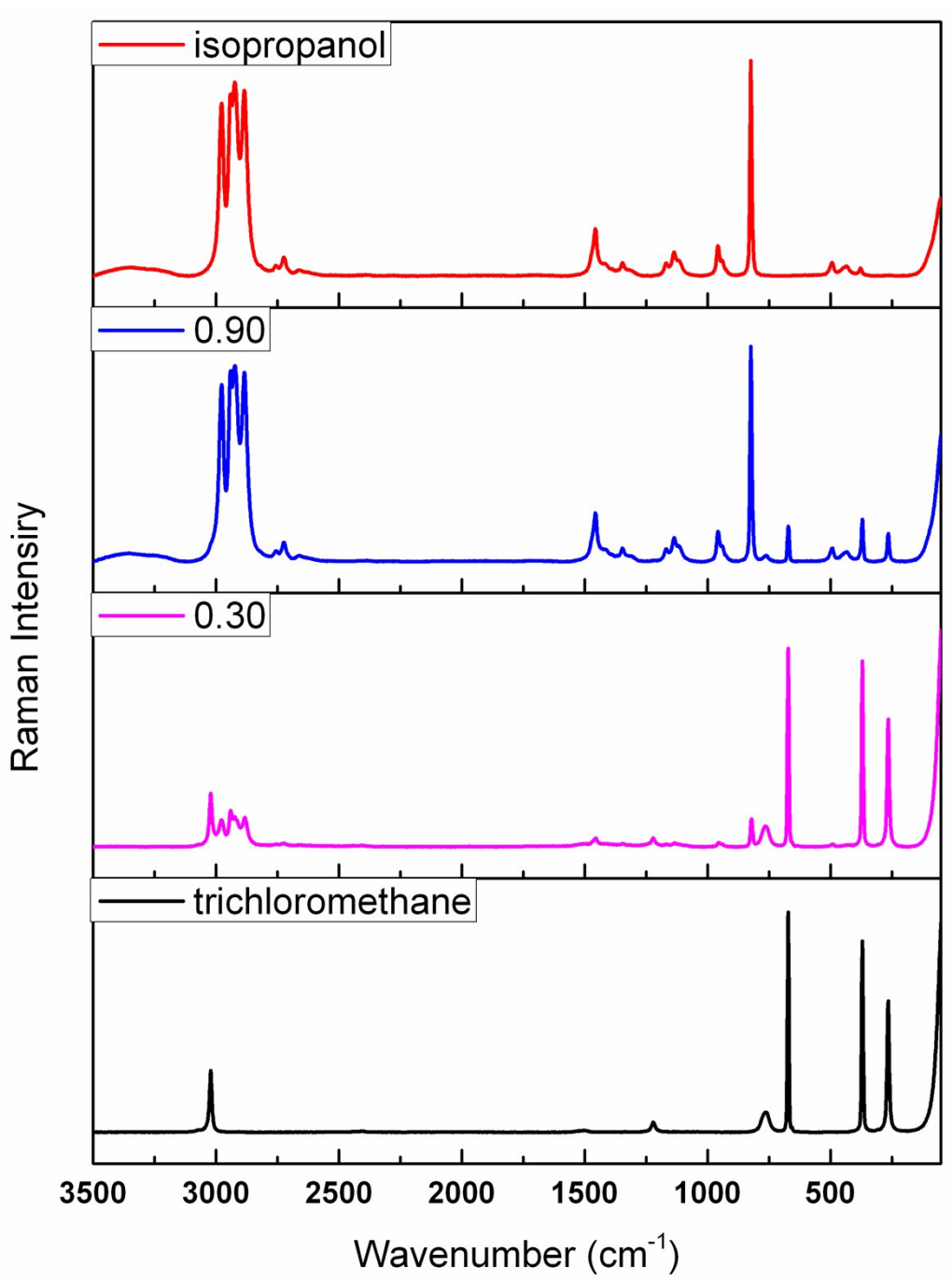

Figure S5. FT-Raman spectra for isopropanol, trichloromethane and the mixtures studied at x_1 = 0.30 and 0.90.