Experimental measurement and Thermodynamic Model of Liquid Liquid Equilibrium for the Ternary System of 1-Dodecanol + Phenol + Water

*Meiling Jiang, Shuai Shen, Yun Chen**

Department of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou, 510640, P.R.China

Supporting Information

1. Internal standard curve of phenol

Table S1 The mass of phenol and 3,4-xylenol in the internal standard sample and the corresponding peak areas in GC [c].

Sample	m_i [a]	A_i [b]	m_{std} [a]	A_{std} [b]	m_i/m_{std}	A_i/A_{std}
1	0.02365	1.21117	0.02404	1.29832	0.98378	0.93287
	0.02365	1.09654	0.02404	1.34592	0.98378	0.81471
2	0.02354	1.11597	0.04605	2.65408	0.51118	0.42047
	0.02354	1.16757	0.04605	2.54708	0.51118	0.45840
3	0.02655	1.18240	0.07889	4.15987	0.33654	0.28424
	0.02655	1.17899	0.07889	4.29128	0.33654	0.27474
4	0.05408	2.63533	0.04870	2.69846	1.11047	0.97661
	0.05408	2.68106	0.04870	2.67945	1.11047	1.00060
5	0.11406	6.11677	0.04993	2.69846	2.28440	2.26676
	0.11406	6.41551	0.04993	2.92044	2.28440	2.19676

6	0.15497	7.98230	0.05309	2.98753	2.91899	2.67187
	0.15497	7.71113	0.05309	2.69868	2.91899	2.85737
7	0.23073	11.35542	0.05445	2.91929	4.23747	3.88979
	0.23073	11.15650	0.05445	2.88039	4.23747	3.87326
8	0.25031	10.67729	0.04763	2.08199	5.25530	5.12841
	0.25031	11.15512	0.04763	2.27793	5.25530	4.89704
9	0.33598	14.18839	0.05652	2.48963	5.94444	5.69900
	0.33598	15.05181	0.05652	2.70436	5.94444	5.56576
10	0.02555	1.23021	0.14560	7.83594	0.17548	0.15700
	0.02555	1.26551	0.14560	8.14265	0.17548	0.15542
11	0.02307	0.99956	0.18298	8.58587	0.12608	0.11642
	0.02307	1.02069	0.18298	9.60312	0.12608	0.10629
12	0.04597	1.99374	0.06448	3.24044	0.71293	0.61527
	0.04597	2.04998	0.06448	3.32143	0.71293	0.61720

[a] m_i is the mass of phenol; m_{std} is the mass of 3,4-xylenol.

[b] A_i is the area of phenol; A_{std} is the area of 3,4-xylenol.

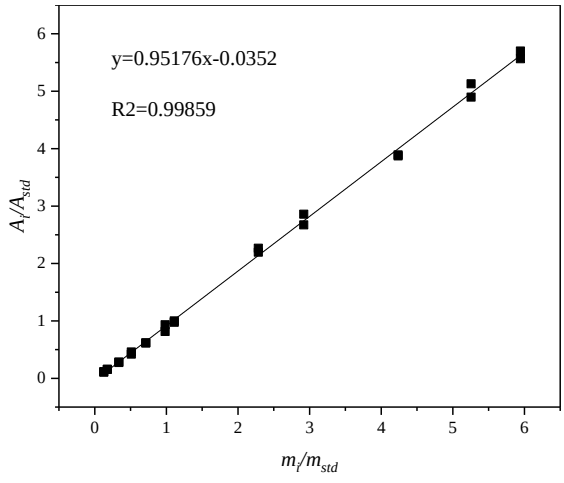

Fig.S1. Standard curve of phenol

2. Internal standard curve of 1-dodecanol

Table S2 The mass of 1-dodecanol and 1-tetradecanol in the internal standard sample and the corresponding peak areas in GC [c].

Sample	m_i[a]	A_i[b]	m_{std}[a]	A_{std}[b]	m_i/m_{std}	A_i/A_{std}
1	0.02519	1.42719	0.02939	1.46720	0.85709	0.97273
	0.02519	1.44513	0.02939	1.53110	0.85709	0.94385
2	0.09230	5.77088	0.02861	1.55057	3.22614	3.72178
	0.09230	5.76912	0.02861	1.54933	3.22614	3.72362
3	0.02085	1.18486	0.05218	2.66082	0.39958	0.44530
	0.02085	1.17267	0.05218	2.65029	0.39958	0.44247
4	0.04305	1.79671	0.05747	2.11432	0.74909	0.84978
	0.04305	2.35212	0.05747	2.85119	0.74909	0.82496
5	0.10476	3.30564	0.05228	1.44839	2.00383	2.28229
	0.10476	3.13918	0.05228	1.34338	2.00383	2.33678
6	0.09413	4.98765	0.09061	4.58700	1.03885	1.08734
	0.09413	2.91369	0.09061	2.52731	1.03885	1.15288
	0.09413	5.29626	0.09061	4.90591	1.03885	1.07957
7	0.02245	1.37895	0.10028	5.23972	0.22384	0.26317
	0.02245	1.22137	0.10028	5.27288	0.22384	0.23163
8	0.04585	1.37849	0.10498	2.87053	0.43675	0.48022
	0.04585	2.59150	0.10498	5.83029	0.43675	0.44449
9	0.10473	5.66182	0.10024	5.22623	1.04479	1.08335
	0.10473	3.86019	0.10024	3.58475	1.04479	1.07684
10	0.17688	8.94454	0.10967	5.42030	1.61284	1.65019
	0.17688	9.01588	0.10967	5.43148	1.61284	1.65993
11	0.25802	7.58287	0.10556	2.80600	2.44430	2.70238
	0.25802	13.93796	0.10556	5.43148	2.44430	2.56614
12	0.29917	13.85221	0.10409	4.60495	2.87415	3.00811
	0.29917	11.39129	0.10409	3.77533	2.87415	3.01730

[a] m_i is the mass of 1-dodecanonl; m_{std} is the mass of 1-tetradecanol.

[b] A_i is the area of 1-dodecanol; A_{std} is the area of 1-tetradecanol.

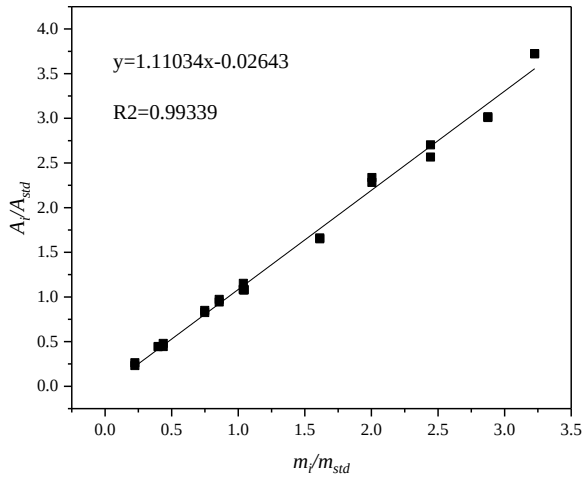

Fig.S2. Standard curve of 1-dodecanol

3. Standard uncertainty evaluation

u(w_2^O) was taken as an example. w_2^O represents mole fraction of phenol in the organic phase and u(w_2^O) is standard uncertainty of w_2^O. The standard deviation expression of the mean value $S(\overline{X}_i)$ is as follows.

$$\overline{X}_i = \frac{1}{n}\sum_{k=1}^{n} X_{i,k} \tag{1}$$

$$S(X_{i,k}) = \left[\frac{1}{n-1}\sum_{k=1}^{n}(X_{i,k} - \overline{X}_i)^2\right]^{1/2} \tag{2}$$

$$u(x_i) = S(\overline{X}_i) = \frac{S(X_{i,k})}{\sqrt{m}} \tag{3}$$

where $X_{i,k}$ is n times equal precision measurement column; $\overline{X}_i$ is the mean value; m is the number of samples; $S(X_{i,k})$ is experimental standard deviation of the mean $X_{i,k}$; $S(\overline{X}_i)$ is experimental standard deviation. Equation (3) is an expression for the Type A uncertainty, $x_i = \overline{X}_i$. The result of u(w_2^O) is shown in Table S3.

Table S3 Calculation of the standard uncertainty of w_2^O

i	Three repeated measurements(k)	$\overline{X}_i$	$S(X_{i,k})$

	X_1	X_2	X_3		
1	0.03612	0.03754	0.03633	0.03666	0.00077
2	0.10755	0.10867	0.10810	0.10811	0.00056
3	0.16632	0.16534	0.16472	0.16546	0.00081
4	0.22936	0.23067	0.22981	0.22994	0.00067
5	0.28643	0.28713	0.28729	0.28695	0.00046
5	0.35087	0.35279	0.35159	0.35175	0.00097
7	0.40567	0.40486	0.40543	0.40532	0.00041
8	0.44306	0.44331	0.44284	0.44307	0.00024
9	0.05679	0.05534	0.05583	0.05599	0.00074
10	0.12033	0.12348	0.12029	0.12136	0.00183
11	0.18157	0.18380	0.18178	0.18238	0.00123
12	0.23789	0.24170	0.23779	0.23913	0.00223
13	0.29557	0.28894	0.29099	0.29183	0.00339
14	0.33676	0.34167	0.33950	0.33931	0.00246
15	0.38457	0.37968	0.38232	0.38219	0.00245
16	0.41858	0.42157	0.41957	0.41991	0.00153
17	0.03089	0.03279	0.03199	0.03189	0.00095
18	0.10043	0.09768	0.09606	0.09806	0.00221
19	0.15690	0.15578	0.15637	0.15635	0.00056
20	0.22555	0.22374	0.22427	0.22452	0.00093
21	0.27653	0.27591	0.27591	0.27612	0.00036
22	0.31568	0.30987	0.31095	0.31217	0.00309
23	0.35598	0.35568	0.35501	0.35556	0.00049
24	0.39323	0.38968	0.39372	0.39221	0.00221
25	0.05573	0.05500	0.05501	0.05525	0.00042
26	0.13560	0.12679	0.13352	0.13197	0.00460

27	0.20287	0.19968	0.20127	0.20127	0.00160
28	0.28363	0.27979	0.28312	0.28218	0.00209
29	0.34188	0.33779	0.34110	0.34026	0.00217
30	0.40366	0.39558	0.39939	0.39954	0.00404
31	0.43999	0.44070	0.44096	0.44055	0.00050
32	0.46789	0.46157	0.46814	0.46587	0.00373
33	0.05745	0.05523	0.05540	0.05603	0.00123
34	0.13007	0.12562	0.12730	0.12767	0.00224
35	0.19157	0.19557	0.19013	0.19242	0.00282
36	0.25360	0.25046	0.25077	0.25161	0.00173
37	0.31270	0.30854	0.31234	0.31119	0.00231
38	0.37598	0.37315	0.37569	0.37494	0.00155
39	0.44900	0.44920	0.44901	0.44907	0.00011
40	0.47996	0.47879	0.48048	0.47974	0.00086
u(w_2^O)					**0.01005**