

Supporting information

Production of high purity allyl alcohol by the salting-out method from formic acid-mediated deoxydehydration of glycerol

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Table S1. Experimental (liquid-liquid) equilibrium mass fractions of a salt-free basis for (allyl alcohol + water + salt) at the given total mass fraction of a salt, temperature $T = 298.15$ K, and pressure $P = 101.3$ kPa (for Figures 3–5)^a

salt	organic phase (wt%)		aqueous phase (wt%)	
	allyl alcohol	water	allyl alcohol	water
5%NaCl	70.97	29.03	13.15	86.85
10%NaCl	72.57	27.43	10.95	89.05
15%NaCl	72.89	27.11	10.96	89.04
20%NaCl	73.03	26.97	10.95	89.05
25%NaCl	73.24	26.76	10.94	89.06
5%K ₂ HPO ₄	75.84	24.16	1.66	98.34
10%K ₂ HPO ₄	79.08	20.92	1.05	98.95
15%K ₂ HPO ₄	82.46	17.54	0.76	99.24
20%K ₂ HPO ₄	84.95	15.05	0.57	99.43
25%K ₂ HPO ₄	87.28	12.72	0.45	99.55
30%K ₂ HPO ₄	89.60	10.40	0.40	99.60
35%K ₂ HPO ₄	91.40	8.60	0.35	99.65
40%K ₂ HPO ₄	93.10	6.90	0.34	99.66
5%K ₂ CO ₃	76.72	23.28	1.57	98.43
10%K ₂ CO ₃	85.20	14.80	0.83	99.17
15%K ₂ CO ₃	90.55	9.45	0.55	99.45
20%K ₂ CO ₃	94.30	5.70	0.42	99.58
25%K ₂ CO ₃	96.74	3.26	0.34	99.66
30%K ₂ CO ₃	98.24	1.76	0.32	99.68
35%K ₂ CO ₃	99.01	0.99	0.31	99.69
40%K ₂ CO ₃	99.05	0.95	0.30	99.70

^aStandard uncertainties u are $u(T) = 0.01$ K, $u(p) = 1$ kPa, $u(\text{wt}\%) = 0.01$

Table S2. Experimental (liquid-liquid) equilibrium mass fractions of a salt-free basis for (allyl alcohol + water + salt) at the given (20% + 20%) mass fraction of two salts, temperature $T = 298.15$ K, and pressure $P = 101.3$ kPa (for Table 3)^a

salt	organic phase (wt%)		aqueous phase (wt%)	
	allyl alcohol	water	allyl alcohol	water
20%KCl+20%KCl	70.72	29.28	14.64	85.36
20%KCl+20%NaCl	72.84	27.16	10.45	89.55
20%KCl+20%CaCl ₂	72.74	27.26	10.42	89.58
20%KCl+20%K ₂ CO ₃	85.93	14.07	0.58	99.42
20%KCl+20%Na ₂ CO ₃	85.82	14.18	0.54	99.46
20%KCl+20%Na ₂ SO ₄	73.39	26.61	9.66	90.34
20%KCl+20%K ₂ C ₂ O ₄	73.33	26.67	9.69	90.31
20%KCl+20%KH ₂ PO ₄	72.87	27.13	10.12	89.88
20%KCl+20%NH ₄ H ₂ PO ₄	72.68	27.32	10.35	89.65
20%KCl+20%K ₂ HPO ₄	84.49	15.51	0.67	99.33
20%KCl+20%Mg(NO ₃) ₂	70.89	29.11	14.66	85.34
20%NaCl+20%NaCl	73.21	26.79	10.84	89.16
20%NaCl+20%CaCl ₂	72.32	27.68	11.25	88.75
20%NaCl+20%K ₂ CO ₃	88.24	11.76	0.53	99.47
20%NaCl+20%Na ₂ CO ₃	72.31	27.87	10.46	89.54
20%NaCl+20%Na ₂ SO ₄	73.17	26.83	9.82	90.18
20%NaCl+20%K ₂ C ₂ O ₄	71.75	28.25	13.88	86.12
20%NaCl+20%KH ₂ PO ₄	70.76	29.24	13.45	86.55
20%NaCl+20%NH ₄ H ₂ PO ₄	70.73	29.27	13.63	86.37
20%NaCl+20%K ₂ HPO ₄	82.96	17.04	0.73	99.27
20%NaCl+20%Mg(NO ₃) ₂	70.52	29.48	14.84	85.16
20%CaCl ₂ +20%CaCl ₂	72.72	27.28	10.29	89.71
20%CaCl ₂ +20%K ₂ CO ₃	72.83	27.17	10.21	89.79
20%CaCl ₂ +20%Na ₂ CO ₃	72.28	27.72	10.78	89.22
20%CaCl ₂ +20%Na ₂ SO ₄	72.95	27.05	9.87	90.13

20%CaCl ₂ +20%K ₂ C ₂ O ₄	71.92	28.08	13.65	86.35
20%CaCl ₂ +20%KH ₂ PO ₄	70.14	29.86	15.24	84.76
20%CaCl ₂ +20%NH ₄ H ₂ PO ₄	70.68	29.32	14.64	85.36
20%CaCl ₂ +20%K ₂ HPO ₄	84.39	15.61	0.64	99.36
20%CaCl ₂ +20%Mg(NO ₃) ₂	70.72	29.28	14.62	85.38
20%K ₂ CO ₃ +20%K ₂ CO ₃	99.12	0.88	0.28	99.72
20%K ₂ CO ₃ +20%Na ₂ CO ₃	94.87	5.13	0.32	99.68
20%K ₂ CO ₃ +20%Na ₂ SO ₄	92.52	7.48	0.33	99.67
20%K ₂ CO ₃ +20%K ₂ C ₂ O ₄	92.13	7.87	0.33	99.67
20% K ₂ CO ₃ +20% KH ₂ PO ₄	85.23	14.77	0.62	99.38
20% K ₂ CO ₃ +20% NH ₄ H ₂ PO ₄	86.29	13.71	0.54	99.46
20% K ₂ CO ₃ +20% K ₂ HPO ₄	95.02	4.98	0.33	99.67
20% K ₂ CO ₃ +20% Mg(NO ₃) ₂	76.43	23.57	8.36	91.64
20% Na ₂ CO ₃ +20% Na ₂ CO ₃	70.64	29.36	14.76	85.24
20% Na ₂ CO ₃ +20%Na ₂ SO ₄	70.53	29.47	14.92	85.08
20% Na ₂ CO ₃ +20% K ₂ C ₂ O ₄	72.09	27.91	11.56	88.44
20% Na ₂ CO ₃ +20% KH ₂ PO ₄	72.21	27.79	10.98	89.02
20% Na ₂ CO ₃ +20% NH ₄ H ₂ PO ₄	72.13	27.87	11.53	88.47
20% Na ₂ CO ₃ +20%K ₂ HPO ₄	91.42	8.58	0.35	99.65
20% Na ₂ CO ₃ +20% Mg(NO ₃) ₂	70.36	29.64	15.34	84.66
20% Na ₂ SO ₄ +20% Na ₂ SO ₄	70.44	29.56	15.32	84.68
20% Na ₂ SO ₄ +20% K ₂ C ₂ O ₄	73.31	26.69	9.72	90.28
20% Na ₂ SO ₄ +20% KH ₂ PO ₄	74.62	25.38	8.57	91.43
20% Na ₂ SO ₄ +20% NH ₄ H ₂ PO ₄	75.16	24.84	8.32	91.68
20% Na ₂ SO ₄ +20% KH ₂ PO ₄	91.28	8.72	0.36	99.64
20% Na ₂ SO ₄ +20% Mg(NO ₃) ₂	70.42	29.58	15.37	84.63
20% K ₂ C ₂ O ₄ +20% K ₂ C ₂ O ₄	70.60	29.4	16.16	83.84
20% K ₂ C ₂ O ₄ +20%KH ₂ PO ₄	71.48	28.52	14.89	85.11
20% K ₂ C ₂ O ₄ +20%NH ₄ H ₂ PO ₄	72.03	27.97	11.13	88.87

20% $\text{K}_2\text{C}_2\text{O}_4$ +20% K_2HPO_4	83.12	16.88	0.73	99.27
20% $\text{K}_2\text{C}_2\text{O}_4$ +20% $\text{Mg}(\text{NO}_3)_2$	70.20	29.80	15.38	84.62
20% KH_2PO_4 +20% KH_2PO_4	70.68	29.32	14.72	85.28
20% KH_2PO_4 +20% $\text{NH}_4\text{H}_2\text{PO}_4$	72.51	27.49	10.45	89.55
20% KH_2PO_4 +20% K_2HPO_4	80.93	19.07	1.02	98.98
20% KH_2PO_4 +20% $\text{Mg}(\text{NO}_3)_2$	70.42	29.58	14.34	85.66
20% $\text{NH}_4\text{H}_2\text{PO}_4$ +20% $\text{NH}_4\text{H}_2\text{PO}_4$	71.63	28.37	14.56	85.44
20% $\text{NH}_4\text{H}_2\text{PO}_4$ +20% K_2HPO_4	78.71	21.29	1.45	98.55
20% $\text{NH}_4\text{H}_2\text{PO}_4$ +20% $\text{Mg}(\text{NO}_3)_2$	71.18	28.82	14.68	85.32
20% K_2HPO_4 +20% K_2HPO_4	93.01	6.99	0.34	99.66
20% K_2HPO_4 +20% $\text{Mg}(\text{NO}_3)_2$	78.83	21.17	1.23	98.77
20% $\text{Mg}(\text{NO}_3)_2$ +20% $\text{Mg}(\text{NO}_3)_2$	70.76	29.24	14.56	85.44

^aStandard uncertainties u are $u(T)=0.01$ K, $u(p)=1$ kPa, $u(\text{wt}\%)=0.01$

Table S3. Experimental (liquid-liquid) equilibrium mass fractions of a salt-free basis for (allyl alcohol + water + salt) at the given ($\text{K}_2\text{CO}_3 + \text{K}_2\text{HPO}_4$) mass fraction of two salts, temperature $T = 298.15 \text{ K}$, and pressure $P = 101.3 \text{ kPa}$ (for Table 4)^a

salt	organic phase (wt%)		aqueous phase (wt%)	
	allyl alcohol	water	allyl alcohol	water
35% K_2CO_3 +5% K_2HPO_4	99.02	0.98	0.31	99.69
35% K_2CO_3 +10% K_2HPO_4	99.61	0.39	0.28	99.72
35% K_2CO_3 +15% K_2HPO_4	99.78	0.22	0.27	99.73
35% K_2CO_3 +20% K_2HPO_4	99.89	0.11	0.27	99.73
35% K_2CO_3 +25% K_2HPO_4	99.92	0.08	0.27	99.73

^aStandard uncertainties u are $u(T) = 0.01 \text{ K}$, $u(p) = 1 \text{ kPa}$, $u(\text{wt}\%) = 0.01$