Supporting Information

Study on Precipitation Processes and Phase Transformation Kinetics of Iron Phosphate Dihydrate

Huiqi Wang [1], Mingxia Guo [2], Yue Niu [1], Jiayu Dai [1], Qiuxiang Yin [1,3] and Ling Zhou [1,*]

1   State Key Laboratory of Chemical Engineering, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

2   Department of Chemical Engineering, South Kensington Campus, Imperial College London, London SW7 2AZ, UK

3   The Co-Innovation Center of Chemistry and Chemical Engineering of Tianjin, Tianjin University, Tianjin 300072, China

*   Correspondence: zhouling@tju.edu.cn

Table S1. The value of different parameter at pH range in equations.

	a+b+c	$10^3 \cdot (A+B)$	$10^2 \cdot (C+D)$	$10^3 \cdot E$	$10^3 \cdot F$	$10^2 \cdot G$	$10^4 \cdot H$
1.3	0.15	15.00	61.70	33.10	33.10	120.00	10700.00
1.25	0.13	12.00	49.00	26.30	26.30	85.00	5366.67
1.2	0.12	9.64	38.90	20.90	20.90	60.50	2690.00
1.05	0.09	4.98	19.50	10.50	10.50	21.40	340.00
0.95	0.07	3.23	12.30	6.61	6.61	10.70	85.00
0.85	0.05	2.10	7.76	4.17	4.17	5.35	21.37
0.8	0.05	1.70	6.17	3.31	3.31	3.80	10.70
0.75	0.04	1.38	4.90	2.63	2.63	2.69	5.37
0.7	0.04	1.12	3.89	2.09	2.09	1.91	2.69
0.65	0.03	0.91	3.09	1.66	1.66	1.35	1.35
0.6	0.03	0.74	2.45	1.32	1.32	0.96	0.68
0.55	0.03	0.61	1.95	1.05	1.05	0.68	0.34
0.5	0.02	0.50	1.55	0.83	0.83	0.48	0.17
0.4	0.02	0.34	0.98	0.52	0.53	0.24	0.04
0.35	0.02	0.28	0.78	0.42	0.42	0.17	0.02
0.3	0.02	0.23	0.62	0.33	0.33	0.12	0.01
0.25	0.01	0.19	0.49	0.26	0.26	0.09	0.01
0.2	0.01	0.16	0.39	0.21	0.21	0.06	0.003

Table S2. The concentration of different ions at pH range.

pH	$c(H^+)$ $\cdot 10^{-3}$ /mol$\cdot$L^{-1}	$c(H_2PO_4^-)$ $\cdot 10^{-3}$ /mol$\cdot$L^{-1}	$c(HPO_4^{2-})$ $\cdot 10^{-10}$ /mol$\cdot$L^{-1}	$c(PO_4^{3-})$ $\cdot 10^{-22}$ /mol$\cdot$L^{-1}	$c(Fe^{3+})$ $\cdot 10^3$ /mol$\cdot$L^{-1}	$c(H_3PO_4)$ $\cdot 10^3$ /mol$\cdot$L^{-1}
1.30	0.15	3.17	40.00	348.00	7.72	7.20
1.25	0.16	2.98	33.50	260.00	8.81	7.72
1.20	0.18	2.86	28.60	198.00	9.83	8.45
1.05	0.23	2.43	17.20	84.30	13.65	10.86
0.95	0.28	2.18	12.20	47.60	16.52	12.93
0.85	0.33	1.93	8.61	26.60	19.56	15.47
0.80	0.35	1.80	7.17	19.70	21.23	16.83
0.75	0.38	1.68	5.97	14.70	22.81	18.39
0.70	0.41	1.56	4.93	10.80	24.47	20.01
0.65	0.44	1.45	4.08	7.96	25.99	21.86
0.60	0.47	1.33	3.35	5.82	27.58	23.75
0.55	0.50	1.22	2.73	4.23	29.13	25.75
0.50	0.53	1.12	2.23	3.08	30.41	28.09
0.40	0.58	0.92	1.46	1.60	32.9	32.92
0.35	0.61	0.83	1.17	1.14	33.95	35.58
0.30	0.64	0.74	0.93	0.81	34.85	38.41
0.25	0.66	0.66	0.74	0.58	35.42	41.60
0.20	0.69	0.59	0.59	0.41	35.94	44.63

Table S3. The concentration of different ions at pH range.

| pH	$c(H_3PO_4)$ $\cdot 10^{-3}$ /mol·L^{-1}	$c(FeHPO_4^+)$ $\cdot 10^{-2}$ /mol·L^{-1}	$c(FeH_2PO_4^{2+})$ $\cdot 10^{-2}$ /mol·L^{-1}	$c(FeH_2(PO_4)_2^-)$ $\cdot 10^{-7}$ /mol·L^{-1}	$c(FeH_4(PO_4)_2^+)$ $\cdot 10^{-3}$ /mol·L^{-1}
1.30	7.20	78.49	5.07	29.00	2.47
1.25	7.72	76.36	5.53	24.00	2.57
1.20	8.45	74.04	6.02	20.20	2.73
1.05	10.86	66.20	7.60	11.70	3.14
0.95	12.93	60.20	8.70	7.96	3.40
0.85	15.47	53.82	9.79	5.38	3.63
0.80	16.83	50.46	10.30	4.36	3.71
0.75	18.39	47.05	10.78	3.52	3.78
0.70	20.01	43.63	11.22	2.82	3.81
0.65	21.86	40.22	11.60	2.26	3.84
0.60	23.75	36.84	11.92	1.79	3.82
0.55	25.75	33.51	12.17	1.40	3.77
0.50	28.09	30.31	12.35	1.10	3.72
0.40	32.92	24.25	12.43	0.65	3.48
0.35	35.58	21.49	12.36	0.49	3.34
0.30	38.41	18.91	12.21	0.37	3.17
0.25	41.60	16.53	11.98	0.28	3.00
0.20	44.63	14.30	11.62	0.21	2.78

Table S4. The concentration of different ions at pH range.

pH	$c(FeH_8(PO_4)_4^-)$ $\cdot 10^{-4}$ /mol·L^{-1}	$c(Fe_2HPO_4^{4+})$ $\cdot 10^{-3}$ /mol·L^{-1}	$c(Fe_2H_3(PO_4)_2^{3+})$ $\cdot 10^{-5}$ /mol·L^{-1}	$c(Fe_3H_6(PO_4)_4^{3+})$ $\cdot 10^{-8}$ /mol·L^{-1}
1.30	1.77	4.88	1.27	1.56
1.25	1.68	5.51	1.38	1.59
1.20	1.70	6.06	1.48	1.64
1.05	1.61	8.05	1.78	1.73
0.95	1.56	9.36	1.96	1.73
0.85	1.51	10.63	2.12	1.70
0.80	1.45	11.24	2.17	1.65
0.75	1.40	11.72	2.21	1.58
0.70	1.33	12.20	2.23	1.50
0.65	1.27	12.53	2.23	1.41
0.60	1.18	12.81	2.21	1.31
0.55	1.09	13.00	2.16	1.19
0.50	1.02	13.02	2.10	1.08
0.40	0.83	12.77	1.92	0.83
0.35	0.73	12.51	1.81	0.72
0.30	0.65	12.14	1.69	0.61

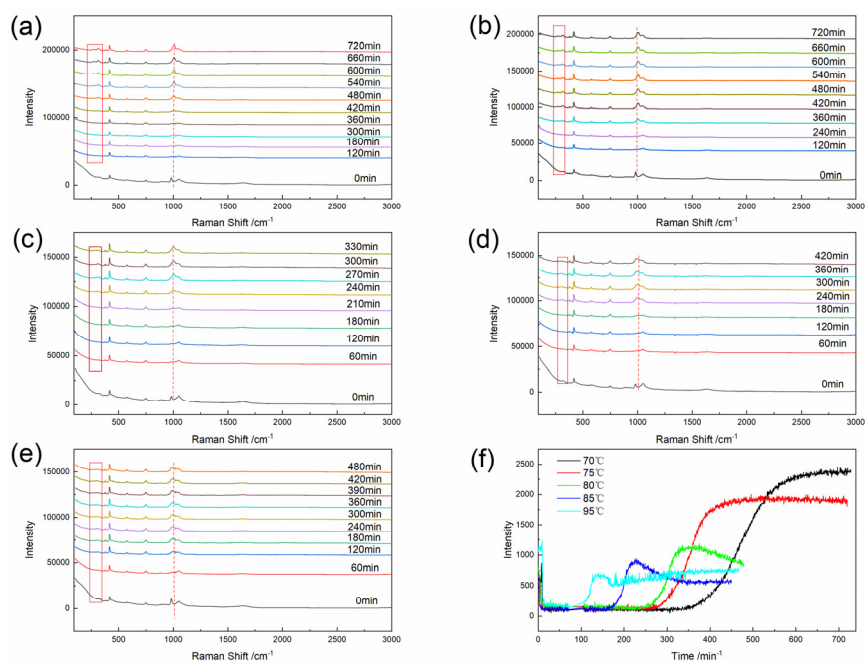| 0.25	0.57	11.62	1.56	0.51
0.20	0.48	11.01	1.42	0.41

Table S5. The content of S and O in precipitation at different time.

Sampling time/min	S (atom %)	O (atom %)
0	2.32	61.90
100	2.42	60.28
320	0.84	56.49
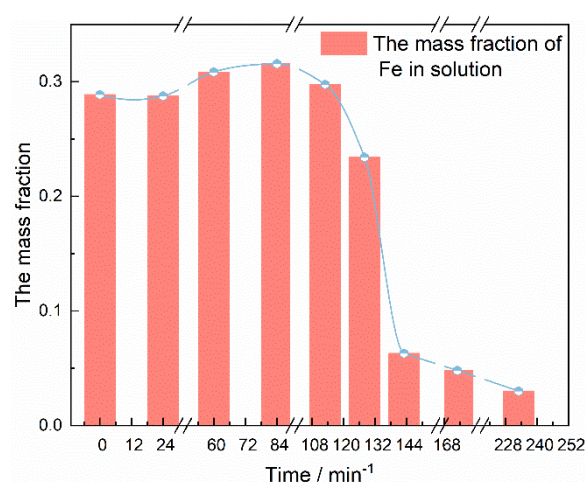
Figure S1. The mass fraction trend of Fe in solution at different time.

Figure S2. Raman spectra of the precipitates at 70 ℃ (a), 75 ℃ (b), 80 ℃ (c), 85 ℃ (d), 95 ℃ (e); (f) the change of characteristic peak at 303 cm^{-1} over time under different temperature.
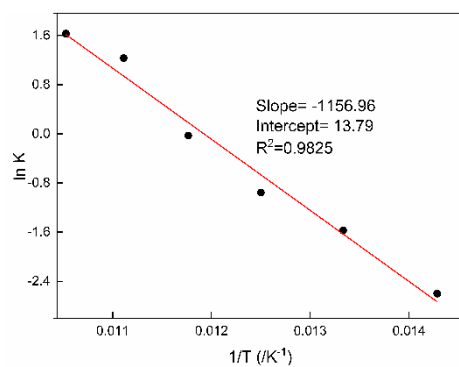
Figure S3. The linear relationship between ln K and (1/T).