

Supporting Information for:

Complexation of arsenate with ferric ion in aqueous solutions

Table S1 The pH values and composition of solution used in figure 1

Solutions in figure 1(a)			Solutions in figure 1(b)		
Concentration (mM)		pH	Concentration (mM)		pH
Fe(NO ₃) ₃	Na ₃ AsO ₄		Fe(NO ₃) ₃	Na ₂ SO ₄	
0.5	0	1.13	0.5	0	1.13
	0.5	1.03		0.5	1.05
	1	1.03		1	1.05
	2	1.06		2	1.05
	4	1.10		4	1.07
	6	1.12		6	1.07
	8	1.17		8	1.08
	10	1.20		10	1.09
	15	1.31		15	1.10
	20	1.43		20	1.12
	25	1.62		25	1.14
0	25	6.09	0	25	1.13

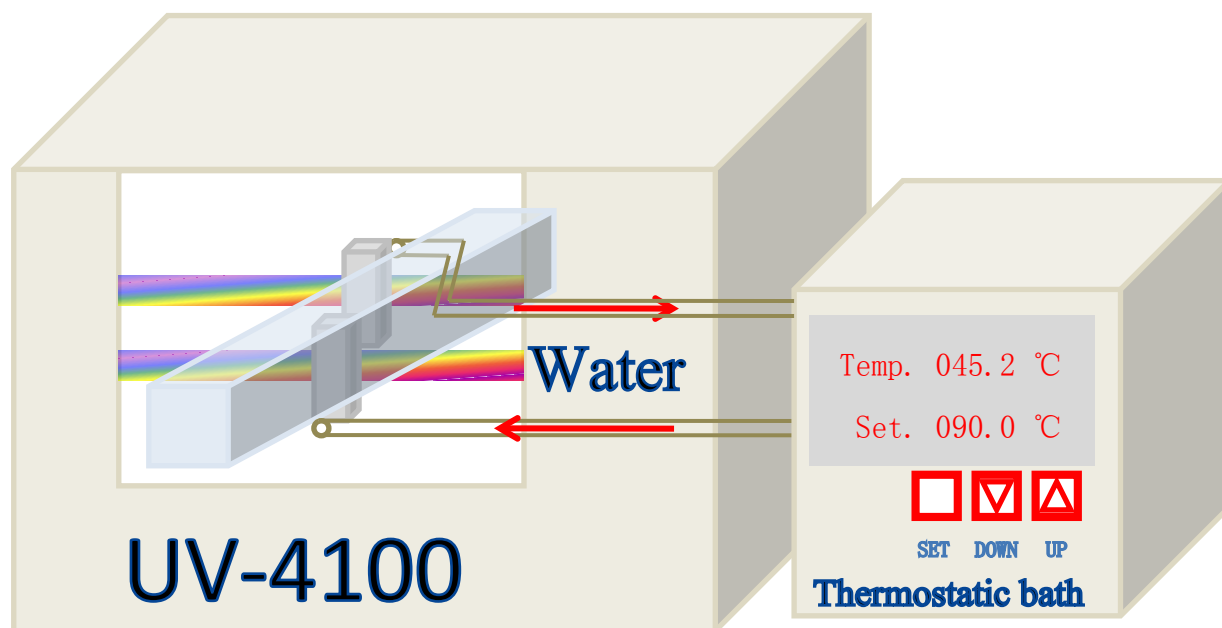


Figure S1 Experimental apparatus of continues heating process (Thermostatic bath THS-10 was purchased from Ningbo Tianheng instrument factory)

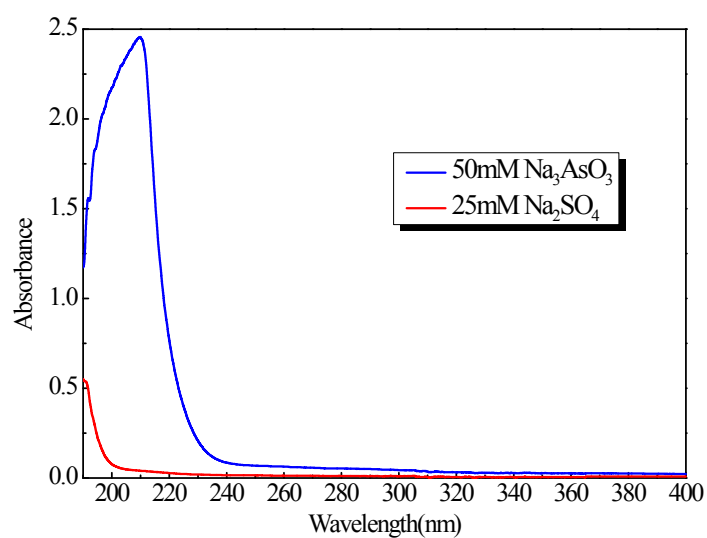


Figure S2 UV-Vis spectra of Na_2SO_4 , Na_3AsO_4 in 0.1 M HClO_4

Table S2 The enthalpy change of hydrolysis reaction of ferric

Reaction	Delta H (kJ/mol)
$\text{Fe}^{3+} + \text{H}_2\text{O} = \text{FeOH}^{2+} + \text{H}^+$	25.1
$\text{Fe}^{3+} + 2\text{H}_2\text{O} = \text{Fe}(\text{OH})_2^+ + 2\text{H}^+$	37.7
$\text{Fe}^{3+} + 3\text{H}_2\text{O} = \text{Fe}(\text{OH})_3 + 3\text{H}^+$	75.3
$\text{Fe}^{3+} + 4\text{H}_2\text{O} = \text{Fe}(\text{OH})_4^- + 4\text{H}^+$	154.8

Table S3 Thermodynamic data of relative species (kJ/mol)

Species	Standard molar enthalpy of formation	Standard molar Gibbs free energy of formation
H_2O	-285.83 ^a	-237.14 ^b
H_3AsO_4	-903.45 ^a	-768.06 ^b
HAsO_4^{2-}	-908.41 ^a	-714.43 ^b
H_2AsO_4^-	-911.42 ^a	-753.07 ^b
AsO_4^{3-}	-890.21 ^a	-642.62 ^b
Fe^{3+}	-49.0 ^c	-17.18 ^b
FeOH^{2+}	-309.73 ^d	-241.96 ^b
$\text{Fe}(\text{OH})_2^+$	-582.96 ^d	-452.198 ^b
$\text{Fe}(\text{OH})_3$	-831.19 ^d	-476.31 ^b
$\text{Fe}(\text{OH})_4^-$	-1037.52 ^d	-849.29 ^b
$\text{FeAsO}_4(\text{s})$	-899.0 ^e	-786.7 ^e
$\text{FeH}_2\text{AsO}_4^{2+}$	-985.95 ^f	-798.75 ^f
FeHAsO_4^+	-972.04 ^f	-787.38 ^f
FeAsO_4	-914.83 ^f	-744.17 ^f
SO_4^{2-}	-909.60 ^b	-744.36 ^b
FeSO_4^+	-931.90 ^b	-772.60 ^b

Source: values with superscript letters a to f are respectively from Ref. 23, HSC 7.0,

Ref. 22, Visual MINTEQ 3.0, Ref. 25 and Ref. 24.

Table S4 XRF of the gel-like material in solid phase

Analyte	Result	Proc-Calc	Line	Net Int.	BG Int.
As	37.2494 %	Quant.-FP	As Kb	439.024	3.048
Fe	30.7726 %	Quant.-FP	Fe Ka	1858.207	3.677
O	30.0135 %	Quant.-FP	O Ka	4.447	0.622
Cl	1.1336 %	Quant.-FP	Cl Ka	17.513	1.705
Na	0.3797 %	Quant.-FP	Na Ka	1.266	0.385
K	0.2660 %	Quant.-FP	K Ka	11.978	2.313
Si	0.1142 %	Quant.-FP	Si Ka	1.590	0.429
S	0.0401 %	Quant.-FP	S Ka	1.406	1.007
Ca	0.0171 %	Quant.-FP	Ca Ka	0.716	3.230
Cr	0.0139 %	Quant.-FP	Cr Ka	0.585	1.166