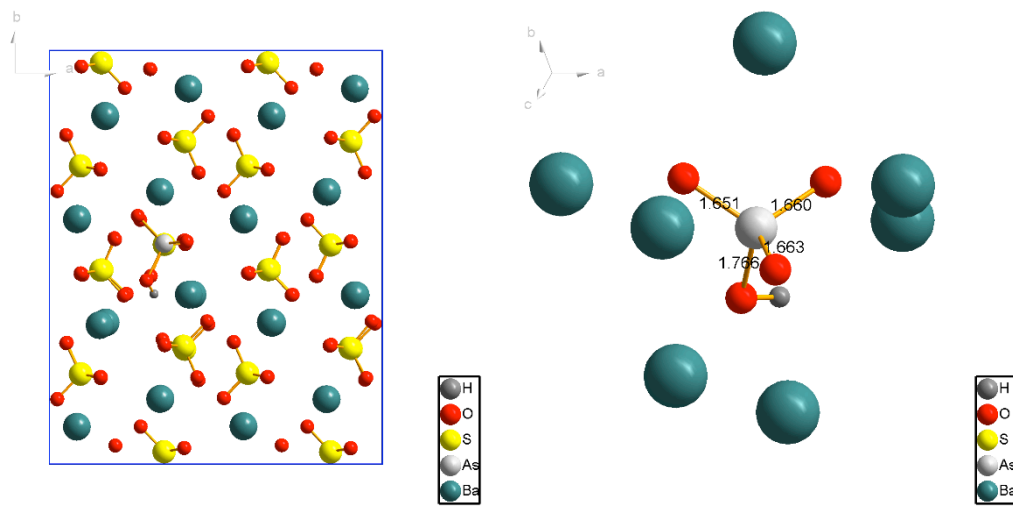# APPENDIX

FIGURE S1. DFT optimized unit cell of $HAsO_4^{2-}$ incorporated barite (left) and the corresponding local structure (right).

TABLE S1. Total mass of solids produced at pH 3-10 and the mass removed after 1M H_2SO_4 treatment. AT and UT mean acid treated and untreated samples, respectively.

Initial As(V) concentration	Sample	pH 3 mg	pH 4 mg	pH 5 mg	pH 6 mg	pH 7 mg	pH 8 mg	pH 9 mg	pH 10 mg
2000 mg /L	UT	1422	1439	1458	1462	1486	1477	1485	1497
	UT - AT	46	70	81	135	151	168	174	286
500 mg/L	UT	1424	1456	1436	1469	1453	1469	1455	1477
	UT - AT	19	61	79	121	140	146	151	159
50 mg/L	UT	1425	1413	1420	1443	1451	1425	1450	1468
	UT - AT	17	19	20	33	42	52	63	74

TABLE S2. Total concentrations of Na^+ and Cl^- in the end of the solution at pH 3-10 and at different initial As(V) 2000 $mg\cdot L^{-1}$, 500 $mg\cdot L^{-1}$ and 50 $mg\cdot L^{-1}$.

Initial As(V) concentration		pH 3 mol	pH 4 mol	pH 5 mol	pH 6 mol	pH 7 mol	pH 8 mol	pH 9 mol	pH 10 mol
2000 $mg\cdot L^{-1}$	Na^+	0.223	0.225	0.256	0.256	0.256	0.256	0.256	0.256
	Cl^-	0.200	0.201	0.201	0.201	0.201	0.201	0.201	0.201
500 $mg\cdot L^{-1}$	Na^+	0.205	0.206	0.207	0.207	0.207	0.207	0.207	0.207
	Cl^-	0.201	0.200	0.200	0.201	0.201	0.201	0.201	0.201
50 $mg\cdot L^{-1}$	Na^+	0.199	0.201	0.201	0.201	0.201	0.201	0.201	0.201
	Cl^-	0.200	0.200	0.200	0.200	0.201	0.201	0.201	0.201

TABLE S3. Unit cell parameters from Rietveld refinement of X-ray data and the goodness of refinements Bragg R-factor and χ^2 of the AT As(V)-barite samples coprecipitated at pH 4, 7, and 10 and an initial As(V) concentration of 2000 mg L^{-1}.

pH	a (Å)	b (Å)	c(Å)	β (°)	Unit cell volume($Å^3$)	Bragg R-factor	χ^2
4	8.881	7.159	5.456	90	346.89	19.4	244
7	8.883	7.161	5.457	90	347.17	17.3	215
10	8.885	7.163	5.459	90	347.43	16.7	188
Barite	8.882	7.157	5.455	90	346.57	15.2	97

TABLE S4. The shell-fit results for the As K-edge EXAFS of the reference materials and the As(V)-doped barite. CN refers to the coordination number. R_{path} is the interatomic distance. σ^2 is the Debye-Waller parameter. ΔE is the energy-shift parameter and χ^2_{red} is the reduced chi-square. R-factor is the mean-square misfit between the measured and the modeled data. The fitted k was set to $3 - 13.5$ Å^{-1}. Accordingly, the number of independent points (N_{idp}) and variables (N_{var}) were 19.75 and 7, respectively. S_0^2 was set 0.95.

Sample	Path	CN	R_{path} (Å)	σ^2 (Å^2)	ΔE (eV)	χ^2_{red}	R-factor
BaHAsO$_4$·H$_2$O	As-O	3	1.68±0.007	0.0016±0.0003	7.5±1.0	93	0.012
	As-OH	1	1.76±0.007	0.0016±0.0003			
	As-Ba1	1	3.65±0.029	0.0113±0.0028			
	As-Ba2	1	3.94±0.029				
	As-Ba3	1	3.98±0.029				
	As-Ba4	1	4.02±0.029				
	As-Ba5	1	4.16±0.029				
Ba$_3$(AsO$_4$)$_2$	As-O	4	1.70±0.006	0.0014±0.001	2.7±2.1	141	0.020
	As-Ba1	3	3.58±0.060	0.0067±0.003			
	As-Ba2	3	3.73±0.060				
AT-pH 3	As-O	4	1.70±0.006	0.0044±0.001	6.8±2.1	25	0.028
	As-Ba1	1	3.03±0.023	0.0317±0.034			
	As-Ba2	1	3.14±0.023				
	As-Ba3	2	3.54±0.023				
AT-pH 7	As-O	4	1.68±0.011	0.0049±0.001	2.7±3.2	117	0.030
	As-Ba1	1	3.00±0.057	0.0229±0.014			
	As-Ba2	1	3.11±0.057				
	As-Ba3	2	3.48±0.057				
AT-pH 10	As-O	4	1.70±0.001	0.0047±0.001	2.7±2.1	114	0.028
	As-Ba1	1	3.01±0.042	0.0178±0.008			
	As-Ba2	1	3.13±0.042				
	As-Ba3	2	3.50±0.042				

TABLE S5. The calculated mean interatomic distance of S-O and As-O of DFT optimized As(V)-doped supercell and barite

Formula	Description	Bond length (Å)	
		S-O	As-O
Ba$_{32}$(SO$_4$)$_{31}$HAsO$_4$	2×2×2 barite supercell with one HAsO$_4^{2-}$ substituting for one SO$_4^{2-}$	1.48±0.011 (1.46-1.49)	1.68±0.05 (As-OH: 1.77)
Ba$_4$(SO$_4$)$_4$	DFT optimized barite unit cell	1.48±0.011 (1.46-1.49)	No data
Ba$_4$(SO$_4$)$_4$	Barite unit cell determined by XRD[a]	1.48±0.017 (1.46-1.49)	No data

[a] The crystallographic data was reported by Jacobsen et al. 1998.