

## **A qualitative and quantitative investigation of partitioning and local structure of arsenate in barite lattice during coprecipitation of barium, sulfate, and arsenate**

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### **ABSTRACT**

Arsenic (As), barium (Ba), and sulfate ( $\text{SO}_4^{2-}$ ), coexisting in natural and mining impacted environments, possibly lead to As-barite coprecipitation. This work investigated the coprecipitation of  $\text{Ba}^{2+}$ ,  $\text{SO}_4^{2-}$ , and  $\text{AsO}_4^{3-}$  [As(V)] and the incorporation of As(V) into the barite structure. The As(V) content in the coprecipitates increased with pH and the initial aqueous As(V) concentration. At  $\text{pH} \leq 5$ , As(V) was dominantly fixed through isomorphic substitution for  $\text{SO}_4^{2-}$  in the barite structure ( $<0.32$  wt%). At  $\text{pH} > 5$ , barium (hydrogen) arsenate constituted an appreciable fraction of As(V)-bearing species in addition to the incorporated As(V). FTIR spectroscopy indicated that As(V) in the coprecipitate occurred as mixed phases and the As(V) species incorporated into the barite structure was dominated by  $\text{HAsO}_4^{2-}$  species. EXAFS analysis gave As-O and As-OH bond lengths of 1.67 and 1.75 Å for  $\text{HAsO}_4^{2-}$  in barite structure, respectively. The FPMS structural refinement reproduced well the As *K*-edge XANES spectrum and gave bond lengths of As-O at 1.63, 1.64, 1.68, and 1.75 Å with an average bond length of  $1.68 \pm 0.05$  Å in  $\text{HAsO}_4^{2-}$  doped barite structure. The findings are of significance for understanding the geochemical cycle of As in As(V),  $\text{Ba}^{2+}$ , and  $\text{SO}_4^{2-}$  coexisting systems.

**Keywords:** Arsenate, barite, coprecipitation, incorporation, local structure, XANES/EXAFS, FTIR, DFT calculation