Chromate Uptake by Calcite: Batch experiments and X-ray absorption spectroscopy analysis

Yuanzhi Tang[1)]* · Evert J. Elzinga[2)] · Young Jae Lee[3)] · Richard J. Reeder[1)]

Abstract

Combined with batch experiments, *in-situ* spectroscopic methods are used to examine chromate uptake by calcite. Partitioning behavior, site-specific distribution of Cr on the surface of calcite single crystal, and local coordination of Cr in the calcite structure are also investigated. It is found that the concentration of Cr incorporated in calcite increases with increasing Cr concentration in solution. The calculated apparent partition coefficient (K_d) is the highest at low Cr solution concentration, and decreases to a constant value with increasing Cr solution concentration. Micro-XRF mapping of the Cr distribution on calcite shows preferential incorporation of Cr into the — steps, which is considered to result from differences in surface structure geometry. XANES spectra confirm that incorporated Cr is hexavalent, and no reduction of Cr(VI) in the X-ray beam was observed. EXAFS best-fit results show the incorporated Cr(VI) has the expected first shell of 4 O at 1.64 ± 0.01 Å, consistent with CrO_4^-. Best-fit results show that the second shell is split with ~2.5 Ca at 3.33 ± 0.05 and ~2.2 Ca at 3.55 ± 0.05 Å, which confirms the incorporation of chromate into calcite. Consideration of possible local coordination indicates that significant distortion or disruption is required to accommodate in the calcite structure.

1) Department of Geosciences and Center for Environmental Molecular Sciences, State University of New York, Stony Brook, NY 11794-2100, USA

2) Institute of Biogeochemistry and Pollutant Dynamics, Department of Environmental Sciences, ETH Zurich, Switzerland

3) Department of Earth and Environmental Sciences, Seoul, Korea 136-701