Investigation of Chromate Coordination on Ferrihydrite by in situ ATR-FTIR Spectroscopy and Theoretical Frequency Calculations: Supporting Information

Chad P. Johnston and Maria Chrysochoou

Department of Civil and Environmental Engineering

University of Connecticut, Storrs CT 06269

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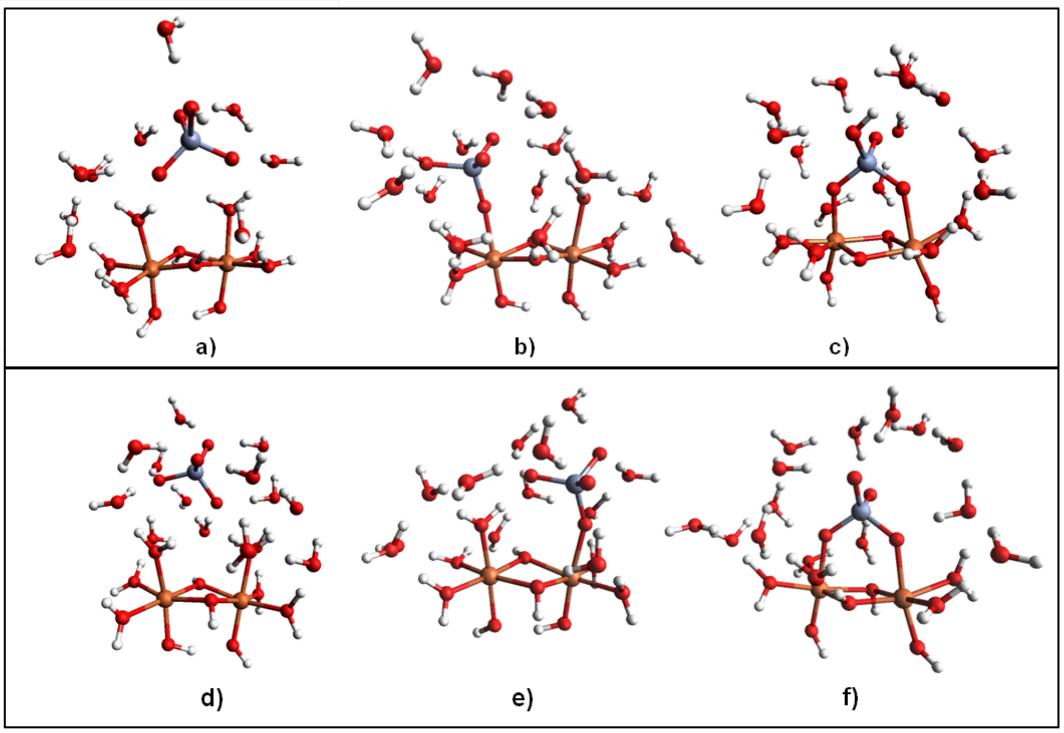

Figure S1. Protonated (top) and nonprotonated (bottom) cluster models used to calculate IR frequencies of chromate coordinated to iron oxide: outer-sphere (a, d), monodentate (b, e), and bidentate (c, f). Some explicit water molecules removed for clarity. Calculations were performed at the BY3LYP/LANL2DZ level of theory and typically converged in 1 to 7 days of computational time.

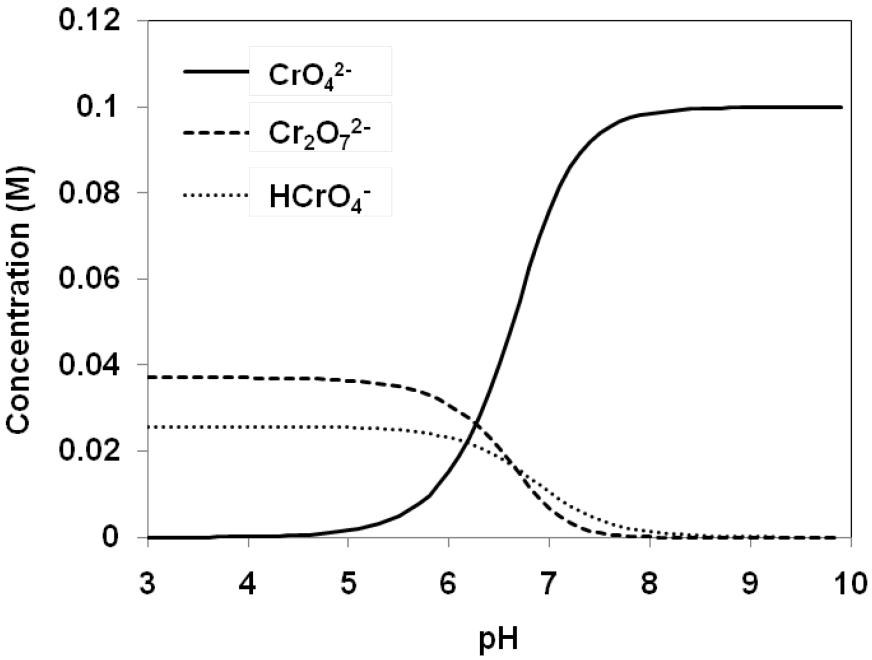

Figure S2. Distribution of chromate species in 100 mM solution as a function of pH.