72 - Glyphosate sorption mechanism at the boehmite/water interface using solid state ^{31}P NMR and P XANES

Wei Li[1], *weili@udel.edu, Xionghan Feng*[1,4], *Paul Northrup*[2], *James D. Kubicki*[3], *Donald L. Sparks*[1]. *(1) Delaware Environmental Institute, University of Delaware, Newark, DE 19713, United States, (2) Department of Environmental Science, Brookhaven National Lab, Upton, NY 11973, United States, (3) Department of Geosciences, Pennsylvania State University, University Park, Pennsylvania 16802, United States, (4) Department of Environmental Science and Engineering, Huazhong Agricuture University, Wuhan, Hubei 430070, China*

The herbicide glyphosate can strongly adsorb on soils, affecting its efficacy as an herbicide and mobility as a contaminant. In this research, we examined the sorption mechanism of glyphosate to boehmite, a variable-charge soil mineral, using ^{31}P solid state NMR, P K-edge XANES, and density function theory (DFT). The ^{31}P NMR spectra contain three resolved peaks, at chemical shifts near 0, 6, and 15 ppm, with relative intensities that vary modestly with pH and reaction time. All three peaks correspond to a P environment with close spatial proximity with Al, as indicated by their nearly identical ^{31}P{^{27}Al} REAPDOR dephasing curves. Comparison of the REAPDOR curves with theoretical simulations, based on the possible structural models (calculated by DFT), suggests that the phosphonate group of glyphosate binds to boehmite via bridging bidentate configurations. These results are consistent with the XANES spectra for glyphosate sorbed on boehmite and pure glyphosate solution.

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