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**Publication history****Published article online:**

22 Jun 2007

**Issue online:**

18 Jul 2007

Received 24 February 2007;  
revised version accepted 14  
May 2007

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Science**

Volume 58 Issue 4 Page 932-944, August 2007

**To cite this article:** J. D. KUBICKI, K. D. KWON, K. W. PAUL, D. L. SPARKS (2007)

Surface complex structures modelled with quantum chemical calculations: carbonate, phosphate, sulphate, arsenate and arsenite

European Journal of Soil Science 58 (4), 932-944.

doi:10.1111/j.1365-2389.2007.00931.x

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 J. Kubicki. E-mail: [kubicki@geosc.psu.edu](mailto:kubicki@geosc.psu.edu)**Summary**

Hybrid molecular orbital/density functional theory (MO/DFT) calculations on molecular clusters were used to model infrared (IR) vibrational frequencies and interatomic distances obtained via extended X-ray absorption fine structure (EXAFS) spectroscopy. Molecular clusters were found to provide good agreement with experimental observations for the oxyanions carbonate, phosphate, sulphate, arsenate and arsenite. The results show a consistent tendency to form bidentate bridging surface complexes at low pH, but the protonation and hydration states play a significant role in the results obtained from calculation as various protonation states of monodentate surface complexes are also predicted to be stable as pH increases (i.e. the number of H<sup>+</sup> ions in the model are decreased). A method for estimating the Gibbs free energy of adsorption ( $\Delta G_{ads}$ ) is discussed to complement the comparisons of experimental and theoretical spectroscopic parameters. Calculated  $\Delta G_{ads}$  values were consistent with the interpretations based on

modelling observed spectra.

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