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Computational Chemistry Applied to Solutions: Anions

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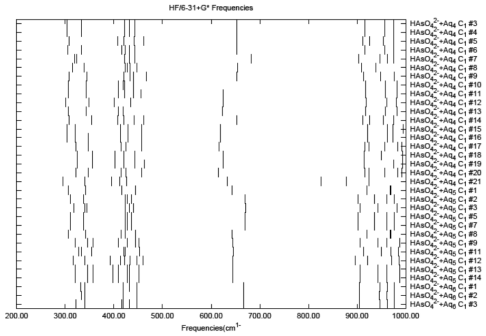

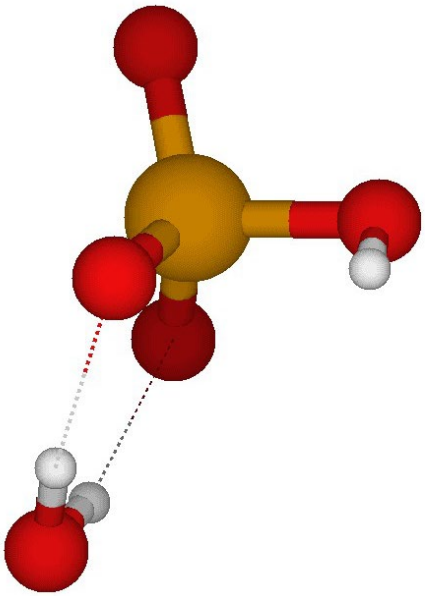

Ab initio computational chemistry has been employed in the past by the author to interpret the vibrational spectra of cations such as Li^{+}[1], Cd^{2+}[2], Mg^{2+}[3], Zn^{2+}[4], Sc^{3+}[5], Al^{3+}[6], Ga^{3+}[7], In^{3+}[8], Bi^{3+}[9], and Be^{2+}[10], Hg^{2+} and Tl^{3+}[11], Cu^{+}[12], and Pb^{2+}[13]; anions such as SO_4^{2-}[14], PO_4^{3-}[15], HPO_4^{2-}[16], $H_2PO_4^{-}$[17], ClO_4^{-}, BrO_4^{-}, SeO_4^{2-}, AsO_4^{3-}, VO_4^{3-}[18], the borates[19], and HSO_4^{-}[20]; and ion pairs/complexes such as LiX (X = F – I)[21], $ScCl_m^{(3-m)+}$ (m = 1 – 6)[22], $ZnCl_m^{(2-m)+}$ (m = 1 – 6)[23], $ZnBr_m^{(2-m)+}$ (m = 1 – 6)[24], and $CuCl_m^{(m-1)-}$ (m = 0 – 6)[25], in aqueous solution.

In this presentation, the author will discuss the microhydration of selected anions and illustrate the relationships between the vibrational spectra of polyatomic anions in the gas-phase and aqueous-phase.

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