Goldschmidt 2024 Abstract
https://doi.org/10.46247/gold2024.21356

Computational Chemistry Applied to Solutions: Anions. II.

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Computational chemistry has been employed by the author to interpret or predict the aqueous vibrational spectra of cations (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], Be^{2+}[10], Hg^{2+}, Tl^{3+}[11], Cu^+[12], Pb^{2+}[13], Sn^{2+}[14], and Sb^{3+}[15]), anions (SO_4^{2-}[16], PO_4^{3-}[17], HPO_4^{2-}[18], $H_2PO_4^-$[19], ClO_4^-, BrO_4^-, SeO_4^{2-}, AsO_4^{3-}, VO_4^{3-}[20], the borates[21], HSO_4^-[22]; $HSeO_4^-$[23]; $HAsO_4^{2-}$[24]; HVO_4^{2-}[25]); and complexes (LiX (X = F – I)[26], $ScCl_m^{(3-m)+}$[27], $ZnCl_m^{(2-m)+}$[28], $ZnBr_m^{(2-m)+}$[29], $CuCl_m^{(m-1)-}$[30]).
I will discuss microhydration of selected anions and illustrate the relationships between the spectra of anions in the gaseous, aqueous, and solid phases.

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