

Molecular ions in steam: experimental and theoretical characterization of solvated metal species and ore fluid implications

KONO H. LEMKE¹

¹Department of Earth Sciences, University of Hong Kong,
Pokfulam Road, Hong Kong, SAR (kono@hku.hk)

Recent advances in experimental techniques, such as FT mass spectrometry, electronic and vibrational spectroscopies, have provided an increasing level of detail regarding the solvation environment around molecular ions, thus providing an important tool for our understanding of ionization and solvation processes in ore fluids. Such experimental studies are also routinely complemented with results from theoretical calculations, e.g. DFT, MP2 and AIMD type simulations. The coupling of FT mass spectrometry and wave-tunable IRMPD spectroscopy has created a new and powerful tool to capture molecular ions and characterize their solvation structure. In particular, use of table-top IRMPD and free-electron lasers now enables one to probe the structure of mass-selected ions in equilibrium with volatiles such as H₂O, NH₃ and H₂S.

Of practical interest to studies of ore vapors are FT-MS and IRMPD studies of molecular clusters, in particular, metal clusters with water solvation shells that reconfigure as the ion core hydrates incrementally and forms a wet nano-scale solid. Previous IRMPD spectroscopy experiments have been successful in probing the water solvation shell around a wide range of clusters, and together with *ab initio* tools have the potential to expand our understanding of metal speciation in ore vapors. The occurrence of metal clusters in a water cluster network also highlights the possibility of metal transport in water nanodroplets. Metal complexes such as AuCl and CuCl would occupy droplet surface or near-surface sites together with ionic species such as H₃O⁺ and larger halides, whereas interior solvation is favored by smaller halides, the hydroxide ion and select metal ions and charged metal complexes. Finally, the propensity of ions to partition to surface or interior regions of a water cluster/droplet has important implications for the ionization and pH of these cluster surfaces and estimates of vapor-phase K_w. Results from ongoing experimental studies and molecular simulations of solvated metal cluster systems will be presented together with an outlook of some experimental challenges that remain to be addressed.