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Theoretical Studies on Synergistic Interactions between Transition Metals and Heavy Metalloids

John Tossell (tossell@chem.umd.edu)

Dept. of Chemistry and Biochemistry, Univ. of Maryland, College Park, MD 20742, USA

Recently we established that the ternary complex CuAsS(SH)(OH) makes a large contribution to the total concentrations of both Cu and As in sulfidic solutions which are in equilibrium with Cu and As sulphide minerals (Tossell, 2000). This complex is unusually stable and has a direct Cu(I)-As(III) bond. We have now established that the complexes of $AsS(SH)(OH)^-$ with Au^+, Hg^{+2} and Pb^{+2} are also very strong. We present calculated structures and gas-phase formation energies for these complexes, obtained at the 2nd order Moller Plesset polarized double zeta ab initio level, along with estimated aqueous formation constants. The Au^+ and Au(SH) complexes of $AsS(SH)(OH)^-$ may be implicated in "invisible gold" in arsenian pyrites. Such synergistic interactions between transitional metals and heavy metalloids may be, through the mechanism of such ternary species, responsible for the numerous transition metal-metalloid element associations observed in sulfidic systems.

Tossell, JA, *Environ. Sci. Tech*, **34**, 1483-1488, (2000).