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Complexation of At⁺ and AtO⁺ with inorganic ligands; a combined experimental and theoretical approach to characterize the formed species

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Astatine (At, Z=85: [Xe]4f145d106s26p5) is below iodine and belongs to the halogen group. One of its isotopes, 211At, is a promising candidate as a therapeutic agent in nuclear medicine [1].
It has been reported that astatine presents a metal-like behavior when existing under the oxidation states +I and +III as At+ and AtO+ species [2]. However, the number of studies dealing with the complexation properties of these cationic forms is limited. Low availability of astatine makes experimental work difficult (usually investigations derived from radiochemical studies at ultra-trace concentrations, typically between 10-12 and 10-15 mol.L-1).
In this work, we propose a combined experimental and theoretical approach to characterize the interaction between these metallic forms and simple inorganic anions (Cl-, Br-, SCN-). A competition method based on solid/liquid separation or liquid/liquid extraction is proposed to determine the equilibrium constants [3]. To assess the reliability of the experimental results, they are compared to theoretical computations. The spin-orbit density functional theory (SO-DFT) approach, which uses two-components relativistic effective core potentials (RECPs), has been used to investigate the spectroscopic properties of At, At2 and HAt species. In conjunction with our own built up basis sets (double and triple zeta augmented with diffuse and polarization functions), SO-B3LYP and SO-M06 functionals offer results in good agreement with that in the literature. In order to compare measured and computed equilibrium constants of the astatine reactions, aqueous solvation effects have been introduced using polarizable continuum models (PCM with UAHF and UAKS cavities). Obtained results show a good agreement between theoretical and experimental values. They also indicate that astatine species have a soft character according to the HSAB theory.

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[3] J. Champion, C. Alliot, S. Huclier, D. Deniaud, Z. Asfari and G. Montavon, Inorg. Chim. Acta, 362 (8), 2654 (2009).

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