Study of the positron affinities of $X^-(H2O)n$ (X=F, Cl, Br) systems

José Mauricio Rodas R.[1,2], **Jorge Charry M.**[1], **Jonathan Romero F.**[3], **Andrés Reyes V.**[1]

[1]*Quantum and Computational Chemistry Group, Universidad Nacional, Bogotá, Colombia*
[2]*Chemistry Department, Universidad de Caldas, Manizales, Colombia*
[3]*Department of Chemistry and Chemical Biology, Harvard University, Cambridge MA, U.S.A.*
email: *areyesv@unal.edu.co*, *mauricio.rodas@ucaldas.edu.co*

Theoretical and experimental research on the positron affinity (PAs) of halides (X-) in gas phase have found that the PAs follows the order[1]:

$$F^->Cl^->Br^-$$

Interestingly, experimental evidence indicates that this trend is reversed in aqueous solution; a behavior that has remained so far unexplained[2]. The positron affinity energy of micro-solvated halides systems ([X-;e+](H2O)n; X=F, Cl, Br, n=0-7) was calculated with the any particle molecular orbital (APMO) approach[3]. The positron affinity of micro-solvated halides were determined using the any particle propagator theory (APMO/PT) and Koopmans approximation to Hartree-Fock level of theory, implemented in the LOWDIN program[4].

The results show that the positron affinity trend effectively is reversed when the systems has five or more water molecules, this behavior could be explained from the positron densities in the systems, these densities show that the oxygen atoms of the water molecules compete with the halide for the positron which weakens the positron-halide binding.

1 P. E. Cade, A. Farazdel, *J. Chem. Phys.* **66**, 2598 (1977)
2 J.R. Andersen, N.J. Pedersen, O.E. Mogensen, P. Christensen, *Chem. Phys. Let.* **63** (1) 171 (1979)
3 S.A. González, N.F. Aguirre, A. Reyes, *Int. J. Q. Chem*. **108** (10) 1742 (2008)
4 J. Romero, J.A. Charry, R. Flores-Moreno, M.T. do N. Varella, A. Reyes, *J. Chem. Phys*. **141**, 114103 (2014)