

Study of the positron affinities of $X^-(H_2O)_n$ ($X=F, Cl, Br$) systems

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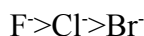
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Theoretical and experimental research on the positron affinity (PAs) of halides (X^-) in gas phase have found that the PAs follows the order¹:



Interestingly, experimental evidence indicates that this trend is reversed in aqueous solution; a behavior that has remained so far unexplained². The positron affinity energy of micro-solvated halides systems ($[X^-; e^+](H_2O)_n$; $X=F, Cl, Br, n=0-7$) was calculated with the any particle molecular orbital (APMO) approach³. 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 program⁴.

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.

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