

Positron Binding Energies for Alkali Hydrides

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Abstract

Ab initio multireference single- and double-excitation configuration interaction (MRD-CI) calculations are carried out to study the interactions of positrons with the members of the alkali hydride class of molecules. A new computer program has been constructed for this purpose that makes use of the Table-Direct-CI method for construction of the required Hamiltonian matrices and electronic/positronic wave functions. The calculations indicate that the binding energy (positron affinity PA) of a single positron to these systems increases by an increment of 0.2-0.3 eV as the atomic number of the alkali atom is increased. It is found that the positron prefers a location in the more electronegative regions of such molecules, similarly as has been found in earlier calculations for the urea and acetone molecules. The positron orbital possesses a diffuse charge distribution with relatively small expectation values of the kinetic energy in all four systems considered. Each of the four positronic molecules is stable with respect to formation of either positronium (Ps) or HPs according to the present calculations. The potential curves of the latter systems are compared with their neutral counterparts and it is found that relatively large changes in the equilibrium bond distance of the hydrides occur as a result of the positron interaction. The importance of bond dipole moments in producing the binding of positrons to molecules is discussed, as well as the role that the electronegativity of the constituent atoms plays in determining the magnitude of the PA for a given system.

April 29, 2005