**Abstract**

Density functional theory calculations have been carried out to analyze the effect of hydrogen halides and H2O molecule interactions with the three lowest energy isomers the ring, bowl and cage of C20 fullerene. The single-point energy calculations have also been performed at MP2/6-31+G\*//B3LYP/6-31G\* level of theory. The complexes (C20⋯H–X and H2O, where X = F, Cl, and Br) are bounded by two interactions namely: (i) very weak X–H⋯π H-bond interactions and (ii) long range van der Waals interactions of H–X⋯C type. These interactions produced negligible distortion in the structures and a good correlation between electron density and stabilization energy of the complexes is found. The counterpoise correction to the interaction energies and the study of topology of the electron density for all the complexes have been performed. The charge transfer and the maneuver of resonance interaction in the interacting orbitals have been investigated by natural bond orbital (NBO) approach.