Theoretical Chemistry Accounts

Volume 138, Issue 43, 2019, Pages 1-14

Quantitative and qualitative analyses of intermolecular interactions in neutral/deprotonated aspirin@?-CD inclusion complexes: QTAIM and NBO analyses

Belgacem BEZZINA, Rayenne Djemil, Nadjia Bensouilah

Abstract: Most of the researches in supramolecular chemistry area are focused on the conventional hydrogen bonds without taking into account unconventional intermolecular interactions. The nature and strength of the conventional and unconventional interactions in inclusion complexes formed between neutral aspirin (ASA) and its deprotonated form (ASA?) with ?-cyclodextrin (?-CD) have been studied. It was conducted through combining atoms in molecules (AIM) theoretical criteria suggested by Koch and Popelier and natural bond orbital (NBO) analyses by means of dispersion-corrected density functional theory (DFT-D3) with the functional B3LYP using cc-pvdz basis set in the gas phase. We have found fve intermolecular closedshell interaction groups responsible for neutral ASA:?-CD and deprotonated ASA?:?-CD inclusion complexes stability: One is conventional O–H···O bond group. The four C–H···O, C–H···C, O–H···H–C and C–H···H–C groups are nonconventional. Also, with respect to the Koch and Popelier criteria, some of them present the properties of a hydrogen bond, while others do not. The non-covalent interaction energies are calculated using Espinosa approach. Finally, according to the AIM and NBO analyses, the topological parameters (electron density ?band its Laplacian ?2?b), estimated interaction energies (Eint), and the stabilization energy E(2)of both complexes were correlated with the intermolecular bond lengths

Keywords : ?-Cyclodextrin, Aspirin, Inclusion complex, DFT-D3, QTAIM, NBO