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Document Title	:	*Theoretical Investigation Of The Electronic Structure Of Some Anti AIDS Deriven Nucleosides* *دراسة نظرية للتركيب الإلكتروني لبعض النيكليوسيدات المضادة لمرض الإيدز*
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Abstract	:	The present work presents a theoretical investigation of the electronic structure and a conformational preference of a series of nucleoside-analogs, namely, 2`,3`-dideoxyinosine (DDI), 2`,3`-dideoxycytidine (DDC), 2`,3`-didehydro-3`-deoxythymidine (D4T), 3`-azido-3`-deoxythymidine (AZT) and 3`-azido-3`-dideoxyuridine (AZDDU). These molecules are potentially effective therapeutic agents for the treatment of the acquired immune deficiency syndrome (AIDS). The geometry of all the studied composite molecules and their subsystems were fully optimized at the HF-level of theory using the split valence 6-31G* basis set. All the studied nucleoside-analogs are much better electron-donors than any of their subsystems and all these molecules are highly polar having dipole moments of ? 7 D units. The direction of these dipole moments are all pointing away from the glucoside subsystems. Gas-phase proton detachment energies (PDE), for the studied series of drugs, were computed at 298 K? and 1 atmospheric pressure. In general, deprotonation causes general changes in the type and extent of interaction between the two subsystems. The mechanism of action of the studied series of drugs is believed to start by phosphorylation to the corresponding triphosphate. The efficiency of this step, which might very well determine the activity of the drug, has been investigated and discussed. The introduction of PO4 group into the glucoside moiety causes major variations, which are common to all studied drugs.
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