

A COMBINED QUANTUM CHEMICAL, CHEMOMETRIC AND STRUCTURAL STUDY ON AROMATIC BONDS IN NUCLEOSIDES

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Rapid growth of life sciences including modifications of nucleic acids at atomic level¹, and also the exponential increase of number of nucleobase containing crystal structures necessarily is followed by various studies on both standard², non-standard and modified nucleobases. This work studies aromatic C-C, C-N and C-O bonds of seven standard², and more than forty non-standard and modified nucleobases. The best crystal structures (crystallographic $R < 6.0\%$, e.s.d.'s 0.005 \AA , published after 1974, no disorder) were retrieved from Cambridge Structural Database³ as source of high-quality experimental bond lengths d . Bond descriptors were calculated: Pauling π -bond order p_P , weighted π -bond order p_w (HOSE approach⁴), π -bond orders with maximal and overall packing effects p_{cr} and p_{cm} , number of non-hydrogen atoms around the bond n , and the sum of atomic numbers Q . Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) were performed to study relationships among the bonds and variables. Partial Least Squares (PLS) were used to model and predict the bond lengths based upon the variables. Pauling potential curves, semi-empirical PM3 and *ab initio* HF 6-31G** were employed also for bond length calculation. PCA shows that the bond lengths of nucleobases are three-dimensional phenomena. There is a clear clustering of the bonds both in PCA and HCA due to the bond type and other structural characteristics. PLS ($r > 0.9$) and *ab initio* shows to predict/calculate d 's better than PM3 and Pauling potential curve. Detailed results will be discussed.

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