A MOLECULAR AND QUANTUM MECHANICAL STUDY OF INDOLE-3-ACETIC ACID

Rudolf Kiralj (PQ) and Márcia M. C. Ferreira (PQ), Instituto de Química, Universidade Estadual de Campinas, Campinas, SP, 13083-970, Brazil. rudolf@iqm.unicamp.br

Indole-3-acetic acid is the most important auxin, a plant hormone with simple molecular structure. All the attempts to quantify its structure-biological activity relationship were not much successful up to date, mostly due to missing knowledge about some intrinsic molecular properties responsible for intermolecular interactions. Low temperature crystal structure of indole-3-acetic acid[1] is a good reference point for systematic theoretical studies. In this work, the experimental geometry was optimized using molecular mechanics (MMF, Sybil), semi-empirical methods (MINDO/3, MNDO, AM1, PM3) and *ab initio* (about fifteen DFT and RHF basis sets). Bond length matrix *m*x*n* (*m* = number of bonds, *n* = number of calculations) and its transpose (*n*x*m*) were analyzed utilizing Principal Component Analysis (PCA) and Hierachical Cluster Analysis (HCA). A carboxylic acid cyclic H-bond dimer from crystal structure was optimized using various methods. In general, *ab initio* bond lengths are closer to experimental ones than those from semi-empirical and molecular mechanics. All the methods do not reproduce well C-OH bond which is the most one affected by dimer's H-bonds. Detailed PCA on both matrices shows that bond lengths are described at most by six Principal Components. The data clustering is similar in PCA and in HCA. Characteristic molecular fragments are recognized among the scores, while similar basis sets of *ab initio* and also methods of the same level of accuracy (*e.g*. molecular mechanics, semi-empirical, *ab initio*) are distinguished in loadings. Bond lengths of optimized cyclic H-bond dimer are closer to experimental values than those of isolated indole-3-acetic acid, especially considering the carboxylic chain (by more than 0.01 Å). The optimized dimer structures show that the carboxyl group geometry is closely related to H-bond geometry.

1 B. Nigovi• , S. Antoli• , B. Koji• -Prodi• , R. Kiralj, V. Magnus, B. Salopek-Sondi, *Acta Cryst.* **B56** (2000) 94 - 111.

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