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Some crystallographic aspects of indole derivatives

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Abstract: In this paper, main aim is to carry out crystallographic comparison of some geometrical and structural features for a series of indole derivatives. Some bond distances, bond angles and torsion angles are discussed in detail, along with their medicinal importances. This study is based on some basic indole derivatives having maximum of two substituents. In compound I & II, the substituent is simply a carboxylic acid whereas in the last two (i.e., III & IV) the substituents are carboxylic acids along with halogens.

Keywords: Indole, bond distances, bond angles, torsion angles.

1. Introduction

Indole is an aromatic heterocyclic organic compound with formula C_8H_7N. It has a bicyclic structure, consisting of a six-membered benzene ring fused to a five-membered nitrogen-containing pyrrole ring. Indole is widely distributed in the natural environment and can be produced by a variety of bacteria. As an intercellular signal molecule, indole regulates various aspects of bacterial physiology[1], including spore formation, plasmid stability, resistance to drugs, biofilm formation[2], and virulence [3]. The amino acid tryptophan is an indole derivative and the precursor of the neurotransmitter serotonin [4].

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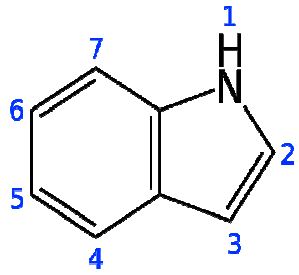

Figure 1. Basic structure of Indole

Indole and its derivatives are especially important aromatic chemicals both in man-made and natural systems, and the aromatic indole ring often acts as an active center in many bioactive chemicals [5][6]. Indole-3-carboxylic acid and its derivatives are important chemical materials, because they are excellent auxins for plants [7] and drug intermediates for many pharmaceutical products [8].

3. Results and Discussion

The structure of all the four derivatives of indole studied, are given in Figure 2. In first two compounds, the side chain is of carboxylic acid whereas in the last two there is one halogen atom attached to the benzene ring in addition to the carboxylic acid. The double bond C=O distance for all the four derivatives are 1.24(1)Å, 1.2272(1)Å, 1.19(3)Å, and 1.2394(2)Å for compound I, II, III, and IV, respectively. The C-O single bond distances in carboxylic acid group in compound I, II, III, IV are 1.3216(1)Å, 1.3258(1)Å, 1.2916(2)Å, 1.34(3)Å, respectively. The O-H distance of carboxylic acid for compound I, II, III, IV respectively are 0.8200Å, 0.951(1)Å, 0.8200Å, 0.8200Å. The N-H distances for compound I, II, III, IV are

0.8600Å, 0.968(1)Å, 0.86(2)Å and 0.91(2)Å, respectively.

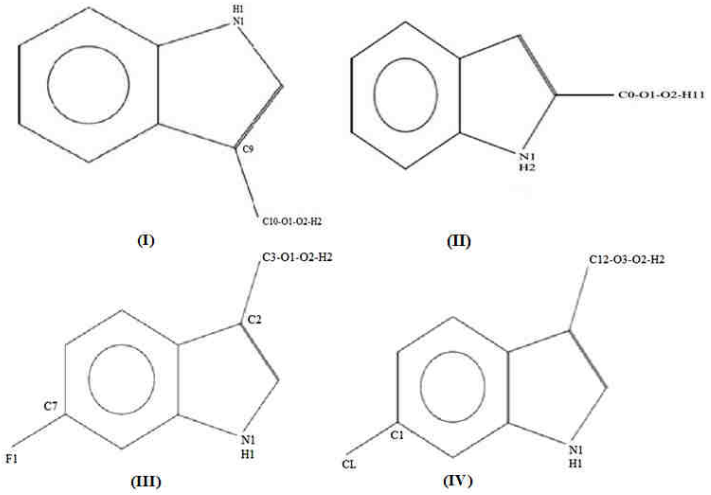

Figure 2. Structure of the four derivatives of Indoles selected for crystallographic studies.

The C-F and C-Cl distances in compound III and IV are 1.351(2)Å and 1.77(4)Å. The value of bond angle O=C-O in compound I, II, III, IV are 122.44(1)°, 121.56(9)°, 122.44(1)°, 122(2)° respectively (Table 1 & 2). The C-O-H bond angle in order in all the four are 109.5°, 116.0(6)°, 109.5° and 109.5°, respectively. All the values of bond distances and bond angles agree with the standard values [9].

Table 1. Reference code and name of the studied indoles derivatives.

Molecule	Reference Code	Chemical Name	Chemical Formula	Molecular Weight (*amu*)
I	ENIVIG	1H-indole-3-carboxylic acid	$C_9H_7NO_2$	161.16
II	ISORUD	Indole-2-carboxylic acid	$C_9H_7N_1O_2$	322.31
III	ZARCAY	6-Fluoro-1H-indole-3-carboxylic acid	$C_9H_6FNO_2$	179.15
IV	ZIFDID	6-Chloro-1H-indole-3-carboxylic acid	$C_9H_6ClNO_2$	195.60

Table 2. The crystal data and structure refinement for compounds I-IV

Compound	I	II	III	IV
Formula	$C_9H_7NO_2$	$C_9H_7N_1O_2$	$C_9H_6FNO_2$	$C_9H_6ClNO_2$
Formula Weight	161.16	322.31	179.15	195.60
Crystal System	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space Group	P 2 1/n	$Pna2_1$	P21/c	P21/c
a (Å)	4.41890(5)	30.144(6)	7.0054(14)	7.2608(15)
b (Å)	10.48312(13)	6.4660(10)	11.699(2)	11.973(2)
c (Å)	16.03096(17)	3.8190(10)	9.2947(19)	9.6567(19)
α (°)	90.00	90.00	90.00	90.00
β (°)	95.3299(10)	90.00	104.15(3)	98.88(3)
γ (°)	90.00	90.00	90.00	90.00
V $Å^3$	739.405(15)	744.4(3)	738.7(3)	829.4(3)
Z	4	4	4	4
T(K)	293(2)	293(2)	293(2)	293(2)
μ (mm^{-1})	0.863	0.103	0.132	0.419
Cryst dimensions	0.4x0.3x0.2	0.3x0.2x0.2	0.5x0.3x0.1	0.3x0.3x0.2
No. of observed reflns	1343	996	1418	461
No. of unique reflns	1448	1392	1693	494
R-factor	0.0341	0.0414	0.0427	0.1691
S	1.027	0.899	1.076	1.187

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