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Crystallographic Analysis of some Structures of Indole Derivatives

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Abstract—*This paper is about the crystallographic comparison of some geometrical and structural features for a series of indole derivatives (Figure 1). The main crystallographic properties which are compared are bond distances, bond angles and torsion angles etc. are discussed in detail, along with their other important properties. This study is based on some basic indole derivatives having two substituents (methyl group and acetic acid). In the entire four compounds, the substituents are same but there crystallographic aspects are entirely different.*

1. INTRODUCTION

Indoles continue to be of great interest to the pharmaceutical industry and at the current time several thousand specific new derivatives are reported annually. Research has been driven by the wide range of indole derivatives which occur in nature and through the biological activity of many indole derivatives, of both natural and synthetic origin. Indole and its derivatives have occupied a unique place in the chemistry of nitrogen heterocyclic compounds [1]. The indole derivatives were known for their dying properties. Many compounds of indole derivatives having the structural resemblance to the ancient dye indigo are known in the literature. A large number of naturally occurring compounds, like alkaloids, were found to possess indole nucleus. The recognition of the plant growth hormone, heteroauxin [2] , the important amino acids, tryptamine [3] and tryptophan [4], antiinflammatory drug, indomethacine [5] and anticancer drug, isatin derivative [6][7]are the important derivatives of indole which have added stimulus to this research work. Reference code and name of the studied indoles derivatives are given in Table 1.

2. RESULTS AND DISCUSSION

2.1. Biological activity predictions using PASS software

Biological activity of indoles is one of the most important reasons for their synthesis and structural characterization. It is the result of chemical compound's interaction with biological activity that a total matrix of activities caused by the compound is generated which is generally referred to as the *biological activity spectrum of the substance*. It is a concept that is crucial to PASS (Prediction of Activity Spectra for Substances) software which provides the rationale for predicting many activity types for different compounds [8-9]. The structural formula of a molecule is presented as a *mol* file and the predictions result in the form of a table containing the list of biological activities on a scale of probability ranging from 0-1. Two values are computed for each activity: P_a - the probability of the compound being active and P_i - the probability of the compound being inactive for a particular activity. Activities with $P_a > P_i$ are retained as the most probable and predicted ones for a given compound. The P_a and P_i values for the molecules (I-IV) are presented in Table 2.

2.2. Comparative Geometrical Parameters

The structure of all the four derivatives of indole studied, are given in Figure 2. In the entire compound studied, the side chain of indole consists of a methyl group and an acetic acid group. The double bond C=O distance for all the four derivatives are 1.217(3) Å, 1.2252(2) Å, 1.223(5) Å, 1.211(3) Å for compound I, II, III, IV respectively. The C-O single bond distances in carboxylic acid group in compound I, II, III, IV are 1.3(3) Å, 1.323(2) Å, 1.306(5) Å, and 1.308(3) Å respectively. The O-H distance of carboxylic acid for compound I, II, III, IV respectively are 1.01(3) Å, 0.87(2) Å, 1.10(5) Å, 0.851(2) Å which shows that the O-H bond distance in I & III and II & IV are nearly same. The N-H distances for compound I, II, III, IV are 0.90 Å, 0.88(2) Å, 0.75(3) Å and 0.877(1) Å respectively. The bond distance value of C-C corresponding to the carbon atom of the ring and methyl group of the side chain is nearly equal to the standard C-C single bond distance [8]. The value of bond angle O=C-O in compound I, II, III, IV are 122.1(2) 122.56(1) 122.0(4), 123.1(2) respectively. The C-O-H bond angle in order in all

the four are 110.0(2), 111.6(1) 116(2) and 106.8(9) respectively. The hydrogen attached to the nitrogen in all the four derivatives makes an angle near to 120°. The crystallographic data are summarized in Table 3.

On comparing the activities as given in the Table 2, it is quite interesting to note that most of indole derivatives possess high a*ntihypertensive* and *calcium regulator* activities. There appears to a quite large probability for all the molecules to exhibit *antiinfertility, female and urological disorder treatment* activity. The $P_a > P_i$ indicates that the molecule [M-III] possess high value of *antiviral* activity.

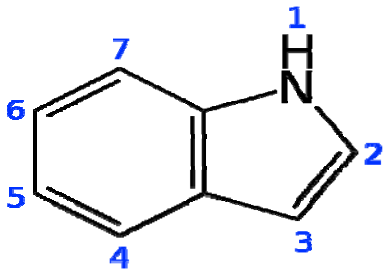
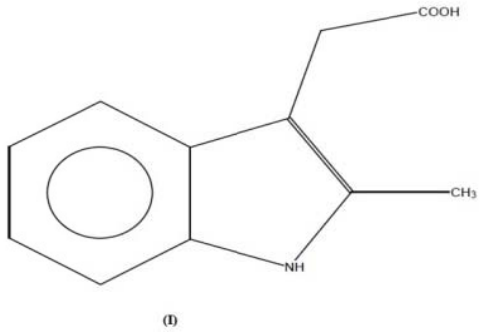
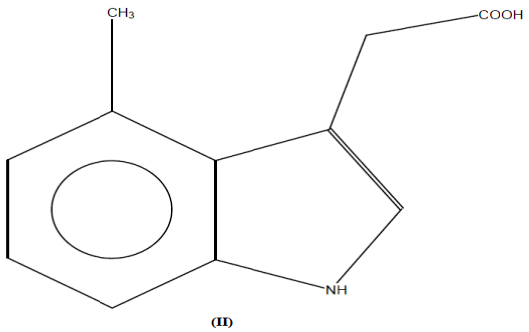
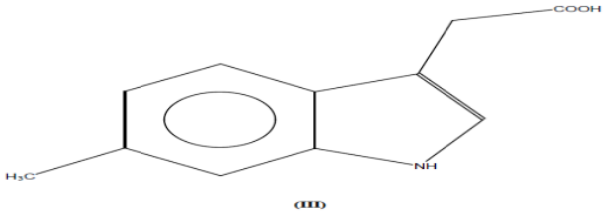


Figure 1: Basic structure of Indole







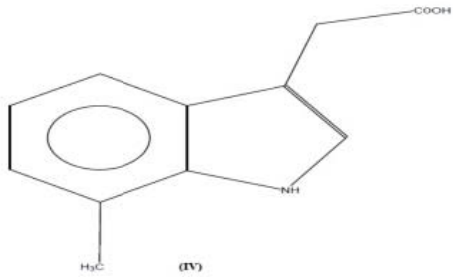


Figure 2: Structure of the four derivatives of Indoles selected for crystallographic studies.

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

Molecule	Reference Code	Chemical Name	Chemical Formula	Molecular Weight (amu)
I	CUVQAL	2-methyl-idole-3-acetic acid	C11H11NO2	189.21
II	CUVQEP	4-methyl-indole-3-acetic acid	C11H11NO2	189.21
III	CUVQIT	6-Methyl-indole-3-acetic acid	C11H11NO2	189.21
IV	CUVQOZ	7-Methyl-indole-3-acetic acid	C11H11NO2	189.21

Table 2. Predicted activities (Pa and Pi) for the molecules (M-I-M-IV)

Molecule	Antiviral	Antihypertensive	Urologic disorder treatment	Calcium regulator	Antiinfertility, female
M-I	0.323>0.076	0.626>0.009	0.448>0.008	0.484>0.017	0.475>0.008
M-II	0.218>0.182	0.646>0.008	0.748>0.004	0.546>0.008	0.383>0.022
M-III	0.405>0.085	0.767>0.005	0.542>0.005	0.552>0.007	0.372>0.024
M-IV	0.308>0.082	0.682>0.006	0.705>0.004	0.495>0.014	0.396>0.019

Table 3: The crystal data and structure refinement for compounds I-IV

Compound	I	II	III	IV
Formula	C11H11NO2	C11H11NO2	C11H11NO2	C11H11NO2
Formula Weight	189.21	189.21	189.21	189.21
Crystal System	Monoclinic	Monoclinic	Orthorhombic	Monoclinic
Space Group	P 2 1/n	P21/n	P b c a	P21/c
a (Å)	8.5420(10)	8.6800(10)	6.2160(10)	19.3530(10)
b (Å)	13.4080(10)	7.6240(10)	38.6270(10)	5.0740(10)
c (Å)	8.6380(10)	15.0440(10)	8.0310(10)	10.2750(10)
α (°)	90	90	90	90
β (°)	99.700(10)	101.870(6)	90	109.000(6)
γ (°)	90	90	90	90
V Å3	975.18(8)	974.27(8)	1928.29(18)	954.00(9)
Z	4	4	8	4
T(K)	297	103	297	297
μ (mm-1)	0.09	0.09	0.09	0.09
Cryst dimensions	0.4x0.3x0.2	0.3x0.2x0.2	0.5x0.3x0.1	0.3x0.3x0.2
No. of observed reflns	1052	1434	970	1038
No. of unique reflns	1467	1619	1398	1461
R-factor	0.039	0.035	0.049	0.041
S	1.027	0.41	0.99	0.47

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