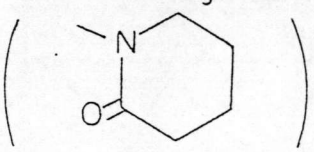
CHAPTER IV

DISCUSSION

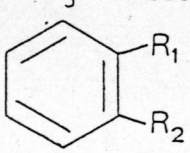
1 Discussion of the isolated alkaloids

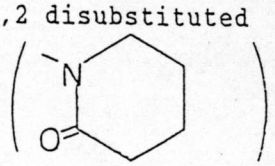
PC_3

The alkaloid (PC_3) was obtained as colorless prism. It is soluble in chloroform but slightly soluble in methanol, UV spectrum of PC_3 gave a series of indole chromophores similar to the alkaloid strychnine.

Infrared spectrum of PC_3 indicated the presence of a lactam carbonyl  at 1660 cm^{-1}. The aromatic C-H stretching can be observed at 1600 cm^{-1}, while the signal representing ether (C-O) vibrations can be seen at 1480, 1400 and 1100 cm^{-1}.

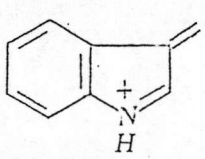
A system of 1,2 disubstituted benzene ring is represented by a moderate vibrational peak at 760 cm^{-1}. From infrared spectrum we can summarize as follows :-

PC_3 molecule consists of a 1,2 disubstituted benzene ring 

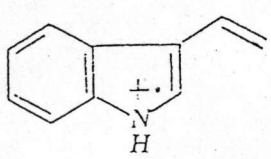
, a lactam carbonyl  and an ether (C-O) function.

Further important information of the molecular structure come from its mass spectrum. The molecular ion is at 344 which is corresponding to the formula $C_{21}H_{22}N_2O_2$ while the unsubstituted indole fragment ions are observed at δ 130, 143, 144 amu.

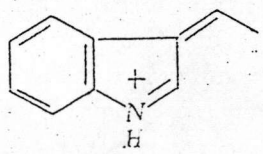
The indole fragments are shown below.



m/z 130



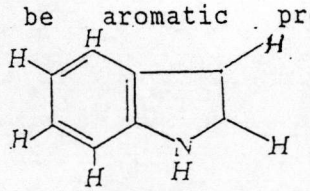
m/z 143



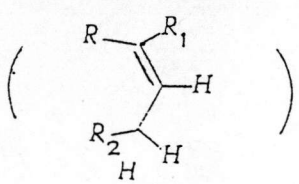
m/z 144

Proton nuclear magnetic resonance spectrum of PC_3 shows the presences of rather complex signals, due to the low resolution instrument (90 MHz). However, the prominent signals obtained are very valuable in the elucidation of the structure of PC_3.

There are 4 protons located in the aromatic region which promptly assume to be aromatic protons of the unsubstituted indole nucleus.



An ill-defined triplets observed at δ 5.89 ppm. is clearly representing an ethylidene function



in the molecule of PC_3.

From the above informations, the alkaloid PC_3 is very similar to the alkaloid strychnine in every respects and so identified as strychnine.

Further comfirmation is conducted by comparison between PC_3 and strychnine on their chromogenic and Rf properties on many TLC solvent systems.

Thus the PC_3 is identified as strychnine.

PC_{4-1}

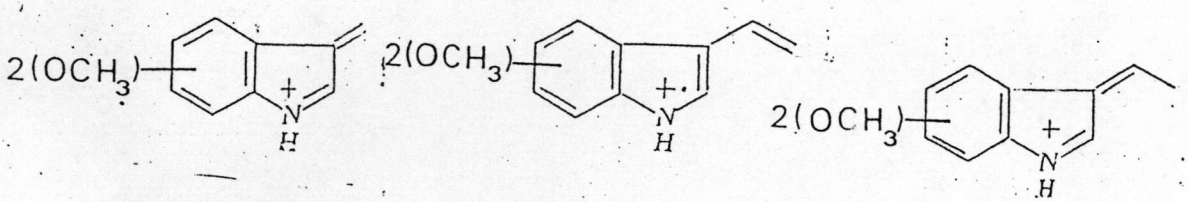
PC_{4-1} is a base obtained as colorless prism. The UV spectrums of PC_{4-1} shows the presence of a disubstituted indole chromophore.

Infrared spectrum of PC_{4-1} gave a lactam carbonyl vibration at 1650 cm^{-1}, while ether (C-O) function are seen at 1500, 1400 and 1110 cm^{-1}.

The 1,2,4,6 tetra-substituted benzene nucleus are observed at 850 and 750 cm^{-1}.

The molecular weight of PC_{4-1} is 394 which presumably obtained from molecular ion peak in mass spectrum. Further more, mass spectrum of PC_{4-1} shows the presence of dimethoxy substituted indole part by producing a series of fragment ions

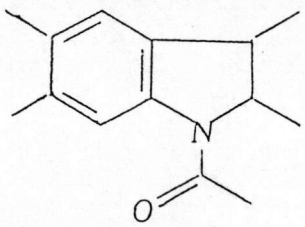
such as *m/z* 190, *m/z* 203 and *m/z* 204 amu which may be written as follows.



m/z 190 *m/z* 203 *m/z* 204

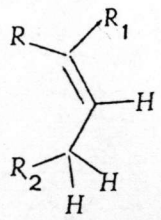
Proton nuclear magnetic resonance of PC_{4-1} indicated the presence of 2 aromatic protons both of which appear as singlets. This indicated that the 2 non-coupled protons must be placed in the para positions to each other.

Thus at this stage a part of PC_{4-1} molecule must consist of a 2,3 disubstituted indole nucleus plus a lactam carbonyl (X) from the IR information as follow.



(X) partial structure of PC_{4-1}

Further informations from proton nuclear magnetic resonance come from an ill-defined triplets, resonating at 5.89 ppm coupled with a multiplets center at δ 4.10 ppm. both of which indicated that there is an ethylidene function in PC_{4-1} molecule.



ethylidene function

From the above informations, the alkaloid PC_{4-1} is very similar to the alkaloid brucine in every respects and so identified as brucine.

The TLC properties of PC_{4-1} and the authentic brucine are similar.

From the above reasons, PC_{4-1} can be identified as brucine.

2. General Discussions

Strychnine and brucine are alkaloids in the Strychnan group which are commonly found in the Section Strychnos eg. *Strychnos ignatii* Berg., not only brucine but also strychnine are found in leaf, pericarp, root bark, root wood, stem, stem bark, and twig, only strychnine is found in fruit. In *S. lucida* R.Br., both brucine and strychnine are found in branch, leaf, root bark and stem bark, only brucine is found in fruit, stem and twig. In *S. nux-vomica* Linn., brucine and strychnine are found in bark, fruit, leaf, pericarp, root bark, root wood, stem, stem bark and stem wood. *S. rupicola* Pierre ex Dop., such as stem contained brucine and strychnine ; *S. wallichiana* Steud ex DC contained brucine and strychnine in branch, leaf, root bark,

root wood, stem, stem bark, small branch, stem wood while *S. nux-blanda* A.W. Hill contained strychnine and brucine in leaf and stem, but for the stem bark, these two alkaloids have never been investigated. The biosynthesis of brucine and strychnine originated from secologanin and tryptophan. Recently secologanin was found in the unripe fruit of *S. nux-blanda* A.W. Hill (Dr.Verpoorte personal communication). Therefore, indole alkaloid may be expected to be found in this plant. But strychnine and brucine content in the stem bark of this plant was low may be due to the secologanin content of the bark is low and strictosidine synthase enzyme is not in the proper condition for the catalytic reaction to obtain the indole alkaloid as the condition found in *S. nux-vomica* Linn. We can differetiate *S. nux-blanda* A.W. Hill and *S. nux-vomica* Linn. by using thin-layer chromatography solvent system 2 (page 92). Alcoholic extract at concentration 50 mg/ml of S. nux-blanda A.W. Hill the brucine and strychnine spots after spraying with Dragendorff is not found but in *S. nux-vomica* Linn. at the same concentration brucine and strychnine spots are appeared.(figure 23 page 133)