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# Physical Sciences Section

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## HOME COMPUTER IN MOLECULAR ORBITAL CALCULATION

### *Part II. The Iterative Methods: W-Technique and SCF Methods*

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(Received November 5, 1988; revised December 9, 1989)

Computer programs in BASIC language for iterative molecular orbital methods:  $\omega$ -technique and self consistent field (SCF) methods have been developed for home computer. These programs can be used for pedagogical as well as research purposes.  $\omega$ -Technique program can be used for both open and closed shell system while the SCF program can only be used for ground state singlet system. The programs are simple and tractable and can be used by nonprofessionals. Sample calculations are carried out on allyl and pyridine system.

**Key words:** Home computer, M.O. program,  $\omega$ -technique, SCF calculations, BASIC programs.

## DIPOLE MOMENTS OF PENTACOORDINATED SILICON DERIVATIVES

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(Received March 11, 1989; revised February 27, 1990)

Dipole moments of  $[(CH_3)_2N]C_{10}H_6SiX_3$  where  $X=CH_3, OCH_3, Cl^-$  in different solvents and at different temperatures indicate that the intramolecular  $N \longrightarrow Si$  coordinate bond is correlated with the strength of the  $Si-X$  bond.

**Key words:** Dipole moment, Silicon derivatives.

## SOME REACTIONS OF 3-CHLOROKETONES

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(Received January 14, 1989; revised October 8, 1989)

3-Chloro-3-(*p*-substitued phenyl) propiophenones (I) were allowed to react with diethyl malonate and ethyl acetoacetate in the presence of slight excess of sodium ethoxide to give the corresponding ethyl 2-carbethoxy-3-aryl-4-benzoylbutyrate (III), and ethyl 3-hydroxy-3-phenyl-5-aryl-cyclohexane-1-one-6-carboxylate IV, respectively. The same products were isolated, when *p*-substitued benzalacetophenones were used instead of the 3-chloroketones. This indicated that, the former reactions proceed by an elimination-addition mechanism. The structure of the products were established.

**Key words:** Carbanions, Chloroketones, Elimination-addition

**ORGANIC REACTIONS IN THE AQUEOUS MEDIUM (1,2)**  
***Part-III. Reactions of Hexamethylenetetramine with Active Methylene Compounds***

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(Received August 5, 1989; revised February 15, 1990)

Reactions of hexamethylene tetramine with active methylene compounds like ethyl acetoacetate, acetylacetone, dimedone and dibenzoylmethane have been thoroughly investigated. These investigations have led to the successful development of simple, convenient and economical methods for the synthesis of pure diethyl 1,4-dihydro-2, 6-dimethyl-3, 5-pyridinedicarboxylate (I) and 3,5-diacetyl-1,4-dihydro-2,6-dimethylpyridine (II) in 74.5 and 53.1% yields respectively, under mild aqueous conditions. The yields of these dihydropyridines have been related to the extent of keto forms of ethyl acetoacetate and acetylacetone in the aqueous medium, where intramolecular hydrogen-bonding cannot operate. Conditions have also been developed for the synthesis of dihydropyridine derivative of dimedone, along with its methylene-*bis*-compound and its formation rationalised through its enol-chelate stabilization. The failure of dibenzoylmethane to go beyond its methylene-*bis*-compound has been interpreted in terms of its preferred *anti*-configuration. The structure of the compounds synthesised have been elucidated using i.r. n.m.r. and mass spectra.

**Key words:** Active methylene compounds, Dihydropyridine derivatives, Methylene-*bis*- ( $\beta$ -diketones).

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## SYNTHESIS OF HETERO-BICYCLIC-COMPOUNDS

### *Part-VII. Formation of 2,2-Diphenyl-4, 5-Dioxopyridino-(4,3-d)-(1,3)-Dioxins*

M. ASLAM BUTT\*, RASHID KEMAL, A. SALAM AND AUSAF AKHTAR

*PCSIR Laboratories, Complex, Karachi-39, Pakistan*

(Received December 7, 1989)

Aminopyranodioxins derived from benzophenone isomerise to yield 6 substituted 1,2-dihydropyridino-dioxins (III). The I.R., U.V. data and chemical conversions supported the structure (II) and (III).

**Key words :** Pyrano-dioxin, Pyridino-dioxin

Introduction

product with other gave 7 ables 2,2 diphenyl 4,5 dioxo

## SYNTHESIS OF NITROGENOUS COMPOUNDS. *Part II*

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(Received April 22, 1989; revised February 15, 1990)

2,4-dioxohexenoates have been prepared by the condensation of ketones with ethyl oxalate to obtain new heterocycles for the study of structure activity relationship. A number of trisubstituted pyrazoles have been synthesized to study their potential use as antimicrobial and/or hypoglycemic agent.

**Key words :** Synthesis-Heterocyclic compounds.

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## THE DETERMINATION OF THIAMINE CONTENT IN SEAWEEDS

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(Received October 31, 1988; revised February 20, 1990)

Determination of Thiamine in Seaweeds was carried out using improved technique with the help of three different Spectrophotometers. This method was applied on standard sample of thiamine (98.5-101.5%) and seven different species of Seaweeds belonging to Red and Brown family: *Botryocladia microphysa*, *Carpogonia florideae*, *Dictyota dichotoma*, *Tetrasporangia*, *Iyengaria stellata*, *Samia indica* and *Hypnea musciformis*. The method was also compared with other methods such as U.S.P., B.P, Pak. Pharmacopeae.

**Key words:** Thiamine, Seaweeds, Improved method



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## CHEMICAL COMPOSITION OF *BRASSICA* OILSEED MEAL

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(Received October 15, 1988; revised February 28, 1990)

The nutritional composition and glucosinolate content of *Brassica* oilseed meal were determined and compared with soybean meal. The latter contained more crude protein (47.5%) than the former (38.3%). However, *Brassica* protein scored higher than soya protein when compared with whole egg protein. Iso-leucine was the limiting amino acid in *Brassica* protein, while methionine and cystine were deficient in soya protein. Although *Brassica* meal contained better quality protein, the presence of glucosinolates (0.9 to 5.6%) impedes its efficient utilization. *Brassica napus* cv. 'Tower' was found better in this respect and its meal could be used as a good protein supplement in livestock rations.

**Key words:** Utilization, Brassica meal, Livestock feed.

## GEOCHEMICAL AND MINERALOGICAL EVALUATION OF PRECIOUS METAL BEARING IRON ORES OF CHILGHAZI, BALUCHISTAN

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(Received March 18, 1989, revised July 17, 1989)

The Chilghazi iron ores were found to contain 0.42-0.9 % copper, 0.1-0.22 ppm gold, 1.5-3.1 ppm silver and 1.5-1.7 ppm platinum. These metals were found as matrix minerals in magnetite. The results of mineral separation and analyses of product showed that Au, Ag and Pt were associated in chalcopyrite probably by substitution of Cu. The DTA of chalcopyrite showed an endothermic peak at 510° and exothermic peaks at 450, 520 and 765° in addition to the peaks of pyrite at 140 and 330°.

**Keywords:** Precious metal, Iron Ores, Chilghazi (Baluchistan).

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## COMPARATIVE BIOAVAILABILITY STUDIES OF SOME COMMERCIAL CHLORAMPHENICOL SUSPENSIONS

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(Received September 27, 1989; revised February 19, 1990)

Plasma chloramphenicol levels were compared in six adult healthy human volunteers. Single oral doses of chloramphenicol palmitate suspensions equivalent to 500 mg of chloramphenicol base were administered. Taking product I as standard, the peak plasma concentrations were found to be lower in products II and III; relative bioavailability of product II and III being 62% and 27.8% respectively. The time for peak plasma concentration was the same i.e. 180 min. for three products. The reduced bioavailability of II and III can be attributed to poor formulation of chloramphenicol palmitate suspensions.

**Key words:** Bioavailability, Chloramphenicol, Suspension.

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## A COMPARATIVE STUDY ON THE OCCURRENCE OF SEED-BORNE MYCOFLORA OF RICE IN PUNJAB AND SINDH

NASREEN SULTANA, S.A.J. KHAN, A.K. KHANZADA AND M. ASLAM

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(Received June 24, 1989; revised January 31, 1990)

Forty seed samples of rice collected from different places of Punjab and Sindh were analysed for the fungal flora in the laboratory. A total of 47 species of fungi were isolated using standard blotter method. Forty-five species of fungi were found to be associated with the samples collected from Sindh, while 36 with those collected from Punjab. *Aspergillus flavus* (7.5-8%), *A. niger* (7-8.5%), *Chaetomium globosum* (13.5-15%), *Curvularia lunata* (15-16%), *Drechslera hawaiiensis* (17.5-18%), *D. oryzae* (13.5-15.5%), *D. rostrata* (20.5-22%), and *Trichoconis padwickii* (27.5-30%) were recorded in higher frequencies in both Punjab and Sindh.

**Key words:** Rice, Seed-borne fungi, Sindh, Punjab.

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**Key words:** Rice, Seed-borne fungi, Sindh, Punjab.

***Short Communication***

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**Determination of Critical Dose of  
Apomorphine for Induction of Emesis in Dogs**

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MARYAM MIRZA

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## Technology Section

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### STUDY OF VITAMINS IN SELECTED SEaweEDS OF KARACHI COAST

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(Received June 30, 1988; revised February 2, 1990)

Eight different species of seaweeds belonging to Rhodophytes and Phaeophytes family - *Tetrasporangia* (Padina), *Botryocladia microphyta*, *Carpogonia florideae*, *Dictyota dichotoma*, *Iyengaria stellata*, *Samia indica*, *Hypnea musciformis* and *Sargassum vulgare* were studied for their contents of vitamins.

**Keywords:** Vitamins, Seaweeds



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## ENERGY CONSERVATION IN INDUSTRIAL DRYING

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(Received March 27, 1988; revised January 29, 1990)

In this study, several ways have been suggested, which could result in considerable saving, by conserving energy in the industrial dryers.

**Key words:** Energy, Conservation of energy, Industrial drying.

***Short Communication***

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**A NOVEL METHOD FOR THE  
SEPARATION OF HUSK AND KERNEL  
FROM THE SEEDS OF *PEGANUM  
HARMALA***

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(Received December 14, 1989; revised February 22, 1990)

*Peganum harmala* (Zygophyllaceae), which grows in