

# GLOBAL JOURNAL

OF SCIENCE FRONTIER RESEARCH: B

## Chemistry

Classification of Elements

Characteristic Graph of the Atom

Highlights

Compounds of Endemic Nepeta

Screening of Therapeutic Potential

Discovering Thoughts, Inventing Future

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CHEMISTRY

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## Charting Atomic Characteristics: A Pathway to Element Classification

By Ousmane BARRY, Mamadou Yaya BALDE, Souleymane BALDE, Lamine KABA  
& Aboubacar Safie SYLLA

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**Abstract-** The classification of elements serves as a rich source of knowledge in chemistry. This article explores the atomic model based on wave mechanics, represented by a graph characterizing the atom, to elucidate both periodic and ordered classifications of elements. Three types of classifications emerge from this graph: periodic, ordered, and hybrid classifications, with the latter resembling periodic tables but incorporating elements of the ordered form. The periodic table stands out as one of the most profound and unifying concepts in modern science. New illustration methods, such as condensed tables with orders and periods, are introduced. The results underscore the conclusiveness of the findings, revealing that classifications extend beyond periodicity, encompassing ordered types of tables as well. This research sheds light on the diverse approaches to classifying elements and opens avenues for further exploration in the field of chemistry.

**Keywords:** *periodic table, chemical element, period, affine equation, quantum number, order, wave mechanics, classification, hybrid classification, electronic structure.*

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# Charting Atomic Characteristics: A Pathway to Element Classification

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& Aboubacar Safie SYLLA <sup>¥</sup>

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## 1. INTRODUCTION

In any chemistry class or laboratory, there is almost always a periodic table hanging on the wall. This table, which includes all the known elements, provides a lot of information on each. As one progresses in the study of chemistry, the usefulness of the periodic table becomes more and more obvious[1].

Atoms were first suggested by the Greek philosophers Democritus and Leucippus around 400 BC, the concept was primarily based on a hunch. In fact, for several centuries thereafter, no convincing experimental evidence was available to support the existence of atoms. The first real scientific data were collected by Lavoisier and others from quantitative measurements of chemical reactions. Thus around 1790 the scientist was already able to identify 33 chemical elements. The results of these stoichiometric experiments allowed John Dalton to propose the first systematic atomic theory. This one, although crude, has stood the test of time extremely well. Once atoms were admitted, logically a number of questions arose such

as: What is the nature of an atom? How is it composed? What are the constituent parts, their properties etc.?

The most striking phenomenon in chemistry was very early the discovery of an analogy and the periodic repetition of the properties of the elements with each other. Several groups of elements with great similarities in their chemical behavior were identified. This is how the need to classify the elements arose. During the first 30 years of the 20th century, the appearance of a new theory, quantum mechanics, made it possible to explain the behavior of atoms under the effect of light. This so-called modern theory made it possible to develop the electronic structure of atoms. This confirmed the periodic behavior of chemical elements in terms of electronic configuration and then the properties of atoms.

In 1817 Döbereiner succeeded in relating the atomic mass of certain elements to their properties. He noticed the existence of similarities between elements grouped in threes which he called "triads". He highlighted the fact that the mass of one of the three elements of the triad was the intermediate (the average) of the other two. In 1850, we could count more than twenty triads to arrive at a first coherent classification.

In 1862 Chancourtois, a French geologist, highlighted a certain periodicity between the properties of the elements of the table. Later the English chemist Newlands announced that "the eighth element which follows a given element resembles the first as the eighth note of the octave resembles the first". But this law could not apply to elements beyond calcium: "The notions of transition elements were unknown". This classification therefore remained insufficient, but the periodic table was beginning to take shape.

In 1869 and 1870 respectively, Dmitri Mendeleev and Lothar Meyer claimed that the properties of elements could be represented as periodic functions of their atomic weight and presented their ideas in the form of a periodic table. As new elements have been discovered, the original form of the periodic table has been significantly modified and it is now recognized that periodicity is a consequence of variation in ground state electronic configurations. A modern periodic table emphasizes blocks of 2, 6, 10, and 14 elements that result from filling the s, p, d, and f atomic orbitals, respectively. An exception is He, which for chemical reasons is placed in the rare group [2].

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The most famous of the periodic classifications was that of MENDELEEV in 1869. It is to him that the merit goes to having presented the first, a well-structured and coherent classification of all the elements known at his time. He then realized the periodic trend in the properties of these placed in increasing order of their atomic masses [3]. This table had 6 columns with short periods with empty boxes according to his manuscript. This intuition of the scientist was confirmed by the later discovery of these new tenants corresponding to his prediction. More than a century after the death of the main founder of the periodic system, different types of periodic tables have emerged. It is time to revisit the origins, the precursors and even the status of this classification which has had a profound influence on the development of chemistry and modern physics. Scientists today are still debating the best possible presentation of the periodic table [4].

The American chemist Glenn T. Seaborg, Lawrence Berkeley National Laboratory, Berkely, California, United States of America whose only address is composed of five chemical elements (Sg, Lr, Bk, Cf, and Am respectively seaborgium, lawrencium, berkelium, californium and americium) had the merit of completing MENDELEEV's periodic table of elements with the addition of Actinides in 1945 [5]. From Lavoisier in 1790 to Glenn T. Seaborg, nearly two centuries of scientific exchange and research have led to several types of classifications, all periodic. It only differs in the mode of presentation.

In 1990 FERNANDO Dufour proposed a three-dimensional classification which he called "element tree" or "tree of elements" also called "periodic tree".

In 1995 PIERRE Demers of the University of Montreal proposed a classification system called "Québecium", a pyramid with 4 faces and 4 levels; the upper level made up only of 2 elements of the "s" block (1st period); the next is composed of the elements of the "s and p" blocks including 4 of "s" and 12 of "p" (the 2nd and 3rd periods), the penultimate level includes the elements of the "s, p and d" blocks » including respectively 4, 12 and 20 elements (periods 4 and 5) and the last level the base containing the elements of the four blocks "s, p, d and f" respectively 4, 12, 20 and 28 components of periods 6 and 7. The atomic number values  $Z$  provide an undeniable if not sufficient ordering principle. A classification called modern, somewhat analogous to the Quebec system but more explicit, is also presented as a pyramid of 7 levels, each corresponding to a period. From the top "the 1st period" to the base "the 7th period" of the pyramid, lines evolve from top to bottom materializing the identity of the valence electrons, that is to say the families (columns) of the periodic table of elements [6].

Eric SCERRI, for the sake of greater regularity, proposes a table in which the hydrogen and helium of the 1st period are brought back to the 2nd period

respectively at the level of halogens and rare gases with the columns  $np^5$  and  $np^6$  of block p cut and moved to the right, this leads to a disrupted periodic table of elements, with a regularity of the type 8 8 18 18 32 32 2 as opposed to 2 8 8 18 18 32 32 [7].

All these classifications present a certain discontinuity from one period to the next according to certain researchers, this seems to mark a disagreement with the logical sequence of the usual ordination of natural numbers in which the atomic numbers  $Z$  of the atoms would be found ( $Z$  ranging from 1 .....118).

This reason indicated above (mentioned) aroused concern and caught the attention of other researchers and served as a reference for them to promote new types of classification. Thus were born the spiral classifications. Professors PHILIP Steaward and JAN Scholten each proposed a spiral classification model, periodic spiral systems or "periodic tables" which according to them respect the natural ordination of atomic numbers. Théodor BENFEY's snail system from the 1960s and others are also of the spiral model. It should be noted that the difference between these presentation models is the simple notion of parallel and spiral linear chains. Periodicity is the only criterion for all these classifications. The period is an instantaneous phenomenon, it is the time that a phenomenon takes to complete the phases of its duration, it is the time interval at the end of which a phenomenon reproduces under the same conditions, such as the properties of the elements chemical; In chemistry periodicity is examined in terms of the number of elements with which identical properties recur from one group to another. It is this phenomenon that the English chemist Newlands wanted to explain with his famous quote: "the eighth element which follows a given element resembles the first as the eighth note of the octave resembles the first".

In 1989 Ouahès, R. made a proposal for a new periodic table of elements. This other table is still called periodic of 8 periods: He explains his table in these terms: "This means, in terms of atomic structure, that each period corresponds to the filling of shells and subshells according to  $n + l = k$  ( $k$ : constant) where  $n$  and  $l$  are the principal and azimuthal quantum numbers. The constant  $k$  is the rank of the period. The results are given in table 1. The number of periods is 8 instead of 7."

*This article will answer questions such as:*

- Can we explain the periodic classification using a more practical vision than that, entirely empirical, of Mendeleev?
- How does the distribution of electrons in an atom help explain periodic properties?
- Is this other table periodic?
- Is the number of periods greater than 7?

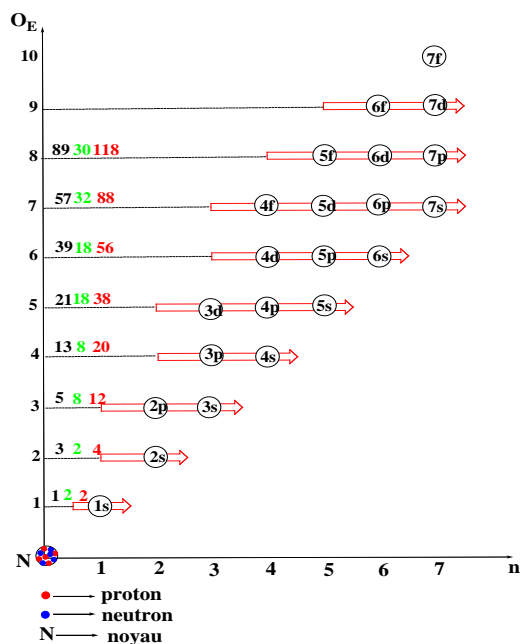
In general, the electronic structure gives all the information about an element, mainly its coordinates in

the different tables. Its physical and chemical properties also depend on it. Valence electrons provide the main concepts of chemical language. They open the way to forms of classification of elements, hence the different methods of illustrating the classification [8]. Obtaining specific graphs from the characteristic graph of the atom was explained in the methodology section. The types of classification of chemical elements were illustrated and discussed and a conclusion was drawn.

## II. METHODOLOGY

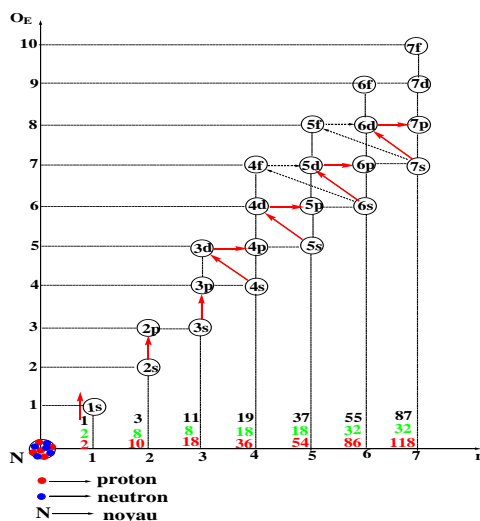
The specific graphs describing the orders and periods concretely explain the principles of stability,

- Electronic structure according to order (y-axis)



Graph 1: Electronic structure of elements according to order

- Electronic structure along the period axis



Graph 2: Electronic structure of elements according to period

aufbau, and in general the Kletchkovsky rule [9]. The distribution of the electrons of the different atoms along the axes of these graphs (abscissa and ordinate) by the periods and the orders respectively make it possible to explain each classification model in the literature and even to propose new methods of illustrating the classifications of the elements. A new criterion for classification of chemical elements becomes the order of the energy level " $O_E$ ", absolutely different from the period " $n$ ", has even emerged, it leads to a new classification called the ordered classification of the elements [10].





The ordered tables are obtained according to *graph 1*. The classification is made according to the ordinate axis "O<sub>E</sub>" which becomes the new classification criterion leading to tables of a new type called ordered tables, the set of ordered tables is summarized by a so-called condensed order table. This goes without saying for all periodic classifications, the only classic

classification criterion of which is the period "n" according to *graph 2* and are all also summarized by a condensed period table. These two condensed tables are analogous but different, the energy order "O<sub>E</sub>" is different from the period "n". See below the respective condensed forms which are effectively new methods of illustrating the classifications.

Table 1: Condensed table to order

Order	1	2	3	4	5	6	7	8
Underlays	1s	2s	2p3s	3p4s	3d4p5s	4d5p6s	4f5d6p7s	5f6d7p...
Z	1- 2	3- 4	5- 12	13- 20	21- 38	39- 56	57- 88	89-118...
Type of tables	2	2	8	8	18	18	32	30.....

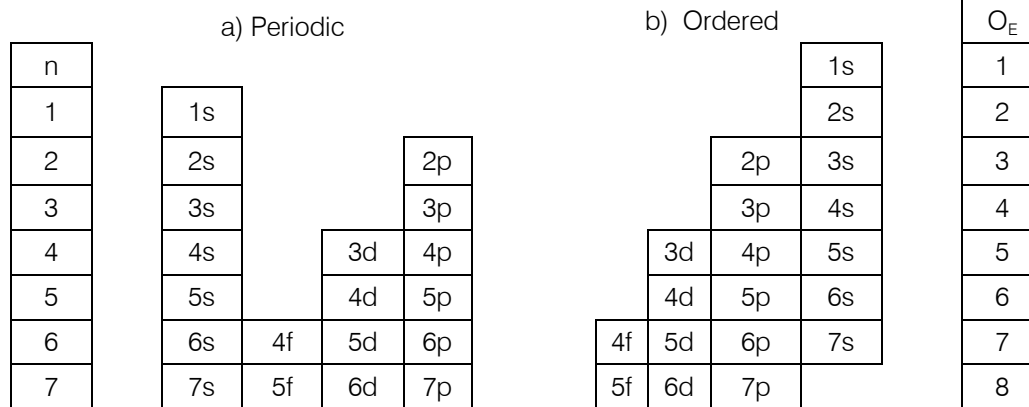
Table 2: Condensed period table

Periods	1	2	3	4	5	6	7
Underlays	1s	2s2p	3s3p	4s3d4p	5s4d5p	6s4f5d6p	7s5f6d7p...
Z	1- 2	3- 10	11- 18	19- 36	37- 54	55- 86	87-118...
Type of tables	2	8	8	18	18	32	32....

### III. RESULTS

To make the classification, whether periodic or ordered, it is enough to arrange vertically the stacks of the different sub-layers in each case. Give each block the number of columns corresponding to its electronic capacity: 2 for block "s", 6 for "p", 10 for "d" and 14 for "f". The classifications are either short, medium and long depending on the stacks chosen as a basis. The main stacks are "sp / ps" for tables with 8 columns "sdp / dps" for those with 18 columns and finally "sfdp/fdps" for long classifications with 32 columns.

The vertical arrangements of the sublayers by stacking the periods and/or order offer the appearance of tables: the periodic tables are fairly well-known emblematic figures which adorn quite a few scientific circles today. Ordered tables constitute a completely new classification model and appear in the form of stairs with regular steps. The longest ordered arrays are made up of four steps corresponding to the four blocks of elements. These stairs start from block "f" via those of "d, p" and end with that of "s", from bottom to top respectively.



Comparing these two classifications, it appears that the order is obtained by the transfer of the "s" block from the left of Mendeleev's periodic table to its right with a shift of one level upwards; which allows you to go from 7 periods to 8 orders. Orders always end with "s" while periods begin with "s" and are composed respectively as follows:  $(n-3) f (n-2) d (n-1) p ns$  and  $ns (n-2) f (n-1) d np$ .

The ordered classification puts the transitional elements, blocks f and d, of group "B" before the non-transitional elements, blocks s and p, of group "A". This

leads to a more regular, coherent presentation, compared to the periodic system which inserts transition elements between normal and non-normal ones. In the



Graphs 1 and 2 depict the composition of the electron cloud elements in order and period respectively. The arrangement of the sublayers from 1s to 7p is practically done according to the increasing order of the energy level either by the ordinate "O<sub>E</sub>" or by the abscissa "n" in the usual ordination of natural numbers.

The structure of an order according to the accepted values is (n-3) f (n-2) d (n-1) p ns and that of the period is ns (n-2) f (n-1) d np, it is remarkable that the order ends with the sublayer "ns" while it can start with any sublayer even with ns if the order is short as for the cases: n = 1 and 2. Practically the orders go from 1 to 8. For the periods, they start with "ns" and end with "np", the coefficients of the intermediate sublayers are counted from "n" to the limit values. The order is then different from the period, the periods go from 1 to 7. The coefficients of the sublayers in each case are linked to O<sub>E</sub> and/or n, knowing that for the block "s" O<sub>E</sub> = n. Thus, it is enough to be able to count from 1 to 7 and/or from 1 to 8 to develop the rule of stability.

Table 3: Group of sublayers according to the order of energy (Graph 1)

Orders « O <sub>E</sub> »	1	2	3	4	5	6	7	8
Underlays	1s	2s	2p 3s	3p 4s	3d 4p 5s	4d 5p 6s	4f 5d 6p 7s	5f 6d 7p ...

Table 4: Group of sub-layers according to the period (Graph 2)

Periods « n »	1	2	3	4	5	6	7
Underlays	1s	2s 2p	3s 3p	4s 3d 4p	5s 4d 5p	6s 4f 5d 6p	7s 5f 6d 7p

These two tables sufficiently express the difference between an "O<sub>E</sub>" order and a "n" period, but these two criteria are well linked.

Table 5: Relationship between period and order (Graphs 1 & 2)

Periods « n »	1		2		3		4		5		6		7	
Underlays	1s	2s	2p	3s	3p	4s	3d4p	5s	4d5p	6s	4f5d6p	7s	5f6d7p...	
Orders « O <sub>E</sub> »	1	2	3		4		5		6		7		8	

These two very similar tables are different. For block "s", O<sub>E</sub> = n, the order is identical to the period and for the others the orders are greater than the period by one unit. The condensed period form confirms all current periodic classifications of the elements. It is the summary of all the classic period processes developed according to the abscissa axis "n" whatever the two or three dimensional model, spiral or not.

The condensed ordered table is also another classification process leading to entirely new forms of tables which are far from being periodic. They are ordered or ordered tables of the elements, obtained along the "O<sub>E</sub>" ordinate axis. These resulting paintings are presented in the form of a staircase also with 8, 18 and 32 columns. If for the periodic system the classification criterion is the period "n", the ordered tables are carried out around a new classification criterion, namely the order "O<sub>E</sub>". Except that they are not periodic. The word "period" or its adjective "periodic" was not accidentally used by the founding father of the classification system. This choice expressed the behavior of the properties of the groups of elements which were born, evolved then diminished and canceled after a certain number of elements which make up said period. An order is a combination of the elements of two successive periods.

## V. CONCLUSION

This new classification conforms to the electronic structures of the elements according to order and period. It can have historical and educational interest, because it is based on simple to understand concepts.

This work demonstrated that all classifications in the literature are not only periodic. The characteristic graph of the atom made it possible to confirm the existence of the two classification criteria leading to fairly classic periodic tables built around the period "n going from 1 to 7" and completely new ordered or ordered tables which carry out around the order of the increasing level of energy order of the sublayers "O<sub>E</sub> starting from 1 to 8" following the ordinate of the graph. The ordered table corresponds to the transfer of the "s" block from the left of the periodic table of elements to its right with the tilting of the latter one level upwards from 7 stacks to 8 others. A third classification intermediate to the other two was envisaged by the reduction of the block "s" of the ordered form by one level downwards from 8 stacks to 7 others, hence a periodic classification in the image of the ordered form. A new illustration of the classification of elements.

We hope to soon provide a rigorous proof of atomistic terminology using the equation of the line,

such as the deduction of valence electrons, the electronic transition and the relationship between the nucleus and the electron cloud of an atom.

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## Screening of Therapeutic Potential and Compounds of Endemic *Nepeta pilinux* P.H. Davis in Kew Bull. from Şanlıurfa

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**Abstract-** *Nepeta pilinux* P.H. Davis in Kew Bull. was recently recorded as an endemic species in Birecik, Şanlıurfa. The essential oils were obtained from air-dried aerial parts by hydrodistillation and their composition was investigated using GC-FID and GC/MS. Determination of antioxidant capacity, and urease and xanthine oxidase inhibitions of the methanolic extracts were performed with HPLC-DAD and spectrophotometry. 34 compounds were identified constituting 89.2% of the total essential oil compounds. The major components were determined as T-cadinol (31.1%),  $\gamma$ -muurolene (14.4%) and 14-nor-cadin-5-en-4-one isomer A (11.0%) in the oil. Mainly rosmarinic acid, chlorogenic acid, and caffeic acid derivatives were quantified together with apigenin, luteolin and tangeretin derivatives in the extracts by HPLC-DAD. The total phenolics of the extract from leaf and flower parts, 50.81 mg GAE.g<sup>-1</sup>, was higher than the extract from stem part, and the radical scavenging activity of this extract was also stronger. While, the leaf and flower extract had significant urease and xanthine oxidase inhibitory activities (62.47 and 48.48  $\mu$ g.mL<sup>-1</sup>), stem extract had low inhibition on both enzymes.

**Keywords:** *nepeta pilinux*, essential oil, rosmarinic acid, GC-FID, GC/MS, HPLC-DAD.

**GJSFR-B Classification:** LCC: QK898.L42



*Strictly as per the compliance and regulations of:*



# Screening of Therapeutic Potential and Compounds of Endemic *Nepeta pilinix* P.H. Davis in Kew Bull. from Şanlıurfa

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**Abstract-** *Nepeta pilinix* P.H. Davis in Kew Bull. was recently recorded as an endemic species in Birecik, Şanlıurfa. The essential oils were obtained from air-dried aerial parts by hydrodistillation and their composition was investigated using GC-FID and GC/MS. Determination of antioxidant capacity, and urease and xanthine oxidase inhibitions of the methanolic extracts were performed with HPLC-DAD and spectrophotometry. 34 compounds were identified constituting 89.2% of the total essential oil compounds. The major components were determined as T-cadinol (31.1%),  $\gamma$ -muurolene (14.4%) and 14-nor-cadin-5-en-4-one isomer A (11.0%) in the oil. Mainly rosmarinic acid, chlorogenic acid, and caffeic acid derivatives were quantified together with apigenin, luteolin and tangeretin derivatives in the extracts by HPLC-DAD. The total phenolics of the extract from leaf and flower parts, 50.81 mg GAE.g<sup>-1</sup>, was higher than the extract from stem part, and the radical scavenging activity of this extract was also stronger. While, the leaf and flower extract had significant urease and xanthine oxidase inhibitory activities (62.47 and 48.48  $\mu\text{g.mL}^{-1}$ ), stem extract had low inhibition on both enzymes.

**Keywords:** *nepeta pilinix*, essential oil, rosmarinic acid, GC-FID, GC/MS, HPLC-DAD.

## I. INTRODUCTION

The genus *Nepeta* is distributed over a large part of Central and Southern Europe, and West, Central, and Southern Asia as a multi-regional genus of the Lamiaceae (labiatae or mint) family, consisting of approximately 300 taxa (1, 2). 34 species (40 taxa) of the genus *Nepeta* were recorded in the Flora of Turkey (3, 4). According to the revision of this genus, it is represented by 39 species (46 taxa) in Turkey with recent studies. Endemism rate on the basis of this species is 44% (5). *Nepeta* species are usually named

as catmint or catnip due to the sedative effects on cats and they are commonly used as diuretic, spasmolytic, diaphoretic, bronchodilator, antitussive, anti-asthmatic and sedative agents in Turkey. Due to their antiseptic properties, they are used topically in the treatment of children with skin rashes, and in snake and scorpion bites as well. *Nepeta caes area*, an endemic species in Turkey, has folkloric uses in southern Anatolia and is used as a herbal tea to treat gastric disorders (6,7). Some *Nepeta* species have been known their feline attractant activity since they have nepetalactone and its derivatives which are responsible for attractant properties (1,7). Nepetalactones have been reported to effect on insects compare to DEET (N, N-diethyl-m-toluamide) (8-10). Nepetoideae is essential oil-rich genera of the Lamiaceae, therefore has potential economic interest (11).

According to the various studies on the essential oil composition of *Nepeta* species the essential oil composition depends on the species, place of cultivation, climatic conditions and method of analysis (12-26). The most comprehensive study on 22 *Nepeta* species was performed by Baser et al. (2000). They were classified into two groups according to composition of essential oil of these species; nepetalactone-containing and nepetalactone-less. Nepetalactone-containing species have 4 $\alpha$ -7 $\alpha$ -7 $\alpha$  nepetalactone as the most frequently contained nepetalactone. *Nepeta cadmea* Boiss., *Nepeta cataria* L., *Nepeta caesarea* Boiss. and *Nepeta pilinix* P.H. Davis contained 4 $\alpha$ -7 $\alpha$ -7 $\alpha$  nepetalactone while *Nepeta racemosa* Lam. contained 4 $\alpha$ -7 $\alpha$ -7 $\beta$ -nepetalactone as major compound in their oils. Caryophyllene oxide or 1,8-cineole/linalool were identified in the essential oils of Nepetalactone-less species as the major components. As main compounds,  $\beta$ -pinene,  $\alpha$ -terpineol, germacrene-D, and spathulenol were respectively determined in the oil of *Nepeta phylloclamys* P.H. Davis, *Nepeta viscida* Boiss., *Nepeta sorgerae* Hedge et Lamond, and *Nepeta trachonitica* Post which are out of the two groups (1).

Being a type of the most popular antioxidant secondary metabolites, phenolic compounds were investigated in the *Nepeta* species as well. Rosmarinic

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acid, epicatechin, chlorogenic acid, caffeic acids, quercetin, rutin, ellagic acid, thymusin, luteolin, and apigenin which are well-known as antioxidant compounds were found in the extracts of *Nepeta cadmea* Boiss., *Nepeta nuda* subsp. *albiflora*, *Nepeta asterotricha* Rech., *Nepeta rtanjensis* Diklic & Milojević (27-30).

Ureases, a nickel-dependent metalloenzymes, are synthesized by plants, some bacteria, algae and fungi. The jack bean urease (urea amidohydrolase EC 3.3.1.5) catalyzes the hydrolysis of urea to form ammonia and carbon dioxide (31). *Helicobacter pylori*, a gram-negative microaerophilic pathogen survivable in a limited pH (4.0–8.2) range. This pathogen can successfully colonize and persist in the mucous layer of the human stomach since its urease activity which produces ammonia to reduce stomach acidity. Since antibiotic-resistant strains of *H. pylori* can emerge against antibiotics, it is believed that plant-derived urease inhibitors would be more beneficial against gastroduodenal disease associated with this pathogen (32, 33).

Xanthine oxidase (EC 1.2.3.2.) produces hydrogen peroxide and superoxide anion, which are reactive oxygen species (ROS) during the oxidation of hypoxanthine and xanthine to uric acid. Under physiological conditions, ROS is kept at a low level by the antioxidant system. Disruption of the balance of ROS and antioxidants due to some diseases causes tissue and DNA damage due to the increase in metabolism of ROS. Inhibition of xanthine oxidase reduces the amount of uric acid and ROS in the bloodstream to prevent both hyperuricemia and oxidation stress (34). Inhibitory effects of some flavonoids such as diosmetin, luteolin, chrysoeriol, apigenin, kaempferol on xanthine oxidase have been reported in various in vitro studies (35-37).

*Nepeta pilinux* P. H. Davis in Kew Bull. is an endemic species of *Nepeta* genus growing in the Southwestern Anatolia (Antalya: Alanya) (3). However, in recent flora research, *Nepeta pilinux* was encountered in Şanlıurfa, Birecik district and was recorded as new endemic species for Şanlıurfa flora. *Nepeta pilinux* is named as 'top pisik otu'. In Şanlıurfa, the fresh aerial parts of the plant are used to heal mouth sores (38).

There is no knowledge about the essential oil and phenolic composition of *Nepeta pilinux* endemic species from Şanlıurfa. Chemical compositions of the polar and apolar extracts from *Nepeta pilinux* were determined by HPLC-DAD and GC/MS respectively for the first time in this study. Radical scavenging activities against DPPH and ABTS radicals and enzyme inhibition activities on urease and xanthine oxidase were investigated in vitro to elucidate the bioactivities which may have developed by this species depending on its chemical composition.

## II. EXPERIMENTAL

### a) Materials

*Nepeta pilinux* was collected from Şanlıurfa: Birecik, Kelaynak area in Turkey in 5 May 2018. The voucher specimen has been deposited at the Herbarium in the Recep Tayyip Erdoğan University (RTEUB 6079), Rize, Turkey (Voucher specimen no: FABAK 1702). The plant material was identified by Prof. Dr. Vagif ATAMOV (Recep Tayyip Erdogan University, Faculty of Science and Literature, Department of Biology, Rize, Turkey). All standards of phenolic compounds were obtained from Sigma-Aldrich (St. Louis, MO, USA) but quercetin from Fluka Chemie GmbH (Switzerland). Na<sub>2</sub>CO<sub>3</sub> and K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> were provided from Sigma-Aldrich (St. Louis, MO, USA). HPLC grade acetonitrile, methanol, acetic acid, Folin ciocalteau, 2,2-Diphenyl-1-picrylhydrazyl (DPPH), and 2,2'-Azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) diammonium salt (ABTS) were supplied by Merck (Darmstadt, Germany).

### b) Isolation of the Essential Oil

Aerial parts of the plant were water distilled for 3 h using a Clevenger-type apparatus. The essential oil was stored at 4°C in the dark until analyzed.

### c) Extraction of Phenolic Compounds

The aerial parts of the plant were divided into two parts. The leaves and flowers were combined in one part and the stems were separated into the other part. The part consisting of leaves and flowers was called NP-LF for short, and the part consisting of stem is called NP-S. These parts were finely ground and 0.5 grams of each were defatted by using 10 mL of hexane. The plant residues were dried at 40 °C for 30 min after removing the hexane extract. 20 mL methanol were added to these residues for the extraction of phenolic compounds. Extraction was continued overnight at 37 °C in the dry thermo-shaker cabinet at 352 rpm, then the extracts were centrifuged at 5000 rpm and supernatants transferred into the falcon tube. This procedure was repeated by adding 10 mL of methanol in the residue. All extract was concentrated until 5 mL by using rotary evaporator at 35 °C. 500 and 1500 µL of these extracts were stored at -20 °C for HPLC-DAD analysis, antioxidant and enzyme inhibition tests. Remaining 3 mL of extract was evaporated to calculate the concentration of the extracts. NP-LF and NP-S extracts concentration were 23.17 and 23.50 mg.mL<sup>-1</sup> respectively.

### d) Gas Chromatography (GC) and Gas Chromatography-Mass Spectrometry (GC/MS) analysis of essential oil

The oil was analyzed by capillary GC and GC/MS using an Agilent GC-MSD system.

#### i. GC/MS analysis Conditions of Essential Oils

The oil was analyzed by capillary GC/MS using an Agilent GC-MSD system (Agilent Technologies Inc.,

Santa Clara, CA). HP-Innowax FSC column (Hewlett-Packard-HP, U.S.A.) (60 m × 0.25 mm i.d., with 0.25 µm film thickness) was used for separation of components in the oil and helium as a carrier gas (0.8 mL/min). The GC oven temperature was kept at 60°C for 10 min and programmed to 220°C at a rate of 4°C/min, and kept constant at 220°C for 10 min and then programmed to 240°C at a rate of 1°C/min. The split flow was adjusted at 40 mL min<sup>-1</sup> with 40:1 split ratio. The injector temperature was set at 250 °C. Mass spectra were taken at 70 eV with the mass range *m/z* 35-450.

ii. *GC Analysis Conditions of Essential Oils*

The GC analysis was done with Agilent 6890N GC system fitted with a FID detector set at a temperature of 300°C. To obtain the same elution order with GC/MS, simultaneous auto-injection was done on a duplicate of the same column applying the same operational conditions. Relative percentage amounts of the separated compounds were calculated from FID chromatogram.

iii. *Identification of Essential Oils*

Identification of essential oil components were performed by comparison of their mass spectra with those in the Baser Library of Essential Oil Constituents, Wiley GC/MS Library, Adams Library, MassFinder Library (39-41) and confirmed by comparison of their retention indices. A homologous series of *n*-alkanes were used as the reference points in calculation of relative retention indices (RRI) (42). The relative percentages of the separated compounds were calculated from FID chromatograms. The analysis results are expressed as mean percentage as listed in Table 1.

e) *HPLC-DAD Analysis Conditions of Methanol Extracts*

The chromatographic analyses were performed using a Dionex (Thermo scientific, Germering, Germany) Ultimate 3000 high performance liquid chromatography (HPLC) system equipped with an Ultimate 3000 diode array detector (DAD).

A Thermo acclaim C30 column (150mm. 3mm id. 3µm pd) was used with Macherey Nagel (3mm id) guard column. Gradient elution was used with mobil phases; A: 2% acetic acid in water and B: 70%acetonitrile-30% water. Flow rate was 0.37 mL/min and injection volume was 10 µL. Column temperature was 25°C. Following 24 phenolic standards were used to calibration and validation of HPLC-DAD analysis method: Gallic acid, protocatechuic acid, *p*-hydroxy benzoic acid (*p*-OH benzoic acid), vanillic acid, catechin, chlorogenic acid, caffeic acid, syringic acid, vanillin, epigallocatechin gallate (EGCG), epicatechin, *p*-coumaric acid, ferulic acid, chicoric acid, rutin, luteolin-7-glycoside, hesperidin, apigenin-7-glycoside, rosmarinic acid, luteolin, quercetin, hesperetin, apigenin, and tangeretin. They were diluted from their stock

solution into nine different concentration at 0.3125; 0.625; 1.25; 5.0; 10.0; 25.0; 40.0 mg.L<sup>-1</sup> in 1:1 methanol-water solution. External calibration method was used and their regression coefficient were found at least 0.999. Repeatability of the retention time and peak areas were measured as coefficient of variation (CV) which was under 0.93 for retention times and 6.02 for areas of the peaks. Limit of detection and quantification values of the peaks were under 0.11 and 0.37 µg.mL<sup>-1</sup> for all standards. Chromatograms were processed at 254, 280, 315, and 370 nm with DAD which operated 200-400 nm. The identification of the peaks was carried out by comparing the retention times and UV spectra with those of standard phenolic compounds. Some peaks had the same or very similar UV spectra as some standards, but with different retention times. They were defined as derivatives of standards with similar UV spectrum and quantified as equivalent of those standards.

f) *Determination of Total Phenolic Content*

Total phenolic content was determined by using the yellow colored Folin-Ciocalteu's phenol reagent, which was reduced to its blue complex in the presence of reducing agent such as phenolic compounds (43). Gallic acid and quercetin were used as phenolic standards to generate standard curves in a range of 0.0156 and 0.500 mg/mL at 6 concentration levels (*r*<sup>2</sup> = 0.998). The optical density of the extracts with phenol reagent in the alkaline solution was measured at 760 nm with a UV-Vis detector (Thermo Scientific Multiskan Go, USA). The results were expressed in mg of gallic acid (GAE) and quercetin equivalent (QE) per gram of extracts. All concentration point of the extracts was analyzed in triplicate.

g) *DPPH Free-Radical Scavenging Activity Assay*

The free-radical scavenging activity was determined based on the reduction of the purple colored 2,2-diphenyl-1-picrylhydrazyl (DPPH•) radical to the yellow colored DPPH-H form by the effect of an antioxidant species such as phenolic compounds in the extracts. It was spectrophotometrically performed at 517 nm (44). Briefly, 0.15 mL of plant extract was mixed with 0.15 mL 0.1 mM daily prepared DPPH in methanol and incubated for 30 min in the dark. Gallic acid and quercetin were used as standards to compare with the methanol extracts. Results are reported as SC<sub>50</sub> values, demonstrating the concentration of extract (µg extract per mL methanol) necessary to scavenge 50% of DPPH•. All concentration point of the extracts was analyzed in triplicate.

h) *ABTS Radical Scavenging Assay*

7 mM of ABTS solution and 2.4 mM of potassium persulfate solution were mixed in equal quantities and allowing to oxidation reaction of ABTS by K<sub>2</sub>S<sub>2</sub>O<sub>8</sub> for 18 h at room temperature in the dark to form



the ABTS<sup>•+</sup> radical. Obtained radical solution was then diluted with methanol 25 times to obtain an ABTS<sup>•+</sup> solution has optical density of 0.700 ± 0.01 at 734 nm (45). 50 µL plant extracts were allowed to react with 250 µL of the ABTS<sup>•+</sup> radical solution and the absorbance was measured at 734 nm after 30 min using a spectrophotometer. The ABTS<sup>•+</sup> scavenging capacity of the extracts were compared with that of gallic acid and quercetin and reported with SC<sub>50</sub> values (µg extract/ mL methanol). All concentration point of the extracts was analyzed in triplicate.

i) Urease Inhibitory Assay

Urease inhibition of the extracts were performed according to the phenol-hypochlorite method developed by Weatherburn (1967) (46). Jack bean urease was used as a model enzyme. Optical density of the resulting blue-navy colored mixture at 625 nm were recorded on a spectrophotometer (1601UV-Shimadzu, Australia). To calculate the IC<sub>50</sub> values of the polar extracts, different concentrations of the extracts or inhibitory compounds were prepared. Acetohydroxamic acid, well-known inhibitor of urease, were used as positive control.

j) In Vitro Anti-Xanthine Oxidase Assay

The inhibition of xanthine oxidase was measured by UV spectroscopy technique at 295 nm which is attributed to the released uric acid from xanthine. The inhibitory activity of the extract was determined using a slight modification of the reference methods (34). Briefly, the reaction mixture consisted of 500 mL of the extract solution, (diluted in DMSO), 770 mL of phosphate buffer (pH 7.8) and 70 mL of bovine milk xanthine oxidase (0.4 U/mL, Sigma Aldrich, St. Louis, USA) was prepared. The reaction was initiated by the addition 660 mL of xanthine solution (0.4 mM) into the mixture after incubation at 25°C for 15 min. The assay mixture was incubated at 25°C for 15 min again. The reaction was stopped by adding 200 mL of 0.5 N HCl and the absorbance was measured at 295 nm using UV/vis spectrophotometer (1601UVShimadzu, Australia). A well-known XO inhibitor (XOI), allopurinol (Sigma Aldrich, St. Louis, USA) was used as a positive control. XO activity was expressed as percent inhibition of xanthine oxidase, calculate as (1-B/A) x 100, where A is the change in absorbance of the assay without the test samples. (Δ abs with enzyme - Δ abs without enzyme),

and B is the change in absorbance of the assay with the test sample (Δ abs with enzyme - Δ abs without enzyme). The assay was done in triplicate. The IC<sub>50</sub> value was determined as the concentration of the extract that gave 50% inhibition of maximal activity.

III. RESULTS AND DISCUSSION

a) GC And GC/MS Analysis of Essential Oils

Essential oil yield in the sample was calculated as 0.26%. Thirty-four compounds comprising about 89.2% of the essential oil were identified. Identified essential oil components were compared with literature polar column retention times. The major components were determined as T-cadinol (31.1%), γ-muurolene (14.4%) and 14-nor-cadin-5-en-4-one isomer A (11.0%) in the oil. *Nepeta pilinux* essential oil has oxygenated sesquiterpenes (44.6%), sesquiterpenes hydrocarbons (17.3%), oxygenated monoterpenes (10.1%), monoterpene hydrocarbons (2.3%) and others (14.9%). The analysis results were shown in Table 1.

Our results were not similar to the classification of *Nepeta* species reported by Baser et al. (2000) (1). *Nepeta pilinux* which was collected from Antalya, Alanya district was in the group containing nepetalactone, an iridoid monoterpene according to their report. Although 89.2% of the essential oil was determined in *Nepeta pilinux* from Şanlıurfa, nepetalactone was not detected. The determination of different essential oil compositions from *Nepeta pilinux* from different regions may have resulted from the difference in locality.

The major constituent of water-distilled essential oils of *Nepeta heliotropifolia* and *Nepeta congesta* subsp. *cryptantha* was determined by GC/MS and GC-FID and found to be germacrene D (36.7% and 38.5%, respectively). Their main aroma component was determined as eucalyptol (48.0% and 24.7%, respectively) (47). Although the major essential oil and aroma compounds of these two species were quite different from the main essential oils of *Nepeta pilinux*, the compositions of these three species had lots of common compounds such as α and β-pinene, γ-muurolene, myrtenal, pinocarveol, caryophyllene oxide, cubenol, T and α-cadinol ect. The presence of more or less components may be due to differences between species, as well as environmental conditions and the harvesting time of the plant.

Table 1: Composition of the Essential Oil of *Nepeta Pilinux*

RRI <sup>a</sup>	RRI <sup>b</sup>	Components	%	IM
1032	1032 <sup>c</sup>	α-Pinene	2.3	t <sub>R</sub> , MS
1118	1118 <sup>c</sup>	β-Pinene	tr	t <sub>R</sub> , MS
1213	1213 <sup>d</sup>	1,8-Cineole	tr	t <sub>R</sub> , MS
1376		trans-Muurola-3,5-diene	0.3	MS
1499	1499 <sup>e</sup>	α-Campholenal	0.7	MS
1535	1535 <sup>e</sup>	Pinocamphone	0.1	MS



1553	1553 <sup>d</sup>	Linalool	2.3	t <sub>R</sub> , MS
1577	1577 <sup>e,g</sup>	α-Cedrene	0.3	MS
1586	1586 <sup>c</sup>	Pinocarvone	0.7	MS
1617	1613 <sup>g</sup>	β-Cedrene	tr	MS
1648	1648 <sup>e</sup>	Myrtenal	0.6	MS
1670	1670 <sup>d</sup>	trans-Pinocarveol	1.3	t <sub>R</sub> , MS
1684	1684 <sup>e</sup>	trans-Verbenol	4.4	MS
1694	1693 <sup>g</sup>	β-Acoradiene	tr	MS
1704	1704 <sup>c,d</sup>	γ-Murolene	<b>14.4</b>	MS
1706	1706 <sup>d</sup>	α-Terpineol	tr	t <sub>R</sub> , MS
1726	1725 <sup>e</sup>	Verbenone	tr	t <sub>R</sub> , MS
1747	1740 <sup>e</sup>	p-Mentha-1,5-dien-8-ol	tr	MS
1751	1751 <sup>d</sup>	Carvone	tr	t <sub>R</sub> , MS
1797	1804 <sup>d</sup>	Myrtenol	tr	MS
1845	1845 <sup>d</sup>	trans-Carveol	tr	t <sub>R</sub> , MS
1853	1849 <sup>d</sup>	cis-Calamenene	1.8	MS
2008	2008 <sup>c</sup>	Caryophyllene oxide	0.6	t <sub>R</sub> , MS
2050	2050 <sup>e</sup>	(E)-Nerolidol	0.4	t <sub>R</sub> , MS
2080	2080 <sup>d</sup>	Cubenol	3.7	MS
2089		6-Methyl-5 (3-methyl phenyl)-2-heptanone	0.8	MS
2187	2187 <sup>d</sup>	<b>T-Cadinol</b>	<b>31.3</b>	MS
2256		epi-α-Bisabolol	0.3	t <sub>R</sub> , MS
2257	2233 <sup>f</sup> 2256 <sup>e</sup>	Cadalene	0.5	MS
2258	2219 <sup>c</sup> 2255 <sup>d</sup>	α-Cadinol	1.4	t <sub>R</sub> , MS
2264	2264 <sup>e</sup>	4,7-dimethyl-1-tetralone	0.8	MS
2320	2324 <sup>c</sup>	<b>14-Nor-cadin-5-en-4-one isomer A</b>	<b>11.0</b>	MS
2349	2349 <sup>e</sup>	Cadina-4, 10 (15)-dien-3-one	6.1	MS
2931	2931 <sup>c</sup> 2913 <sup>f</sup>	Hexadecanoic acid	3.1	MS
		Monoterpene hydrocarbons	2.3	
		Oxygenated monoterpenes	10.1	
		Sesquiterpenes hydrocarbons	17.3	
		Oxygenated sesquiterpenes	44.6	
		Others	14.9	
		Total %	<b>89.2</b>	

RRI<sup>a</sup>: RRI Relative retention indices experimentally calculated against *n*-alkanes; RRI<sup>b</sup>: RRI from literature [c (48); d (49); e (50); f (51); g (52)] for polar column values; % calculated from FID data; tr; Trace (<0.1 %); Identification Method (IM): t<sub>R</sub>, Identification based on comparison with co-injected with standards on a HP Innowax column; MS, identified on the basis of computer matching of the mass spectra with those of the libraries.

#### b) HPLC-DAD Analysis of Phenolic Compounds in the Methanol Extracts

The list of standard phenolic compounds has a wide range of phenolic standards such as 5 benzoic acids (gallic, protocatechuic, *p*-OH benzoic, vanilic, and syringic acid), 1 hydroxybenzaldehyde (vanillin), 5 cinnamic acids (caffeic, *p*-coumaric, ferulic, chicoric and chlorogenic acid), 3 flavanols (catechin EGCG, epicatechin), 1 flavonol with its 1 glycoside (quercetin

and rutin), 3 flavones with 2 sugar attached derivatives, (luteolin, apigenin, tangeretin, luteolin-7-glucoside, apigenin-7-glucoside), 1 flavanone with its 1 glycoside (hesperidin and hesperetin), and rosmarinic acid which is a caffeic acid ester (*supp. Table 1*).

A total 6.9 g and 2.1 g of phenolic compounds per 100 g of NP-LF and NP-S, respectively, were quantified by HPLC-DAD (*Table 2*). The stem part of the plant had at least 3 times less amount of phenolic compounds than the leaf and flower parts (NP-LF). Rosmarinic acid (RA) was found to be the major compound at 3.1 g per 100 g of NP-LF (3.1%) as expected from Lamiaceae family members. The peaks which had same UV spectrum as RA but eluted earlier were identified as RA derivatives (der.) and quantified as equivalent of RA (*Fig. 1*). They could be the sugar or other functional groups attached to the RA causing this early elution. Total ratio of RA derivatives in the extracts

were 4.3% for NP-LF and 0.3% for NP-S (Table 2). Caffeic acid and derivatives including RA covered 4.5% of the NP-LF.

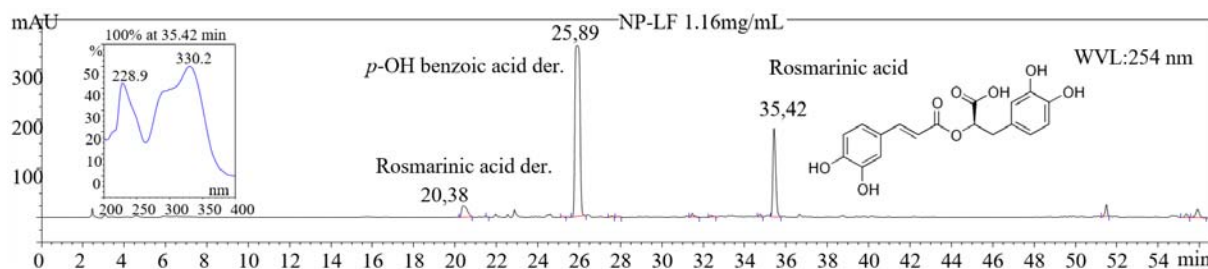


Figure 1: HPLC-DAD chromatogram of the extract from leaf and flower parts of *Nepeta pilinux*

Protocatechuic, chlorogenic, caffeic, *p*-coumaric, chicoric acids and luteolin-7-glycoside were also determined in the extracts by comparing the retention time and UV spectrum of the peaks with those of the standard phenolics. There was extremely large peak among others in the chromatograms at 254 nm which was eluted at around 25.9 min and had overlaying two compounds with 243 and 257 nm maximum wavelengths. These peaks were identified as *p*-OH benzoic acid der. and quantified as its equivalent (Fig. 1 and Table 2). The peak eluting at 21.4 min. and having

max. absorbance at 293 nm was identified as *p*-OH benzaldehyde (4-hydroxybenzaldehyde) since its elution order and UV spectrum were consistent with this phenolic aldehyde (53). The regression equation of vanillin which is the 4-hydroxy-3-methoxybenzaldehyde was used to quantified *p*-OH-benzaldehyde due to their structural and spectral similarity. Four tangeretin derivatives were identified tentatively by comparing UV spectrum of these peaks with that of tangeretin. Since tangeretin has 5 methoxy groups without hydroxyl group, it is eluting in the last part of the chromatogram from

Table 2: The amount and spectral details of phenolic compounds determined in the extracts by HPLC-DAD

	RT		Maximum Wavelength		Compounds	mg/100g extract	
	NP-LF	NP-S	λ max			NP-LF	NP-S
1	ND	8.6	259-292		protocatechuic acid	ND	5.5
2	15.8	15.3	232-284		catechin der.	83.8	57.7
3	20.4	20.3	330-300sh-232		rosmarinic acid der.	1055.9	164.9
4	21.4	21.2	293		<i>p</i> -OH benzaldehyde	2.8	16.2
6	22.0	21.7	326-295sh-237		chlorogenic acid	86.9	6.7
7	22.9	ND	328-295-242		caffeic acid	75.9	ND
8	ND	22.9	315-230		<i>p</i> -coumaric acid der.	ND	14.2
9	23.7	ND	333-243		chicoric acid der.	2.8	ND
10	ND	23.9	281-229		syringic acid der.	ND	5.4
11	24.5	24.3	329-302sh-249		rosmarinic acid der.	84.3	31.9
12	25.2	25.0	330-300sh-243		rosmarinic acid der.	29.0	6.7
13	25.9	25.7	243 and 257 mix		<i>p</i> -OH benzoic acid equivalent	2204.7	1605.3
14	26.8	26.6	229-310		<i>p</i> -coumaric acid	3.7	2.4
15	27.1	26.8	352-255		luteolin-7-glycoside der.	12.7	5.7
16	28.9	ND	312-295-228		<i>p</i> -coumaric acid der.	11.6	ND
17	29.2	29.0	329-305sh-243		chicoric acid	3.7	2.1
18	ND	30.8	329-233		rosmarinic acid der.	ND	3.7
19	31.5	31.2	338-253-225		apigenin-glycoside der.	54.4	3.9
20	ND	31.4	342-246-226		luteolin-glycoside der.	ND	2.5
21	32.4	ND	327-228 and 347-270		ferulic acid der. and luteolin-7-glycoside	mix	ND
22	ND	32.4	320-244		caffeic acid der.	ND	1.2
23	33.2	33.0	228-278		syringic acid der.	31.4	20.1

24	33.4	33.2	228-278	syringic acid der.	17.8	17.3
25	ND	33.4	331-275	apigenin-glycoside der.	ND	3.2
26	ND	34.1	338-275	apigenin-glycoside der.	ND	5.6
27	35.4	35.3	330-290sh-229	rosmarinic acid	3099.7	59.1
28	ND	35.7	314-230	<i>p</i> -coumaric acid der.	ND	2.7
29	36.6	ND	328-300sh-234	caffeic acid der.	21.6	ND
30	ND	38.3	319-230-295sh	ferulic acid der.	ND	6.8
31	38.7	38.6	328-277-226	tangeretine der.	10.7	43.6
32	39.4	39.2	329-277	chicoric acid der.	6.3	1.6
33	ND	39.4	338-276	apigenin der.	ND	5.6
34	39.8	ND	327-300sh-239	chlorogenic acid der.	8.4	ND
35	ND	41.6	267-340	apigenin der.	ND	6.4
36	ND	42.0	324-270	tangeretin der.	ND	1.6
38	ND	45.1	328-277-214	tangeretin der.	ND	1.4
39	ND	49.8	327-275-223	tangeretin der.	ND	7.4
40	ND	50.3	316	<i>p</i> -coumaric acid der.	ND	16.2
41	50.4	50.6	315-214	<i>p</i> -coumaric acid der.	11.5	0.9
				total	6919.7	2135.2
				total rosmarinic acids	4269.0	266.3

Since *Nepeta pilinux* is an endemic species and newly recorded in Şanlıurfa flora, there is not any scientific report for its phenoreverse phase chromatography (Table 2). Tangeretin derivatives may differ from each other in the number of hydroxyl and methoxyl groups and the presence of sugar or other functional groups. Thymusin which is the 5,6,4'-Trihydroxy-7,8-dimethoxyflavone (5,6,4' demethyl-tangeretin) and isothymusin were determined in *Nepeta asterotricha* Rech. (29). Therefore, two of the tangeretin der. could be thymusin and isothymusin. Apigenin and luteolin derivatives, determined in the extracts based on their UV spectra, were identified and quantified as apigenin, apigenin glycoside der. or luteolin glycoside der. based on their elution orders.

lic composition. On the other hand, there are some reports for chemical composition of the other species of *Nepeta* genus to compare with. For instance, epicatechin, caffeic acids, chlorogenic acid, quercetin and ellagic acid, well-known as antioxidant compounds were found in the ethanol extract of *Nepeta cadmea* Boiss. by HPLC-DAD (27). They couldn't have determined RA because it was not in their standard compound list. Unlike their results, epicatechin, quercetin and ellagic acid were not detected in *Nepeta pilinux* extracts (Table 2). Observation of similar but different phenolic compounds in species shows that differences between species also cause differences in metabolic product synthesis. In addition, different derivatives of phenolic compounds can be observed in samples of the same species grown in different geographical conditions. RA, apigenin, and quercetin were determined as major compounds in the ethanol

extract of *Nepeta nuda* subsp. *albiflora* (28). Isolation of some iridoid glycosides such as nepetamoside, nepetaracemoside B, nepetonic acid and some polyphenol and flavonoid components such as RA and its methyle ester, thymusin, luteolin and apigenin from *Nepeta asterotricha* Rech. were performed by Goldansaz et al. (2019) (29). Methanolic extracts from *Nepeta rtanjensis* Diklic & Milojević which is an endemic perennial plant, in a very limited area in Southeast Serbia were investigated in a scientific study (30). The presence of high levels of chlorogenic acid, RA and rutin in these extracts was thought to be the reason for their antigenotoxicity.

RA, which is the main component in these extracts, is synthesized by the phenylpropanoid pathway starting with L-phenylalanine and L-tyrosine. From L-phenylalanine, *t*-cinnamic acid, *p*-coumaric acid and *p*-coumaroyl-CoA are successively produced, while *p*-hydroxyphenylpyruvic acid, *p*-hydroxyphenyllactic acid are successively produced from L-tyrosine. Then, the production of *p*-coumaroyl-*p*-hydroxy-phenyllactic acid by condensation of *p*-coumaroyl-CoA and *p*-hydroxyphenyllactic acid is followed by RA synthesis (54). Chlorogenic acid is synthesized by the condensation of *p*-coumaroyl-CoA with quinic acid (55). These metabolites which were found in the *Nepeta pilinux* extracts, support the survival of plants against harsh environmental conditions, therefore they have been seen by humans as a remedy for various diseases for many years. It has been reported that RA, chlorogenic acid and its metabolite caffeic acid have a neuroprotective effect due to their antioxidant capacity (56, 57).

c) *Total Antioxidant Characterization of the Methanol Extracts*

Total phenolic content (TPC) and radical scavenging activities (RSA) against DPPH and ABTS radical were evaluated to characterize the antioxidant capacity of the extracts and results were presented in Table 3. TPC of the NP-LF and NP-S extract from *Nepeta pilinux* was 50.81 and 13.37 mg GAE/g respectively. Consistent with the TPC of NP-LF which was found around fourfold of NP-S, RSA of NP-LF were higher (433.18 and 82.29 µg / mL for DPPH and ABTS respectively) than NP-S as expected (Table 3). The antioxidant capacity of this species was found to be quite consistent comparing with other species in the literature reports. Antioxidant activity of methanolic extracts from flower and leaf parts of *Nepeta itanjensis* were reported by Bošnjak-Neumüller et al. (2017). They have found that the leaf extract had higher antioxidant capacity with TPC of 62.73 mg of GAE/g and IC<sub>50</sub> value

of RSA against DPPH as 112.59 µg/mL than those of flower extract. The antioxidant activities of ethanol, methanol, acetone, and water extracts from *Nepeta cadmea* were presented by Kaska et al. (2018). They have found that the water extract had the highest RSA (IC<sub>50</sub> value of DPPH as 25.54 µg/mL and ABTS, 14.51 µg/mL) in these four extracts. Highest TPC with 79.84 mg GAE/g, was found in the methanol extract while the highest total flavonoids with 77.09 mgQE/g was in the acetone extract. It was reported by Teber and Bursal (2020) that ethanol and water extracts of *Nepeta nuda* subsp. *albiflora* had strong antioxidant effects with IC<sub>50</sub> values of DPPH as 54.4 and 113.0 µg/mL, respectively. The TPC of flowers, leaves and roots methanol extracts of *Nepeta humulis* were found as 123.18, 66.20 and 54.77 mg GAE/g extract, respectively. Flower extract which had the highest TPC displayed best RCA with IC<sub>50</sub> of 1290 and 350 µg.mL<sup>-1</sup> against DPPH and ABTS respectively (58).

Table 3: Total phenolic content, radical scavenging activity and enzyme inhibition of the extracts

Samples and standards	TPC <sup>a</sup>		RSA <sup>b</sup>		Enzyme inhibition	
	mgGAE/g	mgQE/g	DPPH SC <sub>50</sub>	ABTS SC <sub>50</sub>	urease IC <sub>50</sub>	XO IC <sub>50</sub>
NP-LF	50.81±1.50	35.40±1.06	433.18±12.74	82.29±0.98	62.47±0.10	48.48±0.10
NP-S	13.37±0.34	9.03±0.24	523.49±5.82	381.58±5.15	230.59±0.23	222.67±0.13
Gallic Acid			1.52±0.06	3.29±0.09		
Quercetin			5.87±0.13	8.52±0.16		
Acetohydroxamic acid					24.56±0.29	
Allopurinol						0.54±0.04

GAE, Gallic acid equivalent; QE, quercetin equivalent; SC<sub>50</sub>, value of the concentration of extract required to scavenge 50% of DPPH and ABTS radicals (µg extract per mL methanol); IC<sub>50</sub>, value of the concentration of extract required to inhibit 50% of *Jack bean* urease and bovine milk xanthine oxidase enzymes (µg extract per mL methanol). <sup>a</sup>Total phenolic contents are expressed in mg GAE/g extract and mg QE/g extract. <sup>b</sup>Radical Scavenging Activity

d) *Urease and Xanthine oxidase inhibitions of the methanol extracts*

The urease enzyme inhibition of the NP-LF with IC<sub>50</sub> value of 62.47 µg.mL<sup>-1</sup> was only three times lower than the inhibition of acetohydroxamic acid (24.56 µg.mL<sup>-1</sup>) which is standard medicine (Table 3). NP-S had low inhibition against to this enzyme with IC<sub>50</sub> value of 230.59 µg.mL<sup>-1</sup>. The xanthine oxidase inhibition of the NP-LF and NP-S extracts, 48.48 and 222.67 µg.mL<sup>-1</sup> respectively, were quite lower comparing to the inhibition of allopurinol (0.54 µg.mL<sup>-1</sup>) which is standard medicine reducing the production of uric acid in the body caused by certain cancer medications and kidney stones. Akdeniz et al. (2020) were screened urease inhibition effect of the essential oils and ethanolic

extracts of *Nepeta heliotropifolia* and *Nepeta congesta* subsp. *cryptantha* comparing with the standard thiourea. They reported that none of them exhibited urease inhibitory activity (47). In another study, ethyl acetate sub fraction of *Nepeta praetervis* showed significant urease inhibitory activity (68%) (59). The structure-activity relationship revealed that the planar flavones and flavonols with a 7-hydroxyl group such as chrysin, luteolin, kaempferol, quercetin, myricetin, and isorhamnetin inhibited xanthine oxidase activity at low concentrations, while the nonplanar flavonoids, isoflavones and anthocyanidins were less inhibitory (35). Although the inhibitory effects of the extracts cannot compete with acetohydroxamic acid and allopurinol, the fact that they are a natural herbal inhibitor source shows that these extracts are more suitable for use.

IV. CONCLUSION

This was the first investigation on the chemical composition and bioactivities of the *Nepeta pilinux*. The polar and apolar extracts of aerial parts had high amount of phenolic and essential oil compounds and demonstrated the potential antioxidant capacities. The polar extract with 3.1% rosmarinic acid had urease and

xanthine oxidase inhibition as well. This comprehensive evaluation of *Nepeta pilinux* revealed that this endemic plant could be the source of valuable therapeutic compounds. Besides, this report would be the incentive for further works on this plant's metabolites.

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#### Disclosure Statement

No potential conflict of interest was reported by the authors

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## Dispersion Devices using a Fourier Analyzer

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**Abstract-** The paper considers the possibility of optimizing the parameters of dispersion devices for gas analysis, which use correlation reception of the useful signal and are used for the analysis of gas mixtures in the visible and UV regions of the spectrum. The factors affecting the optimal filtering of the useful signal in the electronic path of the device are determined, and methods of eliminating this influence, including the background component of the signal, are proposed. As an example of the use of gas analysis devices with correlated selection of a useful signal in the electronic path of the analyzer, the structural diagram of the device for the analysis of SO<sub>2</sub> in the gases of thermal power plants is described.

**Keywords:** *gas analyzer; correlation signal selection; electronic channel.*

**GJSFR-B Classification:** *FOR Code: 030101*



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# Dispersion Devices using a Fourier Analyzer

## ДИСПЕРСІЙНІ ПРИЛАДИ З ВИКОРИСТАННЯМ ФУР'Є АНАЛІЗАТОРА

V. Kozubovskyi <sup>α</sup> & Yu. Bllak <sup>σ</sup>

**Abstract-** The paper considers the possibility of optimizing the parameters of dispersion devices for gas analysis, which use correlation reception of the useful signal and are used for the analysis of gas mixtures in the visible and UV regions of the spectrum. The factors affecting the optimal filtering of the useful signal in the electronic path of the device are determined, and methods of eliminating this influence, including the background component of the signal, are proposed. As an example of the use of gas analysis devices with correlated selection of a useful signal in the electronic path of the analyzer, the structural diagram of the device for the analysis of SO<sub>2</sub> in the gases of thermal power plants is described.

**Keywords:** gas analyzer; correlation signal selection; electronic channel.

**Абстрактний:** В роботі розглянута можливість оптимізації параметрів дисперсійних приладів газового аналізу, які використовують кореляційний прийом корисного сигналу і застосовуються для аналізу газових сумішей у видимій та УФ областях спектру. Визначено фактори, які впливають на оптимальну фільтрацію корисного сигналу в електронному тракті приладу, запропоновано методи усунення цього впливу, в тому числі і фонові складові сигналу. Як приклад використання приладів газового аналізу з кореляційним виділенням корисного сигналу в електронному тракті аналізатора описана структурна схема приладу для аналізу SO<sub>2</sub> у газах теплових електростанцій.

### 1. ВСТУП

Зазначеними даними по Україні основними забруднювачами атмосфери міст є пил і викиди автотранспорту — в основному важкі вуглеводні, формальдегід, бензопірен, діоксид азоту, а також важкі метали. Адже саме ці речовини, за словами лікарів, є одними з основних збудників онкологічних захворювань.

Серед інших причин забруднення повітря міст фахівці називають скорочення площі зелених насаджень. Забезпечення надійного та однозначного контролю викидів небезпечних речовин у навколишнє середовище є одним з найбільш актуальних завдань для екології.

Серед методів контролю викидів газоподібних речовин найбільш перспективними і широко вживаними методами є оптичні абсорбційні методи. Вони демонструють високу точність, надійність

метрологічних параметрів, хороші експлуатаційні характеристики.

Для підвищення селективності абсорбційних оптичних приладів часто використовуються методи кореляційного аналізу.

Останнім часом стали широко використовувати кореляційні типи приладів з виділенням корисного сигналу в електронному тракті. Вони основані на скануванні з великою частотою вузького спектрального діапазону (20-40) нм, у якому перебувають смуги поглинання досліджуваних газів, що мають характерну структуру і дозволяють ідентифікувати велику кількість газових компонентів, лінії поглинання яких лежать в межах області спектра, що сканується і мають характерну структуру внаслідок коливальних (для УФ області спектру) або обертальних (для ІЧ області) рухів молекули. Такі прилади, як правило, використовують для наукових досліджень при вивченні процесів, що швидко протікають [1]. Сканування спектру здійснюється швидким переміщенням дифракційної решітки, поворотного дзеркала монохроматора, плоскопаралельної пластини, встановленої на шляху його променів, вихідної щілини монохроматора [2]. При детектуванні спектру, що сканується за допомогою фотоприймача, періодичний електричний сигнал тієї або іншої форми в залежності від наявності газу, що визначається в атмосферному повітрі, надходить у систему реєстрації. Ідентифікація газових компонентів за характерними особливостями періодичного сигналу проходить найчастіше за рахунок формування синхроімпульсів, які поступають в систему реєстрації з визначеною частотою в залежності від періоду структури досліджуваного газового компонента [3,4,5]. Однак можливий і інший шлях - фільтрація корисного електричного сигналу в системі реєстрації за допомогою нечутливих до зміни форми сигналу фільтрів [6]. На цьому принципі були створені прилади для аналізу SO<sub>2</sub> в газоподібних викидах теплових електростанцій і NH<sub>3</sub> при технологічних процесах [7,8].

Електронні смуги поглинання, наприклад, SO<sub>2</sub> мають яскраво виражену характерну коливальну структуру (див.рис.1). Тому у вихідній площині поліхроматора, при наявності в робочій кюветі SO<sub>2</sub>, буде спостерігатися спектр SO<sub>2</sub> у вигляді "світлих" і "темних" смуг, що чергуються (в максимумах поглинання спектру випромінювання послаблюється, в мінімумах - залишається без істотних змін). При скануванні цього спектру з частотою  $\omega_p$  за

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допомогою, наприклад, нарізаних на обертовому диску радіальних вихідних щілин (число щілин вибирається з умови, щоб у зоні сканування в кожний момент часу знаходилася тільки одна щілина), на виході фотоприймача (фотоелектронного помножувача - ФЕП) з'являється електричний сигнал з певною "резонансною" для  $\text{SO}_2$  частотою  $\omega_0$ . Амплітуда цього електричного сигналу пропорційна концентрації  $\text{SO}_2$ .

Частота  $\omega_0$  залежить від частоти сканування  $\omega_p$  і кількості  $n$  ліній поглинання на ділянці спектру аналізованого газу (див.рис.1).

Співвідношення цих частот  $\omega_0/\omega_p = n$ . В електронному тракті приладу здійснюється фільтрація отриманого сигналу. Як видно з рис.1, сигнал має складову з частотою  $\omega_p$ , пов'язану з наявністю інтегрального поглинання випромінювання, яке збільшується зі зменшенням довжини хвилі.

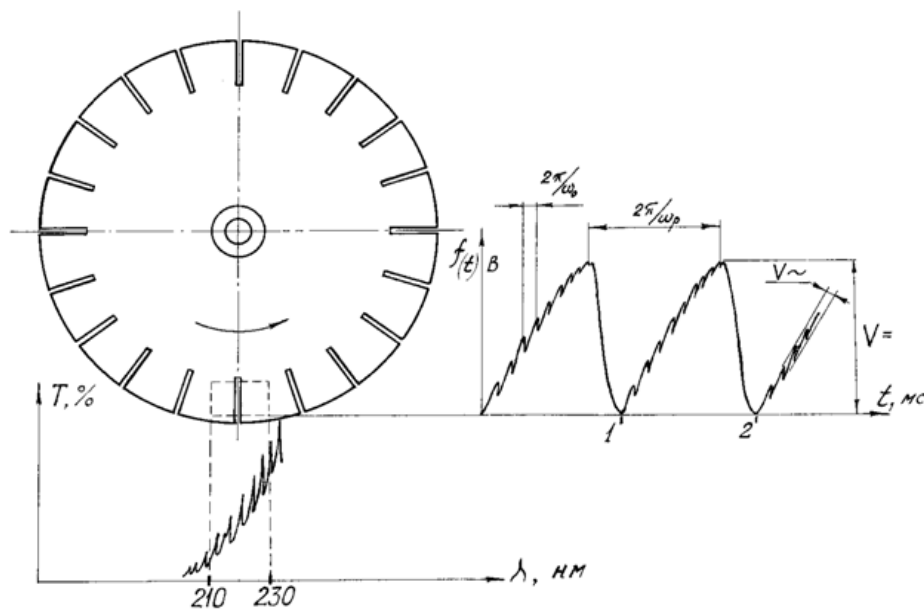


Рис. 1: Сканування спектру поглинання  $\text{SO}_2$  у вихідній площині спектрометра за допомогою вихідної щілини, що обертається

Тому корисний сигнал на частоті  $\omega_0$  спостерігається на фоні пілоподібного сигналу з частотою  $\omega_p$ . Амплітуди  $I_{\omega_0}$ ,  $I_{\omega_p}$  обох частотних складових залежать від інтенсивності світлового потоку, що надходить на фотоприймач, від величини інтегрального поглинання аналізованим газом, неселективних втрат випромінювання. Амплітуда сигналу на частоті  $\omega_0$  залежить ще й від величини диференціального поглинання в лініях тонкої структури спектру. Таким чином, відношення амплітуд сигналів  $I_{\omega_0}/I_{\omega_p}$  визначається тільки диференціальним поглинанням випромінювання аналізованим газовим компонентом і не змінюється при варіаціях інтенсивності джерела випромінювання, неселективних втрат, зміні рівня інтегрального поглинання за рахунок наявності, наприклад, газових компонент, що заважають.

На рис.2 наведені ділянки спектрів  $\text{NO}$ ,  $\text{NH}_3$ ,  $\text{SO}_2$  в області 200-230 нм і  $\text{NO}_2$  в області 430-450 нм. Як бачимо, спектри мають характерну структуру. Ділянки спектрів  $\text{NO}$ ,  $\text{SO}_2$ ,  $\text{NH}_3$  знаходяться на краю інтенсивних електронних смуг поглинання, тому інтегральне поглинання значно змінюється зі зменшенням довжини хвилі. Одержані в результаті

розрахунків гармонічні склади часових сигналів, що знімаються з фотоприймача при скануванні, наведені на рис.2.а, ділянки відповідних спектрів зображені на рис.2.б. Отримані розрахункові залежності перевірялися експериментально за допомогою скануючого з великою  $\omega_0$  ділянки (наприклад,  $\text{NH}_3$ ,  $\text{SO}_2$ ) у спектрі електричного сигналу присутні дві основні гармоніки - перша відповідає частоті  $\omega_p$ , і друга ( $n$ -та) -  $\omega_0$ , де  $n$  - кількість ліній поглинання на сканованій ділянці спектру. Так, при скануванні ділянки спектру  $\text{NH}_3$  200-220 нм частота  $\omega_0$  відповідає п'ятій гармоніці, і дев'ятій гармоніці ( $n = 9$ ) при скануванні ділянки 210-225 нм  $\text{SO}_2$ . Якщо ж сканується не ціле число періодів структури спектру, наприклад  $n = 4,5$ , то інтенсивними є 4 і 5 гармоніки спектру електричного сигналу.

Для  $\text{NO}$  на спектральній ділянці 200-230 нм спостерігається всього 3 вузьких піки поглинання. Однак, оскільки лінії поглинання мають вигляд дельта-функцій, то окрім 3-ої гармоніки спостерігається ряд інтенсивних більш високих гармонік.

У разі ж  $\text{NO}_2$  на ділянці 433-450 нм знаходяться найбільш інтенсивні чотири лінії



поглинання, ширина і форма яких різні і тому поряд з гармонікою  $n = 4$  спостерігається ряд інтенсивних більш високих гармонік.

Отже, у разі аналізу газових компонентів з аперіодичною структурою спектра (наприклад,  $\text{NO}_2$ ),

або з ширинами ліній поглинання значно меншими періоду структури (лінії поглинання  $\text{NO}$  мають вигляд дельта-функцій) спектр електричного сигналу, що знімається з фотоприймача є досить складним і містить низку гармонік.

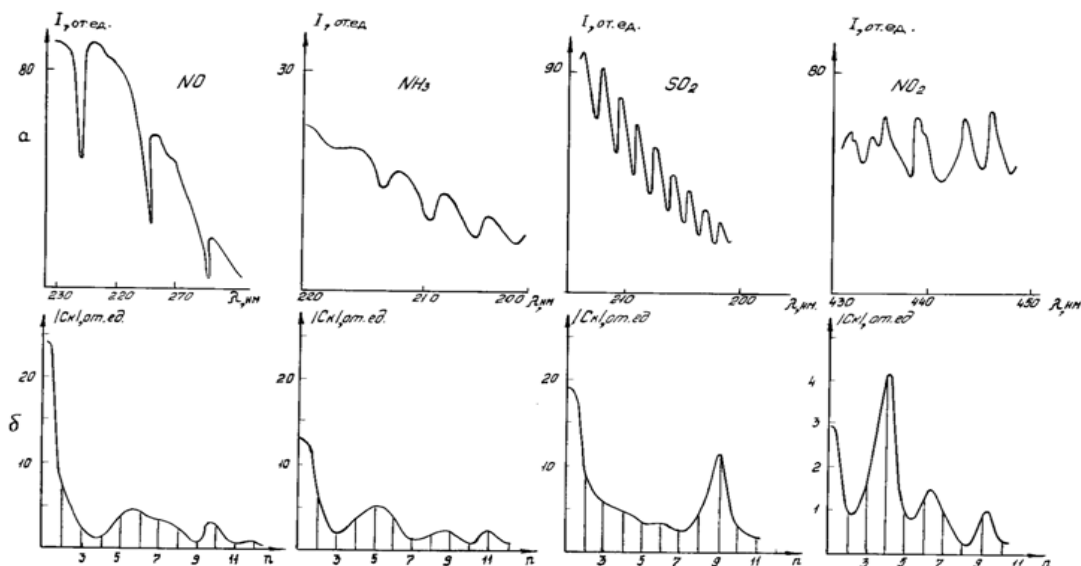


Рис. 2: Залежність світлового потоку від довжини хвилі у вихідній площині спектрометра для різних газів (а) та спектри електричних сигналів, що знімаються з фотоприймача спектрометра при скануванні вихідної щілини (б)

Якщо ж структура спектра має хорошу періодичність ( $\text{SO}_2$ ,  $\text{NH}_3$ ), то спостерігається, в основному, тільки одна  $n$ -та гармоніка, амплітуда якої залежить від концентрації аналізованого компонента в газовій суміші.

*Вплив на спектр корисного сигналу параметрів скануючого спектрометра.*

Досліджувався вплив на гармонічний склад корисного сигналу зміни ширини щілин скануючого монохроматора, концентрації досліджуваного газу, зміщення в площині вихідної щілини спектру досліджуваного газу, вибору ширини ділянки спектру, що сканується. Як буде показано нижче, всі ці параметри мають істотний вплив на гармонічний склад і величину корисного сигналу.

Експериментальна установка складалася з освітлювача на основі дейтерієвої лампи ДДС-30 (оптичної лампи ОП8-9), кварцової кювети довжиною  $L = 100\text{мм}$ , монохроматора МДР-3 зі зворотною лінійною дисперсією  $1,3\text{ нм/мм}$  в області  $(0,2-0,6)\text{ мкм}$ , фотоприймача ФЕП-142 (ФЕП-86) підключеного до самописця через узгоджувальний підсилювач.

У кювету напускалися газові суміші  $\text{NH}_3$  в азоті різної концентрації.

*Зміна ширини вхідної і вихідної щілини монохроматора.* Ширина щілин змінювалась у межах від  $0,1$  до  $0,25\text{ мм}$ . Концентрація в кюветі дорівнювала  $1000\text{ млн}^{-1}$ . При цьому спектральна ширина щілин була значно менше періоду  $D$  структури спектру поглинання

$\text{NH}_3$ . У таких умовах знімався спектр поглинання  $\text{NH}_3$  в області від  $190$  до  $230\text{ нм}$ . Для розрахунків вибиралась ділянка спектру  $(200-220)\text{ нм}$  і визначався гармонічний склад корисного сигналу при послідовному скануванні цієї ділянки.

Результати розрахунків наведено на рис. 3. Як бачимо, при збільшенні ширини щілин величина корисного сигналу (6-ої гармоніки) збільшується. Збільшується і відношення амплітуд гармонік  $|C_6|/|C_1|$ , величина  $[|C_6| - (|C_5| + |C_7|)]/2 / |C_1|$ , тобто корисний сигнал з врахуванням фонові складової, віднесеної до основної гармоніки частоти сканування.

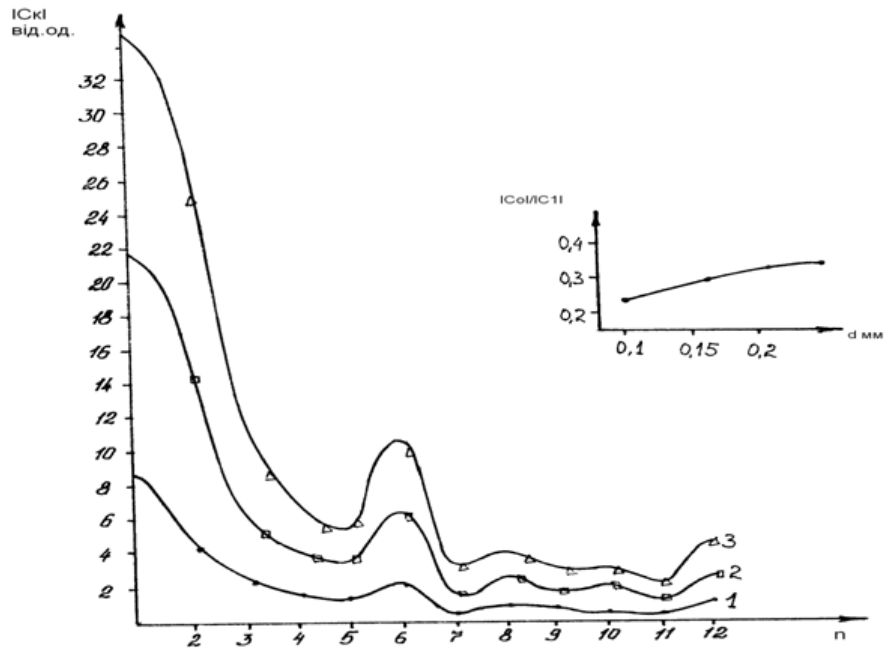


Рис. 3: Зміна амплітуд гармонік електричного сигналу при зміні ширини  $d$  вхідної і вихідної щілин скануючого спектрометра

До яких же меж необхідно збільшувати ширину щілин? Спектральна ширина щілин повинна бути:

$\Delta\lambda = 0,5D$  для досягнення максимальної величини сигналу;

{ (1)

$\Delta\lambda = 0,371D$  для отримання максимального відношення сигнал/шум (СШВ).

Підставляючи параметри спектру поглинання  $\text{NH}_3$  і монохроматора МДР-3 у вираз для спектральної ширини щілин [9]:

$$d\lambda = D_e \Delta x, \quad (2)$$

де  $D_e$  - зворотна лінійна дисперсія, і враховуючи (2), отримуємо оптимальне значення геометричної ширини щілин:

$$\Delta x_{\max} = 1.5 \text{ мм}; \quad \Delta x_{\text{сшв}} = 1.15 \text{ мм}.$$

Тобто збільшення до цих меж ширин вхідної і вихідної щілин буде приводити до зростання величини корисного сигналу (ширини вхідної і вихідної щілин зазвичай вибирають рівними).

Зміна гармонічного складу корисного сигналу при збільшенні концентрації досліджуваного газу. В газову кювету послідовно напускались концентрації  $\text{NH}_3$  рівні  $\chi_1 = 250 \text{ млн}^{-1}$ ,  $\chi_2 = 800 \text{ млн}^{-1}$ ,  $\chi_3 = 1600 \text{ млн}^{-1}$ . Для кожного значення концентрації знімався спектр у діапазоні довжин хвиль від 190 до 230 нм і за допомогою перетворення Фур'є визначався гармонічний склад корисного сигналу. Результати експерименту наведено на рис. 4. Як видно з рис. 4, зі збільшенням

концентрації досліджуваного газу максимум розподілу гармонік корисного сигналу зміщується в бік більш низькочастотних гармонік.

Це, мабуть, пов'язано з тим, що зі збільшенням концентрації досліджуваного газу лінії поглинання ширшають і структура спектру  $\text{NH}_3$  стає ближчою до синусоїдальної, що і призводить до зменшення вкладу високочастотних гармонік в корисний сигнал.

З наведеного експерименту випливає, що для вимірювання концентрації досліджуваного газу в широких межах необхідно детектувати корисний сигнал на декількох близьких гармоніках, пов'язаних з наявністю структури смуги поглинання досліджуваного газу.

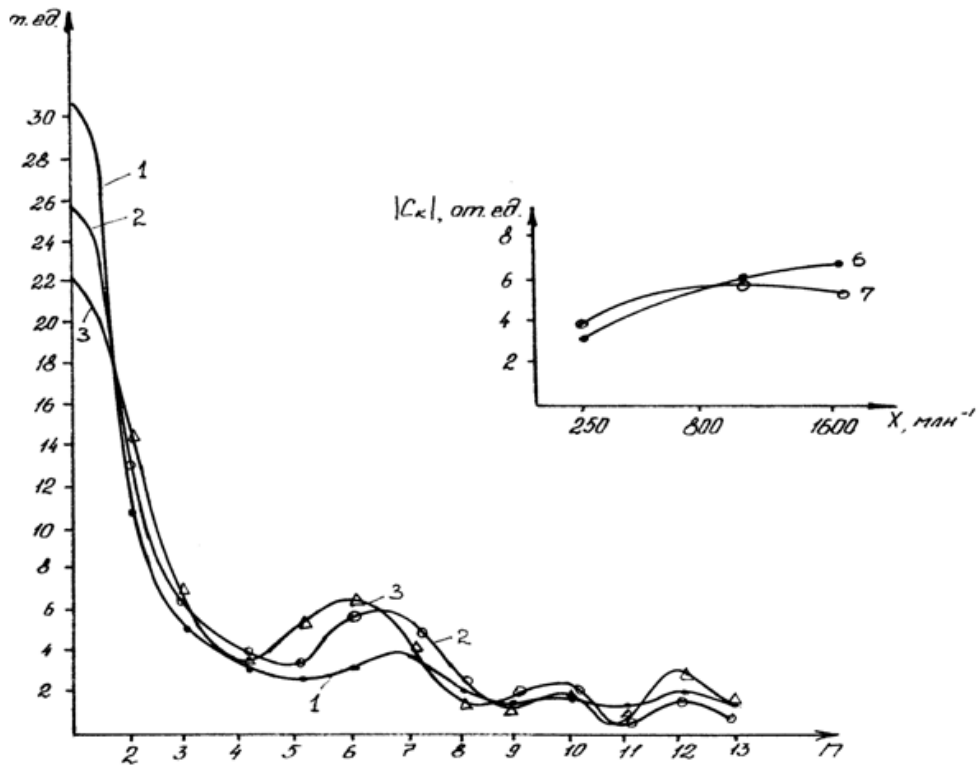


Рис. 4: Перерозподіл амплітуд гармонік корисного сигналу при збільшенні концентрації  $\chi \text{NH}_3$

Зсув ділянки спектру, що сканується. Дослідження проводилися при використанні концентрації  $\text{NH}_3$  або  $\text{NO}_2$  в кюветі рівній  $1000 \text{ млл}^{-1}$ . Знімався спектр поглинання  $\text{NH}_3$  в області (190-230) нм та  $\text{NO}_2$  в області (430-460) нм. З отриманих спектрів вибиралися зміщені один відносно одного більш вузькі ділянки спектра і проводилося обчислення їхніх Фур'є образів.

На рис.5 наведено перерозподіл амплітуд гармонік в разі зміщення спектру  $\text{NH}_3$  (а), структура якого квазіперіодична, і  $\text{NO}_2$  (б), що має значну аперіодичність структури. Як бачимо, зсув сканованої ділянки спектру призводить до значного перерозподілу амплітуд гармонік.

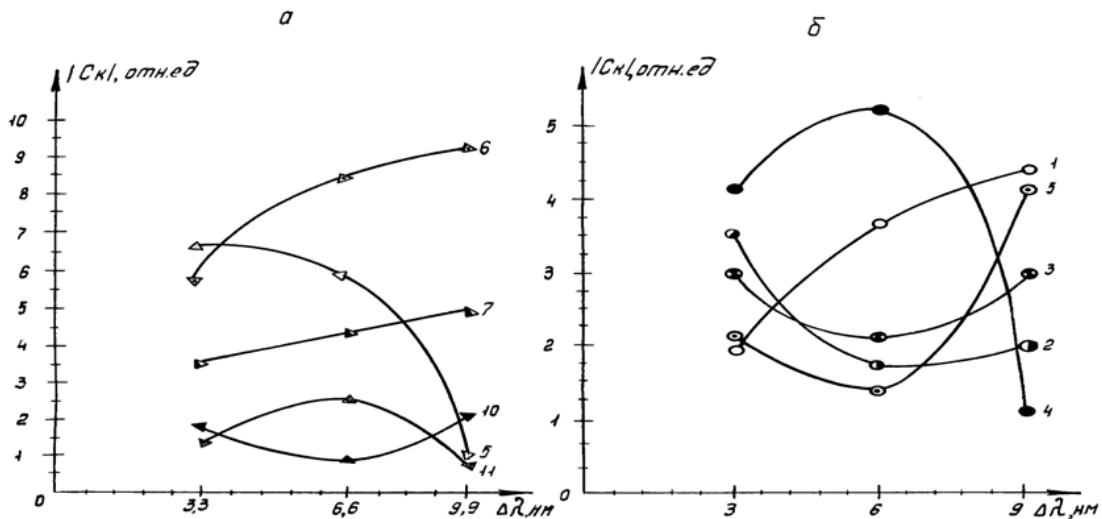


Рис. 5: Перерозподіл амплітуд гармонік корисного сигналу у випадку зміщення спектрів  $\text{NH}_3$  (а) та  $\text{NO}_2$  (б) у вихідній площині спектрометра

Причому у другому випадку амплітуди гармонік зазнають суттєвих змін вже починаючи з першої гармоніки, в першому - значно змінюються амплітуди тільки більш високих гармонік. З рис. 5 випливає, що при ретельному виборі ділянки спектру можна значно збільшити амплітуду гармоніки, пов'язану з наявністю досліджуваного газу в кюветі, а значить, і підвищити відношення сигнал/шум при вимірах корисного сигналу. Тому, вибору ділянки спектра і стабільності його положення в площині вихідної щілини монохроматора слід приділяти значну увагу.

*Вибір ширини ділянки спектра, що сканується.*

При середньоквадратичному детектуванні корисного сигналу, що зазвичай прийнято в газоаналітичних приладах, його величина визначається площею, що знаходиться під обвідною корисного сигналу. Причому ця площа залежить, при нецілому числі сканованих періодів  $D$  структури спектру смуги поглинання, від початкової фази (початкової довжини хвилі) сканування.

Дійсно, нехай, наприклад, сканується  $m = 4,5$  періодів  $D$  структури спектру  $\text{NH}_3$ . При незначних концентраціях  $\text{NH}_3$  в кюветі сканований спектр може

бути представлений у вигляді позитивних напівперіодів синусоїди. Тоді сигнал, що знімається з ФЕП, може бути записаний у вигляді:

$$I_0 \sin \pi t / \tau, \text{ при } 2n\tau < t < (2n+1)\tau \quad I(t) = \begin{cases} I_0 \sin \pi t / \tau, & \text{при } 2n\tau < t < (2n+1)\tau \\ -I_0 \sin \pi t / \tau, & \text{при } (2n+1)\tau < t < 2(n+1)\tau \end{cases} \quad (3)$$

де  $n = 0, 1, 2 \dots k$ ;  $\tau = D / \Delta \lambda f_0$  - період сигналу, що відповідає періоду структури, досліджуваного газу;  $f_0$  - частота сканування спектральної ділянки  $\Delta \lambda = m D$ .

Зазвичай досліджувана ділянка спектру виділяється діафрагмою, спектральна ширина якої дорівнює  $\Delta \lambda$  і розміщеної у площині вихідної щілини (в безпосередній її близькості). Тоді, у разі вимірювання положення спектру щодо діафрагми, можливий випадок, коли сканується 4 цілих періоди структури спектра і 0,5 періода, і коли сканується 4 цілих періоди і два по 0,25 періоди (див. рис.6). У першому випадку величина сигналу після детектування буде дорівнювати:

$$I_1 = 4I_0 \int_0^{\tau} \sin \pi t / \tau dt + I_0 \int_0^{\tau/2} \sin \pi t / \tau dt = 9 I_0 \tau / \pi \quad (4)$$

у другому:

$$I_2 = 4I_0 \int_0^{\tau} \sin \pi t / \tau dt + 2I_0 \int_0^{\tau/4} \sin \pi t / \tau dt = 8,6 I_0 \tau / \pi \quad (5)$$

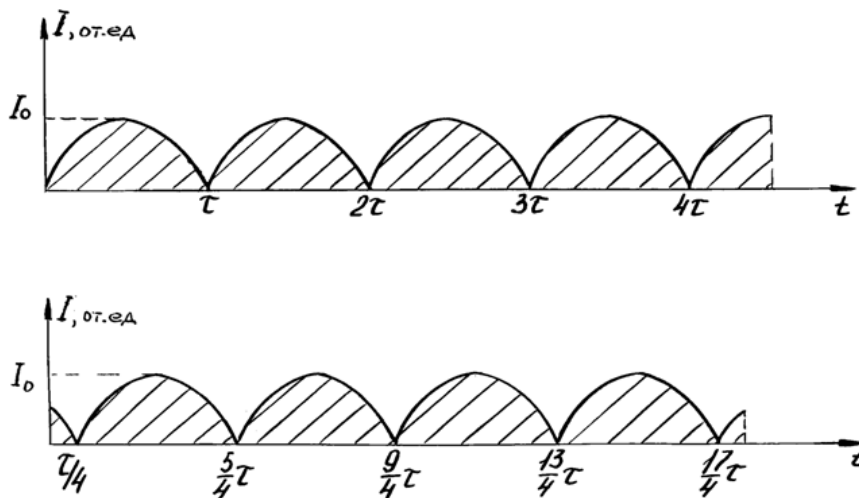


Рис. 6: Величина корисного сигналу при скануванні  $(4+0,5)$  періодів структури спектру аналізованого газу (а) та  $(4+2 \cdot 0,25)$  (б)

Таким чином, відносна зміна сигналу при зсуві спектру досліджуваного газу щодо діафрагми дорівнюватиме:

$$\Delta = (I_1 - I_2)/I_{cp}100\% = 4,5\%, \quad (6)$$

де  $I_{cp} = (I_1 + I_2)/2$ .

Такі коливання корисного сигналу призводять до значних похибок вимірювання. Так, якщо максимальна концентрація досліджуваного газу дає ослаблення сигналу на 30% (таке значення зазвичай вибирають для досягнення лінійності шкали

газоаналізатора), то інструментальна похибка приладу при зазначених коливаннях корисного сигналу не може бути краще 15%.

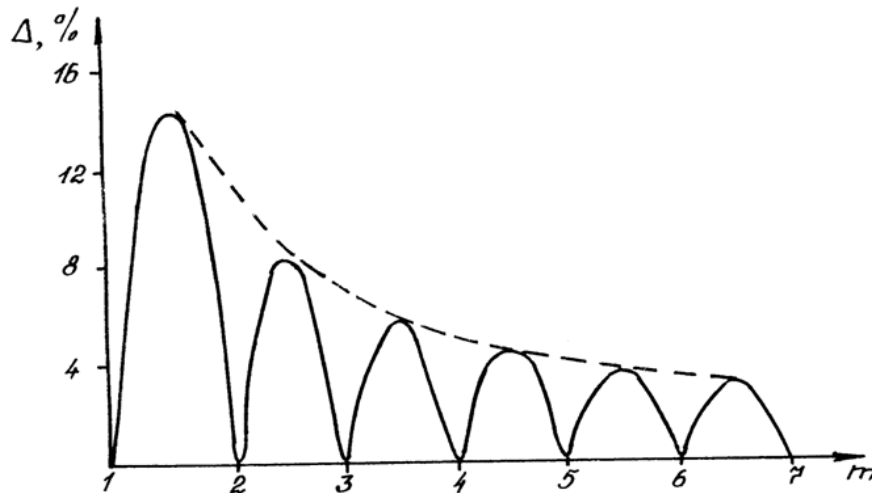


Рис. 7: Зміна величини корисного сигналу при зміщенні спектру аналізованого газу у вихідній площині спектрометру в залежності від кількості періодів спектру, що сканується

Легко бачити, що якщо  $m$  дорівнює цілому числу періодів структури спектру, наприклад  $m = 4$ , то при будь-якому положенні спектру щодо діафрагми величина детектованого сигналу буде одна й та ж:

$$I_1 = I_2 = 4I_0 \int_0^{\tau} \sin \pi t / \tau dt = 8 I_0 \tau / \pi \quad (7)$$

Тобто зміщення спектру досліджуваного газу щодо діафрагми, встановленої за вихідною щілиною і ділянкою спектру, рівне цілому числу періодів структури цього спектру, не призводить до появи додаткової похибки вимірювань.

Звичайно, зі збільшенням числа  $m$  відносний внесок нецілих частин  $\Delta$  зменшується. На рис. 7 показана теоретична залежність відносної зміни корисного сигналу при зсуві спектру досліджуваного газу в площині вихідної щілини в залежності від  $m$ . Як бачимо, зменшення  $\Delta$  при збільшенні  $m$  спочатку

відбувається досить швидко, а далі ця зміна насичується.

*Виділення корисного сигналу в електронному тракті приладу*

Отже, при вимірі концентрації аналізованого газу, що має хорошу періодичність структури спектру, за допомогою приладу на основі скануючого монохроматора необхідно відфільтрувати кілька гармонік корисного сигналу, близьких до  $\pi$ -ої, від інших гармонійних складових електричного сигналу, що знімається з фотоприймача. Для цієї мети може служити узгоджений з сигналом фільтр. Справді, кожен ділянку зображеного на рис. 1 електричного сигналу, можна розглядати як незалежний, окремий відрізок синусоїди з частотою  $\omega_0$ , обмеженою тривалістю і з випадковою фазою. Спектр цього сигналу можна знайти за допомогою перетворення Фур'є. Якщо відрізок синусоїди представити у вигляді:

$$\Omega(t) = \begin{cases} 0, & \text{при } t < 0 \\ \sin \omega_0 t, & \text{при } 0 < t < 2\pi / \omega_0 \\ 0, & \text{при } t > 2\pi / \omega_0 \end{cases} \quad (8)$$

то його спектр буде мати вигляд:

то його спектр буде мати вигляд:

$$\Phi(\omega) = \int_0^{2n\pi/\omega_0} \sin \omega_0 t \exp(i\omega t) dt = 2i\omega_0 / (\omega_0^2 - \omega^2) (-1)^n \sin n\pi\omega/\omega_0 \quad (9)$$

Отриманий спектр зображений на рис 8. Він являє собою центральний максимум, в якому зосереджена основна частина енергії і ряд незначних бічних максимумів.

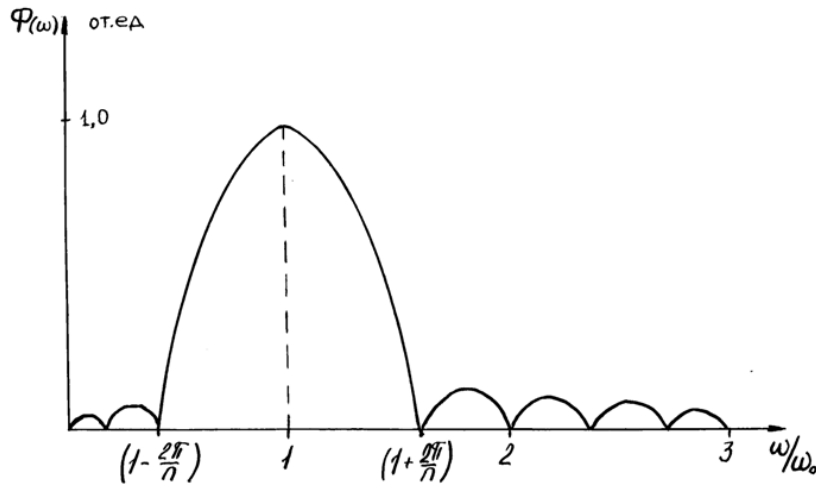


Рис. 8: Спектр електричного сигналу, що знімається з фотоприймача при скануванні  $n$  періодів синусоїдальної структури спектру аналізованого газу

Ширина основного максимуму звужується в міру збільшення кількості періодів синусоїди у пузі і може бути визначена з виразу (9) або, використовуючи відоме співвідношення:

$$\Delta\nu \cdot \Delta t = 1 \quad (10)$$

У даному випадку вона дорівнює:  $\Delta\omega/\omega_0 = 1/n$ .

Тобто, нам необхідно відфільтрувати отриманий спектр від спектру фонового сигналу, пов'язаного, наприклад, з наявністю компонентів, що заважають. У відповідності з теорією оптимальної фільтрації, в разі перешкод з рівномірним спектром передатна функція такого фільтру з точністю до постійного множника повинна бути комплексно спряженою функцією щодо спектра  $\Phi(\omega)$  аналізованого сигналу:

$$k(i\omega) = k \Phi(i\omega). \quad (11)$$

Тобто передатна функція повинна з точністю до постійного множника збігатися зі спектром сигналу, що виділяється. В цьому випадку їх кореляційна функція (відгук фільтру) дорівнює максимально можливій величині:

$$R(\omega)_{max} = \int_{-\infty}^{\infty} \Phi(\omega') \Phi^*(\omega' - \omega) d\omega \quad (12)$$

Таким чином виділення корисного сигналу в електронному тракті кореляційного аналізатора відбувається за рахунок кореляції спектру цього сигналу з еталонним, записаним в пам'ять приладу.

Експериментально вивчається спектр корисного сигналу при скануванні з частотою  $\omega_p = 1$  кГц ділянки смуги поглинання  $\text{SO}_2$  від 210 до 230 нм. Суміш  $\text{SO}_2$  в  $\text{N}_2$  концентрацією 200 млн<sup>-1</sup> напускалася у внутрішню кювету оптичного блоку приладу ФГ 01-1. З ФЕП-142 оптичного блоку знімався часовий сигнал, зображений на рис. 1. Цей сигнал подавався далі на селективний вольтметр В6-9 і з його допомогою вивчався спектральний склад корисного сигналу. Експериментально отриманий спектр сигналу зображений на рис. 9. Максимум на 10-ій гармоніці обумовлений наявністю  $\text{SO}_2$ .



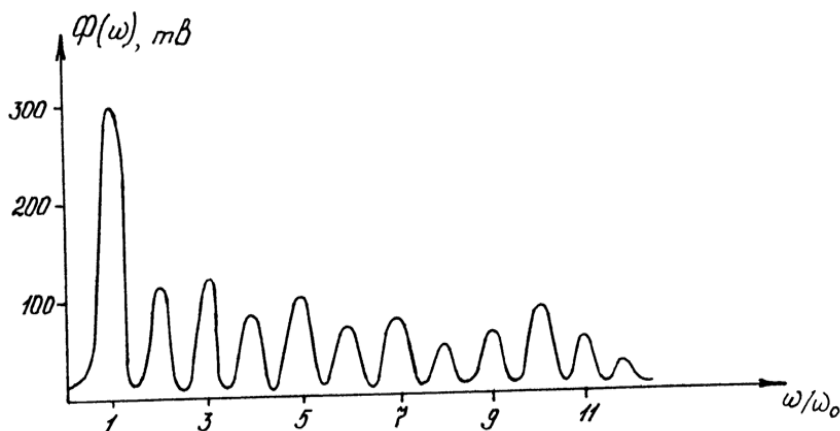


Рис. 9: Спектр електричного сигналу, що знімається з ФЕП 142 оптичного блоку приладу ФГ01-1 при концентрації  $\text{SO}_2$   $x=200\text{млн}^{-1}$

Як бачимо, непарні гармоніки мають більшу амплітуду ніж парні. Це пов'язано, можливо, з биттям диску сканованої вихідної щілини. Ширина гармонійних складових дорівнює  $\approx 200$  Гц.

## II. СТРУКТУРНА СХЕМА АНАЛІЗАТОРА ДИОКСИДУ СІРКИ

Структурна схема кореляційного аналізатора вибиралася, виходячи з таких передумов[1]:

- аналізатор  $\text{SO}_2$  повинен бути переносним приладом для інспекційного контролю викидів ТЕС;
- вимірювання повинні проводитися в газоході для виключення можливості втрат інформації в системі пробо підготовки;
- внаслідок сильної запиленості газів, що відходять, необхідний захист оптичних елементів від впливу пилу, сажі, золи, вологи.

Враховуючи ці вимоги, структурна схема приладу отримала вид, зображений на рис. 10. Потік випромінювання від дейтерієвої лампи 1 типу ДДС-30 формується за допомогою конденсора 2 і направляєтся в газохід. Оскільки коефіцієнт поглинання  $\text{SO}_2$  в УФ області досить великий, то довжина кювети для аналізу необхідних концентрацій  $\text{SO}_2$  повинна бути 45мм для діапазону 0-5,46 г / м<sup>3</sup> і 15мм для діапазону виміру 0-16 г / м<sup>3</sup>. У той же час вимірювання  $\text{SO}_2$  в газоході повинні проводитися на відстані не менше 300мм від внутрішньої стіни газоходу для виключення можливості перепадів концентрації по перерізу газоходу. У зв'язку з цим відкрита кювета, через яку проходить досліджувана речовина, утворена плоскопаралельною кварцевою пластиною 3 і призмою 4, встановленою на кінці зонда, який жорстко кріпиться до приладу і вводиться в газохід. Довжина зонду досягає 1м.

Газова проба надходить в кювету внаслідок наявності газового потоку в газоході і шляхом природної дифузії через металокерамічний кожух, у

який вона встановлюється. Відбившись від призми, потік випромінювання повторно проходить через кювету і повертається в аналізатор. За допомогою об'єктива 5 випромінювання фокусується на вхідну щілину 6 монохроматора і заповнює увігнуту дифракційну решітку 7, радіусом 250 мм і з кількістю штрихів на 1 мм рівною 2400. Дифракційна решітка розкладає по спектру падаюче випромінювання і фокусує його на вихідну рухливу щілину 8. Вихідні щілини 8 нарізані на диск діаметром 76 мм за його радіусом. Загальна кількість нарізаних щілин дорівнює 20. Диск встановлений на осі синхронного двигуна 9 типу ДС-12. Якщо у газоході присутній  $\text{SO}_2$ , то у фокальній площині решітки спостерігається його спектр поглинання. Діафрагма 10 обмежує величину сканованої ділянки спектру, рівної (210-230) нм (див.рис. 1). На цій ділянці спектра присутні 10 максимумів поглинання  $\text{SO}_2$ .

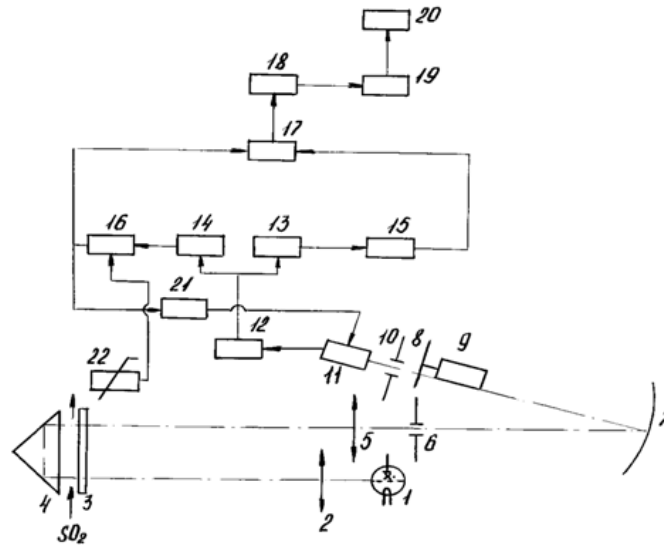


Рис.10: Структурна схема приладу для аналізу  $\text{SO}_2$

Щілини 8 на диску нарізані таким чином, щоб  $n$ -та щілина, закінчивши сканування спектру  $\text{SO}_2$ , вийшла за межі діафрагми 10, а  $(n+1)$ -ша увійшла. Таким чином, при обертанні диска відбувається безперервне сканування спектру  $\text{SO}_2$  в спектральному діапазоні (210-230) нм. Як приймач випромінювання 11 використовується сонячно-сліпий ФЕП 142. Сигнал з фотоприймача 11 надходить на попередній підсилювач 12. Оскільки тільки частина випромінювання поглинається  $\text{SO}_2$  в зазначеному діапазоні довжин хвиль, то з ФЕП знімається як змінна  $V_{\sim}$ , так і постійна  $V_{\equiv}$  складова сигналу.

Форма сигналу, що знімається з ФЕП після посилення в попередньому підсилювачі 12 зображена на рис. 1. Величина постійної складової  $V_{\equiv}$  залежить від концентрації в газозоді  $\text{SO}_2$  і інших поглинаючих випромінювання в цій області спектру компонентів, від параметрів джерела випромінювання та ФЕП. Тобто в ній міститься корисна інформація, яка може бути використана при обробці сигналів. Тому  $V_{\equiv}$ ,  $V_{\sim}$  посилюються відповідними підсилювачами 13, 14, детектуються детекторами 15, 16 і подаються на вхід АЦП 17. У АЦП величина  $V_{\equiv}$  використовується в якості опорної напруги, а  $V_{\sim}$  надходить на інформаційний вхід. Таким чином в АЦП відбувається перетворення аналогових сигналів в цифрову форму і одночасно береться відношення  $V_{\sim} / V_{\equiv}$ . Сигнал з АЦП поступає в постійно запам'ятовуючий пристрій (ПЗП) 18, де записана залежність концентрації аналізованого газу ( $\text{SO}_2$ ) від відношення сигналів робочого і опорного каналів і далі в блок виводу інформації 19. Блок виведення інформації розподіляє інформацію у відповідній формі між блоком індикації 20, виходом на цифро-друкуючий пристрій (ЦДП), виходом на самописець. У блоці індикації 20 здійснюється динамічна індикація результатів вимірювання на

трьохрозрядному світлодіодному індикаторі. Для врахування залежності показів аналізатора від його температури встановлений датчик температури 22 (термоопір), з'єднаний зі схемою компенсації нуля детектора. У залежності від температури аналізатора, змінюється величина корисного сигналу, що поступає на інформаційний вхід АЦП 17.

Оскільки на опорний канал АЦП має подаватися певне значення постійної напруги (10 В), величина постійної складової  $V_{\equiv}$ , що надходить на АЦП, підтримується на цьому рівні за рахунок регулювання підсилення ФЕП за допомогою ланцюга зворотного зв'язку, що включає блок живлення ФЕП 21. Таким чином, при зміні величини постійної складової сигналу  $V_{\equiv}$ , викликаному поглинанням  $\text{SO}_2$  в газозоді, запиленістю оптичних елементів, зростає напруга на ФЕП, не перевищуючи допустимого значення (2,2 кВ). Інші блоки живлення (лампи ДДС-30, електроніки) на рис. 10 не показані.

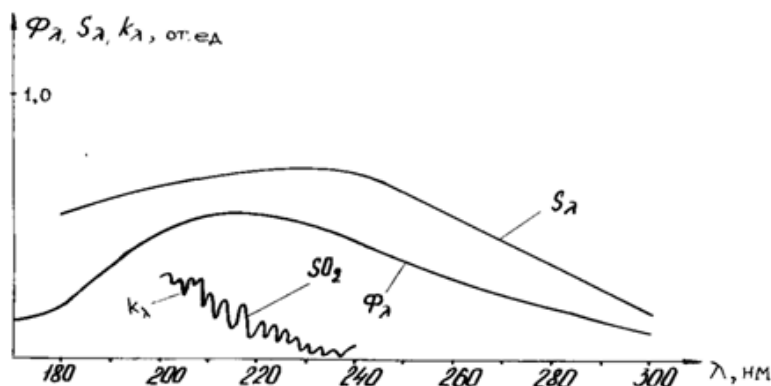


Рис. 11: Спектральні залежності чутливості фотокаатода  $S_{\lambda}$  ФЕП 142 світлового потоку  $\Phi_{\lambda}$  лампи ДДС-30 і коефіцієнта поглинання  $K_{\lambda}$   $\text{SO}_2$

Щодо вибору області аналізу  $\text{SO}_2$  - (210-230) нм, то вона обумовлена спектральними характеристиками обраної елементної бази (ФЕП-142, лампи ДДС-30), а також відносно невеликим інтегральним поглинанням  $\text{SO}_2$  в цій області.

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*Оптимизация параметров сканирующего спектрометра для анализа газов*

В работе приведены результаты оптимизационного расчета параметров дисперсионных приборов газового анализа в УФ и видимой областях спектра, которые используют корреляционное выделение полезного сигнала в его электронном тракте. Предложены методы оптимального выбора этих параметров. Как пример использования этих типов приборов описана структурная схема газоанализатора  $\text{SO}_2$  в отходящих газах тепловых электростанций.

*Optimisation of parameters of a scanning spectrometer for the gas analysis*

In the article results of optimization calculation of parameters of scanning spectrometer for the gas analysis in UV and visible fields of a spectrum are considered. The correlation selection of the useful signal in its electronic path is used. The methods of optimum choice of these parameters are offered. The block-diagram of gas analyzer  $\text{SO}_2$  in exit gases of thermal power stations is described as an example of use of these types of devices.

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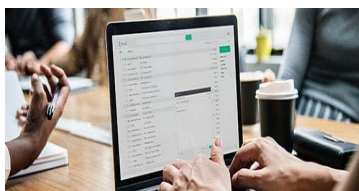
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Global Journals follows the definition of authorship set up by the Open Association of Research Society, USA. According to its guidelines, authorship criteria must be based on:

1. Substantial contributions to the conception and acquisition of data, analysis, and interpretation of findings.
2. Drafting the paper and revising it critically regarding important academic content.
3. Final approval of the version of the paper to be published.

### Changes in Authorship

The corresponding author should mention the name and complete details of all co-authors during submission and in manuscript. We support addition, rearrangement, manipulation, and deletions in authors list till the early view publication of the journal. We expect that corresponding author will notify all co-authors of submission. We follow COPE guidelines for changes in authorship.

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### Appealing Decisions

Unless specified in the notification, the Editorial Board's decision on publication of the paper is final and cannot be appealed before making the major change in the manuscript.

### Acknowledgments

Contributors to the research other than authors credited should be mentioned in Acknowledgments. The source of funding for the research can be included. Suppliers of resources may be mentioned along with their addresses.

### Declaration of funding sources

Global Journals is in partnership with various universities, laboratories, and other institutions worldwide in the research domain. Authors are requested to disclose their source of funding during every stage of their research, such as making analysis, performing laboratory operations, computing data, and using institutional resources, from writing an article to its submission. This will also help authors to get reimbursements by requesting an open access publication letter from Global Journals and submitting to the respective funding source.

## PREPARING YOUR MANUSCRIPT

Authors can submit papers and articles in an acceptable file format: MS Word (doc, docx), LaTeX (.tex, .zip or .rar including all of your files), Adobe PDF (.pdf), rich text format (.rtf), simple text document (.txt), Open Document Text (.odt), and Apple Pages (.pages). Our professional layout editors will format the entire paper according to our official guidelines. This is one of the highlights of publishing with Global Journals—authors should not be concerned about the formatting of their paper. Global Journals accepts articles and manuscripts in every major language, be it Spanish, Chinese, Japanese, Portuguese, Russian, French, German, Dutch, Italian, Greek, or any other national language, but the title, subtitle, and abstract should be in English. This will facilitate indexing and the pre-peer review process.

The following is the official style and template developed for publication of a research paper. Authors are not required to follow this style during the submission of the paper. It is just for reference purposes.



### ***Manuscript Style Instruction (Optional)***

- Microsoft Word Document Setting Instructions.
- Font type of all text should be Swis721 Lt BT.
- Page size: 8.27" x 11", left margin: 0.65, right margin: 0.65, bottom margin: 0.75.
- Paper title should be in one column of font size 24.
- Author name in font size of 11 in one column.
- Abstract: font size 9 with the word "Abstract" in bold italics.
- Main text: font size 10 with two justified columns.
- Two columns with equal column width of 3.38 and spacing of 0.2.
- First character must be three lines drop-capped.
- The paragraph before spacing of 1 pt and after of 0 pt.
- Line spacing of 1 pt.
- Large images must be in one column.
- The names of first main headings (Heading 1) must be in Roman font, capital letters, and font size of 10.
- The names of second main headings (Heading 2) must not include numbers and must be in italics with a font size of 10.

### ***Structure and Format of Manuscript***

The recommended size of an original research paper is under 15,000 words and review papers under 7,000 words. Research articles should be less than 10,000 words. Research papers are usually longer than review papers. Review papers are reports of significant research (typically less than 7,000 words, including tables, figures, and references)

A research paper must include:

- a) A title which should be relevant to the theme of the paper.
- b) A summary, known as an abstract (less than 150 words), containing the major results and conclusions.
- c) Up to 10 keywords that precisely identify the paper's subject, purpose, and focus.
- d) An introduction, giving fundamental background objectives.
- e) Resources and techniques with sufficient complete experimental details (wherever possible by reference) to permit repetition, sources of information must be given, and numerical methods must be specified by reference.
- f) Results which should be presented concisely by well-designed tables and figures.
- g) Suitable statistical data should also be given.
- h) All data must have been gathered with attention to numerical detail in the planning stage.

Design has been recognized to be essential to experiments for a considerable time, and the editor has decided that any paper that appears not to have adequate numerical treatments of the data will be returned unrefereed.

- i) Discussion should cover implications and consequences and not just recapitulate the results; conclusions should also be summarized.
- j) There should be brief acknowledgments.
- k) There ought to be references in the conventional format. Global Journals recommends APA format.

Authors should carefully consider the preparation of papers to ensure that they communicate effectively. Papers are much more likely to be accepted if they are carefully designed and laid out, contain few or no errors, are summarizing, and follow instructions. They will also be published with much fewer delays than those that require much technical and editorial correction.

The Editorial Board reserves the right to make literary corrections and suggestions to improve brevity.





## FORMAT STRUCTURE

***It is necessary that authors take care in submitting a manuscript that is written in simple language and adheres to published guidelines.***

All manuscripts submitted to Global Journals should include:

### **Title**

The title page must carry an informative title that reflects the content, a running title (less than 45 characters together with spaces), names of the authors and co-authors, and the place(s) where the work was carried out.

### **Author details**

The full postal address of any related author(s) must be specified.

### **Abstract**

The abstract is the foundation of the research paper. It should be clear and concise and must contain the objective of the paper and inferences drawn. It is advised to not include big mathematical equations or complicated jargon.

Many researchers searching for information online will use search engines such as Google, Yahoo or others. By optimizing your paper for search engines, you will amplify the chance of someone finding it. In turn, this will make it more likely to be viewed and cited in further works. Global Journals has compiled these guidelines to facilitate you to maximize the web-friendliness of the most public part of your paper.

### **Keywords**

A major lynchpin of research work for the writing of research papers is the keyword search, which one will employ to find both library and internet resources. Up to eleven keywords or very brief phrases have to be given to help data retrieval, mining, and indexing.

One must be persistent and creative in using keywords. An effective keyword search requires a strategy: planning of a list of possible keywords and phrases to try.

Choice of the main keywords is the first tool of writing a research paper. Research paper writing is an art. Keyword search should be as strategic as possible.

One should start brainstorming lists of potential keywords before even beginning searching. Think about the most important concepts related to research work. Ask, "What words would a source have to include to be truly valuable in a research paper?" Then consider synonyms for the important words.

It may take the discovery of only one important paper to steer in the right keyword direction because, in most databases, the keywords under which a research paper is abstracted are listed with the paper.

### **Numerical Methods**

Numerical methods used should be transparent and, where appropriate, supported by references.

### **Abbreviations**

Authors must list all the abbreviations used in the paper at the end of the paper or in a separate table before using them.

### **Formulas and equations**

Authors are advised to submit any mathematical equation using either MathJax, KaTeX, or LaTeX, or in a very high-quality image.

### **Tables, Figures, and Figure Legends**

Tables: Tables should be cautiously designed, uncrowned, and include only essential data. Each must have an Arabic number, e.g., Table 4, a self-explanatory caption, and be on a separate sheet. Authors must submit tables in an editable format and not as images. References to these tables (if any) must be mentioned accurately.



## Figures

Figures are supposed to be submitted as separate files. Always include a citation in the text for each figure using Arabic numbers, e.g., Fig. 4. Artwork must be submitted online in vector electronic form or by emailing it.

## PREPARATION OF ELETRONIC FIGURES FOR PUBLICATION

Although low-quality images are sufficient for review purposes, print publication requires high-quality images to prevent the final product being blurred or fuzzy. Submit (possibly by e-mail) EPS (line art) or TIFF (halftone/ photographs) files only. MS PowerPoint and Word Graphics are unsuitable for printed pictures. Avoid using pixel-oriented software. Scans (TIFF only) should have a resolution of at least 350 dpi (halftone) or 700 to 1100 dpi (line drawings). Please give the data for figures in black and white or submit a Color Work Agreement form. EPS files must be saved with fonts embedded (and with a TIFF preview, if possible).

For scanned images, the scanning resolution at final image size ought to be as follows to ensure good reproduction: line art: >650 dpi; halftones (including gel photographs): >350 dpi; figures containing both halftone and line images: >650 dpi.

Color charges: Authors are advised to pay the full cost for the reproduction of their color artwork. Hence, please note that if there is color artwork in your manuscript when it is accepted for publication, we would require you to complete and return a Color Work Agreement form before your paper can be published. Also, you can email your editor to remove the color fee after acceptance of the paper.

## TIPS FOR WRITING A GOOD QUALITY SCIENCE FRONTIER RESEARCH PAPER

Techniques for writing a good quality Science Frontier Research paper:

**1. Choosing the topic:** In most cases, the topic is selected by the interests of the author, but it can also be suggested by the guides. You can have several topics, and then judge which you are most comfortable with. This may be done by asking several questions of yourself, like "Will I be able to carry out a search in this area? Will I find all necessary resources to accomplish the search? Will I be able to find all information in this field area?" If the answer to this type of question is "yes," then you ought to choose that topic. In most cases, you may have to conduct surveys and visit several places. Also, you might have to do a lot of work to find all the rises and falls of the various data on that subject. Sometimes, detailed information plays a vital role, instead of short information. Evaluators are human: The first thing to remember is that evaluators are also human beings. They are not only meant for rejecting a paper. They are here to evaluate your paper. So present your best aspect.

**2. Think like evaluators:** If you are in confusion or getting demotivated because your paper may not be accepted by the evaluators, then think, and try to evaluate your paper like an evaluator. Try to understand what an evaluator wants in your research paper, and you will automatically have your answer. Make blueprints of paper: The outline is the plan or framework that will help you to arrange your thoughts. It will make your paper logical. But remember that all points of your outline must be related to the topic you have chosen.

**3. Ask your guides:** If you are having any difficulty with your research, then do not hesitate to share your difficulty with your guide (if you have one). They will surely help you out and resolve your doubts. If you can't clarify what exactly you require for your work, then ask your supervisor to help you with an alternative. He or she might also provide you with a list of essential readings.

**4. Use of computer is recommended:** As you are doing research in the field of science frontier then this point is quite obvious. Use right software: Always use good quality software packages. If you are not capable of judging good software, then you can lose the quality of your paper unknowingly. There are various programs available to help you which you can get through the internet.

**5. Use the internet for help:** An excellent start for your paper is using Google. It is a wondrous search engine, where you can have your doubts resolved. You may also read some answers for the frequent question of how to write your research paper or find a model research paper. You can download books from the internet. If you have all the required books, place importance on reading, selecting, and analyzing the specified information. Then sketch out your research paper. Use big pictures: You may use encyclopedias like Wikipedia to get pictures with the best resolution. At Global Journals, you should strictly follow here.



**6. Bookmarks are useful:** When you read any book or magazine, you generally use bookmarks, right? It is a good habit which helps to not lose your continuity. You should always use bookmarks while searching on the internet also, which will make your search easier.

**7. Revise what you wrote:** When you write anything, always read it, summarize it, and then finalize it.

**8. Make every effort:** Make every effort to mention what you are going to write in your paper. That means always have a good start. Try to mention everything in the introduction—what is the need for a particular research paper. Polish your work with good writing skills and always give an evaluator what he wants. Make backups: When you are going to do any important thing like making a research paper, you should always have backup copies of it either on your computer or on paper. This protects you from losing any portion of your important data.

**9. Produce good diagrams of your own:** Always try to include good charts or diagrams in your paper to improve quality. Using several unnecessary diagrams will degrade the quality of your paper by creating a hodgepodge. So always try to include diagrams which were made by you to improve the readability of your paper. Use of direct quotes: When you do research relevant to literature, history, or current affairs, then use of quotes becomes essential, but if the study is relevant to science, use of quotes is not preferable.

**10. Use proper verb tense:** Use proper verb tenses in your paper. Use past tense to present those events that have happened. Use present tense to indicate events that are going on. Use future tense to indicate events that will happen in the future. Use of wrong tenses will confuse the evaluator. Avoid sentences that are incomplete.

**11. Pick a good study spot:** Always try to pick a spot for your research which is quiet. Not every spot is good for studying.

**12. Know what you know:** Always try to know what you know by making objectives, otherwise you will be confused and unable to achieve your target.

**13. Use good grammar:** Always use good grammar and words that will have a positive impact on the evaluator; use of good vocabulary does not mean using tough words which the evaluator has to find in a dictionary. Do not fragment sentences. Eliminate one-word sentences. Do not ever use a big word when a smaller one would suffice.

Verbs have to be in agreement with their subjects. In a research paper, do not start sentences with conjunctions or finish them with prepositions. When writing formally, it is advisable to never split an infinitive because someone will (wrongly) complain. Avoid clichés like a disease. Always shun irritating alliteration. Use language which is simple and straightforward. Put together a neat summary.

**14. Arrangement of information:** Each section of the main body should start with an opening sentence, and there should be a changeover at the end of the section. Give only valid and powerful arguments for your topic. You may also maintain your arguments with records.

**15. Never start at the last minute:** Always allow enough time for research work. Leaving everything to the last minute will degrade your paper and spoil your work.

**16. Multitasking in research is not good:** Doing several things at the same time is a bad habit in the case of research activity. Research is an area where everything has a particular time slot. Divide your research work into parts, and do a particular part in a particular time slot.

**17. Never copy others' work:** Never copy others' work and give it your name because if the evaluator has seen it anywhere, you will be in trouble. Take proper rest and food: No matter how many hours you spend on your research activity, if you are not taking care of your health, then all your efforts will have been in vain. For quality research, take proper rest and food.

**18. Go to seminars:** Attend seminars if the topic is relevant to your research area. Utilize all your resources.

**19. Refresh your mind after intervals:** Try to give your mind a rest by listening to soft music or sleeping in intervals. This will also improve your memory. Acquire colleagues: Always try to acquire colleagues. No matter how sharp you are, if you acquire colleagues, they can give you ideas which will be helpful to your research.



**20. Think technically:** Always think technically. If anything happens, search for its reasons, benefits, and demerits. Think and then print: When you go to print your paper, check that tables are not split, headings are not detached from their descriptions, and page sequence is maintained.

**21. Adding unnecessary information:** Do not add unnecessary information like "I have used MS Excel to draw graphs." Irrelevant and inappropriate material is superfluous. Foreign terminology and phrases are not apropos. One should never take a broad view. Analogy is like feathers on a snake. Use words properly, regardless of how others use them. Remove quotations. Puns are for kids, not grunt readers. Never oversimplify: When adding material to your research paper, never go for oversimplification; this will definitely irritate the evaluator. Be specific. Never use rhythmic redundancies. Contractions shouldn't be used in a research paper. Comparisons are as terrible as clichés. Give up ampersands, abbreviations, and so on. Remove commas that are not necessary. Parenthetical words should be between brackets or commas. Understatement is always the best way to put forward earth-shaking thoughts. Give a detailed literary review.

**22. Report concluded results:** Use concluded results. From raw data, filter the results, and then conclude your studies based on measurements and observations taken. An appropriate number of decimal places should be used. Parenthetical remarks are prohibited here. Proofread carefully at the final stage. At the end, give an outline to your arguments. Spot perspectives of further study of the subject. Justify your conclusion at the bottom sufficiently, which will probably include examples.

**23. Upon conclusion:** Once you have concluded your research, the next most important step is to present your findings. Presentation is extremely important as it is the definite medium through which your research is going to be in print for the rest of the crowd. Care should be taken to categorize your thoughts well and present them in a logical and neat manner. A good quality research paper format is essential because it serves to highlight your research paper and bring to light all necessary aspects of your research.

## INFORMAL GUIDELINES OF RESEARCH PAPER WRITING

### **Key points to remember:**

- Submit all work in its final form.
- Write your paper in the form which is presented in the guidelines using the template.
- Please note the criteria peer reviewers will use for grading the final paper.

### **Final points:**

One purpose of organizing a research paper is to let people interpret your efforts selectively. The journal requires the following sections, submitted in the order listed, with each section starting on a new page:

*The introduction:* This will be compiled from reference matter and reflect the design processes or outline of basis that directed you to make a study. As you carry out the process of study, the method and process section will be constructed like that. The results segment will show related statistics in nearly sequential order and direct reviewers to similar intellectual paths throughout the data that you gathered to carry out your study.

### **The discussion section:**

This will provide understanding of the data and projections as to the implications of the results. The use of good quality references throughout the paper will give the effort trustworthiness by representing an alertness to prior workings.

Writing a research paper is not an easy job, no matter how trouble-free the actual research or concept. Practice, excellent preparation, and controlled record-keeping are the only means to make straightforward progression.

### **General style:**

Specific editorial column necessities for compliance of a manuscript will always take over from directions in these general guidelines.

**To make a paper clear:** Adhere to recommended page limits.



### *Mistakes to avoid:*

- Insertion of a title at the foot of a page with subsequent text on the next page.
- Separating a table, chart, or figure—confine each to a single page.
- Submitting a manuscript with pages out of sequence.
- In every section of your document, use standard writing style, including articles ("a" and "the").
- Keep paying attention to the topic of the paper.
- Use paragraphs to split each significant point (excluding the abstract).
- Align the primary line of each section.
- Present your points in sound order.
- Use present tense to report well-accepted matters.
- Use past tense to describe specific results.
- Do not use familiar wording; don't address the reviewer directly. Don't use slang or superlatives.
- Avoid use of extra pictures—include only those figures essential to presenting results.

### **Title page:**

Choose a revealing title. It should be short and include the name(s) and address(es) of all authors. It should not have acronyms or abbreviations or exceed two printed lines.

**Abstract:** This summary should be two hundred words or less. It should clearly and briefly explain the key findings reported in the manuscript and must have precise statistics. It should not have acronyms or abbreviations. It should be logical in itself. Do not cite references at this point.

An abstract is a brief, distinct paragraph summary of finished work or work in development. In a minute or less, a reviewer can be taught the foundation behind the study, common approaches to the problem, relevant results, and significant conclusions or new questions.

Write your summary when your paper is completed because how can you write the summary of anything which is not yet written? Wealth of terminology is very essential in abstract. Use comprehensive sentences, and do not sacrifice readability for brevity; you can maintain it succinctly by phrasing sentences so that they provide more than a lone rationale. The author can at this moment go straight to shortening the outcome. Sum up the study with the subsequent elements in any summary. Try to limit the initial two items to no more than one line each.

*Reason for writing the article—theory, overall issue, purpose.*

- Fundamental goal.
- To-the-point depiction of the research.
- Consequences, including definite statistics—if the consequences are quantitative in nature, account for this; results of any numerical analysis should be reported. Significant conclusions or questions that emerge from the research.

### **Approach:**

- Single section and succinct.
- An outline of the job done is always written in past tense.
- Concentrate on shortening results—limit background information to a verdict or two.
- Exact spelling, clarity of sentences and phrases, and appropriate reporting of quantities (proper units, important statistics) are just as significant in an abstract as they are anywhere else.

### **Introduction:**

The introduction should "introduce" the manuscript. The reviewer should be presented with sufficient background information to be capable of comprehending and calculating the purpose of your study without having to refer to other works. The basis for the study should be offered. Give the most important references, but avoid making a comprehensive appraisal of the topic. Describe the problem visibly. If the problem is not acknowledged in a logical, reasonable way, the reviewer will give no attention to your results. Speak in common terms about techniques used to explain the problem, if needed, but do not present any particulars about the protocols here.



*The following approach can create a valuable beginning:*

- Explain the value (significance) of the study.
- Defend the model—why did you employ this particular system or method? What is its compensation? Remark upon its appropriateness from an abstract point of view as well as pointing out sensible reasons for using it.
- Present a justification. State your particular theory(-ies) or aim(s), and describe the logic that led you to choose them.
- Briefly explain the study's tentative purpose and how it meets the declared objectives.

#### **Approach:**

Use past tense except for when referring to recognized facts. After all, the manuscript will be submitted after the entire job is done. Sort out your thoughts; manufacture one key point for every section. If you make the four points listed above, you will need at least four paragraphs. Present surrounding information only when it is necessary to support a situation. The reviewer does not desire to read everything you know about a topic. Shape the theory specifically—do not take a broad view.

As always, give awareness to spelling, simplicity, and correctness of sentences and phrases.

#### **Procedures (methods and materials):**

This part is supposed to be the easiest to carve if you have good skills. A soundly written procedures segment allows a capable scientist to replicate your results. Present precise information about your supplies. The suppliers and clarity of reagents can be helpful bits of information. Present methods in sequential order, but linked methodologies can be grouped as a segment. Be concise when relating the protocols. Attempt to give the least amount of information that would permit another capable scientist to replicate your outcome, but be cautious that vital information is integrated. The use of subheadings is suggested and ought to be synchronized with the results section.

When a technique is used that has been well-described in another section, mention the specific item describing the way, but draw the basic principle while stating the situation. The purpose is to show all particular resources and broad procedures so that another person may use some or all of the methods in one more study or referee the scientific value of your work. It is not to be a step-by-step report of the whole thing you did, nor is a methods section a set of orders.

#### **Materials:**

*Materials may be reported in part of a section or else they may be recognized along with your measures.*

#### **Methods:**

- Report the method and not the particulars of each process that engaged the same methodology.
- Describe the method entirely.
- To be succinct, present methods under headings dedicated to specific dealings or groups of measures.
- Simplify—detail how procedures were completed, not how they were performed on a particular day.
- If well-known procedures were used, account for the procedure by name, possibly with a reference, and that's all.

#### **Approach:**

It is embarrassing to use vigorous voice when documenting methods without using first person, which would focus the reviewer's interest on the researcher rather than the job. As a result, when writing up the methods, most authors use third person passive voice.

Use standard style in this and every other part of the paper—avoid familiar lists, and use full sentences.

#### **What to keep away from:**

- Resources and methods are not a set of information.
- Skip all descriptive information and surroundings—save it for the argument.
- Leave out information that is immaterial to a third party.





**Results:**

The principle of a results segment is to present and demonstrate your conclusion. Create this part as entirely objective details of the outcome, and save all understanding for the discussion.

The page length of this segment is set by the sum and types of data to be reported. Use statistics and tables, if suitable, to present consequences most efficiently.

You must clearly differentiate material which would usually be incorporated in a study editorial from any unprocessed data or additional appendix matter that would not be available. In fact, such matters should not be submitted at all except if requested by the instructor.

**Content:**

- Sum up your conclusions in text and demonstrate them, if suitable, with figures and tables.
- In the manuscript, explain each of your consequences, and point the reader to remarks that are most appropriate.
- Present a background, such as by describing the question that was addressed by creation of an exacting study.
- Explain results of control experiments and give remarks that are not accessible in a prescribed figure or table, if appropriate.
- Examine your data, then prepare the analyzed (transformed) data in the form of a figure (graph), table, or manuscript.

**What to stay away from:**

- Do not discuss or infer your outcome, report surrounding information, or try to explain anything.
- Do not include raw data or intermediate calculations in a research manuscript.
- Do not present similar data more than once.
- A manuscript should complement any figures or tables, not duplicate information.
- Never confuse figures with tables—there is a difference.

**Approach:**

As always, use past tense when you submit your results, and put the whole thing in a reasonable order.

Put figures and tables, appropriately numbered, in order at the end of the report.

If you desire, you may place your figures and tables properly within the text of your results section.

**Figures and tables:**

If you put figures and tables at the end of some details, make certain that they are visibly distinguished from any attached appendix materials, such as raw facts. Whatever the position, each table must be titled, numbered one after the other, and include a heading. All figures and tables must be divided from the text.

**Discussion:**

The discussion is expected to be the trickiest segment to write. A lot of papers submitted to the journal are discarded based on problems with the discussion. There is no rule for how long an argument should be.

Position your understanding of the outcome visibly to lead the reviewer through your conclusions, and then finish the paper with a summing up of the implications of the study. The purpose here is to offer an understanding of your results and support all of your conclusions, using facts from your research and generally accepted information, if suitable. The implication of results should be fully described.

Infer your data in the conversation in suitable depth. This means that when you clarify an observable fact, you must explain mechanisms that may account for the observation. If your results vary from your prospect, make clear why that may have happened. If your results agree, then explain the theory that the proof supported. It is never suitable to just state that the data approved the prospect, and let it drop at that. Make a decision as to whether each premise is supported or discarded or if you cannot make a conclusion with assurance. Do not just dismiss a study or part of a study as "uncertain."



Research papers are not acknowledged if the work is imperfect. Draw what conclusions you can based upon the results that you have, and take care of the study as a finished work.

- You may propose future guidelines, such as how an experiment might be personalized to accomplish a new idea.
- Give details of all of your remarks as much as possible, focusing on mechanisms.
- Make a decision as to whether the tentative design sufficiently addressed the theory and whether or not it was correctly restricted. Try to present substitute explanations if they are sensible alternatives.
- One piece of research will not counter an overall question, so maintain the large picture in mind. Where do you go next? The best studies unlock new avenues of study. What questions remain?
- Recommendations for detailed papers will offer supplementary suggestions.

**Approach:**

When you refer to information, differentiate data generated by your own studies from other available information. Present work done by specific persons (including you) in past tense.

Describe generally acknowledged facts and main beliefs in present tense.

## THE ADMINISTRATION RULES

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*Written material:* You may discuss this with your guides and key sources. Do not copy anyone else's paper, even if this is only imitation, otherwise it will be rejected on the grounds of plagiarism, which is illegal. Various methods to avoid plagiarism are strictly applied by us to every paper, and, if found guilty, you may be blacklisted, which could affect your career adversely. To guard yourself and others from possible illegal use, please do not permit anyone to use or even read your paper and file.



CRITERION FOR GRADING A RESEARCH PAPER (COMPILATION)  
BY GLOBAL JOURNALS

Please note that following table is only a Grading of "Paper Compilation" and not on "Performed/Stated Research" whose grading solely depends on Individual Assigned Peer Reviewer and Editorial Board Member. These can be available only on request and after decision of Paper. This report will be the property of Global Journals.

Topics	Grades		
	A-B	C-D	E-F
<i>Abstract</i>	Clear and concise with appropriate content, Correct format. 200 words or below	Unclear summary and no specific data, Incorrect form  Above 200 words	No specific data with ambiguous information  Above 250 words
<i>Introduction</i>	Containing all background details with clear goal and appropriate details, flow specification, no grammar and spelling mistake, well organized sentence and paragraph, reference cited	Unclear and confusing data, appropriate format, grammar and spelling errors with unorganized matter	Out of place depth and content, hazy format
<i>Methods and Procedures</i>	Clear and to the point with well arranged paragraph, precision and accuracy of facts and figures, well organized subheads	Difficult to comprehend with embarrassed text, too much explanation but completed	Incorrect and unorganized structure with hazy meaning
<i>Result</i>	Well organized, Clear and specific, Correct units with precision, correct data, well structuring of paragraph, no grammar and spelling mistake	Complete and embarrassed text, difficult to comprehend	Irregular format with wrong facts and figures
<i>Discussion</i>	Well organized, meaningful specification, sound conclusion, logical and concise explanation, highly structured paragraph reference cited	Wordy, unclear conclusion, spurious	Conclusion is not cited, unorganized, difficult to comprehend
<i>References</i>	Complete and correct format, well organized	Beside the point, Incomplete	Wrong format and structuring



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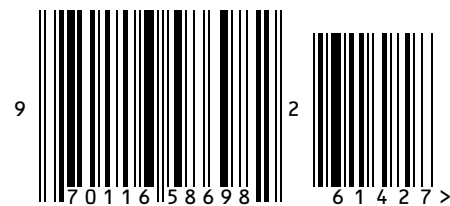
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