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Solving Some Issues of Sensory Ecology

Nadira B. Khonkhodjayeva[1], Mahina A. Isabekova[2]

[1]*Associate Professor of the Tashkent State Pedagogical University named after Nizami, Republic of Tashkent, Uzbekistan*
[2]*Senior lecturer of the Tashkent State Pedagogical University named after Nizami, Tashkent, Uzbekistan*

Abstract: This article discusses the prospects for the use of pheromones in agriculture as a method of pest control and their advantages over pesticides from an ecological point of view. This article shows the concept of pheromones, their specific meaning, as well as their significance for biological species, ways of their possible use for human needs, as well as the influence of external physical environmental factors on pheromones. In modern environmental conditions, this issue is most acute, and research in this area is very promising. Pheromones are one of the types of external stimuli that affect the behaviour and physiological state of humans and animals, a complex of special olfactory signals. These are biological markers of a kind, volatile chemosignals that control neuroendocrine behavioral reactions, developmental processes, as well as processes related to social behavior and reproduction. Pheromones contribute to changing the behavior, physiological and emotional state or metabolism of other individuals of the same species. Pheromones have found their application in agriculture. In combination with traps of various types, pheromones that lure insects can destroy a significant number of pests. [2]

Keywords: physical environmental factors, pheromones, environmental problems, perspective, research, scaly-winged insects, light, methods of quantum theory, adsorption, temperature.

1. Introduction

"The problem of environmental safety has gone beyond the national and regional and has become a global problem for all mankind ... Humanity has really felt the threat it is facing, as a result of which there is an anthropogenic impact on the environment." Intensive human economic activity has brought the world to the brink of an ecological catastrophe. The human impact on the environment is multifaceted. The main anthropogenic factors that destroy the habitat are: urban growth, mining, automobile transport, industry and the chemicalization of agriculture.

An ecological trap is a case when organisms choose a poor-quality habitat instead of the best available one due to an incorrect assessment of the quality of the habitat.[6] Artificial landscapes represent a new habitat for organisms. In addition, artificial materials can be mistaken for natural ones, which causes some organisms to choose substandard habitats rather than higher-quality ones. Sensory ecology can be used to mitigate the effects of these environmental traps by finding out what specific information organisms use to make "bad" decisions.

2. The Main Results and Findings

Organisms often mistake artificial surfaces, such as asphalt and solar panels, for natural surfaces. Solar panels, for example, reflect horizontally polarized light, which many insects mistake for water. Since insects lay eggs in water, they will try to lay eggs on solar panels. This leads to the mass death of young solar-powered insects.[7] To mitigate the effects of this ecological trap, the researchers changed the shape of the solar core on the panels. At the same time, the panels became less attractive to insects, which led to a decrease in mortality.[7] A number of bat species also fall victim to environmental traps that result from artificial surfaces. A recent study by Greif and Simers[8] showed that bats determine the location of a reservoir by the smoothness of the surface, and not by the actual presence of water. Thus, bats try to drink from smooth surfaces that are not actually water, such as glass. As a result, bats waste energy and time, which can lead to a decrease in physical fitness.[8] Bird species are also often exposed to ecological traps as a result of their sensory ecology. One of the recent areas of focus for sensory ecology of birds has been the study of how birds can perceive large wind turbines and other buildings. Every year countless birds die as a result of collisions with power lines, fences, wind turbines and buildings.[9] Flight paths around these structures act as forms of ecological traps; while birds may perceive areas around buildings as "good habitat" and viable corridors for flight, they may actually increase bird mortality due to collisions. Sensory ecologists have linked these ecological traps to the sensory ecology of birds. The researchers found that although human vision is binocular, bird vision is much weaker. In addition, birds do not have high-resolution frontal vision.[9] As a result, birds may not see large structures directly in front of them, which leads to collisions.

Several solutions to this problem have been proposed. One study showed that the response of birds to different lighting schemes at airports is different and that the number of bird strikes can be reduced by changing the lighting scheme.[10] Other researchers have suggested that warning sounds or visual cues placed on the ground may help reduce collisions with birds.10] By regulating other sensory signals of birds, ecologists can help reduce the presence of bird ecological traps around these structures.

In the deterioration of the environment, chemical exposure is in the first place. The role of chemical objects in human life is difficult to overestimate. They are assigned one of the important places in the fight against pests, diseases and weeds of agricultural crops, but the actions of pesticides are never unambiguous. Pesticides used in agriculture are organic compounds that are toxic not only to pests, but also to humans and animals. Humans use pesticides to destroy a limited number of organisms that make up no more than 0.5% of the total number of species inhabiting the biosphere, while pesticides, when used, affect all living organisms. When carrying out protective measures, pesticides are always directed against the population.[2]

This article examines the influence of physical environmental factors on pheromones, provides examples of studies of this kind of influence on the pheromones of scaly-winged insects, as well as prospects for the use of pheromones in agriculture.

President of the Republic of Uzbekistan Sh. M. Mirziyoyev, speaking at the meeting of the heads of the founding states of the International Fund for Saving the Aral Sea, noted that it is necessary to begin the introduction of environmentally friendly technologies, lay the foundations for the comprehensive introduction of green economy, environmentally friendly, energy and water-saving technologies. The Head of State also initiated the organization next year of a conference with the support of the United Nations, the World Bank, the Asian Development Bank and the Global Environment Facility, at which negotiations will be held on practical issues of creating a zone of environmental innovations and technologies in environmentally disadvantaged regions of the world. This is provided for in the action strategy for the five priority areas of development of the Republic of Uzbekistan for 2017-2025 in subparagraph 3.3. Modernization and intensive development of agriculture refers to the implementation of investment projects for the construction of new, reconstruction and modernization of existing processing enterprises, the widespread introduction of intensive methods in agricultural production, primarily modern water and resource-saving agricultural technologies, the use of high-performance agricultural machinery; expansion of research work on the creation and introduction into production of new breeding varieties of crops resistant to diseases and pests, adapted to local soil, climatic and environmental conditions, and animal breeds with high productivity [4].

The content of the article. Insect pheromones, discovered more than fifty years ago, can now become a safe and harmless substitute for pesticides and other harmful chemicals that are currently used in the fight against harmful insects that cause huge damage to agriculture.

The question arises, what is the essence of pheromones? How do they act on insect pests? How do external environmental factors affect them, and most importantly, what are the prospects for the use of pheromones in agriculture.

Pheromones are biologically active substances, products of external secretion released into the external environment by insects, fish, animals and humans. Pheromones, providing chemical communication between organisms of the same species, are some kind of volatile chemosignals capable of controlling neuroendocrine behavioral reactions, developmental processes, social behavior and reproduction. Pheromones change the behavior, physiological and emotional state, and even the metabolism of different individuals of the same species. These substances are means of regulation, play an important role in the communication of many insect species, for example, ensuring the rapprochement of males and females during the breeding season, the concentration of insects on forage plants and in wintering areas, or controlling the behavior and physiological processes in working individuals of social insects. Pheromones are found in animals of various systematic groups, from invertebrates to mammals. Currently, insect pheromones are considered the most studied.

There are two main types of pheromones that differ in their effects: releasers and primers. The first type is relizers, capable of prompting an individual to take immediate action, for example, pheromones that transmit danger signals between individuals of the same species. Usually relizers are highly volatile substances that spread through the air. The second type is primers, designed to form a special behavior and influence other individuals, an example is the pheromones secreted by the queen bee, in order to suppress the sexual development of female bees, turning them into ordinary worker bees. Primers are most often distributed by contact. Relizers are currently studied better than primers, several subtypes of pheromones can be distinguished on their basis, such as: attractants – these include sexual pheromones and aggregation pheromones that stimulate the accumulation of insects; repellents – repelling pheromones; stimulants – pheromones that cause activity, for example, anxiety pheromones; determinants – inhibiting the reaction, etc [5].

The source of the pheromone in insects can be individual secretory cells scattered throughout the body or groups of them that form a special organ – the pheromone gland. The ducts of the pheromone glands open on the surface of the body or in cavities communicating with the external environment. Insects secrete a pheromone in micro quantities: thus, the female apple fruit moth (Cydia pomonella) secretes only 9 nanograms of pheromone per hour. However, this amount is enough for the male fruitworm to smell and find a female in the crown of the tree. Insects perceive the smell of pheromones with the help of chemoreceptor sensors – special receptors in the form of hairs, bristles or bumps located on the antennae; their number on one antennae can reach 15 thousand. For the insect's response, the presence of a very small amount of pheromone in the air is sufficient [4].

Usually pheromones are not a single substance, but a mixture of the main, predominant component by weight with small additives (minor components): they may contain more than 10 components. One substance can have several different functions. Pheromone molecules are highly volatile, decompose rapidly under the influence of oxygen, air, moisture and light. By chemical composition, insect pheromones belong to various classes of organic compounds, such as alcohols, esters, terpenoids, steroids, aldehydes, heterocyclic compounds and others.

Knowing the chemical composition of the insect pheromone, it is possible to synthesize it in the laboratory. It is these synthetic analogues of sexual and aggregation pheromones that can be used to protect plants from pests. The advantage of synthetic pheromones, which are used in microdoses, is high species specificity and attractiveness. They are completely harmless to humans and the environment, and also act directly on the target insect pest species.

There are two main areas of application of synthetic pheromones against harmful insects: The first is monitoring. This suggests that the use of pheromones provides an opportunity to record such processes as the number of pests, to obtain data on their numbers, or even the ability to determine the range of quarantine pests. The second is pest control. Having saturated the air with synthetic pheromone, it is possible to prevent males from finding females, attract insects and catch or destroy them before they can detect the natural source of the pheromone. In both cases, the reproduction of pests is blocked.

However, in addition to the influence of pheromones on pests, it is necessary to consider the influence of environmental factors on the pheromones themselves. Taking into account the huge species diversity of insect pests and the complexity of the composition of pheromones, an urgent task is to develop universal methods for the study of pheromone communication, which allow saving material, labor and time resources.

It is important to pay attention to another aspect of the possible use of pheromones - the establishment of the species composition of insects in a particular area. This is most clearly seen in the example of a scoop. Analogues of sexual pheromones of many types of scoops have been synthesized. A sample of the synthesis of VNIIHSZR was selected. Observations were carried out in the cotton crop rotation of three farms of the Yangiyul district, as well as in the fields of the research Institute of vegetable and melon crops of the Tashkent district of the Tashkent region. We used pheromones of two- and three-component winter scoops (OC-77 and OC-8), exclamation scoops (BK-23 and BK-137), C-black scoops (SCH-72), convolutional scoops (Cons-21), cotton scoops (CS), meadow scoops (MS). Pheromone dispensers were

they were placed in triangular traps made of laminated paper, which were placed in the fields at the rate of 1 trap per 1 ha at a height of 25 cm above the plants. The dispensers were updated every 10 days. Observations were carried out for three years in the fields of cotton, kenaf, corn, alfalfa, red pepper, tomatoes and pumpkin. Based on the number of males of each species trapped in pheromone traps, we calculated the relative abundance of the species [4].

In the surveyed cotton crop rotation fields (cotton, kenaf, corn, alfalfa), the scoop complex, determined by the presence of pheromones, is usually of the same type. However, in some years there were differences, which mainly concerned small species. So, in all areas, the dominant species was the convolvulus scoop, subdominant - exclamation and winter. There was no carradrina and leaf corn in the corn and cotton fields. (Leucanialorrhea). Convovulus, winter, exclusion, cotton, meadow (Mythimnaunipuncta) scoops, as well as gamma scoop, C-black scoop, upsilon scoop were identified in the cotton field. The species diversity of scoops in the cornfield was somewhat less: there was no cotton scoop and there was no epsilon scoop. In the alfalfa field, all kinds of scoops were identified, the pheromones of which were used. In the fields of vegetable crops, all types of scoops were also found, the pheromones of which were used during observations, with the exception of caradrins and corn leaf scoops. On the vegetable crops of the Tashkent region, the number of scoops was generally higher than on the cotton crop rotation fields in the Yangiyul district. In vegetable crops, as well as in agrocenoses of cotton crop rotation, the dominant species was the convolvulus scoop, subdominant-exclamation and winter scoops. So, a day after installing pheromone traps, 14.7 individuals were caught on red pepper, and 11 individuals were caught on tomatoes and alfalfa. At the same time, in the fields of alfalfa, tomatoes and red pepper, it was found on traps with winter pheromones of 6, 7.7 and 10.7 individuals, respectively. According to available data, the generalized economic threshold of harmfulness is considered to be catching, on average, 5 or more butterflies of winter scoops per day (night), which corresponds to a caterpillar density of 2.6 - 4.0 individuals per 1 m2.

In the fields of vegetable crops studied by us, the number of winter owl butterflies exceeded the above-mentioned EVP. With the help of pheromones of other scoops, a large number of other species that are not inferior to the winter scooper were identified; the total number of detected scoops significantly exceeded the generalized damage threshold set for only one species.

Thus, the use of gender (sexual) analogues of pheromones makes it possible to establish the specific composition of scoops in the fields of various crops, as well as to identify the total number of pests in a separate field and signal the need for protective measures to regulate their numbers. [3]

Pheromones, in particular, changes in their structure (destruction) from a physical point of view are influenced by the values of the electric dipole moment (μ, D) and the wavelengths corresponding to the absorption maximum (λmax, nm). For oxygen-containing pheromones, the values of the electric dipole moment are in the range of 1.23–2.71 D, for unsaturated hydrocarbons - in the range from 0.29 to 0.49. Pheromones, in which partial positive and partial negative charges are located on different parts of the molecule, are mutually oriented in space in such a way that there are other polar molecules nearby – components of air, for example, water molecules whose dipole moment is 1.85 D. Coulomb interaction between polar fragments of molecules can create favorable conditions for their mutual orientation, flow chemical reaction and, as a consequence, for the destruction of the pheromone.

Modeling of photoexcitation processes has shown that the absorption wavelengths are affected by the presence, number and mutual arrangement of multiple bonds in the molecule. For pheromones that do not contain multiple bonds, the maximum absorption lies in the range of 136-144 nm, for unsaturated hydrocarbons and unsaturated oxygen–containing pheromones – in the range of 157-204 nm, for oxygen-containing pheromones with conjugated double bonds - in the range of 226-230 nm. The intensity of the pheromone signal will decrease when exposed to light radiation, since the excited state is unstable, the molecule goes into the ground state, losing energy due to radiation, vibrations or when colliding with other molecules.

Exposure to electromagnetic radiation leads to changes in the electronic and atomic structure of pheromones. Most pheromones of lepidoptera insects belong to unsaturated compounds containing up to three double bonds in the structure. Analysis of the electronic structure of pheromone molecules shows that, regardless of the presence and type of oxygen-containing functional group, the redistribution of electron density during light absorption occurs in the region of the location of double bonds and corresponds to the transition of an electron from π-binding to π*-loosening orbitals. The change in bond lengths occurs only in the area of the location of multiple bonds and does not affect oxygen-containing functional groups. Such a change in the bond length is unlikely to lead to the destruction of the initial atomic structure of molecules only under the influence of electromagnetic radiation, but it will increase their reactivity and promote the flow of chemical reactions when interacting with air components. For bicyclic pheromones, during the transition to an excited state, an increase in the length of one of the bonds included in both cycles is observed, which can lead to the opening of one of the cycles of the molecule and the destruction of the pheromone molecule.

Evaluation of the resistance of pheromones to thermal effects using the results of first-principle calculations showed that the lengths of single bonds in non-cyclic and monocyclic molecules are most likely to change during thermal exposure, while light radiation primarily affects multiple bonds, leading to an increase in their lengths. For bicyclic unsaturated pheromones, exposure to light radiation and thermal exposure lead to similar structural changes – an increase in the length of a single bond included in both cycles, which can lead to its rupture and the opening of one of the cycles in the structure of the molecule.

Factors that can deactivate pheromone molecules can be adsorption on the surface of plants, exposure to temperature, light and chemical interaction with substances-components of air. Water molecules that are present in the air can interact with polar pheromone molecules, which will lead to a decrease in their concentration. Exposure to light radiation of the ultraviolet part of the spectrum converts pheromone molecules into an excited state, while bond lengths and valence angles change in the molecules. Linking the considered process of molecule excitation with insect communication, it can be assumed that the pheromone molecule in the excited state may not be detected by insect sensors, since the efficiency of pheromone binding inside the receptor depends on its atomic structure, that is, the intensity of the pheromone signal will decrease.

Pheromone molecules must have certain physical characteristics in order to remain in the air stream for some time sufficient for the signal to propagate, but they should not accumulate in the territory in order to carry up-to-date information about the position of the signal source. The huge species diversity of insect pests, the multicomponent composition of pheromones, complex multi-stage processes of obtaining pheromones from insects in laboratory conditions lead to the need to develop alternative non-experimental methods for studying the properties of pheromones and mechanisms of chemical communication. We can consider the properties of insect pest pheromone molecules by investigating them using the methods of quantum condensed matter theory.

The application of quantum theory methods makes it possible to obtain the basic physical characteristics of pheromone molecules and assess their resistance to external factors such as thermal and light effects without the use of expensive experimental techniques. This approach is universal for different types of pheromone molecules of various insect species, which is very important, given the multicomponent composition of pheromones and the species diversity of insect pests.

Establishing the relationship between the search behavior of insects and the physical characteristics of pheromone molecules can be used to obtain information about the search behavior of insects based on data on the chemical composition of the pheromone. Data on the resistance of pheromone molecules to environmental factors obtained using the first-principle methods of quantum theory can be used to modernize and improve the effectiveness of insect population control methods based on the use of pheromone preparations.6

Theoretical modeling and calculation of the physical characteristics of pheromone molecules was carried out within the framework of the density functional theory using the B3LYP functional, using basic packages 6-31G** and cc-pVDZ implemented in the GAMESS-US program. The calculation of absorption spectra and optimization of molecules in the excited state was carried out by the Time Dependent method. The assessment of the effect of thermal exposure on pheromone molecules was carried out using a method based on the calculation of modes of normal oscillations.

The geometry of lepidopteran insect pheromones makes it possible to form conformers by rotating parts of the molecule relative to each other around σ-bonds, therefore, at the first stage of the study, modeling and calculation of the properties of pheromones in various conformations other than the linear structure were performed. The energy and structural characteristics in the ground and excited states were determined for all conformers, and the absorption spectra of electromagnetic radiation were calculated. Analysis of the obtained data showed that a change in conformation leads to a change in the total energy of the molecules by no more than 24 kJ/mol, which is less than 0.001% of the total energy of the molecules. On average, the difference between the total energy of the conformers is 6 kJ/mol. A slight difference in energy between the conformers suggests that the formation of certain conformations is not characteristic of the pheromones of lepidoptera insects. Figure 2 shows examples of pheromones in linear (K1) and twisted (K2) conformations with corresponding values of the linear dimensions of the molecule, the electric dipole moment and the wavelength corresponding to the absorption maximum.

The influence of the geometry of molecules on the value of the electric dipole moment and the absorption spectra of pheromones was considered. For oxygen-containing pheromones, a change in conformation leads to a change in the dipole moment by an average of 30% relative to the linear structure (Figures 2A and 2B), for hydrocarbons, an increase in the dipole moment during the transition from the linear conformation to the maximum twisted is up to 50%.

The values of the dipole moment and the wavelengths corresponding to the absorption maximum for different types of pheromone molecules are given in Table 1.

For oxygen-containing pheromones, the values of the electric dipole moment are in the range of 1.23–2.71 D, for unsaturated hydrocarbons - in the range from 0.29 to 0.49. Pheromones, in which partial positive and partial negative charges are located on different parts of the molecule, are mutually oriented in space in such a way that there are other polar molecules nearby – components of air, for example, water molecules whose dipole moment is 1.85 D.

Table 1.

Calculated values of the electric dipole moment (μ, D) and the wavelengths corresponding to the absorption maximum (λmax, nm) for lepidopteran insect pheromones

Pheromone Type	μ, D	λ_{max}, нм
A pheromone that does not contain multiple bonds	1,76-2,04	136-144
Unsaturated hydrocarbons	0,29-0,49	1 9
Unsaturated oxygen-containing pheromones	1,23-2,65	168-204
Unsaturated	1,50-2,71	224-227

Coulomb interaction between polar fragments of molecules can create favorable conditions for their mutual orientation, the course of a chemical reaction and, as a consequence, for the destruction of the pheromone. Considering the high polarity of molecules as a factor contributing to the chemical interaction of pheromones with polar components of the medium, it can be concluded that for oxygen-containing pheromones, the probability of destruction as a result of chemical reactions will be higher than for hydrocarbon pheromones, whose dipole moment is significantly less than 1 D, in all possible conformations.

All calculated lepidopteran pheromones absorb radiation corresponding to the ultraviolet part of the spectrum in the range from 130 to 230 nm. A change in the geometry for some pheromones leads to a shift in the absorption maximum, but not more than 8 nm, that is, not more than 6%. The analysis of spectral characteristics showed that the maximum absorption of pheromones depends primarily on the presence and mutual arrangement of multiple bonds and practically does not depend on the type of oxygen-containing functional group. The greatest energy is required to excite the limiting epoxide, the minimum – for pheromones with conjugated double bonds. As noted earlier, a change in the conformation of the molecule does not lead to a significant shift in the absorption maximum.

Exposure to electromagnetic radiation leads to changes in the electronic and atomic structure of pheromones. For disparlure, a pheromone of an unpaired silkworm that does not have multiple bonds in the structure, the change in electron density during radiation absorption occurs in the region of the epoxy ring for all conformers. The calculation of the geometry of the disparlure in the excited state shows similar structural changes for all conformations: the values of the valence angles change in the epoxy ring, one of the C-O bonds increases to an average of 0.9 Å, which can further lead to its rupture and, as a consequence, to the opening of the cycle and the destruction of the pheromone. Most pheromones of lepidoptera insects belong to unsaturated compounds containing up to three double bonds in the structure. Analysis of the electronic structure of pheromone molecules shows that, regardless of the presence and type of oxygen-containing functional group, the redistribution of electron density during light absorption occurs in the region of the location of double bonds and corresponds to the transition of an electron from π-binding to π*-loosening orbitals (Figure 3).

The change in bond lengths occurs only in the area of the location of multiple bonds and does not affect oxygen-containing functional groups. Similar structural changes occur in all unsaturated pheromones of lepidoptera. The increase in the lengths of double bonds occurs on average by 0.1 Å. Such a change in the bond length is unlikely to lead to the destruction of the initial atomic structure of molecules only under the influence of electromagnetic radiation, but it will increase their reactivity and promote the flow of chemical reactions when interacting with air components. The interaction of the pheromone with the protein of the insect's olfactory receptor occurs according to the "key-lock" principle, that is, in addition to the chemical composition of the pheromone, its geometric correspondence with the protein plays an important role. Therefore, the course of chemical reactions or a significant change in the initial geometry of the molecule will lead to the deactivation of the pheromone as a carrier of information.

The calculated characteristics of lepidoptera pheromones were compared with the data on the search activity of insects.

The pheromone of the unpaired silkworm consists of one component – disparlure, the pheromone of the pine silkworm includes four components, the structure of the molecules is shown in Figure 4. One can see obvious differences in the intensity and wavelengths of absorption of pheromones of these two species. It is known that the unpaired silkworm, whose pheromone absorbs in the region of 130 nm with very low intensity, is characterized by searching behavior throughout the day, while the pine silkworm is characterized by activity in the evening and at night, in the absence of solar radiation. For the pheromones of the Siberian silkworm and moths, the absorption spectra lie in the same range as for the pine silkworm and have similar values of the intensity of electronic transitions. The traceable relationship between the spectral characteristics of molecules and data on the time of summer suggests that the physical properties of pheromones to some extent determine the time of insect search activity.[6]

3. Conclusion

The efficiency of information transmission using pheromone molecules is determined by several factors, for example, such as the resistance of pheromones to the effects of the external environment on them, that is, to their physico-chemical characteristics. The purpose of pheromones and the principle of their action is based on their preservation of their composition and structure, for a certain time, which should be enough to spread in the air, and to reach individuals who should receive a chemical signal. And the use of highly resistant molecules as pheromones can lead to clogging of the information channel and disorientation of individuals receiving signals.

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