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CHEMICAL MIXING SYSTEM

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The modern era of microelectronics allows creating not only flexible but also less resource-intensive control systems, in comparison to existing similar ones. Options of component set for task solving appearing, the possibility of creating a chemical mixing control system has become available. The rapidly changing economic situation has led to a rethink of the resource saving importance. This factor has increased the demand for automated resource control and management systems.

Keywords: Raspberry Pi, Arduino, chemical mixing, fertilizer, automation system.

An automated system allows you to optimize resource consumption, ensure data reliability, increase comfort by informing and automatic resources managing. Thus, it is possible not only to see the current consumption of resources, but also in case of abnormal consumption, to automatically cut it of.

The object of the study is to consider the possibility of creating a chemical mixing system as a separate module of a plant growing system.

The subject of the study is the use of a modern Arduino Uno R3 Microcontroller board in the system of control and management of chemical mixing.

Mineral fertilizers can be simple and complex. Each simple fertilizer contains one element (e.g. nitrogen or phosphorus), while complex fertilizers consist of two or more components [1].

A chemical mixing system (hereinafter ChMS) is an integrated chemical dosing control system in a closed water circuit which is implemented with automatic operation system, and with a possibility of manual control as well.

The purpose of ChMS is to develop a chemical mixing control and automation system.

The ChMS tasks are:

– to facilitate chemical dosing control;

– resource saving;

– to create an information base on chemical mixing systems.

The composition of the chemical mixing system includes:

– the centralized management of all peristaltic pumps;

– pH and EC measurement;

– a set of dosing sketches depending on the crop grown.

The management of dosing is centralized according to pre-configured sketches.

Sketches are defined programs with manual or automatic activation. By controlling the sketches, each pump can be activated, and the appropriate dosage and response time for each individual pump can be set.

ChMS technical resources:

– a Raspberry Pi Microcomputer;

– a set of peristaltic pumps;

– a set of sensors;

– Arduino Uno R3.

ChMS information resources:

– Raspbian operating system;

– a web resource (information management site);

– a monitoring system;

– a set of managing sketches.

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QUANTUM-CHEMICAL CALCULATIONS OF NEW AZOMETHINE COMPOUNDS WITH ANTIOXIDANT ACTIVITY

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This publication represents theoretical calculations applied to newly synthetized azometine compounds to de-fine their optimized state, predicts its free energy, and distinguishes molecular orbitals that involved in spectrum for-mation.

Keywords: PM6, B3LYP, semi-empirical, theoretical calculations.

Materials and methods

For calculations we used a personal computer with an Intel core i7 processor (2.21 GHz CPU), with the installed Ubuntu 18.04 operating system. When calculating the starting geometry of the molecule with an azomethine base, we selected the method of molecular mechanics (MM+) of the HyperChem 08 software package. The choice of the MM+ method is justified by the fact that it has developed for organic molecules, takes into account potential fields generated by all atoms of the calculated system, and allows you to flexibly modify the calculation parameters depending on the specific task. Starting geometry of the molecule was additionally optimized in a solvent medium of N, N-dimethylformamide (DMF) using the semi-empirical PM6 method of the Gaussian 16 software package to achieve a global minimum of the total energy of the systems under study. To find the global energy minimum and the most stable conformers, we analyzed all the stationary points on the surface of the potential energy of the molecules.

Full optimization and calculation of the electronic structure was carried out by the non-empirical DFT / B3LYP method in the basis 6-311++G. This method is used to calculate optimized geometries, electronic absorption spectra, total energy and heat of formation and we used to calculate the electronic absorption spectrum of azomethine mole-cules. Electronic spectrum of the molecule 4-((Z)-((4-((E)-phenyldiazenyl)phenyl)imino)methyl)benzoic acid ($C_{20}H_{15}N_3O_2$) was calculated for 20 single-electron excitations in the region of 242.29 - 514.56 nm in the basis of 6-31G *.

The theoretical absorption spectrum of the optimized molecule in a solvent medium was calculated using the Gaussian 16 software package using the theory level RB3LYP / 6-311 ++ G. The average scaling factor of the program in calculating the UV spectra is 0.99 [1,2].

Results and discussion

Using the PM6 method we had found optimized geometric configurations.

The maximum wavelength with a high oscillator strength was observed at $\lambda = 479.15$ nm и f = 2.0107 (Table 1, Fig. 2,3). The calculation showed that the strongest electron transition is observed at an absorption maximum of 479.15 nm, which refers to the transition of an electron to an excited singlet state $S_0 \rightarrow S_2$. The remaining transitions have a small value of f and forbidden by symmetry.

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