gramming of the system node interaction, C / C ++, Java, and Android frameworks will be used. The database management system is MySQL.

The second part of the proposed system is the design of an aircraft capable of carrying a mini-weather station. It is proposed to use an airship as an aircraft. Attaching a mini-weather station to an aircraft will allow receiving data from the most hard-to-reach regions, including areas exposed to chemical or radioactive contamination.

At this stage, the system requirements are being determined and a working draft of an aircraft for the installation of a mini-weather station is being developed.

QUANTUM-CHEMICAL CALCULATION AND SYNTHESIS OF NEW ANTHRAQUINONE COMPOUNDS FOR BIOLOGICAL APPLICATIONS

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A number of anthraquinone compounds have been calculated and predicted by non-empirical chemical-quantum calculations. Their equilibrium geometric parameters, electronic, IR and NMR spectra have been predicted and discussed. Antioxidant properties of them have been calculated.

Keywords: non-empirical method, antioxidant activity, anthraquinone, UV/Vis, optimization.

Anthraquinones are a group of functionally diverse aromatic compounds structurally related to anthracene, also known as 9,10-anthraquinone, 9,10-anthracenedione, anthradione and anthracene-9,10-quinone [1]. They are moderately strong and chemically stable, have provoked broad investigation of anthraquinones based structures as dyes and colorants [1].

Computational methods

A Pentium IV personal computer (CPU at 4.80 GHz) with the Windows 10 operating system was used. The initial geometry optimization of title compounds was performed with HyperChem (Version 8.0 Hypercube, Inc., Alberta, Canada). For all the ab initio calculations, Gaussian 16 was employed. The molecular properties of the compounds were calculated by PM6 method. Lowest energy structures of the species were computed by conformational analysis. Geometry optimization was performed at the PM6 density functional theory with the same basis set. For the geometry optimization of parent molecules restricted approach was applied, while for the free radicals the unrestricted was used. For computational calculations of radicals H atom was removed from OH groups of optimized most stable structure of the neutral molecules. Harmonic vibrational frequencies were computed at the same level of theory for both neutral molecules and radicals to estimate zero-point energies and vibrational contributions to enthalpy. The O-H bond dissociation enthalpy was calculated at 298.15 K using following formula:

$$BDE = Hr + Hh\text{-}Hn \quad (1)$$

where, Hr is the enthalpy of the radical generated through H-abstraction, Hh is the enthalpy of hydrogen atom [-0.4962 Hartree] and Hn is the enthalpy of neutral molecule. The following formulas were applied to calculate electronic properties of the title molecules and their radicals [1]:

$$IP = -E_{HOMO}\ (eV) \quad (2)$$

$$EA = -E_{LUMO}\ (eV) \quad (3)$$

$$\eta = (IP - EA)/2\ (eV) \quad (4)$$

$$S = 1/2\eta\ (eV) \quad (5)$$

$$\mu = (IP + EA)/2\ (eV) \quad (6)$$

$$\omega = \mu 2/2\eta\ (eV) \quad (7)$$

$$\omega+ = (IP + 3EA)2/16(IP - EA)\ (eV) \quad (8)$$

$$\omega- = (3IP + EA)2/16(IP - EA)\ (eV) \quad (9)$$

$$Eg = E_{LUMO} - E_{HOMO}\ (eV) \quad (10)$$

All the calculations were carried out in N,N- dimethylformamide (DMF) environment with the Polarizable Continuum Model (PCM) using the Integral Equation Formalism variant (IEFPCM) solvation model [1].

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SIMULATION OF INTERACTION OF HIGH ENERGY PROTON BEAM WITH HEAVY TARGETS

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The study of processes occurring in Accelerator Driven system (ADS) is of high interest in the development of innovative projects. The main reason for this interest is using the accelerator as an external source of neutrons which makes such systems safer to operate and makes it easy to control chain fission reaction. Furthermore, ADS seems to be a promising system for energy production and transmutation of spent nuclear fuel.

Keywords: Accelerator Driven system, Monte Carlo method.

An experimental study at potentially dangerous facilities is often costly and difficult to implement. To justify and plan experimental studies on a subcritical system, it is necessary to determine some of its characteristics. Neutronics of ADS can be calculated using modern simulation programs based on the Monte Carlo method.

In this research lead and tungsten targets exposed to high-energy protons were investigated. For this issue the model of the target was developed for calculation by Geant4 code. Standard physics list QGSP_BIC_HP was used for simulation. Different characteristics of radiation coming out of heavy targets were obtained and compared with relevant experimental data [1, 2].

Previously, the neutron yield from the lead and tungsten targets was calculated. Next, energy spectra of emitted secondary particles were obtained for both targets and different source energy. The simulation results are in good agreement with corresponding experimental data and similar calculations using other Monte Carlo codes [1, 2]. Also, the processes occurred in the targets exposed to proton beam were determined.

The development of a full-scale model of ADS is planned for studying its kinetics and experimental research at the Joint Institute for Nuclear Research (Dubna, Russian Federation).

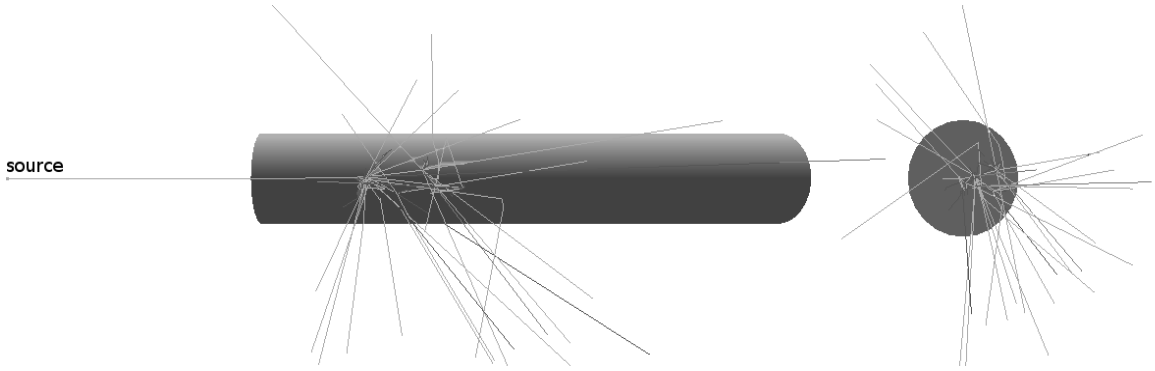

Fig. 1. – Model of lead target irradiated to proton with energy 1,4GeV