

THEORETICAL MODEL OF PHYSISORPTION EFFECT OF CO ON CONIINE AND FURANOCOUMARINS FOR AIR PURIFICATION

V. Cheplya¹, S. Shahab^{1,2,3}, M. Murashko¹

¹Belarussian State University, ISEI BSU,
Minsk, Republic of Belarus
vlad1997.cheplya@gmail.com

²Institute of Physical Organic Chemistry, National Academy of Sciences of Belarus,
Minsk, the Republic of Belarus

³Institute of Chemistry of New Materials, National Academy of Sciences of Belarus,
Minsk, the Republic of Belarus
siyamakshahab@mail.ru

For the first time in the present work, the adsorption properties of the Coniine and Furanocoumarins at the non-bonded interaction with CO was investigated by density functional theory (DFT/B3LYP/MidiX, DFT/M062X/6-311+G* levels of theory) in the solvent water.

Keywords: physisorption, DFT method, Coniine, Furanocoumarins, Air Purification.

For the first time in the present study, the non-bonded interaction of the Coniine and Furanocoumarins with carbon monoxide (CO) was investigated by density functional theory (DFT/B3LYP/MidiX, DFT/M062X/6-311+G*) in the gas phase and solvent water. The adsorption of the CO over C₈H₁₇N was affected on the electronic properties such as E_{HOMO}, E_{LUMO}, the energy gap between LUMO and HOMO, global hardness. Furthermore, chemical shift tensors and natural charge of the C₈H₁₇N and complex C₈H₁₇N/CO were determined and discussed [1]. According to the natural bond orbital (NBO) results, the molecule C₈H₁₇N and CO play as both electron donor and acceptor at the complex C₈H₁₇N/CO in the gas phase and solvent water. On the other hand, the charge transfer is occurred between the bonding, antibonding or nonbonding orbitals in two molecules C₈H₁₇N and CO. We have also investigated the charge distribution for the complex C₈H₁₇N/CO by molecular electrostatic potential (MEP) calculations using the M062X/6-311+G* level of theory. The electronic spectra of the C₈H₁₇N and complex C₈H₁₇N/CO were calculated by time dependent DFT (TD-DFT) for investigation of the maximum wavelength value of the C₈H₁₇N before and after the non-bonded interaction with the CO in the gas phase and solvent water. Therefore, C₈H₁₇N can be used as strong absorbers for air purification and reduce environmental pollution [2].

BIBLIOGRAPHY

1. Shahab, S. Interaction between new synthesized derivative of (E,E)-azomethines and BN(6,6-7) nano-tube for medical applications: Geometry optimization, molecular structure, spectroscopic (NMR, UV/Vis, excited state), FMO, MEP and HOMO-LUMO investigations / S. Shahab [at all] // J. of Molec. Struct. – 2017. – Vol. 1, № 1146. – P. 881–888.
2. Shahab, S. DFT study of physisorption effect of CO and CO₂ on furanocoumarins for air purification / S. Shahab [at all] // J. of Environmental Chemical Engineering. – 2018. – Vol.6, № 4. – P. 4784–4796.

EFFECTIVENESS OF PRENATAL DIAGNOSTICS OF CONGENITAL DEVELOPMENT DISORDERS IN THE REPUBLIC OF BELARUS ACCORDING TO THE DATA OF THE BELARUSIAN REGISTER

S. Chirlina, A. Ershova-Pavlova, N. Kokorina

Belarussian State University, ISEI BSU,
Minsk, the Republic of Belarus
chirlina98@mail.ru

Keywords: congenital malformations, the effectiveness of prenatal diagnosis.

Congenital malformations (CHD) in recent decades have occupied a major place in the world among the causes of stillbirth, infant and child morbidity, disability, and mortality.

Congenital pathology caused by impaired fetal development is observed in approximately 2–3 % of newborns and is the most common cause of neonatal mortality and morbidity. According to the WHO, malformations are diagnosed in 18 % of stillbirths, in 25,6 % of children who died in the perinatal period, in 50 % of children who died during the first year of life.

In Belarus, CDF monitoring is carried out within the framework of the Belarusian Register on the basis of the Republican Scientific and Practical Center "Mother and Child", which is unique in terms of the breadth of coverage of controlled territories and the number of births analyzed. In world practice, similar national registers are available only in Hungary, Sweden and Finland.

The monitoring system allows you to: analyze the number of congenital malformations, population frequencies and the effectiveness of prenatal diagnosis (EPD), which is the basis for taking measures to prevent the birth of children with developmental abnormalities. EPD is defined as the ratio of prenatally diagnosed CMD to the total number of identified abnormalities.

The purpose of this study was to assess the number of congenital malformations and the effectiveness of their prenatal detection for 2005–2016 in Belarus. It was established that, on average, 3540 cases of congenital malformations were detected per 108171 births, incl. in stillborn – 2753, in stillborn – 28; EPD was 21,45 %. The highest level of EPD was observed in the Mogilev (28,20 %) and Gomel (28,15 %) regions. The lowest EPD values were found in Grodno (16,95 %) and Minsk (17,12 %) regions. It should be noted that in the republic for 2012–2016. there is a tendency to increase the EPD of malformations (23,71 %), compared with 2005–2011. (20,47 %), which is largely due to the development and implementation in practice of improved methods for prenatal detection of congenital heart disease, central nervous system, systemic skeletal dysplasias and a number of other defects.

The results of prenatal diagnosis make it possible to prevent the birth of more than 800 children with severe, incurable, disabling, developmental abnormalities annually, which is an indicator of the effectiveness of the preventive activities of the republic's medical and genetic services. Prevention of the birth of such children makes a significant contribution to reducing the incidence of childhood morbidity, disability and mortality.

An analysis of the CD-ROM database and the level of EPD indicates the need for further optimization of the provision of specialized medical care, both in the country and in individual regions, which makes a significant contribution to reducing the incidence of child morbidity, disability and mortality in the country.

BIBLIOGRAPHY

1. *Naumchik, I. V.* Primary prevention of the most common congenital malformations in the Republic of Belarus. Instructions for use / I. V. Naumchik, O. V. Pribushenya, A. A. Ershova-Pavlova, , R. D. Khmel, I. O. Zatsepin. – Minsk. : – 2011. – 8 p.
2. *Vilchuk, K. U.* Monitoring system in the characterization of the number and frequency of congenital malformations of the central nervous system in Belarus / K. U. Vilchuk, A. A. Ershova-Pavlova, G. I. Karpenko, R. D. Khmel, I. V. Naumchik // Achievements of the Medical Science of Belarus. – 2014. – № 19. – P. 49–50.
3. *Ershova-Pavlova, A. A.* Monitoring system of congenital malformations in Belarus / A. A. Ershova-Pavlova, R. D. Khmel, A. A. Lazarevich, G. A. Karpenko, I. V. Naumchik // Theses of the 14th International Scientific Conference Sakharov Readings of 2014: Environmental Problems of the 21st Century. – Minsk, 2014. – P. 78.

ASSESSMENT OF RADIOACTIVE IMPACT ON INDIVIDUAL OBJECTS OF THE BIOTA ON THE LEVEL OF CONTAMINATION IN DIFFERENT TYPES OF LAKES

A. Chuholskiy, M. Pashuk

Belarusian State University, ISEI BSU,

Minsk, Republic of Belarus

Chuholskiy96@mail.ru

mailto:aleynikova-1997@bk.ru

The specific activity of cesium -137 decreased over time for the majority of fish species living in the waters of the national Park Pripyat. In 2016, perchorgans showed a slight increase in the average specific activity of radionuclide. An increase in the accumulation of cesium 137 was detected in 2017 by the organs of some fish. 2018-year fish monitoring showed decrease in the average specific activity of ¹³⁷Cs in all studied fish species.

Keywords: biota, reservoir, nuclear weapons, radionuclides, aquatic ecosystems.