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The article is devoted to the results of the survey of patients from the Minsk Regional Clinical Center "Psychiatry-Narcology". The study involved 49 patients aged up to forty years. In the questionnaire, the authors fo-cused on the main sociological and demographic indicators.

Keywords: alcohol dependence, sociological factors, demographic indicators.

According to statistics from the World Health Organization, about 240 million people in the world are alco-hol-dependent, which makes up about 3,5% of the world's population, and alcohol abuse causes 3,3 million deaths per year (6% of all deaths in the world). Today, alcoholism remains a high priority public health issue, and the med-ical component of this disease goes far beyond the scope of narcology itself, since regular use of alcohol leads to the development of somatic diseases. Alcohol abuse is an acute social issue, leading to an increase in road traffic accidents, work-related injuries, and criminal offenses. The population's alcoholization is not a concern of a single country. It is a common problem of a developed society as it affects many states.

#### Material and methods

The material for the study was the questionnaire data of people suffering from alcoholism, in the amount of forty nine. The questionnaire was completely voluntary and anonymous and was carried out by specialists of the Minsk Regional Clinical Center "Psychiatry-Narcology". The questionnaire was conducted with age restrictions, and patients older than 40 years did not fall into the group of respondents. All data were received in 2019.

#### Results

The study involved men and women suffering from alcohol use disorder. The age of the patients ranged be-tween 19 and 39 years, the mean age was 32 years. In total 29 men (mean age 32 years, range 21–39 years) and 20 women (mean age 31,6 years, range 19-37 years) were surveyed. 57,1% of patients had an alcoholdependent fa-ther, 8,1% of patients had a nicotine-dependent father and 30,6% of patients had an alcoholdependent mother. The numbers can be much larger as the patients didn't always answer the question about their relative's dependen-cy, and some patients didn't know anything about their biological parents. It should be noted that 5,1% of patients have vocational education (28 people), 28,6% of patients have secondary education (14 people), 8,1% of patients have higher education (4 people) and 6,1% of patients have only basic education (3 people). 29 patients were born in a city, 10 - in an urban-type settlement and 10 in a village. 12 respondents grew up in a single-parent family, 3 – without parents at all. 33 of 49 have patients 1–3 children. As far the patient's financial situation is concerned, 16 people earn from 300 to 500 rubles (9 of them work in state enterprises, 1 patient is on maternity leave, and 3 pa-tients work for a private company), 13 people earn from 500 to 700 rubles (4 patients work in state-owned enter-prises and 9 - in private firms), 6 people's earnings range between 700 and 1000 rubles (4 of them work in state enterprises, 2 people work for a private company, 1 patient is an individual entrepreneur), 6 people earn more than 1000 rubles (1 works in a state enterprise, 5 patients work for a private company and 1 is an individual entrepre-neur). 10 patients don't work one of them is a student.

#### **Discussion and conclusions**

From the results obtained, we can conclude that men are more likely to suffer from alcoholism, but at the same time, women are characterized by an earlier onset of regular alcohol use. The assumption that parent's alco-hol dependence contributes to the development of alcohol abuse in children was partially confirmed by us, and in more than half of the cases, people with alcohol use disorder have a parent who also regularly used or uses alcohol. It is also shown that people suffering from alcohol abuse were usually brought up in single-parent families.

According to the National Statistics Committee of Belarus, Belarusian worker's average salary in August amounted to 1117,80 rubles. If we compare this figure with the data we received as a result of the survey, we can see that the material well-being of people suffering from alcoholism is significantly lower than the average level. So only 6 people out of 49 (12,2%) have a monthly salary of 1,000 rubles or more.

It is also worth noting that people suffering from alcohol use disorder in most cases don't have higher educa-tion. So, among our patients only 4 people out of 49 (8,1%) had a higher education, and this percentage is much lower than the average in the Republic of Belarus.

It can be concluded that people's alcohol dependence imposes a burden on society, and the more people suffer from alcohol use disorder, the higher this load is.

## CONIINE, PHYSICO-CHEMICAL PROPERTIES AND ITS APPLICATION IN THE ENVIRONMENTAL INDUSTRY

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For the first time the geometric parameters of the coniine molecule were calculated, the electronic and UV spectrum of coniine was calculated by an ab initio method (M062X). The intermolecular interaction between the molecules of the coniine and the molecules of CO of the air has been established. It has been found that coniine is a powerful absorber of CO air.

Keywords: coniine, adsorption, DFT, non-bonded interaction, NBO analysis.

For the first time in the present study, the non-bonded interaction of the Coniine (C8H17N) with carbon monoxide (CO) was investigated by density functional theory (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 EHOMO, ELUMO, 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. 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 [1].

1. The adsorption energy of CO over C8H17N in the gas phase (-2,67 eV) is greater than solvent water (-1,33 eV).

2. It is found that some geometrical parameters of C8H17N are changed after adsorption process due to the formation of intermolecular non-bonded interaction.

3.NBO analysis predicted a charge transfer from the molecule C8H17N to CO and from CO to C8H17N. It was found that the electronic properties of the molecule C8H17N are sensitive to the adsorption of the CO. The complex C8H17N /CO in the gas phase has a high chemical activity, low chemical stability and it is a soft system rather than complex in the solvent water.

4. The non-bonded interaction between the C8H17N and CO is changed the value of  $\lambda$ max. Therefore, C8H17N may be used for development of filters in order to adsorption of carbon monoxide as environmental pollution [1].

### BIBLIOGRAPHY

1. Sheikhi, M. Interaction between new synthesized derivative of (E,E)-azomethines and BN(6,6-7) nanotube for medical applications: Geometry optimization, molecular structure, spectroscopic (NMR, UV/Vis, excited state), FMO, MEP and HOMO-LUMO investigations / M.Sheikhi, S. Shahab, L. Filippovich, M. Khaleghian, E. Dikusar, M. Mashayekhi, // J. Mol. Struct. – 2017. – No 1146. – P. 881–888.