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QUANTUM CHEMICAL ANALYSIS OF REACTIVITY OF DITHIZONE (DIPHENYLTHIOCARBAZONE) REAGENT

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Abstract. This paper studies methods of lead and zinc metal ions extraction by dithizone from Khondzha wastewater samples. Inorganic metals or ions can act back with dithizone to produce colourful coordination. The dithizone reagent is highly sensitive to the presence of heavy metals such as lead (Pb) and zinc (Zn) as designated in this study. Inorganic metals or ionic can react with dithizone to produce coloured coordination compounds. As a result of studying the "composition-structure-property" system in chemical compounds, it is possible to theoretically predict the properties, composition and molecular structure of complex compounds during research. Such information helps to synthesize complex compounds with selected properties, composition and structure. Creating the basis of theoretical studies of the formation of complex compounds and the possibility of their practical application is one of the urgent problems of the chemistry of coordination compounds in the advanced period of modern science.

Keywords: dithizone, extraction method, Khondzha, lead and zinc metal ions,

КВАНТОВО-ХИМИЧЕСКИЙ АНАЛИЗ РЕАКЦИОННОЙ СПОСОБНОСТИ РЕАГЕНТА ДИТИЗОНА (ДИФЕНИЛТИОКАРБАЗОНА)

Абстрактный. В статье изучены методы извлечения ионов металлов свинца и цинка дитизоном из проб сточных вод Хонджи. Неорганические металлы или ионы могут действовать в ответ на дитизон, создавая красочную координацию. Реагент дитизон очень чувствителен к присутствию тяжелых металлов, таких как свинец (Pb) и цинк (Zn), как указано в этом исследовании.

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Неорганические или ионные металлы могут реагировать с дитизоном с образованием окрашенных координационных соединений. В результате изучения системы «состав-структура-свойство» в химических соединениях можно теоретически прогнозировать свойства, состав и молекулярное строение сложных соединений в ходе исследований. Такая информация помогает синтезировать сложные соединения с выбранными свойствами, составом и структурой. Создание основ теоретических исследований образования комплексных соединений и возможности их практического применения является одной из актуальных задач химии координационных соединений в развитый период современной науки.

Ключевые слова: дитизон, метод экстракции, Хонджа, ионы металлов свинца и цинка,

INTRODUCTION

In addition to the widespread use and economic importance of zinc, lead and related compounds, they are included among the ecotoxicologically dangerous materials. This makes the removal, separation and purification of these metals from various sources an important topic of many fundamental and industrial studies[1].

It is known that liquid-liquid extraction techniques play an important role in the development of processes for the recovery and separation of various metal ions. Undoubtedly, the selectivity and efficiency of these methods are mainly determined by the extracting substances [2]. These heavy metals are non-biodegradable and accumulate in living systems, causing various serious diseases. These metals are widely distributed in the environment and eventually enter the food chain and are released from industrial activities (industrial waste, metal production, incineration plants, electroplating, fuel burning, etc.) and agricultural activities[3]. There are numerous techniques for extracting metals from water, but extracting metals from seawater stands out as particularly challenging due to factors like chloride ions and high salt concentrations. Additionally, this extraction process involves intricate procedures that demand significant manpower, extensive time, and substantial amounts of seawater samples[4].. In this research, the dithizone method was employed for trace metal extraction. Inorganic metals or ions can form colored coordination compounds when they react with dithizone. This dithizone reagent exhibits high sensitivity to heavy

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metals such as lead (Pb), cadmium (Cd), and zinc (Zn), as highlighted in this study. The resulting dithizoneate can then be extracted using organic solvents like carbon tetrachloride (CCl_4). Furthermore, this study entails pH adjustment measures to facilitate dithizoneate production[5].

Experimental part

As a result of studying the "composition-structure-property" system in chemical compounds, it is possible to theoretically predict the properties, composition and molecular structure of complex compounds during research. Such information helps to synthesize complex compounds with selected properties, composition and structure. Creating the basis of theoretical studies of the formation of complex compounds and the possibility of their practical application is one of the urgent problems of the chemistry of coordination compounds in the advanced period of modern science.

Geometric optimization of dithizon was fully optimized using the Popl basis set - RHF/6-311G(d, p) using GaussView 6.0.16 software using the out file generated by the Avogadro software package. Results of GaussView 6.0.16 calculations using the DFT (B3LYP) method The Mulliken method and the frontier molecular orbital (ChegMO) approximation were used to calculate the charges on all atoms[6,7].

Table-1.

Ditison's GaussView 6.0.16 calculated Mulliken charge distribution

№	$Belgi_E$	Zaryad
1	C	-0.234992
2	C	-0.224964
3	C	0.250322
4	C	-0.248240
5	C	-0.229042
6	C	-0.241491
7	H	0.246930
8	H	0.260547
9	H	0.237291
10	H	0.246845
11	H	0.243390
12	C	-0.195050

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13	C	-0.249194
14	C	-0.221005
15	C	-0.247535
16	C	-0.202237
17	C	0.200322
18	H	0.274424
19	H	0.252153
20	H	0.252118
21	H	0.252268
22	H	0.295461
23	N	-0.598566
24	H	0.325167
25	N	-0.523293
26	H	0.345377
27	N	-0.304051
28	C	0.073523
29	S	0.253329
30	N	-0.289805

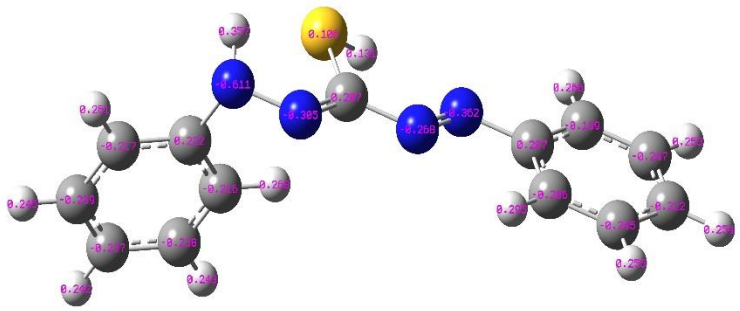

Figure 1. Mulliken charge distribution of dithizone

In reactivity, the distribution of charge on the atoms of the molecule is important, that is, they play an important role in predicting the electrophilic and nucleophilic centers of the molecule. Taking this into account, the total charges of atoms of dithizone molecules were calculated according to the widely used method of charge calculation -

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Mulliken's method. The calculation results show the localization of the largest negative charge on the nitrogen atoms of the dithizone molecule. The largest negative charge is on the nitrogen atom of the amino group and the most mobile hydrogen atom is on the S-H group[8,9].

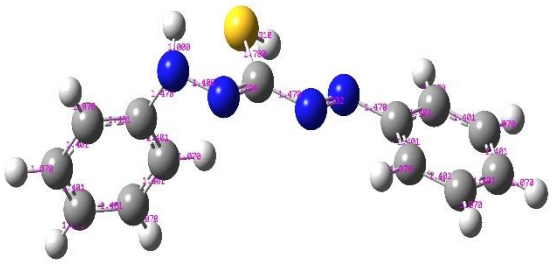

Figure 2. Bond lengths in dithizone molecule

One of the main indices used to evaluate the reactivity of organic compounds is the electron density in marginal MOs (ChegMO). The upper occupied molecular orbital (UMBO) and the lower unoccupied molecular orbital (QBMO) are frontier molecular orbitals. An atom with a high electron density in UBMO is an electron-donating atom and is an electrophilic reaction center. In QBMO, an atom with a high electron density is an electron acceptor atom and a nucleophilic reaction center.

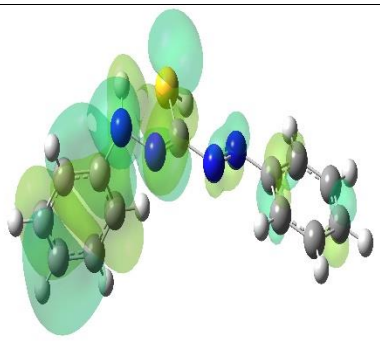	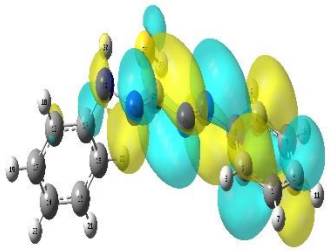
YuBMO = -8,66 eV	QBMO = 1.18 eV

Figure 3. The molecules of the Republic of DIFEN (DIFENILTYOKARTBAZON) Effective charging distribution in donor atoms

The most basic molecular orbital orbital orbital orbital orbital density belongs to the density distribution-band.

The number of sends and Qboma is also important, the difference between orbital

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energy and the difference between them (De = Eqbomo-Eugamo, EV). Among the compounds indicates an increase in the electrical properties of the compound (the elevation of the employed surface direction). Qboma Enterprise sets 90 e-hardy capacity of combustible combination. The hardness (ŋ) and softness of molecules is determined on the basis of CegMo energies. Riddly Ionization Potential (i) and electronic tendencies are equal to 2: ŋ (i-a) / 2; softness is found as follows: s = 1 / 2/. Absolut electrical americity is also found on the basis of the CegMO: (I + A) / 2 = x

It is known that electrostatic potential is used to determine the parts of the molecule and the electronic factor, and very important. The color scale is listed in valuable (minus) and positive (plus) values, and the blue color represents the minimum (excess electronics area) and indicates atoms act as nucleophilic. Red color indicates an electronic deficiency near atoms. The Ditizon Esp Sata has shown that the group-NAN group exists the maximum at the minimum and -s-h band of the group (Figure 4)[10-13].

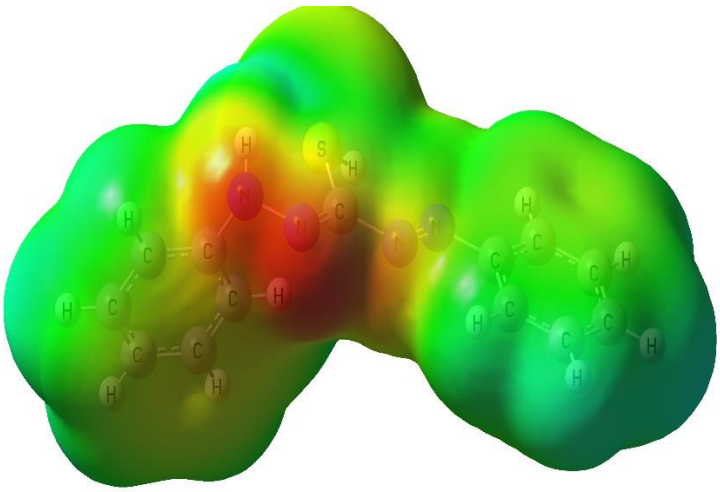

Figure 4. Ditizon (Difeniliokarbazon) electrostatical potential

Table 3.2.

Quant-chemical parameters accrued for DITIZON (DIFENILTYOKARRAZON)

Quantum-chemical parameters	Ditizon
E_{YUBMO}, eV	-8,66
E_{QBMO}, eV	1,18

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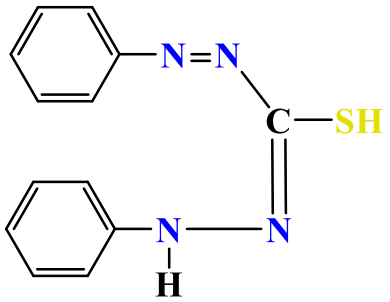
$\|\Delta E\| = E_{QBMO} - E_{YUBMO}$ (eV)	9,85
Ionization potential, $I = -E_{YUBMO}$, (eV)	8,66
Tendency, $A = -E_{QBMO}$, (eV)	-1,18
Electrophonel, $\chi = (I + A)/2$ (eV)	3,74
Chemical hardness, $\eta = (I - A)/2$ (eV)	4,92
Chemical potential, $\mu_p = -(I + A)/2$ (eV)	-3,74
Chemical softness, $\sigma = 1/(2\eta)$ (eV-1)	0,10
Electrophication index, $\omega = \mu_p^2/2\eta$ (eV)	1,42
Dipol moment, μ (Debay)	4,25

With the help of the Chemdrow professional program, the dicy element analysis, the 13C and 13c shows spectrums were studied. The results were given in Figures 4 and 5.



(1*E*)-*N*,2-diphenyldiazene-1-carbohydrazonothioic acid

Chemical Formula: $C_{13}H_{12}N_4S$

Exact Mass: 256,08

Molecular Weight: 256,33

m/z: 256.08 (100.0%), 257.08 (16.4%), 258.07 (4.5%), 258.08 (1.2%)

Elemental Analysis: C, 60.92; H, 4.72; N, 21.86; S, 12.51

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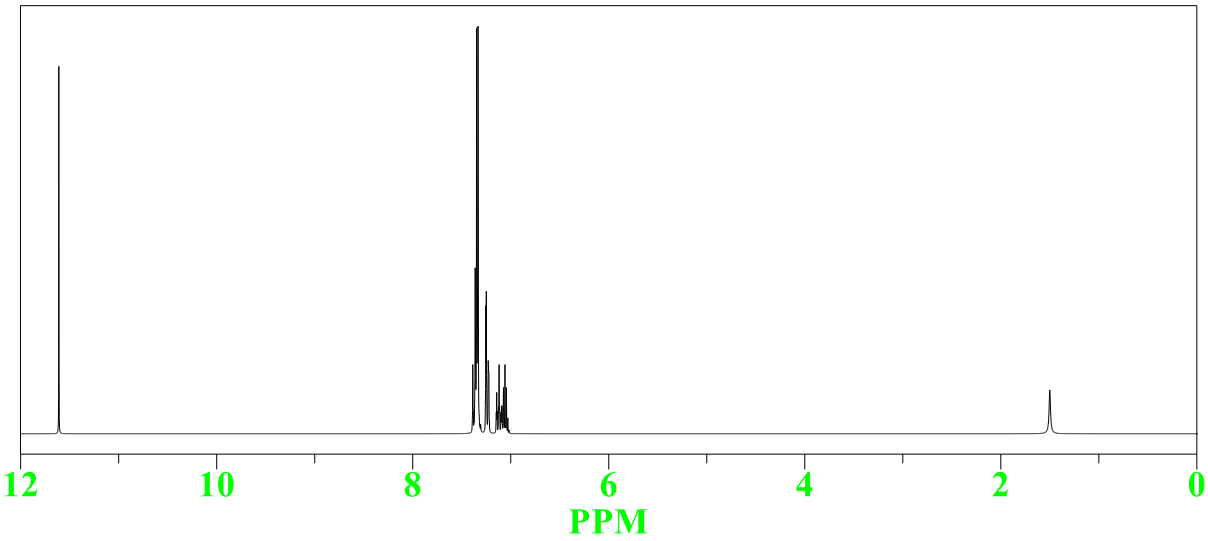
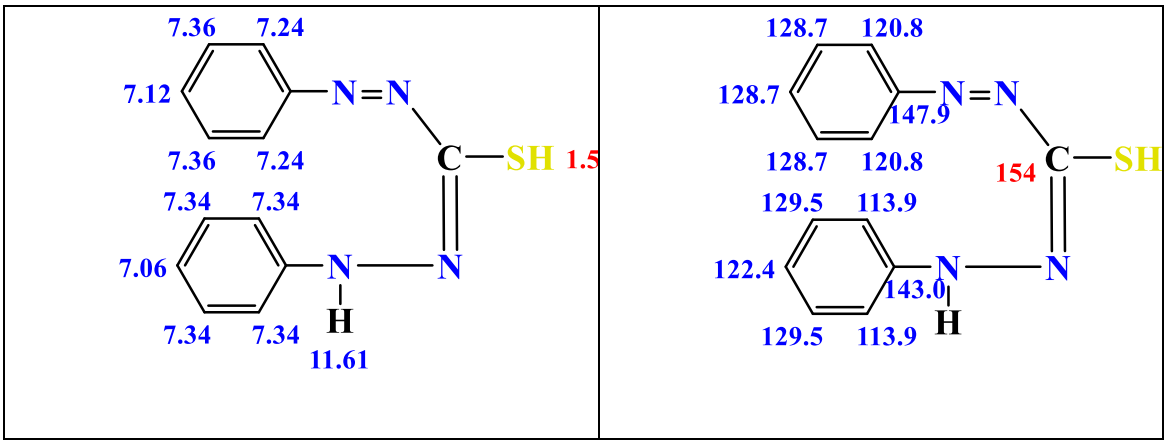
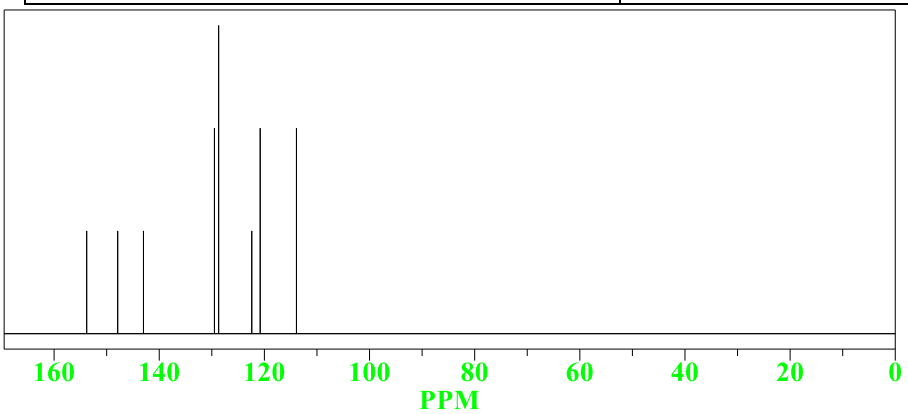


Figure 4. Ditizon the first Spectruit





5-rasm. Ditizonning 13C spektri

CONCLUSION.

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This article analyzed the recovery ability to form a complex crease with lead ions of Dietsia. According to the results of the study, the lead was determined that the reaction molecule was named two ions.

REFERENCES

1. Huang, Y., Peng, J. & Huang, X. Allylthiourea functionalized magnetic adsorbent for the extraction of cadmium, copper and lead ions prior to their determination by atomic absorption spectrometry. *Microchim Acta* **186**, 51 (2019).

2. Aliyari, E., Fathi, A.A., Alvand, M. *et al.* β-Cyclodextrin-grafted magnetic graphene oxide nanocomposites in ultrasound-assisted dispersive magnetic solid-phase extraction for simultaneous preconcentration of lead and cadmium ions. *Res Chem Intermed* **47**, 1905–1918 (2021).

3. Sorouraddin, S.M., Farajzadeh, M.A., Pinou, R. *et al.* Development of a reversed-phase dispersive liquid–liquid microextraction method for the extraction and preconcentration of lead and cadmium ions in some cosmetic products. *Chem. Pap.* **76**, 2085–2092 (2022).

4. Nezhadali, A., Mohammadi, R., Akbarpour, M. *et al.* Application of the Taguchi Method and Central Composite Design for the Highly Selective and Efficient Extraction of Cu(II) ions from an Aqueous Solution Containing Mn(II), Co(II), Ni(II), Zn(II), Cu(II), and Pb(II) ions Mixture Using Benzyl Bis(thiosemicarbazone). *Chemistry Africa* **3**, 1001–1008 (2020).

5. Sorouraddin, S.M., Parvizzad, K. & Farajzadeh, M.A. Development of a pH-induced dispersive solid-phase extraction method using folic acid combined with dispersive liquid–liquid microextraction: application in the extraction of Cu(II) and Pb(II) ions from water and fruit juice samples. *ANAL. SCI.* **39**, 23–31 (2023).

6. Nazokat M., Fayzulla N., Abdulahat J. Flame retardant for cotton fabrics based on phosphate acid-urea polymer //Universum: химия и биология. – 2022. – №. 9-2 (99). – С. 53-56.

7. Muzaffarova N. S., Nurqulov F. N., Jalilov A. T. Pentaeritrit va ammofos asosida antipiren tayyorlash //Kimyo va tibbiyot: nazariyadan amaliyotgacha. 2022. – С. 77-80.

8. Muzaffarova N. S., Nurqulov F. N. Paxta matolari uchun azot va fosfor saqlovchi antipiren sintez qilish //Kimyo va tibbiyot: nazariyadan amaliyotgacha. – 2022. – С. 75-77.

ISSN (E): 2181-4570 ResearchBib Impact Factor: 6,4 / 2023 SJIF 2024 = 5.073/Volume-2, Issue-5

9. Muzaffarova N., Toshtemirova N. Antipirenlar bilan ishlov berilgan tabiiy to ‘qimachilik materiallarning termik barqarorligini tadqiq etish //Theoretical and experimental chemistry and modern problems of chemical technology. – 2023. – Т. 1. – №. 01.

10. Nazokat M., Faizulla N., Abdulahat J. Synthesis of a new flame retardant, high content of phosphorus and nitrogen and its use in cotton fabrics //Universum: технические науки. – 2022. – №. 8-3 (101). – С. 59-62.

11. Muzaffarova, N., & Toshtemirova , N. Antipirenlar bilan ishlov berilgan tabiiy to‘qimachilik materiallarning termik barqarorligini tadqiq etish. *Theoretical and Experimental Chemistry and Modern Problems of Chemical Technology*, *1*(01). Retrieved from https://ojs.qarshidu.uz/index.php/ch/article/view/36.

12. Muratov B.A, Turaev Kh. Kh, Umbarov I.A, Kasimov Sh.A, Nomozov A.K, "Studying of Complexes of Zn(II) and Co(II) with Acyclovir (2-amino-9-((2-hydroxyethoxy)methyl)-1,9- dihydro-6H-purine-6-OH),"*Int. J of Eng. Trends and Tech.* 2024**;** 72(1)**:** 202-208. https://doi.org/10.14445/22315381/IJETT-V72I1P120.

13. Durdubaeva R., Beknazarov S., Nomozov A. Synthesis of 2, 4, 6-Triethanolimine-1, 3, 5-Triazine and its application as a corrosion inhibitor of carbon steel in 0.5 M H2SO4 solution //Science and Innovation. – 2022. – Т. 1. – №. 8. – С. 613-618.