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STUDY OF THE ELECTRONIC STRUCTURE AND QUANTUM CHEMICAL CALCULATIONS OF N,N[1]-HEXAMETHYLENE BIS-[(AMINOAROYL)UREAS]

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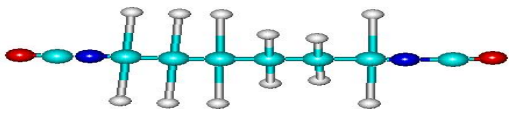
Currently, in the natural sciences, including chemistry, various computer-chemical programs can be used to comprehensively characterize molecules based on the results of quantum chemical and molecular dynamics calculations. Based on these results, it is possible to predict the properties, reactivity, and, most importantly, the reaction centers of the molecules being studied [1]. It should be noted that quantum chemical and, especially, molecular dynamics calculations have not yet received the widespread application they deserve in organic chemistry and chemical engineering.

The results obtained using quantum chemistry methods provide important information on the distribution of electron charge density, total energy, formation energy, heat of formation, electron energy, nuclear energy and dipole moment of the molecules studied.

Furthermore, quantum chemistry is a less expensive, more accessible, and more versatile method for studying the properties of molecules [2,3]. However, it should be noted that we cannot completely abandon chemical experimental research methods, as quantum chemical research relies on key experimental results.

The activity of a molecule in chemical reactions depends primarily on its composition, structure, and energetic characteristics. Predicting the reaction centers of organic molecules is an important and pressing task. Using modern quantum chemical methods, chemists can plan experimental studies and conduct targeted synthesis of important chemical products.

Based on these considerations, we investigated the 3D structures, charge distribution, and electron density of the starting nitrogen-containing compounds: hexane-1,6-diisocyanate, diphenylamine, dibenzylamine, carbazole, isatin, 5-bromoisatin, and p-ferrocenylamine, which were used in the synthesis of urea derivatives. In all the reactions studied, hexane-1,6-diisocyanate was the starting compound. Figure 3.4 shows the 3D structures, charge distribution, and electron density in the hexane-1,6-diisocyanate molecule (Fig. 1).



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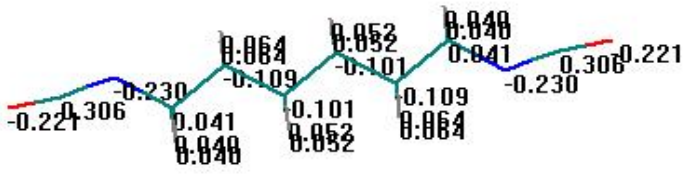

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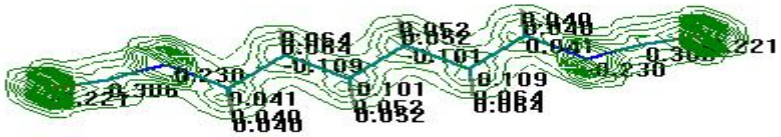

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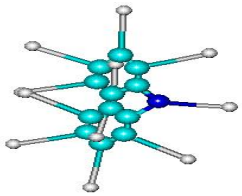
Fig. 1. Structure, charge distribution, and electron density of the compound under study.

a) 3D structure; b) charge distribution; c) electron density distribution in the hexane-1,6-diisocyanate molecule.

Analysis of the obtained results revealed that in the hexane-1,6-diisocyanate molecule, the most negative charge is observed at the nitrogen atom (Fig. 1.b), with a value of -2.30 (the charge of oxygen atom is -2.21). It should be noted that in this molecule, both nitrogen atoms have the same negative charge. Based on these data, it can be assumed that the reaction involving hexane-1,6-diisocyanate occurs at the expense of both nitrogen atoms. The 3D structures, charge distributions, and electron density of the starting heterocyclic amines were also studied.



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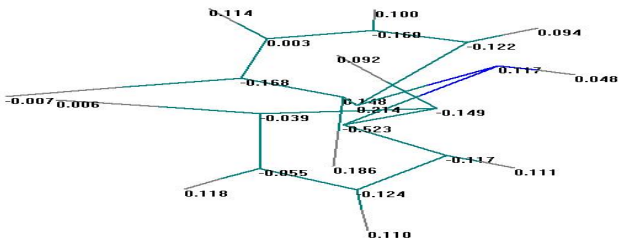

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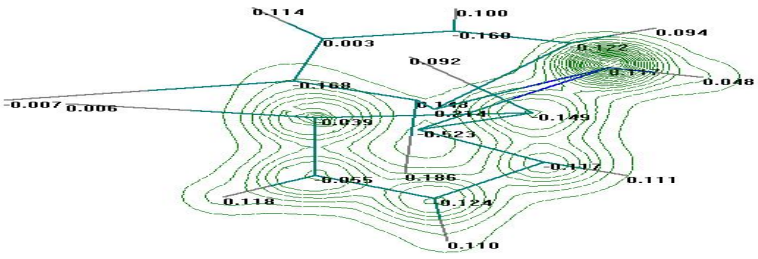

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Fig. 2. Structure, charge distribution, and electron density of the compound under study

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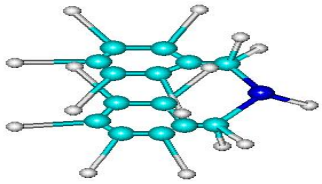
a) 3D structure; b) charge distribution; c) electron density distribution in the diphenylamine molecule

Analysis of the results revealed that the nitrogen atom in the diphenylamine molecule has an sp^3 pyramidal state and is coplanar with the two phenyl rings (Fig. 2.b). The electron density distribution (Fig. 2.c) showed that the greatest concentration of the electron cloud is concentrated around the nitrogen atom, which is the reaction center of the diphenylamine molecule.

In addition, the dibenzylamine molecule, shown in Fig. 3, was also studied.



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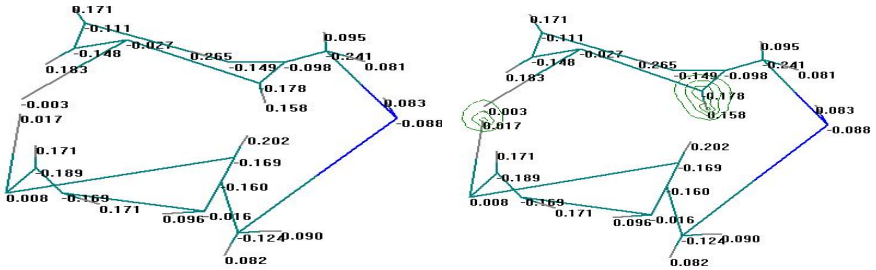

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a) 3D structure; b) charge distribution; c) electron density distribution in the dibenzylamine molecule

Fig. 3. Charge distribution and electron density structures

The quantum chemical characteristics of the studied compounds were also examined. The total energy, formation energy, heat of formation, electron energy, nuclear energy, dipole moment, and atomic charge in the molecules of the starting and target compounds were studied. The results are presented in Table 1.

Data from calculating the quantum-chemical characteristics of the starting compounds are used to determine (predict) the nature and direction of the reaction, as well as the reaction center of the molecule involved. For example, hexane-1,6-diisocyanate is the starting reagent in all studied reactions with secondary amines. In its molecule, the nitrogen atom has a negative charge of -0.230. It can be assumed that this is the reaction center in the nucleophilic addition reaction of aromatic secondary amines to hexane-1,6-diisocyanate.

The second starting compound in the reactions studied are secondary aromatic amines (diphenylamine, dibenzylamine, carbazole, isatin, and 5-bromoisatin). Among these, the nitrogen atom of the dibenzylamine molecule has the highest negative charge, with a value of -0.088 (Table 1). Dibenzylamine is presumably the most reactive of the amines used in reactions with hexane-1,6-diisocyanate.

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It should be noted that the presented considerations regarding the quantum-chemical and molecular-dynamic characteristics of the compounds used are confirmed by the experimental data we obtained.

For example, the reaction of hexane-1,6-diisocyanate with dibenzylamine produces N,N^1-hexamethylene bis-[(dibenzylamino)urea], i.e., the addition occurs via the nitrogen atom of the reactants. The yield of the product with dibenzylamine is higher (94%) than with other amines.

The quantum-chemical and molecular-dynamic properties of the resulting compounds were also studied. The data obtained can be used for further research involving these molecules, as well as as reference data for those working in the field of computational chemistry.**Table 1**

Quantum-chemical calculations of the studied compounds

The nature of chemical compounds	Total energy, kcal/mol	Energy of formation, kcal/mol	Heat of formation, kcal/mol	Electron energy, eV	Nuclear energy, kcal/mol	Dipole moment (D)	Charge of the nitrogen atom
Hexane-1,6-diisocyanate	-47140,61	-2387,79	-50,328	-224669,01	177528,39	9,485	-0,230
Diphenylamine	-40235,48	-2503,60	233,201	-243565,9	203330,42	2,803	0,117
Dibenzylamine	-46848,58	-2780,61	506,37	-243113,26	196264,71	0	-0,088
Carbazole	-39706,68	-2577,76	54,837	-229233,71	189527,04	1,411	0,236
Isatin	-40905,01	-1897,25	-37,511	-191939,35	151034,35	4,585	0,040
5-bromoisatin	-48699,83	-1863,63	-29,253	-223294,96	174595,12	3,996	0,041
N,N^1-hexamethylene bis-[(carbazolyl)urea]	-126500,2031	-7489,5273	113,1304	-1349161,125	1222660,875	6,216	-0,038
N,N^1-dinitroso-N,N^1-hexamethylene bis-[(carbazolyl)urea]	-146693,0938	-7670,8759	172,6961	-1602912,5	1456219,375	7,762	-0,140
N,N^1-hexamethylene bis-[(diphenylamino)urea]	-129320	-7897,5126	121,961	-1422843,875	1293523,875	6,554	-0,041
N,N^1-dinitroso-N,N^1-	-	-8083,720	176,667	-1675196,1	1525678,3	8,709	-0,139

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hexamethylene bis-[(diphenylamino) urea]	149517,75	7	1	25	75		
N,N^1-dichloro-N,N^1-hexamethylene bis-[(diphenylamino) urea]	-143279,0156	-7922,0664	51,18349	-1573909,625	1430630,625	5,426	-0,119
N,N^1-dibromo-N,N^1-hexamethylene bis-[(diphenylamino) urea]	-144996,25	-7916,8642	51,8859	-1573684	1428687,75	5,379	-0,104
N,N^1-diisopropyl-N,N^1-hexamethylene bis-[(diphenylamino) urea]	-150052,75	-9622,1025	47,9366	-1873370,62	1723317,87	1,117	-0,113
N,N^1-diamyl-N,N^1-hexamethylene bis-[(diphenylamino) urea]	-163846,4063	-10743,6484	26,7656	-2152937,75	1989091,25	1,042	-0,130
N,N^1-hexamethylene bis-[(isatinyl)urea]	-128787,1172	-6018,7973	38,1607	-1085994,37	957207,18	9,192	-0,097

Continuation of Table 1

N,N^1-dinitroso-N,N^1-hexamethylene bis-[(isatinyl)urea]	-148978,2188	-6198,3427	99,5294	-1317129,5	1168151,25	11,63	-0,191
N,N^1-hexamethylene bis-[(5-bromoisatinyl)urea	-144379,8281	-5954,6035	51,6305	-1207149	1062769,125	7,571	-0,075

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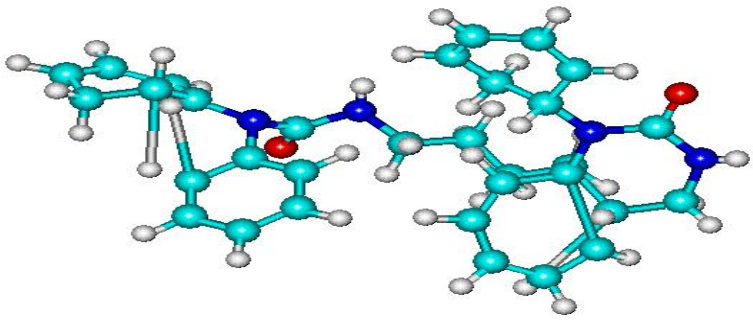
N,N[1]-dinitroso-N,N[1]-hexamethylene bis-[(5-bromoisatinyl)urea	-164568,4531	-6131,684	115,4637	-1449550,5	1284982,125	10,1	-0,184
N,N[1]-hexamethylene bis-[(dibenzylamino)urea]	-142481,7188	-8990,0761	25,5701	-1655439,625	1512957,875	4,074	-0,016
N,N[1]-dinitroso-N,N[1]-hexamethylene bis-[(dibenzylamino)urea]	-162643,5625	-9140,3681	116,1917	-1933932,375	1771288,875	3,841	-0,218



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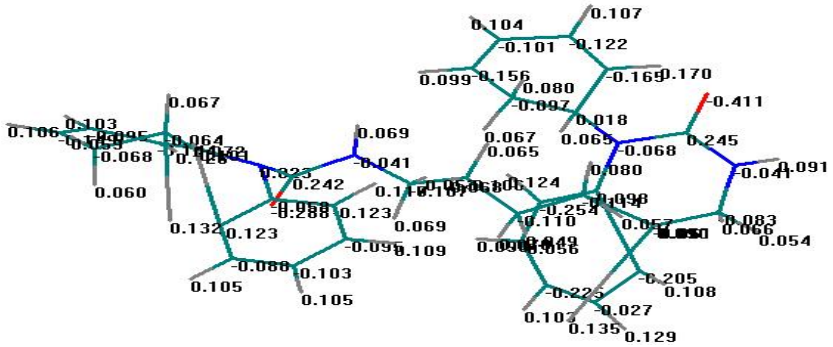

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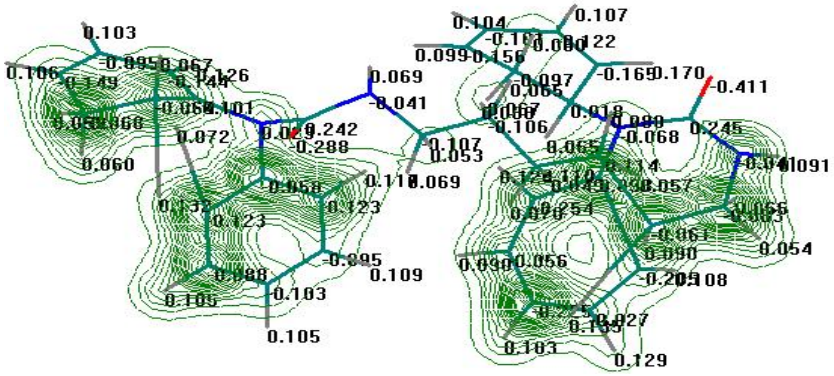

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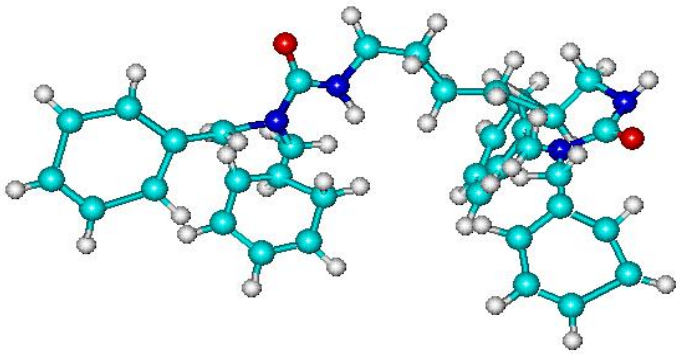
a) 3D structure; b) charge distribution; c) electron density distribution in the N,N[1]-hexamethylene bis-[(diphenylamino)urea] molecule

Fig. 4. Structures, charge distribution, and electron density



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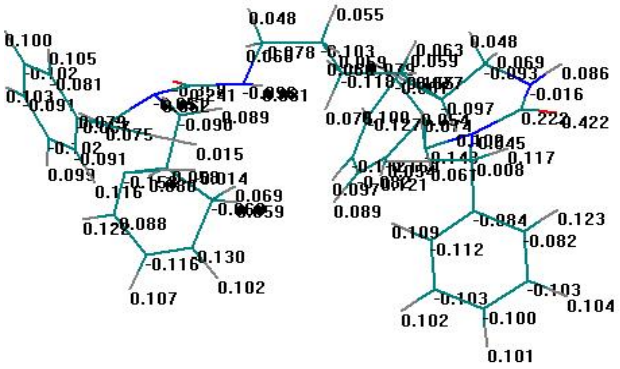

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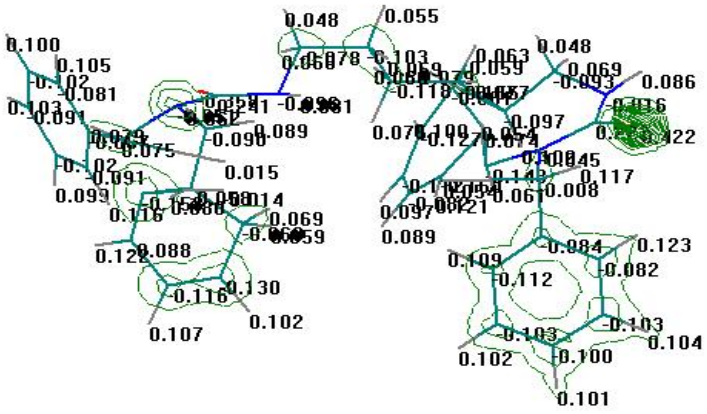

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a) 3D structure; b) charge distribution; c) electron density distribution in the N,N[1]-hexamethylene bis-[(dibenzylamino)urea] molecule

Fig. 5. Structures, charge distribution, and electron density

Thus, the quantum chemical characteristics and molecular dynamics calculations of the studied compounds were studied. Based on these data, a hypothesis was put forward regarding the reaction pathway involving them and the reaction center where the nucleophilic addition process occurs. These ideas were confirmed by the experimental results obtained.

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