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DFT-Based Evaluation of the Drug Dibazol as a Promising Molecular Scaffold Considering Charge State and Solvation Effects

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Abstract

Despite considerable research devoted to the synthesis and biological activity of benzimidazole derivatives, their reactivity as molecular systems remains poorly understood. In particular, for dibazol, one of the best-known representatives of this class, the literature has primarily focused on its pharmacological properties and synthetic approaches, while a systematic analysis of its electronic structure and reactivity is virtually absent. Therefore, the present work aims at a quantum-chemical evaluation of the reactivity of dibazol in the neutral and anionic states, taking into account the influence of the environment, as well as the identification of the key reactive centers of the molecule. The scientific significance of the study lies in the systematic analysis of the influence of anionization and solvation on the electronic and thermodynamic characteristics of dibazol, while the practical significance is associated with the possibility of using the obtained data for the targeted synthesis of its derivatives. The calculations were performed using density functional theory (DFT) at the B3LYP/6-311+G(d,p) level with the SMD solvation model. The results show that the anionic form of dibazol is thermodynamically unstable in the gas phase but is stabilized in a polar medium. Analysis of reactivity descriptors and Fukui functions revealed that the C7, C17, and C21 atoms are the main electrophilic sites susceptible to nucleophilic attack, whereas the C15 and C20 atoms exhibit the most pronounced nucleophilic character. The NH group shows comparatively low reactivity. The obtained results contribute to the application of conceptual DFT to the analysis of heterocyclic compounds and can be used in the rational design of new dibazol derivatives with the pre-set properties.

1. Introduction

Benzimidazole derivatives occupy an important place in modern medicinal and pharmaceutical chemistry due to their broad spectrum of biological activity, including anti-inflammatory, vasoactive, antispasmodic, anticancer and antimicrobial effects [1–3]. The structural feature of the benzimidazole fragment, which combines an aromatic π -system with the nitrogen-containing heteroatoms, determines its high electronic flexibility and the ability to

participate in various types of intermolecular interactions, making this class of compounds a promising basis for the development of new preparations [4–7].

Dibazol (2-(phenylmethyl)-1H-benzimidazole), a benzimidazole derivative, is a well-known and clinically used preparation. It was developed in the USSR in the mid-20th century and introduced into clinical practice as a myotropic antispasmodic and moderate hypotensive agent [8]. In addition to its vasodilatory properties [9], dibazol has been described as having neurotropic effects and an effect on the central nervous system function [10]. It also possesses moderate immunomodulatory effect [11].

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The pharmacological properties of dibazol are largely determined by the electronic structure of the molecule, the distribution of electron density, and the presence of potentially reactive centers. However, despite the long-standing use of dibazol in medical practice, the fundamental aspects of its electronic nature and reactivity remain insufficiently systematized, particularly with regard to the possibility of a targeted chemical modification of the molecule.

Our interest in the dibazol molecule is driven not only by its intrinsic biological properties but also by its the potential to serve as a structural platform for the preparation of new derivatives. The presence of nitrogen-containing centers and a conjugated π -system creates the prerequisites for a targeted chemical modification of the molecule and the variation of its electronic and coordination properties. However, an analysis of the literature shows that the synthesis of dibazol derivatives is most often based on the reconstitution of the benzimidazole framework, while the reactivity of dibazol itself as a complete molecule remains virtually unexplored [12–16]. In this context, studying the electronic structure of dibazol is particularly important as a step preceding the rational design of its new derivatives.

Furthermore, most quantum chemical studies of benzimidazole compounds are limited to neutral forms, while the effect of the charge state and solvation on reactivity has been studied fragmentarily [17, 18]. In the present study, a comparative analysis of the neutral and anionic forms of dibazol in the gaseous and a polar medium has been conducted using density functional theory (DFT). Particular attention is paid to the effect of anionization and solvation on the electronic structure, thermodynamic stability, and distribution of reactive sites in the molecule through global and local reactivity descriptors.

Thus, the relevance of this study is determined by the need for an in-depth study of the electronic nature of dibazol, as well as identifying the factors determining its reactivity under various conditions. This has both theoretical significance for the development of the conceptual density functional theory, and practical significance for the rational design of new derivatives with the pre-set properties. The object of this study is the dibazol molecule in its neutral and anionic states. The subject of the study is the electronic structure and reactivity of dibazol, considered within the frames of the conceptual density functional theory. The aim of the study is to establish patterns of the influence of the charge state and environment on the reactivity of dibazol, based on quantum chemical modeling.

To achieve this aim, the following objectives were formulated:

- optimization of the geometric parameters of the molecule in various environments;
- analysis of the frontier molecular orbitals and energy characteristics;
- study of the molecular electrostatic potential;
- calculation of the global and local reactivity descriptors;
- determination of the most probable reactive centers.

The research methods comprise quantum chemical calculations within the frames of the DFT, including analysis of the frontier orbitals, molecular electrostatic potential, the Fukui function, and conceptual DFT descriptors. Environmental effects were taken into account using a continuum solvation model.

The scientific novelty of the study lies in a comprehensive analysis of the influence of anionization and solvation on the electronic structure and reactivity of dibazol, including a comparison of the global and local descriptors. The practical significance of the study lies in the potential use of the obtained results to predict the directions of a chemical modification of dibazol and the development of new derivatives.

2. Experimental

The quantum chemical calculations were performed using the Gaussian 16 software package. The geometry optimization of the neutral and radical-anionic forms of dibazol in the gas and alcohol phases was performed, using the density functional theory (DFT) with the B3LYP hybrid functional and the 6-311+G(d,p) basis set. For the open-shell radical-anionic systems, the unrestricted UB3LYP approach was used. The B3LYP functional was chosen due to its widespread use in the study of organic heterocyclic compounds and its good balance of accuracy and computational efficiency [19, 20]. The 6-311+G(d,p) basis set provides additional flexibility in describing the electron-density distribution through polarization functions, while the presence of diffuse functions is particularly relevant for the description of the anionic electronic state. Thus, the selected level of theory provides a reasonable balance between computational accuracy and computational cost for the comparative analysis performed in this study. However, the conventional B3LYP functional does not explicitly account for long-range dispersion interactions, which may affect the quantitative description of conformational

changes in flexible molecular systems; therefore, this aspect should be considered a limitation of the present computational approach.

Solvent effect were taken into account using the SMD (Solvation Model based on Density) continuum solvation model for an ethanol medium [21, 22]. The use of the SMD model allows one to take into account the polarization effect of the solvent on the electronic structure of the molecule without explicitly including the solvent molecules in the calculation.

For all optimized structures, the vibrational frequencies were calculated in the harmonic approximation [23]. The absence of imaginary frequencies confirmed that the obtained geometries corresponded to the minimum of the potential energy surface. Using the optimized structures, the bond lengths, bond and dihedral angles, HOMO and LUMO frontier molecular orbital energies, thermodynamic parameters, and atomic charges were calculated, and molecular electrostatic potential (MEP) maps were constructed [24, 25]. Visualization of the molecular orbitals and electrostatic potential maps was performed, using the GaussView.

Atomic charges were determined using the Mulliken method [26] (Table S1).

The global reactivity descriptors were calculated based on the HOMO and LUMO energies, using an approximate interpretation of the Koopmans' theorem [27, 28]. The ionization potential (I) and electron affinity (A) were determined using the following equations:

$$I \approx -E_{HOMO} \quad (1)$$

$$A \approx -E_{LUMO} \quad (2)$$

Based on the obtained values, the electronegativity (χ), chemical potential (μ), chemical hardness (η), softness (S) and electrophilicity index (ω) were calculated:

$$\chi = \frac{I + A}{2} \quad (3)$$

$$\mu \approx -\chi \quad (4)$$

$$\eta = \frac{I - A}{2} \quad (5)$$

$$S = \frac{1}{2\eta} \quad (6)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (7)$$

The local reactivity was investigated, using the Fukui functions and dual descriptors, which allow one to identify the most probable sites of the electrophilic and nucleophilic attack, as well as to evaluate the change in the local reactivity of individual atoms upon the molecule anionization [29].

To analyze the intramolecular redistribution of the electron density and donor-acceptor interactions, a natural bonding orbital (NBO) analysis was performed at the same level of theory.

3. Results and Discussion

To elucidate the influence of anionization and solvation on the reactivity of dibazol, its geometric, thermodynamic, and electronic characteristics have been sequentially analyzed.

Geometric Parameters. The first stage of the study has been to optimize the geometry of the neutral and anionic forms of dibazol in the gaseous and polar environments. An analysis of the geometric parameters allows us to assess the influence of the charge state and solvation on the spatial organization of the molecule, and identify the structural changes, associated with the electron density redistribution. The optimization has been performed using the DFT method at the B3LYP/6-311+G(d,p) level of theory. For the anionic states, the unrestricted UB3LYP approach has been used. The optimized structure of the neutral dibazol molecule in the gas phase is shown in Fig. 1.

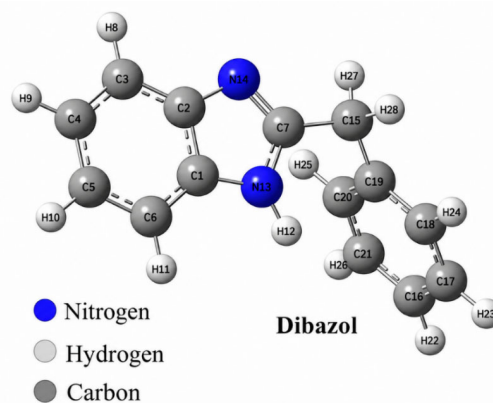


Fig. 1. The optimized DFT B3LYP/6-311+G(d, p) model of the neutral dibazol molecule in the gas phase.

The calculated geometric parameters of the neutral and anionic forms of dibazol in the gas phase are shown in Table 1.

Table 1. The geometric parameters of the optimized neutral and anionic forms of Dibazol in the gas phase

Parameter	Neutral form	Anionic form	Δ^*
Bond lengths, Å			
N13–H12	1.008	1.010	+0.002
N13–C1	1.384	1.382	-0.002
N13–C7	1.380	1.393	+0.013
N14–C2	1.389	1.377	-0.012
N14–C7	1.309	1.329	+0.020
C15–H27	1.092	1.092	0.000
C7–C15	1.502	1.487	-0.015
C15–C19	1.517	1.513	-0.004
Valency angles, °			
H12–N13–C1	127.095	126.769	-0.326
H12–N13–C7	125.340	123.166	-2.174
N14–C2–C7	105.450	106.007	+0.557
H28–C15–H27	106.591	106.910	+0.319
C7–C15–H28	108.775	110.889	+2.114
C7–C15–H27	106.677	106.929	+0.252
C7–C15–C19	104.061	112.262	+8.201
C19–C15–H27	111.019	111.037	+0.018
Dihedral angles, °			
N13–C1–C2–C3	-179.799	-179.372	+0.427
N13–C1–C2–N14	0.587	1.650	+1.063
N13–C1–C6–H11	-0.081	-1.002	-0.921
N13–C7–C15–C19	39.399	48.684	+9.285
H12–N13–C7–C15	-7.560	-17.378	-9.818
C17–C18–C19–C15	179.263	175.291	-3.972
C18–C19–C15–H28	14.230	36.267	+22.037

* Δ = (Anionic form - Neutral form)

An analysis of the optimized structures shows that the electron addition is accompanied by a local redistribution of the electron density, leading to moderate changes in the bond lengths and valency angles without a significant rearrangement of the molecular framework. The most pronounced changes are observed for the bonds involving the nitrogen atoms and the conjugated carbon fragment of the molecule. In the anionic form, the elongation of the N13–C7 and N14–C7 bonds is observed, indicating a decrease in the bond multiplicity and a reduced contribution of the π -conjugation due to an increase in the electron density in the nitrogen-containing fragment. Simultaneously, a slight shortening of the C7–C15 bond indicates a partial

redistribution of the π -electron density in the conjugated system. The changes in the valency angles are generally minor, indicating the preservation of the overall spatial organization of the molecule during anionization. However, an increase in the C7–C15–C19 angle indicates a local geometric relaxation of the conjugated fragment, which occurs during the redistribution of the negative charge. An analysis of the dihedral angles shows that anionization leads to a slight change in the relative orientation of the aromatic and conjugated regions of the molecule, which may be due to a change in the degree of electron delocalization. The geometric parameters of the neutral and anionic forms of dibazol in the alcohol phase are presented in Table 2.

Table 2. The geometric parameters of the optimized neutral molecule and dibazol anion in the alcohol phase

Parameter	Neutral form	Anionic form	Δ^*
Bond lengths, Å			
N13–H12	1.012	1.010	-0.002
N13–C1	1.382	1.376	-0.006
N13–C7	1.371	1.418	+0.047
N14–C2	1.390	1.363	-0.027
N14–C7	1.317	1.366	+0.049
C15–H27	1.096	1.108	+0.012
C7–C15	1.503	1.504	+0.001
C15–C19	1.515	1.515	0.000
Valency angles, °			
H12–N13–C1	126.693	124.613	-2.080
H12–N13–C7	125.596	124.270	-1.326
N14–C2–C7	105.487	107.107	+1.620
H28–C15–H27	106.528	106.070	-0.458
C7–C15–H28	108.218	108.207	-0.011
C7–C15–H27	108.035	110.545	+2.510
C7–C15–C19	114.247	114.119	-0.128
C19–C15–H27	109.521	108.407	-1.114
Dihedral angles, °			
N13–C1–C2–C3	179.772	179.152	-0.620
N13–C1–C2–N14	-0.062	1.444	+1.506
N13–C1–C6–H11	0.357	1.718	+1.361
N13–C7–C15–C19	147.135	159.599	+12.464
H12–N13–C7–C15	-3.036	-40.297	-37.261
C17–C18–C19–C15	179.918	179.709	-0.209
C18–C19–C15–H28	40.803	41.999	+1.196

* Δ = (Anionic form – Neutral form)

In the presence of a polar solvent, the effect of anionization on molecular geometry becomes more pronounced. The most significant changes are observed for the N13–C7 and N14–C7 bonds, whose lengths increase considerably compared with those in the neutral form. This behavior indicates increased delocalization of the negative charge in a polar medium and decreased localization of electron density on individual atoms. At the same time, the increase in the C15–H27 bond length indicates a redistribution of electron density in the hydrocarbon fragment of the molecule. In contrast to the gas phase, more significant changes in the dihedral angles are observed in an alcohol medium, especially for the H12–N13–C7–C15 fragments. This indicates increased conformational mobility of the anionic form under solva-

tion conditions and reflects additional geometric relaxation occurring when the negative charge is stabilized by the solvent. The results obtained demonstrate that a polar environment has a significant effect not only on the energetic stability of the anion but also on the spatial organization of the molecule.

Overall, the geometric optimization results indicate that the dibazol anionization is accompanied by a redistribution of electron density predominantly within the π -conjugated system, while the effect of the solvent leads to the additional charge delocalization and enhanced geometric relaxation of the structure. The obtained data are of fundamental importance for interpreting the reactivity of dibazol and predicting the most likely routes for its chemical modification.

Table 3. The energy characteristics of the dibazol molecule and anion in the gas and alcohol phases

Parameter	Gas phase		Alcohol phase	
	Neutral	Anionic	Neutral	Anionic
Total Electron Energy (EE), eV	-17698	-17698	-17699	-17700
Zero-Point Energy, eV	6.164	5.988	6.159	6.015
Thermal Energy (E), kcal/mol	149.785	145.982	149.649	146.715
Heat Capacity (CV), cal/mol*Kelvin	49.214	51.681	49.140	51.617
Entropy (S), cal/mol*Kelvin	113.770	114.196	114.842	115.674
Gibbs Free Energy (G), eV	-17693	-17693	-17694	-17695

Thermodynamic parameters. The thermodynamic parameters of the neutral and anionic forms of dibazol have been calculated based on a harmonic vibrational analysis of the optimized structures under the standard conditions ($T = 298.15$ K, $p = 1$ atm). The resulting values for the total electronic energy, zero-point energy, thermal energy, heat capacity, entropy, and Gibbs free energy are presented in Table 3.

An analysis of the energy characteristics shows that the stability of the anionic form depends significantly on the environment. In the gas phase, the total electron energy and Gibbs free energy for the neutral and anionic forms are similar, indicating the absence of a pronounced thermodynamic advantage of the anionic state in the absence of solvation. In the polar medium, a noticeable stabilization of the anionic form is observed. The anion exhibits a decrease in the total electron energy and a lower Gibbs free energy compared to the neutral molecule. This indicates the effective solvation stabilization of the negative charge by the polar solvent and confirms the key role of the environment in the stabilization of charged states. Thus, the energetic data indicate a relative stabilization of the anionic state in the polar medium. This conclusion is also consistent with

the electron affinity values discussed below, which reflect the ability of dibazol to accept an additional electron under different conditions. Therefore, solvation effects should be taken into account when modeling the reactivity of benzimidazole systems.

The Molecular Electrostatic Potential. To assess the electron density distribution and identify the potential reactive centers, the molecular electrostatic potential (MEP) maps have been constructed. The MEP reflects the distribution of the electrostatic field, generated by the nuclei, and the electron density of the molecule, and is used for the qualitative and semiquantitative analysis of the reactivity, intermolecular interactions, and charge distribution. The MEP maps allow for the visual identification of the nucleophilic and electrophilic centers, the prediction of the electrophilic and nucleophilic attack directions, and the assessment of the molecule's ability to form the hydrogen bonds and complexes. The corresponding maps of the neutral and anionic forms of dibazol are shown in Fig. 2, where the red areas correspond to the regions with the most negative electrostatic potential, and the blue areas correspond to the most positive potential, while the green regions represent intermediate potential values close to neutral electrostatic potential.

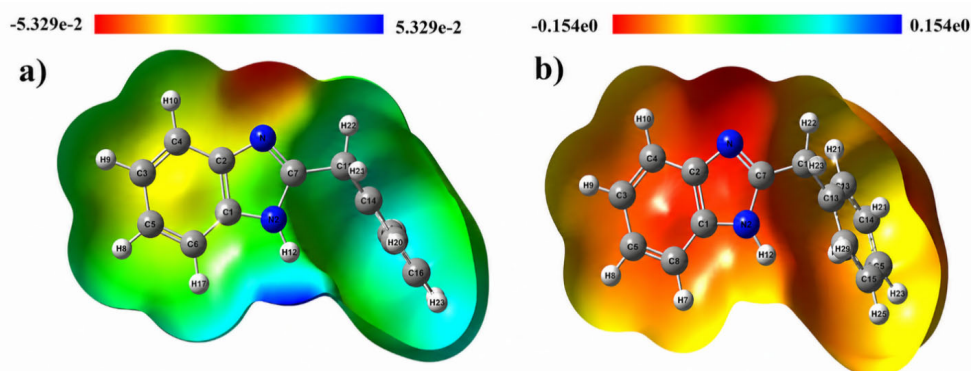


Fig. 2. The molecular electrostatic potential (MEP) maps of the neutral (a) and anionic (b) forms of dibazol. The electrostatic potential values shown on the color scales are given in atomic units (a.u.).

For the neutral molecule, the negative electrostatic potential is predominantly localized around the nitrogen atoms of the benzimidazole fragment, indicating increased electron density in this region and a potential tendency to interact with electrophilic reagents. The positive potential is concentrated primarily on the hydrogen atoms and in the peripheral regions of the hydrocarbon fragment of the molecule. In the anionic form, a significant increase and spatial expansion of the negative potential regions are observed. Moreover, the negative charge is not localized on a single atom but is distributed throughout the conjugated system, including the nitrogen-containing and carbon fragments of the molecule. This delocalization indicates the high polarizability of the anionic state and explains the decrease in the dipole moment compared with that of the neutral form. At the same time, the decrease in the positive potential regions indicates an increase in the overall electron donor capacity of the system. The obtained MEP maps confirm that anionization of dibazol is accompanied by a significant increase in nucleophilicity and the delocalization of the electron density within the π -conjugated system. This is consistent with the results of the geometric analysis, and indicates the important role of the conjugation in stabilizing the charged state of the molecule.

The atomic charges and frontier orbitals. To estimate the redistribution of electron density during the anionization of dibazol, atomic charges were calculated using the Mulliken method [26, 30]. The charge distribution for the neutral and anionic forms is shown in Fig. 3 (Table S2).

Analysis of the charge distribution shows that electron addition is accompanied by pronounced delocalization of electron density across the conjugated system. The most significant increase in negative charge is observed at the C7, C17, and C21 atoms, indicating their involvement in stabilizing the anionic state. Changes in the charges of the N13 and N14 nitrogen atoms also indicate their involvement in electron density redistribution; however, the negative charge is not localized exclusively at the heteroatoms. These results indicate that dibazol anionization leads to a delocalized π -electron system, in which the excess electron is stabilized through conjugation between the aromatic and nitrogen-containing fragments of the molecule. This charge distribution pattern is consistent with the geometric analysis data and molecular electrostatic potential maps.

For a more detailed analysis of the electronic structure, the energies of the frontier molecular orbitals HOMO and LUMO have been calculated. The corresponding energy parameters are provided in Table 4.

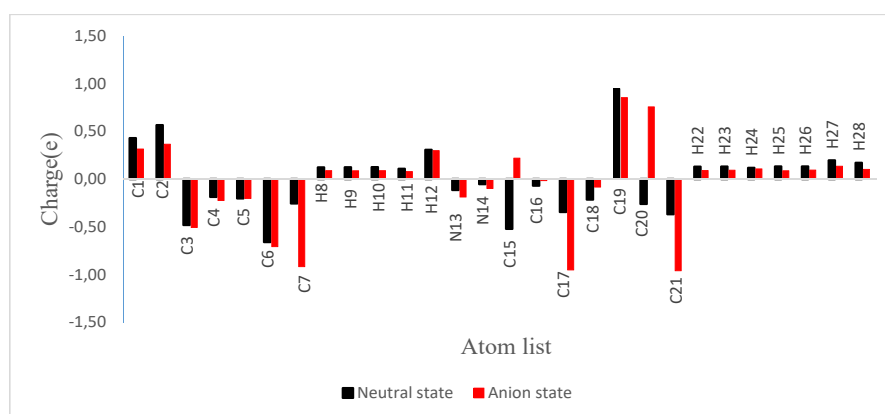


Fig. 3. The Mulliken distribution of the atomic charges during the transition of dibazol from the ground state to the anion.

Table 4. The HOMO and LUMO energies of the dibazol molecule in the neutral and anionic states, in the gas and alcohol phases, optimized, using the DFT B3LYP /6-311+G(d, p) method

Energy, eV	Gas phase		Alcohol phase	
	Neutral	Anionic	Neutral	Anionic
EHOMO(α)	-6.240	1.541	-6.311	-1.895
ELUMO(α)	-0.921	2.539	-0.811	-0.300
EHOMO(β)	—	-2.498	—	-5.110
ELUMO(β)	—	2.500	—	-0.403
$\Delta E(\alpha)$	5.319	0.998	5.5	1.595
$\Delta E(\beta)$	—	4.998	—	4.707

For the neutral form of dibazol in the gas phase, a relatively large HOMO–LUMO energy gap ($\Delta E = 5.319$ eV) is observed, indicating a high electronic stability and moderate reactivity of the system. In the alcohol phase, the ΔE value increases slightly up to 5.5 eV, indicating an additional stabilization of the neutral molecule in the polar medium. The transition to the anionic state is accompanied by a significant change in the electronic structure. In the gas phase, the HOMO(α) energy becomes positive, and the $\Delta E(\alpha)$ energy gap decreases almost fivefold compared to the neutral form. This indicates a significant increase in the electron donor capacity and nucleophilicity of the anion. Simultaneously, the separation of the α - and β -orbitals reflects the spin-polarized nature of

the open-shell system. In the alcohol phase, a partial stabilization of the anionic form is observed: the HOMO(α) energy decreases down to the negative values, and the energy gap increases up to 1.595 eV. Despite the decreased reactivity compared to the gas phase, the anion remains significantly more nucleophilic than the neutral molecule. These results demonstrate the key role of the solvation in stabilizing the charged states, and regulating the electronic structure of dibazol. The spatial distribution of the HOMO and LUMO orbitals for the neutral form of dibazol in the gas and alcohol phases is shown in Fig. 4.

For the anionic form, the α - and β -frontier orbitals have been additionally constructed and are shown in Fig. 5.

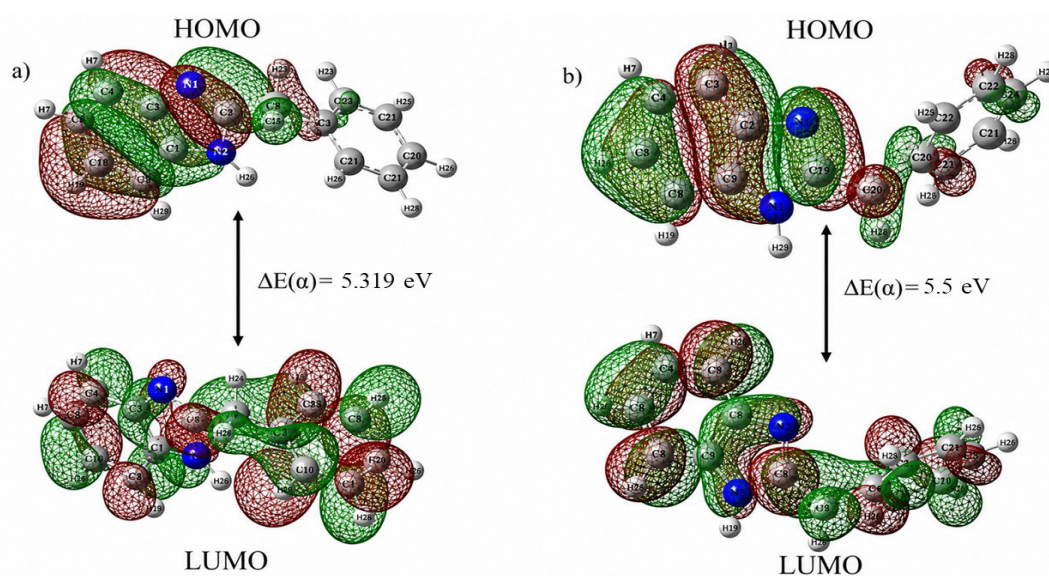


Fig. 4. The visualization of the HOMO and LUMO orbitals of the neutral dibazol molecule calculated, using the DFT B3LYP/6-311+G(d, p) method in the gas phase (a) and alcohol phase (b).

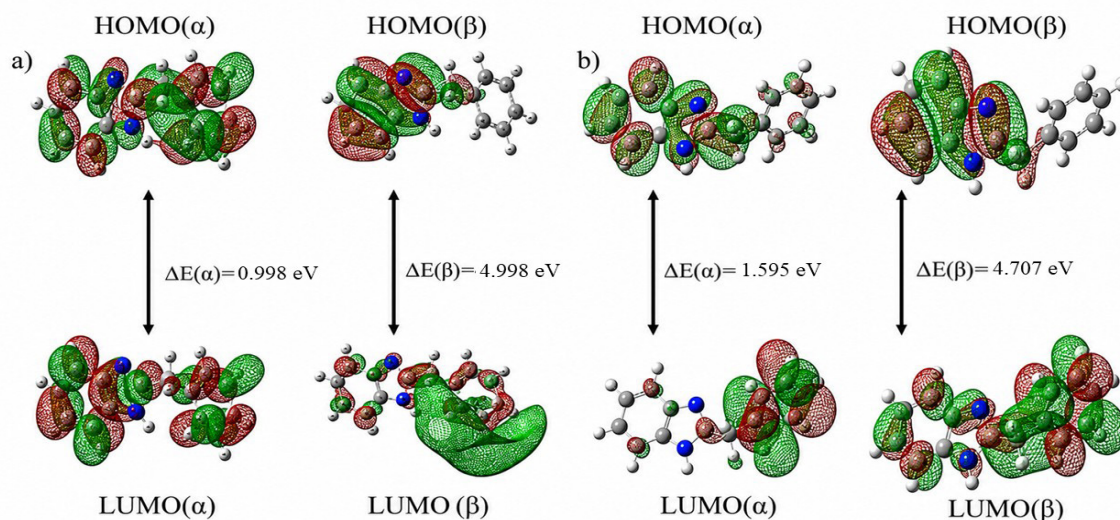


Fig. 5. The visualization of the HOMO and LUMO orbitals of the dibazol anion calculated, using the DFT B3LYP/6-311+G(d, p) method in the gas phase a) and the alcohol phase b).

The orbital visualization reveals that the HOMO is predominantly localized on the conjugated π -system and the nitrogen-containing fragment of the molecule, while the LUMO is distributed across the aromatic framework and conjugated carbon centers. In the anionic form, an increased degree of HOMO delocalization is observed, consistent with the increased nucleophilicity and polarizability of the system. The distribution of the β -orbitals further confirms the open-shell nature of the anionic state.

The global descriptors of the reactivity. To quantitatively assess the reactivity of Dibazol, the global descriptors of the conceptual density functional theory have been calculated, including the electronegativity (χ), chemical potential (μ), chemical hardness (η), softness (S), electrophilicity index (ω), as well as the electron-donating and electron-accepting characteristics of the system. The calculated values are presented in Table 5.

The neutral form of dibazol, in both the gas and alcohol phases, is characterized by relatively high chemical hardness and low softness, consistent with a large HOMO–LUMO energy gap and indicating a relatively stable electronic structure. The electron-donor potential significantly exceeds the electron-acceptor properties, indicating the predominantly nucleophilic nature of the molecule. The anionization is accompanied by a sharp decrease in chemical hardness and an increase in softness of the

system, especially in the gas phase. This change indicates a significant increase in the polarizability and reactivity of the anion. Concurrently, an increase in the chemical potential and a change in electronegativity are observed, reflecting a significant redistribution of the electron density upon the electron attachment. The anomalously high electrophilicity index values are observed for the anionic form in the gas phase. This behavior is associated with the specifics of applying the approximate relationships of the conceptual DFT to the open-shell systems, and has no direct physical interpretation. In the polar medium, the corresponding descriptors are less affected by this limitation due to the stabilization of the additional electron by the solvent, and the anionic form is characterized by a marked decrease in its ability to accept electron density, which is consistent with its increased nucleophilicity.

It should be noted that the spin-resolved descriptors of the open-shell radical anion are used here primarily for qualitative interpretation of the spin-polarized electronic structure. They should not be regarded as strictly equivalent to, or directly quantitatively comparable with, the conventional global descriptors of the closed-shell neutral molecule. In particular, the positive HOMO(α) energy of the gas-phase radical anion indicates limited electronic stability of this state and requires cautious interpretation.

Table 5. The reaction indices of the neutral molecule and dibazol anion, calculated in the gas and alcohol phases

Descriptor, eV	Gas phase		Alcohol phase	
	Neutral	Anionic	Neutral	Anionic
Electron affinity $A(\alpha)$	0.921	-2.539	0.811	0.300
Ionization potential $I(\alpha)$	6.240	-1.541	6.311	1.895
Electronegativity $\chi(\alpha)$	3.581	-2.040	3.561	1.097
Chemical potential $\mu(\alpha)$	-3.581	2.040	-3.561	-1.097
Hardness $\eta(\alpha)$	2.66	0.499	2.750	0.798
Softness $S(\alpha)$	0.36	2.004	0.182	0.627
Electrophilicity $\omega(\alpha)$	2.41	4.17	2.31	0.75
Electron donor potential $\omega^-(\alpha)$	3.66	–	3.62	–
Electron acceptor potential $\omega^+(\alpha)$	0.080	–	0.060	–
Electron affinity $A(\beta)$	–	-2.500	–	0.403
Ionization potential $I(\beta)$	–	2.488	–	5.110
Electronegativity $\chi(\beta)$	–	-0.006	–	2.757
Chemical potential $\mu(\beta)$	–	0.006	–	-2.757
Hardness $\eta(\beta)$	–	2.494	–	2.354
Softness $S(\beta)$	–	0.4001	–	0.212
Electrophilicity $\omega(\beta)$	–	0	–	1.62

To further evaluate the electron-donating ability, the global nucleophilicity index was calculated according to Domingo's empirical method [31, 32] as $N = E_{\text{HOMO}}(\text{Nu}) - E_{\text{HOMO}}(\text{TCE})$, where tetracyanoethylene (TCE) was used as the reference. At the B3LYP/6-311+G(d,p) level, the calculated HOMO energy of TCE was -9.488 eV in the gas phase and -8.870 eV in ethanol using the SMD solvation model. According to the obtained data, the neutral dibazol molecule has a nucleophilicity index of 3.248 eV in the gas phase, indicating strong nucleophilic character, whereas its nucleophilicity decreases to 2.559 eV in ethanol. This indicates a significant influence of solvation on the electron-donating properties of the system. The polar solvent stabilizes the electron density and reduces the molecule's tendency to donate it, which is consistent with an increase in the HOMO-LUMO energy gap and a decrease in the chemical potential in ethanol. Overall, the results of the global descriptor analysis show that anionization leads to a significant increase in the reactivity and polarizability of dibazol, whereas solvation has a stabilizing effect, reducing the electron-donating properties of the system. The obtained data are in good agreement with the frontier molecular orbital analysis and confirm the key

role of the π -conjugated system in determining the reactivity of the molecule.

Local Reactivity and Fukui Functions. To determine the most likely sites of electrophilic and nucleophilic attack, local reactivity descriptors, including Fukui functions and dual descriptors [33–36], were calculated. The calculations were performed using the finite difference method based on the Mulliken atomic charges obtained for the neutral (N), anionic (N+1), and cationic (N-1) states of the molecule. The cationic state was used only as an auxiliary state required for evaluating the condensed Fukui functions and was not included in the comparative analysis of the neutral and radical-anionic forms. For charge-based Fukui functions, the condensed descriptors were evaluated according to the following expressions:

$$f_k^+ = q_k(N) - q_k(N+1) \quad (8)$$

$$f_k^- = q_k(N-1) - q_k(N) \quad (9)$$

$$f_k^0 = \frac{q_k(N-1) - q_k(N+1)}{2} \quad (10)$$

The resulting local descriptor values are presented in Table 6.

Table 6. The local reactivity of the atoms

Atom	f^+	f^-	f^0	Atom	f^+	f^-	f^0
C1	0.113139	0.117667	0.115403	C15	-0.740281	0.136716	-0.301783
C2	0.199078	-0.004904	0.097087	C16	-0.052527	-0.007920	-0.030223
C3	0.025965	-0.043919	-0.008977	C17	0.607493	0.071060	0.339276
C4	0.039134	0.056128	0.047631	C18	-0.130385	-0.087761	-0.109073
C5	0.001083	0.078665	0.039874	C19	0.091970	-0.046215	0.022877
C6	0.048356	0.157616	0.102986	C20	-1.016187	-0.042337	-0.529262
C7	0.662640	-0.131059	0.265790	C21	0.593072	0.094773	0.343923
H8	0.032807	0.060383	0.046595	H22	0.040181	0.026573	0.033377
H9	0.036571	0.059951	0.048261	H23	0.037042	0.024558	0.030800
H10	0.035828	0.070773	0.053300	H24	0.009456	0.017885	0.013671
H11	0.028838	0.060117	0.044478	H25	0.044373	0.003209	0.023791
H12	0.007537	0.061672	0.034604	H26	0.036872	0.023342	0.030107
N13	0.073914	0.062065	0.067990	H27	0.060230	0.033782	0.047006
N14	0.046803	0.087245	0.067024	H28	0.066998	0.059931	0.063465

The Fukui function values indicate that the reactivity of dibazol is unevenly distributed and is determined primarily by the electronic structure of the conjugated π -system. The most pronounced changes in electron density upon electron addition are observed for the C7, C17, and C21 atoms, indicating their high sensitivity to electron redistribution and

their role in stabilizing the anionic state. To provide a clearer interpretation of reactivity, the dual Fukui descriptor Δf was used to simultaneously assess the susceptibility of atoms to electrophilic and nucleophilic attack. The dual descriptor values are presented in Table 7.

Table 7. Dual Fukui descriptors

Atom	Δf	Character	Atom	Δf	Character
C1	-0.004528	Weakly nucleophilic	C15	-0.876997	Strongly nucleophilic
C2	0.203982	Electrophilic	C16	-0.044607	Nucleophilic
C3	0.069884	Electrophilic	C17	0.536433	Strongly electrophilic
C4	-0.016994	Weakly nucleophilic	C18	-0.042624	Nucleophilic
C5	-0.077582	Nucleophilic	C19	0.138185	Electrophilic
C6	-0.109260	Nucleophilic	C20	-0.973850	Strongly nucleophilic
C7	0.793699	Strongly electrophilic	C21	0.498299	Strongly electrophilic
H8	-0.027576	Nucleophilic	H22	0.013608	Weakly electrophilic
H9	-0.023380	Nucleophilic	H23	0.012484	Weakly electrophilic
H10	-0.034945	Nucleophilic	H24	-0.008429	Weakly nucleophilic
H11	-0.031279	Nucleophilic	H25	0.041164	Electrophilic
H12	-0.054135	Nucleophilic	H26	0.013530	Weakly electrophilic
N13	0.011849	Weakly electrophilic	H27	0.026448	Electrophilic
N14	-0.040442	Nucleophilic	H28	0.007067	Weakly electrophilic

An analysis of the dual descriptors reveals that the C7, C17, and C21 atoms exhibit the most pronounced electrophilic character and therefore represent the preferred sites for nucleophilic attack, whereas the C15 and C20 atoms display the strongest nucleophilic character and are expected to be the most favorable sites for electrophilic attack. The N13 and N14 nitrogen atoms exhibit comparatively low local nucleophilicity despite the presence of lone electron pairs. This is due to the involvement of the electron density of the nitrogen atoms in the aromatic conjugation of the benzimidazole moiety, which leads to a decrease in their local reactivity. Prototropic tautomerism between the two nitrogen sites may influence their local electronic properties; however, the present study considers a single tautomeric form and focuses on one-electron attachment rather than proton-transfer or deprotonation

equilibria. The obtained results are in good agreement with the analysis of the molecular electrostatic potential, the Mulliken charge distribution, and the results of the NBO analysis. It should be noted that the predicted reactive sites are based on computational descriptors and have not been directly validated against experimental structural, spectroscopic, or reactivity data; therefore, their experimental verification remains necessary.

The Natural Bond Orbital (NBO). To study the nature of the intramolecular redistribution of electron density and evaluate donor-acceptor interactions, an analysis of the natural bond orbitals (NBOs) was performed at the DFT B3LYP/6-311+G(d,p) level of theory. The solvent effect was taken into account using the SMD model. The key donor-acceptor interactions and the corresponding second-order stabilization energies $E(2)$ are presented in Table 8.

Table 8. The nature of the valency bonds and donor-acceptor interactions of the atoms in the dibazol molecule

No.	Donor (i)	Acceptor (j)	$E(2)$, kcal/mol	Interpretation
1	$\pi(C1-C2)$	$\pi^*(C3-C4)$	19.02	Strong $\pi-\pi^*$ conjugation in the aromatic system
2	$\pi(C1-C2)$	$\pi^*(C5-C6)$	18.80	Density delocalization along the carbon framework
3	$\pi(C3-C4)$	$\pi^*(C1-C2)$	18.20	Reverse $\pi-\pi^*$ conjugation
4	$\pi(C3-C4)$	$\pi^*(C5-C6)$	19.33	Extended conjugation of the π -system
5	$\pi(C5-C6)$	$\pi^*(C1-C2)$	19.62	Density migration along the ring
6	$\pi(C5-C6)$	$\pi^*(C3-C4)$	17.96	Stabilization of the aromatic fragment
7	LP(N13)	$\pi^*(C7-N14)$	53.72	Delocalization of the lone pair N $\rightarrow \pi^*$, decreasing nucleophilicity
8	LP(N13)	$\pi^*(C1-C2)$	34.60	Involvement of an N electron pair into the conjugation
9	LP(N14)	$\pi^*(C7-N13)$	8.60	Conjugation of the second N atom (moderate)
10	$\pi(C7-N14)$	$\pi^*(C1-C2)$	18.70	Bonding of the nitrogen-containing fragment to the π -system

The obtained results indicate a pronounced delocalization of the electron density in the π -conjugated system of dibazol. The most significant interactions correspond to the $\pi \rightarrow \pi^*$ transitions in the aromatic framework, indicating an efficient conjugation of the benzimidazole system. The highest stabilization energy is observed for the $LP(N13) \rightarrow \pi^*(C7-N14)$ interaction, indicating a strong involvement of the lone electron pair of the nitrogen atom in the aromatic conjugation. As a result, the local nucleophilicity of the NH fragment decreases, and the excess electron density is predominantly delocalized along the π -carbon system of the molecule. The results of the NBO analysis are in good agreement with the Fukui functions, charge distribution, and MEP maps, confirming that the reactivity of dibazol is determined predominantly by the π -conjugated carbon framework, rather than the charge localization on the nitrogen atoms. Taken together, the complementary computational descriptors provide a consistent picture of the electronic response of dibazol to anionization and solvation. The MEP and atomic-charge analyses reflect the redistribution of electron density, while the frontier orbitals and global descriptors characterize changes in the overall donor–acceptor properties of the system. The Fukui functions and dual descriptor complement these results at the local level, whereas the NBO analysis relates the observed reactivity patterns to intramolecular conjugation and donor–acceptor interactions.

4. Conclusions

In this paper, a comprehensive study of the electronic structure and reactivity of dibazol in the neutral and anionic states has been performed using the B3LYP/6-311+G(d,p) DFT method, taking into account the influence of the polar environment. It has been found that the electron addition leads to a delocalization of the electron density along the π -conjugated system of the molecule, and is accompanied by the localized changes in the geometric parameters, primarily in the nitrogen-containing and conjugated carbon fragments.

It has been shown that the neutral form of dibazol exhibits a moderate reactivity and is characterized by a relatively high electronic stability due to a large HOMO-LUMO energy gap. In the gas phase, dibazol exhibits the properties of a strong nucleophile, whereas in the polar environment, its nucleophilicity decreases down to medium due to the solvation stabilization of the electron density. The anionization leads to a sharp increase in the reactivi-

ty, increased polarizability and nucleophilicity of the system, and a decrease in the HOMO-LUMO energy gap. The anionic form is thermodynamically stabilized in the polar environment.

The obtained results indicate two potential directions for further investigation of the chemical modification of dibazol: functionalization involving the potentially reactive carbon centers C7, C17, and C21, and N-functionalization under appropriate activation conditions. These directions should be regarded as theoretical predictions based on local reactivity descriptors and require further mechanistic and experimental verification. Thus, the reactivity of dibazol is governed by both the π -conjugated carbon framework and the nitrogen-containing fragment. According to the local reactivity descriptors, the C7, C17, and C21 atoms are characterized by increased electrophilic character, whereas the NH group exhibits reduced local reactivity due to its involvement in aromatic conjugation. However, under appropriate activation conditions, particularly after deprotonation, the NH group may serve as an important site for N-functionalization.

CRedit authorship contribution statement

Alexey Surnin: Methodology, Software, Investigation, Formal analysis, Data curation, Visualization, Writing – original draft. **Assel Ten:** Conceptualization, Methodology, Supervision, Project administration, Funding acquisition, Writing – review & editing. **Valentina Yu:** Validation, Formal analysis, Visualization, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary material

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