PREDICTION OF DETONATION PERFORMANCE AND STABILITY OF NEW CLASS HIGH ENERGETIC MATERIALS

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PURPOSE

The term 'energetic material' is used to describe any material that can react with the rapid release of high amounts of energy in form of heat upon initiation (Klapötke, 2022). This broad category includes common fuels like gasoline and diesel, as well as rocket propellants, pyrotechnics, and high-energy explosives such as gunpowder, dynamite, and TNT (Trinitrotoluene) (Bruce Cranford & AIChE, 2008). The variety and quantity of high-energy materials have expanded significantly over recent decades. In explosive research and development, high performance has always been a crucial criterion. However, the occurrence of catastrophic detonations has prompted the development of explosives with better thermal stability and reduced sensitivity to impact (Sikder & Sikder, 2004; Mathieu, 2017). The origin of these threats can be different, starting with accidents during the transport of dangerous goods, then accidents that occur during the work processes in industry, or laboratories, as well as accidents that happen as a result of weather disasters such as earthquakes and typhoons (Tasić et al., 2021). Typically, less sensitive explosives tend to have lower performance. Currently, there is a strong interest in designing new energetic materials that combine high performance with good stability, surpassing those in current use (Mathieu, 2017). Research using computer programs to explore the relationship between the structure and properties of explosives has led to the design new energetic materials with enhanced performance and reduced sensitivity. Reliable computational methods help scientists safely manage energetic molecules and offer valuable insights into the factors that affect the sensitivity of these compounds (Türker & Variş, 2009). The sensitivity of explosives can be influenced by the positive electrostatic potential at the center of the molecule. Nitroaromatic compounds, like TNT, are well-known explosives that exhibit positive potentials around their central regions because the nitro group attracts electrons. Additionally, C-NO_2 bonds in these compounds are relatively weak and can break easily under external influences, which can lead to detonation (Politzer & Murray, 2014a; Shoaf & Bayse, 2018). Several quantitative measures are used as indicators of detonation performance, including detonation

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velocity (D), detonation pressure (P), brisance (B), and Gurney velocity. Detonation velocity (D) is the stable speed of the shock front, while detonation pressure (P) is the stable pressure behind the front. Brisance refers to the explosive power, primarily indicated by detonation pressure, and Gurney velocity is the speed of metal fragments. Among these, detonation velocity and detonation pressure are crucial for evaluating explosives, with higher values being preferable (Keshavarz et al., 2009; Politzer & Murray, 2017).

Electrostatic potentials on the surfaces of C, H, N, and O atoms in explosives differ significantly from those in typical organic molecules. Energetic compounds often contain atoms or groups like -aza, -nitro, or -nitrito that attract electrons towards the molecule's periphery, creating positive electrostatic potentials in the central regions of the molecule. In contrast, typical organic molecules (excluding hydrocarbons) usually have negative potentials on their surfaces due to lone electron pairs or π-electrons (Politzer & Murray, 2021).

Positive electrostatic potentials in the central regions of high-energy molecules are associated with increased sensitivity to impact, especially within the same class of chemical compounds. For instance, in a specific class of compounds like nitroaromatics, higher positive potentials in the central part of the molecule correlate with greater sensitivity to impact (Politzer & Murray, 2003, 2015a, 2015b).

One hypothesis suggests that very positive electrostatic potentials in the central regions of molecules and at the C-NO_2 and N-NO_2 bond regions of neighboring molecules cause repulsion. This repulsion increases resistance to shearing or sliding, contributing to the formation of "hot spots" and influencing the initiation of detonation, thereby making the explosive more sensitive (Politzer et al., 2017).

On the other hand, it is known that so-called 'trigger linkages,' such as C-NO2 and N-NO2 bonds, influence the positive electrostatic potential, which is crucial for initiating detonation. Even with just one C-NO_2 bond present, positive maxima *Vs(r)* above these bonds can occur (Politzer & Murray, 1999, 2003). The withdrawal of negative charge from the interior of the molecule to the periphery creates a strong positive potential in the center of the molecule and above the C-NO_2 and N-NO_2 bonds. This results in a depletion of charge in the bonds, making them weaker. The stronger the positive potential above the bonds, the weaker the bonds become, and the greater the potential for detonation initiation (Politzer & Murray, 2003).

It has been proven that as the number of aromatic rings in a molecule increases, the electrostatic potential above the central parts of the molecule decreases. This reduction in electrostatic potential suggests that the molecule's sensitivity to detonation decreases (S. Veljković et al., 2021).

By introducing electron-donating or electron-accepting groups as substituents and varying the number of aromatic rings, the electrostatic potential in the central parts of the molecules is altered. This modification directly influences the sensitivity and detonation parameters of the compounds.

DESIGN/METHODS/APPROACH

All calculations for molecular systems were performed using the Gaussian 09 software package utilizing the B3LYP functional, most widely used DFT functional. It has been shown that DFT methods (Maslovara et al., 2019; Ječmenica Dučić et al., 2023), particularly B3LYP (Becke-3 Parameter-Lee-Yang-Parr) as a hybrid DFT method, provide reliable geometries while also requiring less time and computational resources. For geometry optimization, the Dunning correlation-consistent basis set cc-PVDZ was used.

Initially, molecules were drawn in ArgusLab (*ArgusLab*, n.d.) and optimise in Gaussian 09 (*G09 | Gaussian.Com*, n.d.). After completing the calculations, wave function files were obtained and used in the WFA-SAS (Wave Function Analysis - Surface Analysis Suite) program to create electrostatic potential maps (Plasser et al., 2022). The resulting maps were scaled to approximately the same scale and displayed the calculated critical points on the molecular surfaces.

The Kamlet-Jacobs equations, which have demonstrated good accuracy and reliability when compared with experimental values, are of particular importance for the design of explosive compounds (Politzer & Murray, 2011, 2014a).

The detonation pressure is defined by the equation:

$$P_{det} = \rho_0 DW + P_1 \quad (1)$$

where ρ_0 is the density of the explosive, D is the detonation velocity, W is the particle velocity, and P_1 is the initial pressure of the explosive, which is negligible compared to P_{det} .

Kamlet and Jacobs described simple methods for calculating detonation parameters for explosives that contain carbon, hydrogen, nitrogen, and oxygen in their composition. The factors that directly affect D and P are given as Kamlet-Jacobs parameter φ (Politzer & Murray, 2019):

$$\varphi = NM^{0.5}Q^{0.5} \quad (2)$$

where N is the number of moles of gaseous detonation products per gram of explosive, Q is the total heat released by the detonation reaction in calories per gram of explosive, and M is the average molecular weight of the gaseous products. The detonation pressure is then expressed as:

$$P = K\rho_0^2\varphi \quad (3)$$

and the detonation velocity is represented by the equation (Mathieu, 2017):

$$D = A\varphi^{0.5}(1 + B\rho_0) \quad (4)$$

In these equations, ρ_0 is the density of the explosive, and A, B, and K are empirical constants. The final form of these equations is (Politzer & Murray, 2019):

$$P(\text{kbar}) = 15.58\ [NM_{ave}^{0.5}Q^{0.5}\rho^2] \quad (5)$$

$$D(\text{km/s}) = 1.01\ [N^{0.5}M^{0.25}Q^{0.25}(1 + 1.30\rho)] \quad (6)$$

To determine N, M, and Q, it is necessary to predict the detonation products. The detonation process involves a series of reactions and equilibria, resulting in various gaseous compounds. The final products for an explosive containing carbon, hydrogen, nitrogen, and oxygen are usually N_2(g), CO(g), CO_2(g), H_2O(g), H_2(g), и C(s) (Politzer & Murray, 2016, 2017).

However, the proportion of these products depends on external physical factors such as the explosive's loading density, temperature, and other conditions. Gas ratios can be predicted using computer codes or various proposed rules, such as the Kistiakowsky-Wilson, modified Kistiakowsky-Wilson, and Springall-Roberts methods, with the Kamlet and Jacobs rules being the most commonly used (Politzer & Murray, 2014b). These rules predict the formation of N_2(g), CO_2(g), H_2O(g), and C(s), with oxygen more likely to form H_2O(g) rather than CO_2(g). The formation of CO(g) is not predicted by these rules (Politzer & Murray, 2016, 2019).

In practice, it has been confirmed that differences in the assumed compositions of products for a given explosive and loading density have very little effect on D and P. This is due to an unexpectedly balanced counteracting effect (balancing effects apply only to D and P, not to Mave, N, and Q individually, and

can vary significantly depending on the products). For loading densities approaching the densities of pure crystals, the Kamlet-Jacobs rules yield D and P values somewhat closer to experimental results than those obtained from other rules (Politzer & Murray, 2016).

Today, there are many computer programs used for directly calculating detonation parameters. We used the "online molecular modeling platform and resources for atomistic calculations" (Armaković & Armaković, 2023).

FINDINGS

In this paper, nitro derivatives of anthracene, tetracene, and pentacene with formyl, methyl, and fluoro substituents were examined. The values of the total electronic energies were calculated and compared. ESP maps were obtained, and the values of the electrostatic potential above the central parts of the molecules were calculated. Additionally, detonation parameters, D (detonation velocity) and P (detonation pressure), were calculated. Unfortunately, due to the fact that K-J equation was not parametrized for explosives containing atoms other than C, N, O, H, it is only possible to determine the detonation velocity and detonation pressure for molecules that contain only carbon, hydrogen, oxygen, and nitrogen in their structure. Therefore, we were unable to calculate these parameters for the nitro derivatives of these compounds that contain fluorine as a substituent.

RESULTS AND DISCUSSION

Total Electronic Energy of a Molecule

Table 1 provides an overview of the total electronic energies of nitro derivatives of anthracene, tetracene, and pentacene. The compound with the highest stability (lowest energy) is 5,6,11,12-tetraformyl-2,3,8,9-tetranitrotetracene (-1964,52 Eh), while the lowest stability is observed in 9,10-dimethyl-2,3,6,7-tetranitroanthracene (-1436,25 Eh).

Table 1. *Values of the Total Electronic Energies of the Nitro Derivatives of Anthracene, Tetracene, and Pentacene (Expressed in Eh)*

Name of compound	**Energy (Eh)**
9,10-dimethil-2,3,6,7-tetranitroanthracene	-1436,24641607
9,10-diformyl-2,3,6,7-tetranitroanthracene	-1584,21825286
5,6,11,12-tetraformyl-2,3,8,9-tetranitrotetracene	-1964,52546242
6,13- diformyl-2,3,9,10- tetranitropentacene	-1891,51914013
9,10-difluro-2,3,6,7-tetranitroanthracene	-1556,09572199
5,6,11,12-tetrafluoro-2,3,8,9-tetranitrotetracene	-1908,17937930
6,13- difluoro-2,3,9,10- tetranitropentacene	-1863,36162635

By comparing the energy values of the nitro derivatives of anthracene (Table 2), it can be concluded that the energy values are very close, but the molecule with the highest stability is the nitro derivative of anthracene with a formyl group as a substituent.

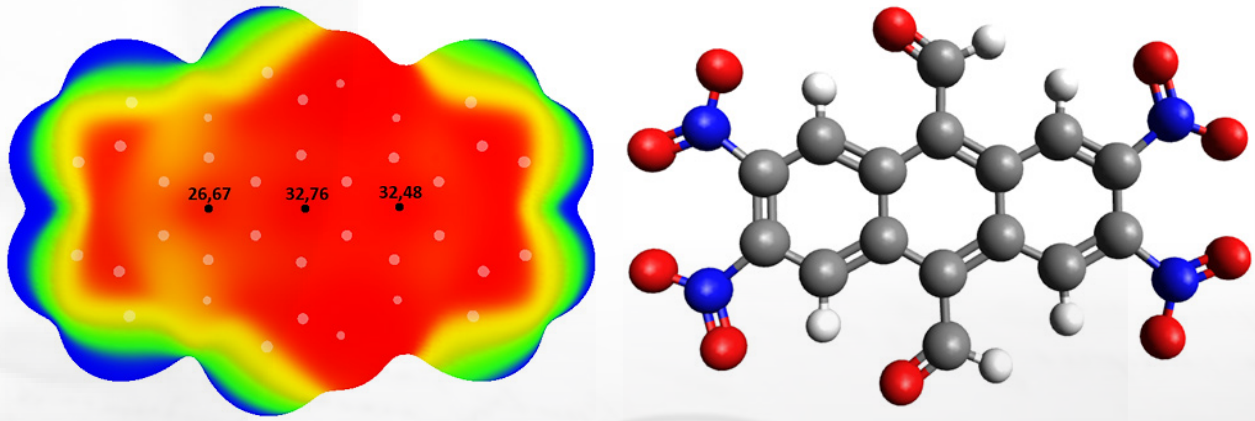
Table 2. *Values of the Total Electronic Energies of the Nitro Derivatives of Anthracene (Expressed in Eh)*

Name of compound	Energy (Eh)
9,10-dimethil-2,3,6,7-tetranitroanthracene	-1436,24641607
9,10-diformyl-2,3,6,7-tetranitroanthracene	-1584,21825286
9,10-difluro-2,3,6,7-tetranitroanthracene	-1556,09572199

Additionally, by comparing the values of the nitro derivatives of tetracene and pentacene, an increase in stability can be observed in molecules that have a formyl group as a substituent. In this case, these are the molecules 6,13-diformyl-2,3,9,10-tetranitropentacene and 6,13-difluoro-2,3,9,10-tetranitropentacene.

Electrostatic Potential Maps

The electrostatic potential map was calculated for the molecule 9,10-diformyl-2,3,6,7-tetranitroanthracene using the previously calculated .wfn file with the B3LYP method and CC-PVDZ basis set, and is shown in Figure 1. The analysis of the charge distribution on the surface of the calculated electrostatic potential for the molecule 9,10-diformyl-2,3,6,7-tetranitroanthracene shows a positive charge at the center of the ring (the energy value at the critical point in the center is 32.76 kcal/mol).

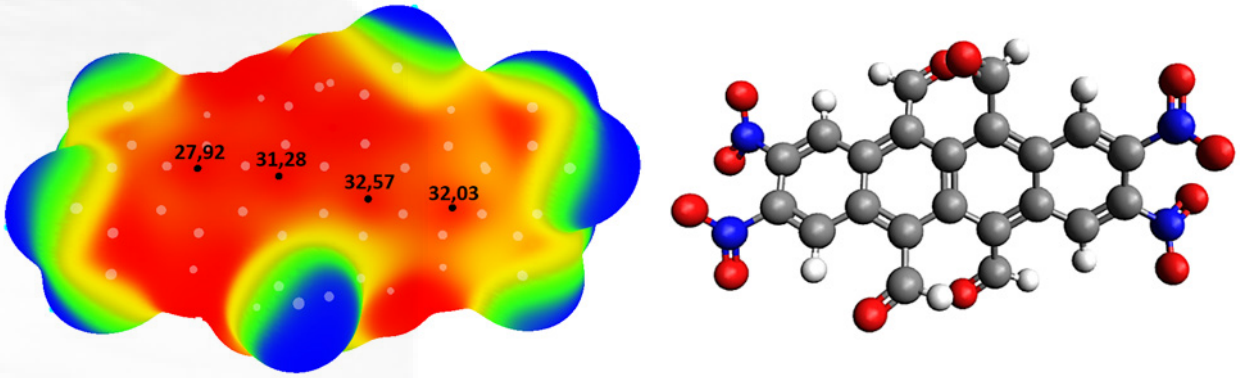


a) b)

Figure 1. *Calculated Electrostatic Potentials on the 0.001 au Surface for A) 9,10-Diformyl-2,3,6,7-Tetranitroanthracene. The Energy Value at the Critical Point Is Expressed in Kcal/Mol. Color Ranges: Red Greater Than 18.82; Yellow from 18.82 to 0; Green from 0 to -9.41; Blue More Negative Than -9.41. The Positions of the Atoms Within the Molecule Are Marked with White Circles. Molecular System Model B) 9,10-Diformyl-2,3,6,7-Tetranitroanthracene.*

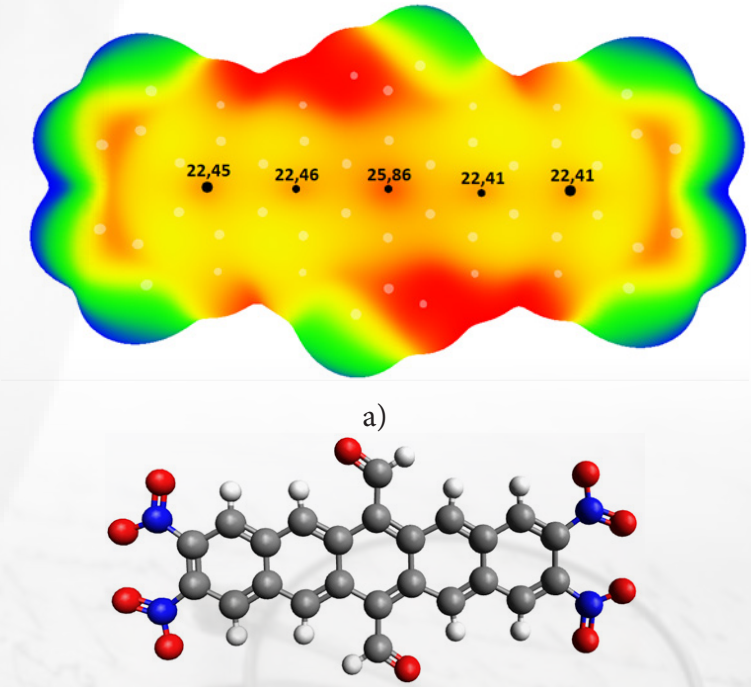
An electrostatic potential map was also calculated for the molecule 5,6,11,12-tetraformyl-2,3,8,9-tetranitrotetracene and is shown in Figure 2. Analysis of the charge distribution on the surface of the calculated electrostatic potential for the molecule 5,6,11,12-tetraformyl-2,3,8,9-tetranitrotetracene indicates that there are two critical points near the center of the molecule. From this, it can be concluded

that the number and arrangement of formyl substituents influence the charge distribution around the center of the molecule.



a) b)

Figure 2. *Calculated Electrostatic Potentials on the 0.001 au Surface for A) 5,6,11,12-Tetraformyl-2,3,8,9-Tetranitrotetracene. The Energy Value at the Critical Point Is Expressed in Kcal/Mol. Color Ranges: Red Greater Than 18.82; Yellow from 18.82 to 0; Green from 0 to -9.41; Blue More Negative Than -9.41. The Positions of the Atoms Within the Molecule Are Marked with White Circles. Molecular System Model B) 5,6,11,12-Tetraformyl-2,3,8,9-Tetranitrotetracene.*

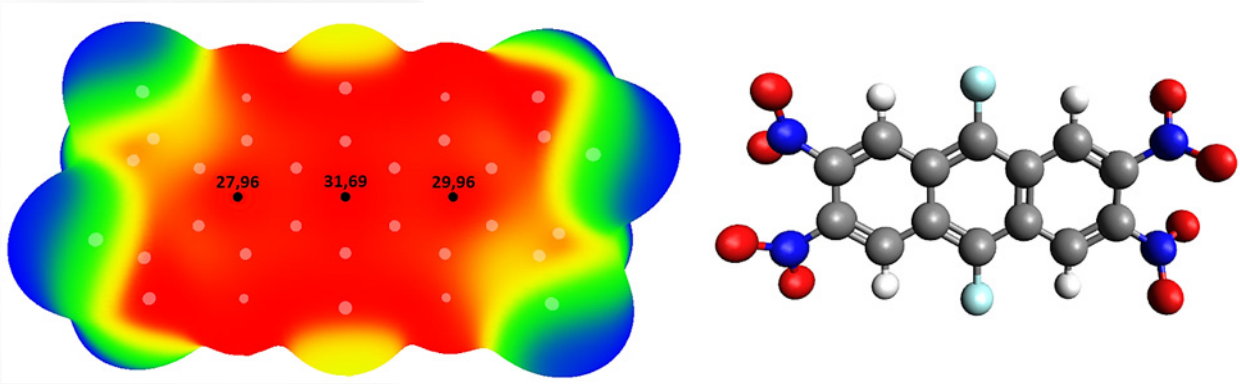


a)

b)

Figure 3. *Calculated Electrostatic Potentials on the 0.001 au Surface for a) 6,13- Diformyl-2,3,9,10-Tetranitropentacene. The Energy Value at the Critical Point Is Expressed in kcal/mol. Color Ranges: Red Greater Than 18.82; Yellow from 18.82 to 0; Green from 0 to -9.41; Blue More Negative Than -9.41. The Positions of the Atoms Within the Molecule Are Marked with White Circles. Molecular System Model b) 6,13-Diformyl-2,3,9,10-Tetranitropentacene.*

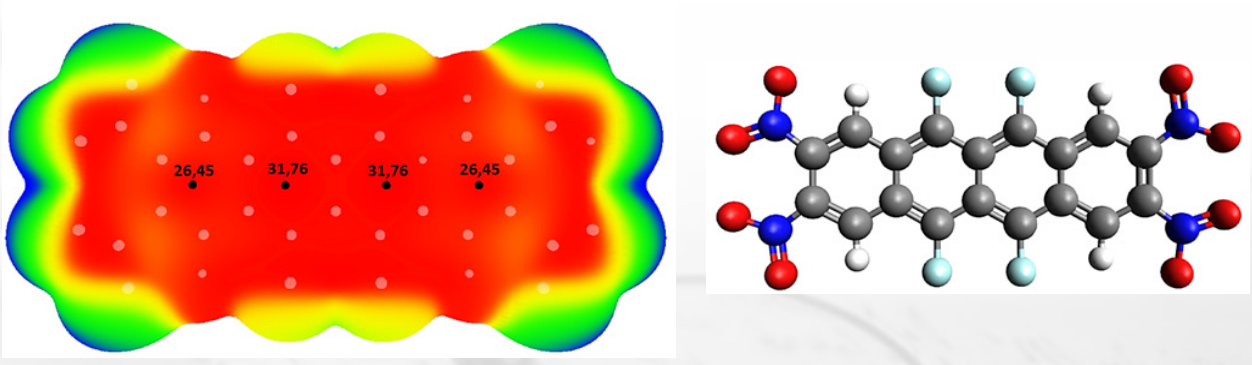
We conducted a comparative overview of the electrostatic potential values above the central parts of the molecules of anthracene, tetracene, and pentacene with a formyl group as a substituent. It can be observed that the highest electrostatic potential value is possessed by the molecule 9,10-diformyl-2,3,6,7-tetranitroanthracene (32,76 kcal/mol). The potential values decrease with the increase in the number of rings in the molecule, so the molecule 6,13-diformyl-2,3,9,10-tetranitropentacene (28,56 kcal/mol) has the lowest electrostatic potential value at the central point of the molecule.



a) b)

Figure 4. *Calculated Electrostatic Potentials on the 0.001 au Surface for A) 9,10-Difluro-2,3,6,7-Tetranitroanthracene. The Energy Value at the Critical Point Is Expressed in Kcal/Mol. Color Ranges: Red Greater Than 18.82; Yellow from 18.82 to 0; Green from 0 to -9.41; Blue More Negative Than -9.41. The Positions of the Atoms Within the Molecule Are Marked with White Circles. Molecular System Model B) 9,10-Difluro-2,3,6,7-Tetranitroanthracene.*

Figure 4 shows the electrostatic potential map for the molecule 9,10-difluoro-2,3,6,7-tetranitroanthracene. As in the previous case, three critical points can be observed above the central parts of the molecule, with the middle one having the highest potential value (31.63 kcal/mol).



a) b)

Figure 5. *Calculated Electrostatic Potentials on the 0.001 au Surface for A) 5,6,11,12-Tetrafluoro-2,3,8,9-Tetranitrotetracene. The Energy Value at the Critical Point Is Expressed in Kcal/Mol. Color Ranges: Red Greater Than 18.82; Yellow from 18.82 to 0; Green from 0 to -9.41; Blue More Negative Than -9.41. The Positions of the Atoms Within the Molecule Are Marked with White Circles. Molecular System Model B) 5,6,11,12-Tetrafluoro-2,3,8,9-Tetranitrotetracene.*

Examples of electrostatic potential maps for the molecules 5,6,11,12-tetrafluoro-2,3,8,9-tetranitrotetracene and 6,13-difluoro-2,3,9,10-tetranitropentacene are shown in Figures 5a and 6a. For the molecule 5,6,11,12-tetrafluoro-2,3,8,9-tetranitrotetracene (26,45; 31,76; 31,76; 26,45 kcal/mol), there are four critical points, with the two around the center of the molecule having the highest value (31,76 kcal/mol).

In the case of the molecule 6,13-difluoro-2,3,9,10-tetranitropentacene (Figure 6), the energy values at the critical points are as follows: 20,73; 20,61; 24,79; 20,72; 20,73 kcal/mol.

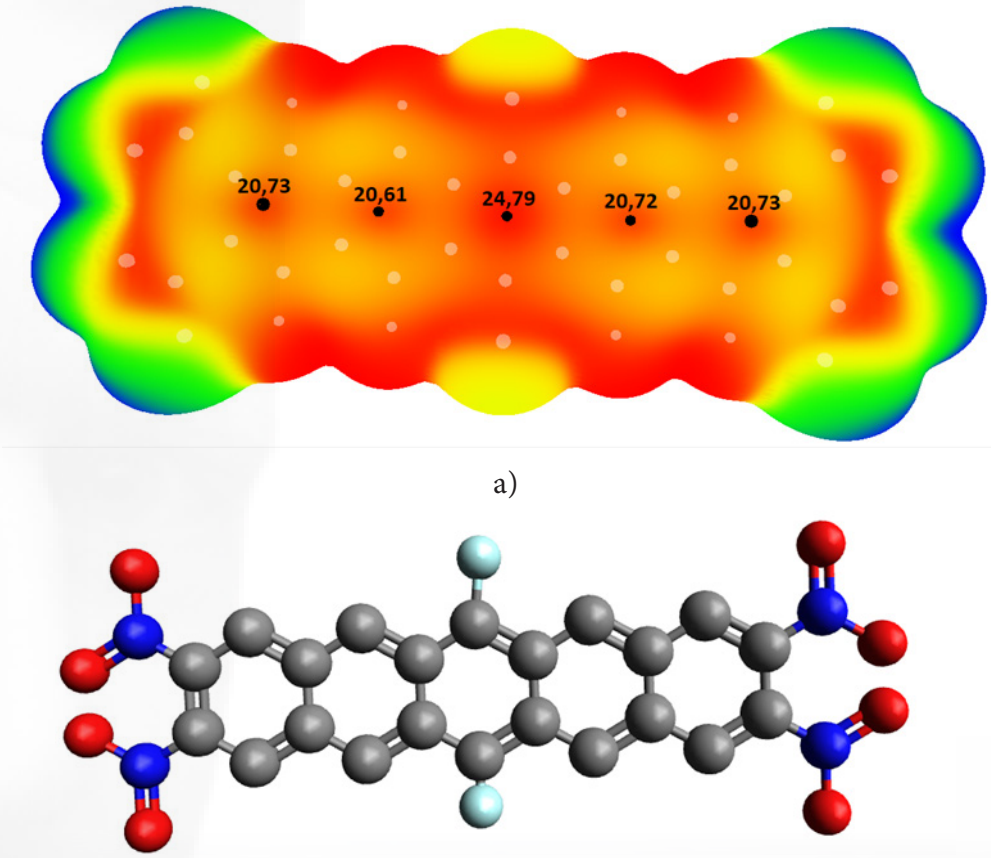
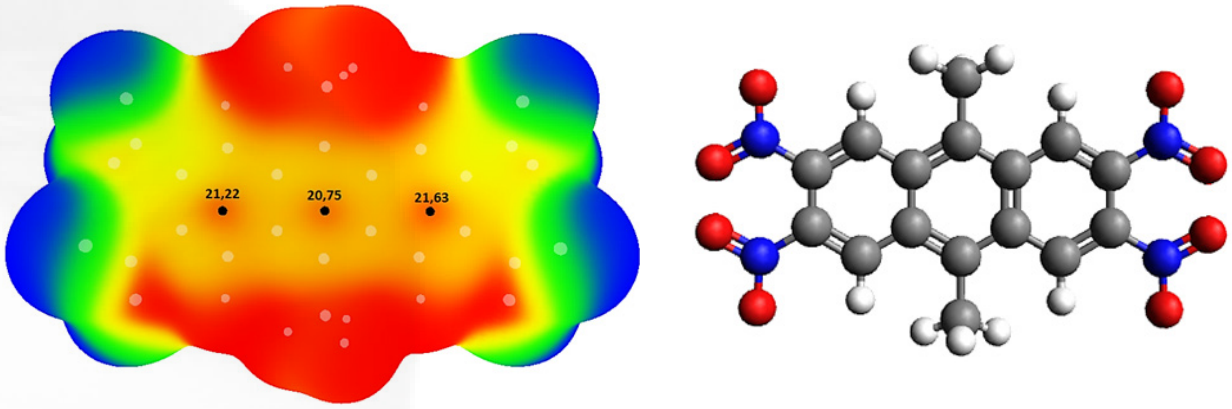


Figure 6. *Calculated Electrostatic Potentials on the 0.001 au Surface for A) 6,13-Difluoro-2,3,9,10-Tetranitropentacene. The Energy Value at the Critical Point Is Expressed in Kcal/Mol. Color Ranges: Red Greater Than 18.82; Yellow from 18.82 to 0; Green from 0 to -9.41; Blue More Negative Than -9.41. The Positions of the Atoms Within the Molecule Are Marked with White Circles. Molecular System Model B) 6,13- Difluoro-2,3,9,10- etranitropentacene.*

It can be observed that, in the case of the molecules 9,10-difluoro-2,3,6,7-tetranitroanthracene (31,69 kcal/mol) and 5,6,11,12-tetrafluoro-2,3,8,9-tetranitrotetracene (31,76; 31,76 kcal/mol), the values at the critical points are very close. In the molecule 6,13-difluoro-2,3,9,10-tetranitropentacene, a decrease in the electrostatic potential value at the center of the molecule is observed (24,79 kcal/mol).



a) b)

Figure 7. *Calculated Electrostatic Potentials on the 0.001 Au Surface for A) 9,10-Dimethil-2,3,6,7-Tetranitroanthracene. The Energy Value at the Critical Point Is Expressed in Kcal/Mol. Color Ranges: Red Greater Than 18.82; Yellow from 18.82 to 0; Green from 0 to -9.41; Blue More Negative Than -9.41. The Positions of the Atoms Within the Molecule Are Marked with White Circles. Molecular System Model B) 9,10-Dimethil-2,3,6,7-Tetranitroanthracene.*

Positive charges also occur in the centers of nitro derivatives of anthracene with a methyl group as a substituent. In the case of the calculated electrostatic potential map for the molecule 9,10-dimethyl-2,3,6,7-tetranitroanthracene (Figure 7), there are three critical points above the central part of the molecule, with potentials of 21,22; 20,75 and 21,63 kcal/mol.

It is noted that the values at the critical points of the molecules 9,10-diformyl-2,3,6,7-tetranitroanthracene (32,76 kcal/mol) and 9,10-difluoro-2,3,6,7-tetranitroanthracene (31,69 kcal/mol) are very similar. The analysis of charge distribution on the surface of the molecule 9,10-dimethyl-2,3,6,7-tetranitroanthracene (Figure 7) indicates that the introduction of the formyl group as a substituent leads to a decrease in the positivity of the potential. The energy value at the critical point around the center of the molecule (20,75 kcal/mol) are lower compared to the molecules 9,10-diformyl-2,3,6,7-tetranitroanthracene and 9,10-difluoro-2,3,6,7-tetranitroanthracene.

Detonation Parameters

Table 3 provides an overview of the calculated values of detonation velocity and detonation pressure for nitro derivatives of anthracene, tetracene, and pentacene with methyl and formyl groups as substituents.

The highest values of detonation pressure and detonation velocity were calculated for the molecule 9,10-dimethyl-2,3,6,7-tetranitroanthracene (335,74 kbar and 8979,49 m/s). Additionally, high values of detonation parameters were observed for the molecule 9,10-diformyl-2,3,6,7-tetranitroanthracene (241,02 kbar and 7354,88 m/s). We can conclude that increasing the number of aromatic rings in the molecule reduces the values of detonation parameters, as seen in Table 3.1, where the molecule 5,6,11,12-tetraformyl-2,3,8,9-tetranitrotetracene has values of (200,84 kbar and 6706,67 m/s), and the molecule 6,13-diformyl-2,3,9,10-tetranitropentacene has values of (164,97 kbar and 6167,89 m/s).

Table 3. *Values of Calculated Detonation Parameters of Nitro Derivatives of Anthracene, Tetracene, and Pentacene*

Name of compound	Detonation Pressure [kbar]	Detonation Velocity [m/s]
9,10-dimethil-2,3,6,7-tetranitroanthracene	335,74	8979,49
9,10-diformyl-2,3,6,7-tetranitroanthracene	241,02	7354,88
5,6,11,12-tetraformyl-2,3,8,9-tetranitrotetracene	200,84	6706,67
6,13- diformyl-2,3,9,10-tetranitropentacene	164,97	6167,89

ORIGINALITY/VALUE

Electrostatic potential plays a crucial role in predicting the sensitivity of explosives. It is well-established that a positive electrostatic potential at the center of the molecules of many C, H, N, O-based explosives correlates with increased sensitivity. For explosive compounds within specific classes, such as nitroaromatics, sensitivity tends to rise as the electrostatic potentials become more positive. The total energies of the investigated molecules were also calculated, and based on that, their stabilities were compared. The results obtained provide valuable insights for predicting detonation parameters and assessing the sensitivity of high-energy molecules. Furthermore, combining experimental and computational methods significantly reduced the volume and time of experimental research, as well as the quantity of chemicals used (Rakić et al., 2023).

CONCLUSION

In this study, we calculated electrostatic potential maps and total electronic energies for nitro derivatives of anthracene, tetracene and pentacene, using the B3LYP functional and the CC-PVDZ basis set in Gaussian 09. We compared the values of critical points at the centers of these molecules.

It is shown that the compound with the highest stability (lowest energy) is 5,6,11,12-tetraformyl-2,3,8,9-tetranitrotetracene (-1964,52 Eh). On the other hand, the lowest stability is observed in the molecule 9,10-dimethyl-2,3,6,7-tetranitroanthracene (-1436,25 Eh).

From the calculated electrostatic potential maps, the molecule with the highest positive potential value above the central region is 9,10-diformyl-2,3,6,7-tetranitroanthracene (32,76 kcal/mol). In accordance with the fact that sensitivity to detonation increases with the positive potential, it is expected that this compound will be the most sensitive.

Additionally, we computed key detonation parameters, including detonation pressure (P) and detonation velocity (D), to evaluate their explosive characteristics.

The compound expected to have the highest values for detonation pressure and detonation velocity is 9,10-dimethyl-2,3,6,7-tetranitroanthracene (335,74 kbar and 8979,49 m/s). However, the introduction of formyl groups resulted in molecules with slightly lower detonation parameters but greater

stability. The increase in the number of aromatic rings led to a decrease in detonation parameters and electrostatic potential.

In conclusion, formyl substitution enhances stability across the nitro derivatives of anthracene, tetracene and pentacene, while increasing the number of rings reduces both detonation properties and electrostatic potential. The balance between charge distribution, stability, and detonation parameters varies significantly with the type of substituent and the number of rings in these compounds.

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