CAN FURANOCOUMARINS BECOME THE NEW PLATFORM FOR HIGH-ENERGY MATERIALS?

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ABSTRACT

Purpose: Furanocoumarins such as angelicin and psoralen, modified by the introduction of nitro groups, were investigated as potential high-energy materials (HEMs). Their structure has been recognized as a suitable basis for the development of new explosive compounds. In the research of high-energy materials, reducing the risk of explosion is desirable, which has led to the use of computational tools for investigating structure–property relationships and designing advanced HEMs by predicting key parameters such as stability and detonation performance prior to synthesis.

Design/Methods/Approach: In this paper, a computational research approach has been applied, which includes molecular modeling, quantum chemical calculations, and comparative analysis of energetic and stability parameters.

Findings: Key properties for the evaluation of the modified furanocoumarin explosives were the detonation velocity and detonation pressure, estimated using the Kamlet–Jacobs equations. DFT methods provided reliable molecular geometries and electronic parameters necessary for the prediction of energetic performance. The obtained results showed that the detonation characteristics of nitro-substituted furanocoumarins are comparable to those of conventional commercial explosives, highlighting their potential as promising candidates for further development.

Originality/Value: In this paper, nitro-substituted furanocoumarins are investigated as potential high-energy compounds, and their properties are compared with those of commercial explosives. The study provides insights into the structural modification of furanocoumarins for the development of energetic materials and lays the foundation for future research.

Keywords: Furanocoumarins, HEM, detonation parameters, molecular modeling

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INTRODUCTION

Coumarins (2H-1-benzopyran-2-ones), according to their chemical structure, belong to the subgroup of lactones and constitute a large class of phenolic derivatives (Hung, Suh, & Wang, 2017). Their structure consists of a benzene ring fused with an α-pyrone ring, forming a π–π conjugated system rich in electrons, which provides good charge delocalization properties (Kontogiorgis et al., 2012; Nikhil et al., 2012). Most compounds are oxygenated at the C-7 position and often contain isoprenoid chains bound to carbon, oxygen, or both. Based on their structural features, coumarins are classified as: (I) simple coumarins, (II) furanocoumarins, (III) pyranocoumarins, or (IV) coumarins substituted on the pyrone ring, including their hydroxylated, alkoxylated, and alkylated derivatives, as well as their glycosides (Del Río et al., 2014). Coumarins are most frequently found in fruits, but also occur in roots, stems, and leaves. Their biosynthesis takes place through the shikimate and phenylpropanoid pathways, with cinnamic acid serving as the key precursor (Eisenbrand, 2007; Scott et al., 1976).

Furanocoumarins represent a specific subgroup of coumarins, formed by the fusion of a furan ring with the benzopyran core, resulting in angular (e.g., angelicin) or linear (e.g., psoralen) isomers depending on the position of the furan ring (Chen et al., 2014; Dugrand-Judek et al., 2015). These compounds, predominantly found in the Apiaceae, Rutaceae, Moraceae, and Leguminosae families, are synthesized by plants as an adaptation to biotic and abiotic stress, particularly as a defense against insects, fungi, and bacteria (Fracarolli et al., 2016; Raunio et al., 2020). Furanocoumarins display a wide range of biological activities, including antioxidant, antimicrobial, anti-inflammatory, analgesic, and even anticancer properties, and are therefore recognized as promising therapeutic agents (Melough et al., 2018). Some compounds from this group have also shown the ability to inhibit the growth of phytopathogenic microorganisms, making them attractive as natural pesticides in agriculture (Fracarolli et al., 2016; Raunio et al., 2020).

Nevertheless, in addition to their usefulness, coumarins – and furanocoumarins in particular – may cause undesirable and potentially harmful effects. Of particular importance are the phototoxic effects of linear furanocoumarins such as psoralen, which, in interaction with human skin and UV radiation, can lead to photosensitization, allergic reactions, and potential carcinogenicity. Furthermore, furanocoumarins can interfere with drug metabolism through the inhibition of cytochrome P450, which makes them highly relevant in the context of drug interactions. (Chen et al., 2014)

Although furanocoumarins are mainly studied for their pharmacological and ecological properties, their structural features – a rigid aromatic system with potential for further functionalization – also make them interesting candidates for applications beyond biomedicine. In particular, the combination of aromatic stability and electron-rich conjugation is a desirable characteristic in the design of high-energy materials (HEMs). In recent decades, both the diversity and production volume of high-energy materials (HEMs) have increased substantially. While superior performance has always been a primary requirement, catastrophic detonations have highlighted the urgent need for explosives with improved thermal stability and reduced sensitivity to external stimuli such as shock or friction (Sikder & Sikder, 2004; Mathieu, 2017). Hazards associated with these substances can arise in various contexts, including accidents during transport, incidents in laboratories or industrial processes, and natural disasters such as earthquakes and typhoons (Tasić et al., 2021). To address these challenges, researchers have increasingly relied on computational tools to investigate the relationship between molecular structure and explosive properties. Such approaches have facilitated the design of new energetic compounds that combine high performance with lower sensitivity. Reliable computational methods not only allow safer handling of energetic molecules but also provide valuable insights into the structural factors governing their sensitivity and stability (Türker & Variş, 2009).

With more than 1,300 coumarins identified and an increasing number of studies confirming both their pharmacological potential and toxicological challenges, coumarins remain one of the most extensively investigated classes of natural compounds in phytochemistry and biomedicine. In this study, we focused on exploring a novel aspect of furanocoumarins – their potential application as new types of high-energy materials. Particular attention was given to psoralen and angelicin derivatives, into whose structures nitro groups were incorporated, resulting in a significant enhancement of their energetic performance. The selection of these compounds was based on the fact that molecules with a higher number of aromatic rings often exhibit increased thermal stability and resistance to external influences, making them suitable candidates for the development of new high-energy materials. (Veljković et al., 2021)

METHODOLOGY

All quantum chemical calculations for the investigated molecular systems were carried out using the Gaussian 09 software package. The B3LYP functional (Becke, three-parameter, Lee–Yang–Parr), one of the most widely employed hybrid density functional theory (DFT) methods, was chosen due to its proven balance between accuracy and efficiency. Numerous studies (Maslovara et al., 2019; Ječmenica Dučić et al., 2023) have demonstrated that DFT methods, and B3LYP in particular, yield reliable molecular geometries while demanding significantly less computational time and resources compared to more advanced post-Hartree–Fock methods. For geometry optimization, the correlation-consistent polarized valence double-zeta (cc-PVDZ) basis set developed by Dunning was applied, ensuring a good compromise between computational cost and accuracy of the obtained structural parameters. The initial molecular geometries were constructed using ArgusLab (ArgusLab, n.d.) and subsequently fully optimized in Gaussian 09 (G09 | Gaussian.Com, n.d.), where vibrational frequency analyses confirmed the absence of imaginary frequencies, indicating that the optimized structures correspond to true minima on the potential energy surface.

The Kamlet–Jacobs equations have long been recognized as one of the most reliable semi-empirical tools for estimating detonation parameters of energetic materials. Numerous studies (Politzer & Murray, 2011, 2014a) have demonstrated their good agreement with experimental data, which makes them particularly important in the design and theoretical evaluation of new explosive compounds.

According to the original formulation of Kamlet and Jacobs, the detonation pressure is defined as:

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

where ρ_0 is the initial density of the explosive, D the detonation velocity, W the particle velocity, and P_1 the initial pressure of the explosive. In practice, P_1 is negligible compared to P_{det}. These equations were initially derived for CHNO-type explosives, i.e., compounds containing carbon, hydrogen, nitrogen, and oxygen.

The key factor influencing detonation velocity and pressure is expressed through the Kamlet–Jacobs parameter φ (Politzer & Murray, 2019):

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

Here, N is the number of moles of gaseous detonation products per gram of explosive, Q is the heat of detonation in cal/g, and M represents the average molecular weight of the gaseous products. Using this parameter, the detonation pressure and velocity can be estimated as:

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

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

where A, B, and K are empirical constants. The final, most widely used form of these equations is given as (Politzer & Murray, 2019):

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

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

To calculate N, M, and Q, it is first necessary to predict the composition of detonation products. The detonation reaction involves multiple equilibria that typically yield gaseous species such as N_2, CO_2, CO, H_2O, H_2, and solid carbon (Politzer & Murray, 2016, 2017). The actual product distribution, however, depends on factors such as initial density, temperature, and confinement. Several empirical rules have been proposed for product prediction, including the Kistiakowsky–Wilson, modified Kis-

tiakowsky–Wilson, and Springall–Roberts methods. Among these, the Kamlet–Jacobs rules are most frequently used (Politzer & Murray, 2014b). They predict formation of N_2, CO_2, C , H_2O, while oxygen is assumed to preferentially generate water rather than carbon dioxide. These rules do not predict the formation of (Politzer & Murray, 2016, 2019).

Interestingly, deviations in the assumed product composition have been shown to have little effect on the calculated values of *D* and *P*. This is attributed to compensating (balancing) effects, although these do not apply to the individual parameters *N*, *M*, and *Q*, which can vary significantly. For loading densities close to those of the pure crystals, the Kamlet–Jacobs rules typically provide results for *D* and *P* that are in somewhat better agreement with experimental data than those obtained from other rules (Politzer & Murray, 2016).

Nowadays, a variety of computer codes are available for direct calculation of detonation parameters. In the present study, we employed the "online molecular modeling platform and resources for atomistic calculations" (Armaković & Armaković, 2023), which allows automated prediction of the necessary thermodynamic quantities and detonation parameters.

RESULTS AND DISCUSSION

The obtained results for five psoralen derivatives are presented in **Table 1** and include the detonation parameters – detonation velocity (D), detonation pressure (P), and the heat of explosion (Q).

Table 1: *Calculated detonation parameters – detonation velocity (D), detonation pressure (P), and heat of explosion (Q) – for nitro derivates of psoralen.*

Compound	D(m/s)	P(kbar)	Q(g/mol)
3',4,8-trinitropsoralen	7739.69	275.13	1528.45
3',4,5,8-tetranitropsoralen	8609.84	353.27	1690.56
3',5,8-trinitropsoralen	7870.21	283.11	1673.81
5,8-dinitropsoralen	7803.45	279.68	1579.42
4,5,8-trinitropsoralen	6774.62	200.22	1398.40

The analysis shows that the detonation velocity ranges from 6774,62 m/s (4,5,8-trinitropsoralen) to 8609,84 m/s (3',4,5,8-tetranitropsoralen). 3',4,5,8-tetranitropsoralen exhibits the highest D value, which is consistent with its maximum heat of explosion (Q = 1690,56 g/mol) and the highest detonation pressure (P = 353,27 kbar). This indicates a clear correlation between the released energy, the energy density of the system, and the ability of the compound to achieve higher detonation performance. On the other hand, 4,5,8-trinitropsoralen displays the lowest values of all parameters (D = 6774,62 m/s, P = 200,22 kbar, Q = 1398,40 g/mol), making it the least efficient compared to the other derivatives. The remaining compounds (3',4,8-trinitropsoralen, 3',5,8-trinitropsoralen, and 5,8-dinitropsoralen) show similar detonation velocities (7800–7900 m/s) and detonation pressures (275–283 kbar), with Q values ranging from 1528 to 1673 g/mol. This group demonstrates uniform performance, suggesting that they share similar structural factors influencing their detonation mechanism. Overall, the results confirm that even slight structural modifications of psoralen derivatives can significantly affect their detonation parameters. 3',4,5,8-tetranitropsoralen stands out as the compound with the most favorable properties, while 4,5,8-trinitropsoralen exhibits substantially weaker performance. The observed trends are consistent with literature reports, which emphasize that an increase in the heat of explosion directly contributes to higher detonation velocity and pressure.

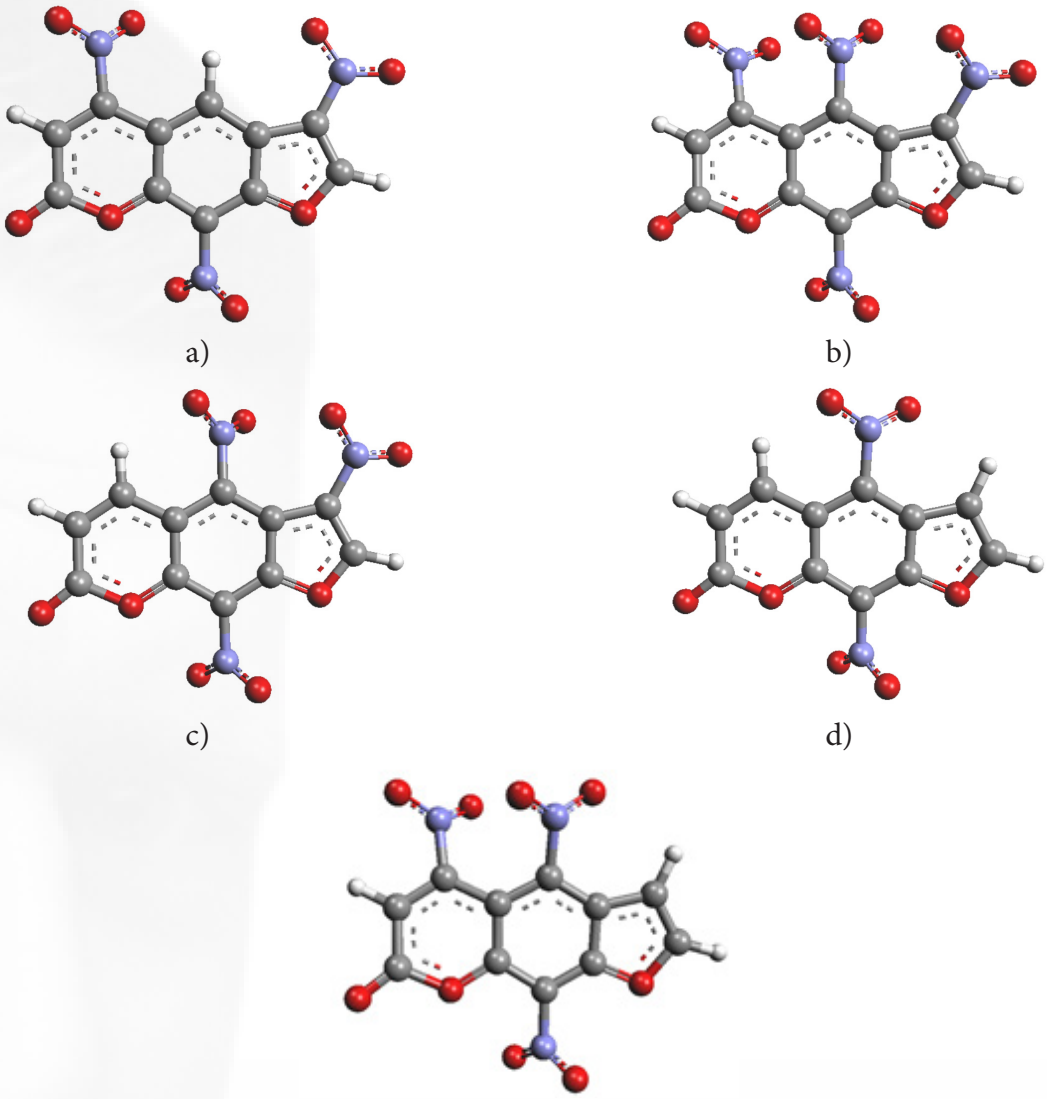

Figure 1: *a) 3',4,8-trinitropsoralen; b) 3',4,5,8-tetranitropsoralen; c) 3',5,8-trinitropsoralen; d) 5,8-dinitropsoralen; e) 4,5,8-trinitropsoralen.*

For the series of nitro derivatives of angelicin, the key detonation characteristics were calculated, and the values are presented in **Table 2**.

Table 2: *Calculated detonation parameters – detonation velocity (D), detonation pressure (P), and heat of explosion (Q) – for nitro derivatives of angelicin*

Compound	D(m/s)	P(kbar)	Q(g/mol)
3',4,6-trinitroangelicin	7795.09	275.68	1670.21
3',4,5,6-tetranitroangelicin	8606.69	353.017	1688.81
3',4,5- trinitroangelicin	7774.76	277.62	1556.34
3'5-dinitroangelicin	6757.13	199.18	1384.02

The most pronounced performance is exhibited by 3',4,5,6-tetranitroangelicin, with the highest detonation velocity (8606.69 m/s) and pressure (353.02 kbar), along with an almost maximum heat of

explosion (1688.81 g/mol). These parameters indicate the significant potential of this derivative compared to the others in the series. In contrast, 3'5-dinitroangelicin displays clearly the weakest characteristics (D = 6757.13 m/s; P = 199.18 kbar; Q = 1384.02 g/mol), confirming that this derivative is energetically less favorable. 3',4,6-trinitroangelicin and 3',4,5- trinitroangelicin occupy an intermediate position – their D and P values (approximately 7775–7795 m/s and 275–278 kbar) suggest a balanced level of stability and explosive power, while their Q values differ to a lesser extent (1556–1670 g/mol). Overall, the results confirm that nitro substitution in angelicin can significantly influence the detonation parameters. Two extremes are clearly distinguished – 3',4,5,6-tetranitroangelicin as the most energetic and 3'5-dinitroangelicin as the least efficient – while the remaining derivatives demonstrate balanced values.

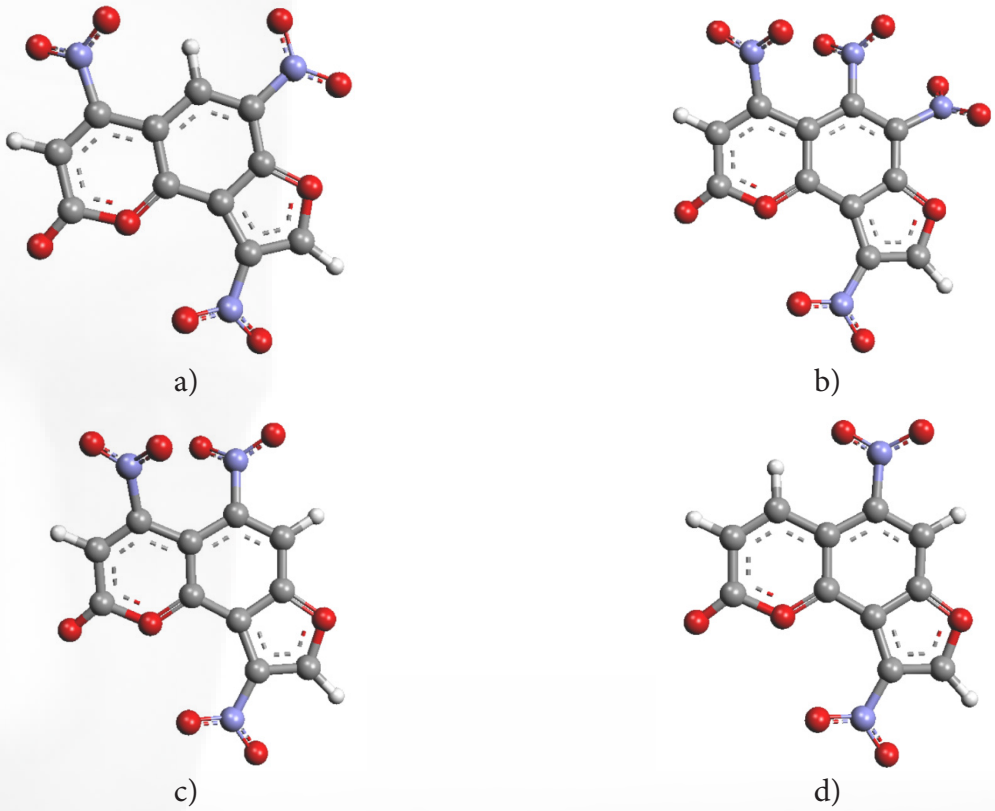

Figure 2: *a) 3',4,6-trinitroangelicin; b) 3',4,5,6-tetranitroangelicin; c) 3',4,5- trinitroangelicin; d) 3'5-dinitroangelicin*

The results show that both psoralen and angelicin derivatives exhibit a similar range of detonation parameters, although certain differences are observed among individual compounds. When the two series are compared, it is evident that psoralens and angelicins share very similar maximum and minimum values, indicating that both types of compounds display comparable energetic potentials. It is particularly interesting that 3',4,5,8-tetranitropsoralen and 3',4,5,6-tetranitroangelicin achieve almost identical values of D and P, while the least efficient derivatives (4,5,8-trinitropsoralen and 3'5-dinitroangelicin) record similarly lower parameters. This suggests that the fundamental difference between the two classes lies not in the extreme values, but rather in the internal distribution and consistency of the parameters. In general, it can be concluded that psoralens are somewhat more widely dispersed in their values (from 6774 to 8609 m/s), while angelicins show a slightly narrower interval (6757–8606 m/s). Nevertheless, both sets of compounds confirm that nitro substitution has a decisive influence on

detonation characteristics and that even minor structural variations can lead to significant differences in performance.

TOTAL ELECTRONIC ENERGY OF A MOLECULE

Table 3: *Calculated total energies (Eh) for nitro derivatives of psoralen*

Compound	Energy (Eh)
3',4,8-trinitropsoralen	-1.46E+11
3',4,5,8-tetranitropsoralen	-1.47E+11
3',5,8-trinitropsoralen	-1.26E+11
5,8-dinitropsoralen	-1.06E+11
4,5,8-trinitropsoralen	-1.26E+11

The obtained total energy values for psoralen derivatives clearly indicate differences in stability and potential explosive properties. The most negative energy was recorded for 3',4,5,8-tetranitropsoralen (–1.47E+11 Eh), confirming that this derivative possesses the most stable molecular structure. This finding is in good agreement with previous analyses of detonation parameters, according to which 3',4,5,8-tetranitropsoralen showed the highest detonation velocity and pressure, as well as the greatest released heat of explosion. Very close is 3',4,8-trinitropsoralen (–1.46E+11 Eh), indicating that both derivatives belong to the group of the most favorable ones in terms of stability and energetic efficiency. At the opposite end is 5,8-dinitropsoralen, with the highest energy (–1.06E+11 Eh), which points to the least favorable configuration and weak stability. This corresponds to its modest detonation performance. 3',5,8-trinitropsoralen and 4,5,8-trinitropsoralen share identical energy values (–1.26E+11 Eh), placing them in the middle of the series, with moderate stability and balanced energetic potential.

Table 4: *Calculated total energies (Eh) for nitro derivatives of angelicin*

Compound	Energy (Eh)
3',4,6-trinitroangelicin	-1.26E+11
3',4,5,6-tetranitroangelicin	-1.47E+11
3',4,5- trinitroangelicin	-1.6E+11
3'5-dinitroangelicin	-1.06E+11

The obtained total energy values for the series of angelicin derivatives show clear differences that can be correlated with the stability and potential energetic performance of the compounds. The lowest (most negative) energy is observed for 3',4,5,6-tetranitroangelicin (–1.47E+11 Eh), indicating the most stable configuration among the investigated derivatives. This is consistent with the results, where 3',4,5,6-tetranitroangelicin has already been identified as the derivative with the highest detonation velocity and pressure, as well as nearly maximal heat of explosion. Thus, the molecular stability is directly reflected in its energetic efficiency. In contrast, 3'5-dinitroangelicin exhibits the highest energy (–1.06E+11 Eh), which indicates a less favorable structure and lower stability. This also corresponds to the calculated detonation parameters, where 3'5-dinitroangelicin shows the weakest performance. 3',4,6-trinitroangelicin and 3',4,5- trinitroangelicin have similar energy values (–1.26E+11 Eh), confirming their comparable stability and balanced detonation characteristics. These results suggest that structural variations within the series of derivatives can lead to significant differences in total energies and, consequently, in the energetic performance of the compounds.

By comparing the energy values of the nitro derivatives of psoralen and angelicin (Tables 3 and 4), it can be concluded that the most stable molecules in both series are the second derivatives (3',4,5,8-tetranitropsoralen and 3',4,5,6-tetranitroangelicin), which show the most negative energy values (–1.47E+11 Eh). Conversely, the least stable compounds are 5,8-dinitropsoralen and 3'5-dinitroangelicin, characterized by the highest energy values (–1.06E+11 Eh). The remaining derivatives (3',4,8-trinitropsoralen, 3',5,8-trinitropsoralen, 4,5,8-trinitropsoralen, 3',4,6-trinitroangelicin, and 3',4,5- trinitroangelicin) exhibit intermediate energy values, indicating moderate stability and balanced energetic potential.

CONCLUSION

This study explored the potential of nitro-substituted furanocoumarins, specifically psoralen and angelicin derivatives, as novel high-energy materials (HEMs). Quantum chemical calculations combined with the Kamlet–Jacobs equations provided key insights into their detonation parameters and total electronic energies.

The results demonstrated that both psoralen and angelicin derivatives exhibit detonation velocities and pressures comparable to conventional explosives. Among the investigated compounds, 3',4,5,8-tetranitropsoralen and 3',4,5,6-tetranitroangelicin were identified as the most stable and energetically efficient derivatives, characterized by the lowest electronic energies and the highest detonation parameters. Conversely, 5,8-dinitropsoralen and 3'5-dinitroangelicin showed the least favorable performance, confirming that the number and position of nitro groups strongly influence the energetic potential of these molecules. When compared to a well-known reference explosive, TNT (Trinitrotoluene), which has a detonation velocity of approximately 6900 m/s and a detonation pressure around 210 kbar, it is evident that several of the studied nitro-furanocoumarins—particularly the tetranitro derivatives—surpass TNT in both velocity and pressure. This highlights their promising potential as next-generation energetic compounds.

Overall, the findings indicate that furanocoumarins, owing to their rigid aromatic scaffold and the possibility of structural modification, can serve as strong candidates for the design of new HEMs. The observed consistency between calculated detonation parameters and total energy values highlights the reliability of computational methods in predicting performance and stability. Future work should involve additional computational studies with more advanced methods to refine these predictions, followed by synthesis and experimental validation to confirm the energetic performance and safety profile of these novel compounds.

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