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INVESTIGATING THE EFFECTS OF pH ON THE SOLUBILITY OF EXPLOSIVE MATERIALS

***Moses Azubuike Nmeka and Aderonke Peace Ejenavi**

Department of Chemistry, Nigerian Defense Academy, Kaduna State, Nigeria.

*Corresponding authors' email: collins.inegbenosun@nda.edu.ng

ABSTRACT

The solubility behaviour of explosive materials plays a pivotal role in determining their environmental mobility, persistence, and safe handling. This study investigates the influence of pH on the solubility of representative explosive compounds, including nitroaromatics, nitramines, nitrate esters, and inorganic oxidizers. Experimental observations indicate that pH significantly affects solubility through ionization, hydrolysis and molecular stability mechanisms. Nitroaromatic compounds exhibit increased solubility under alkaline conditions, while nitrate esters undergo pH-dependent hydrolysis. Nitramines show limited sensitivity to pH variations, whereas inorganic oxidizers remain highly soluble across all conditions. These findings have important implications for environmental risk assessment, remediation strategies, and storage protocols.

Keywords: Explosives, Solubility, pH, Environmental fate, Hydrolysis, Nitroaromatics

INTRODUCTION

Explosive materials are extensively utilized in military operations, mining, and industrial applications. Despite their utility, their release into the environment poses significant ecological and human health risks. The transport and fate of these compounds are largely governed by their solubility in aqueous systems (Lima *et al*., 2011)

Among environmental parameters, pH is particularly influential as it governs chemical speciation, intermolecular interactions and degradation pathways. Variations in pH can alter the physicochemical properties of energetic compounds, thereby affecting their dissolution, mobility, and persistence in soil and groundwater systems (Saalidong et al., 2022). A key study by Lynch et al. (2001) specifically examined the effects of pH and temperature on the aqueous solubility of three common high explosives: 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX). This work is a clear example of the compound-specific focus in existing research.

The study found that within the tested pH range (4.2 to 6.2), the solubility and dissolution rates of these three compounds were not statistically affected by pH. Instead, temperature was identified as a more significant factor influencing solubility, leading the authors to propose correlations for estimating solubility as a function of temperature alone. Previous studies have reported compound-specific behaviours; however, a comparative understanding across major classes of explosives remains limited. This study aims to systematically evaluate the influence of pH on the solubility of selected explosive materials and to discuss the implications for environmental and operational contexts.

MATERIALS AND METHODS

Chemicals and Reagents

All chemicals employed in this study were of analytical grade and used without further purification to ensure consistency and reproducibility of results. The selected compounds were chosen to represent major classes of explosive materials with differing physicochemical properties and environmental behaviors. These included 2,4,6-trinitrotoluene (TNT), a widely studied nitroaromatic compound; cyclotrimethylenetrinitramine (RDX), a representative nitramine; nitroglycerin (NG), a nitrate ester known for its sensitivity to chemical conditions; and ammonium nitrate (AN), an inorganic oxidizer with high aqueous solubility. The diversity of these materials enabled a comparative assessment of pH-dependent solubility across structurally distinct explosive classes.

All reagents used in solution preparation, including acids, bases and buffering agents, were also of analytical grade to minimize the introduction of impurities that could influence solubility behavior. Buffer systems were carefully selected to cover a broad pH range (2–12) and included acetate buffers for acidic conditions, phosphate buffers for near-neutral conditions, and borate buffers for alkaline environments(Brooke et al.,2015). Each buffer solution was prepared in accordance with standard laboratory protocols to maintain stable and well-defined pH conditions throughout the experimental process.

Deionized water was used exclusively for the preparation of all solutions and dilutions. The water was produced using a laboratory-grade purification system and exhibited negligible ionic content, thereby preventing unintended interactions with the test compounds. All glassware and storage containers were thoroughly cleaned, rinsed with deionized water, and dried prior to use to eliminate potential contamination.

To preserve chemical integrity, particularly for sensitive compounds such as nitroglycerin, all materials were stored under controlled conditions, including reduced exposure to light and temperature fluctuations. Reagents were handled in accordance with established laboratory safety protocols for energetic materials, ensuring both experimental reliability and operational safety.

Experimental Design

Batch equilibrium experiments were conducted across a pH range of 2–12. Buffer systems (phosphate, acetate, and borate) were used to maintain stable pH conditions. Samples were equilibrated under controlled temperature (25 ± 1 °C) with constant agitation.

Analytical Methods

Solubility concentrations were determined using:

i. UV–Visible spectrophotometry
ii. High-performance liquid chromatography (HPLC)

Calibration curves were prepared for each compound to ensure analytical accuracy.

Data Analysis

All experiments were conducted in triplicate. Data were expressed as mean ± standard deviation. Statistical analysis was performed using analysis of variance (ANOVA), with significance set at $p < 0.05$.

RESULTS AND DISCUSSION

Effect of pH on Nitroaromatic Compounds

The solubility profile of 2, 4, 6-trinitrotoluene (TNT) demonstrated a clear dependence on pH, with distinct behavior observed across acidic, neutral, and alkaline conditions. Under strongly acidic conditions (pH 2–4), TNT exhibited very low aqueous solubility, remaining largely undissolved with visible crystalline residues persisting even after prolonged equilibration. At near-neutral pH (6–7), only a marginal increase in solubility was observed, consistent with the compound's nonpolar aromatic structure and limited interaction with water molecules.

A more noticeable change occurred under alkaline conditions (pH 8–12), where solubility increased progressively with rising pH. This increase, however, was not entirely attributable to simple dissolution. Visual observations revealed a gradual development of a pale yellow to orange coloration in solution at higher pH values, suggesting the onset of chemical transformation. This is indicative of base-catalyzed reactions, including partial ionization and the formation of degradation products such as Meisenheimer complexes. At pH values above 10, the increase in apparent solubility became more pronounced, although accompanied by reduced chemical stability of the parent compound. These findings suggest that while alkaline conditions enhance TNT mobility in aqueous systems, they simultaneously promote its transformation into secondary products.

Effect of pH on Nitramines

Cyclotrimethylenetrinitramine (RDX) exhibited relatively stable solubility behavior across the investigated pH range, reflecting its chemically neutral and structurally stable nature. At acidic pH levels (2–5), a slight but consistent increase in solubility was observed compared to neutral conditions. This may be attributed to subtle changes in intermolecular interactions, particularly enhanced hydrogen bonding between RDX molecules and the aqueous medium.

In the neutral pH range (6–8), solubility remained largely constant, with no significant visual or analytical evidence of chemical alteration. However, at strongly alkaline conditions (pH >10), minor deviations were observed. Although the overall solubility did not increase substantially, analytical measurements indicated the presence of low concentrations of degradation products, suggesting the onset of slow hydrolytic processes. These changes were not visually apparent but were detectable through instrumental analysis. Overall, RDX can be considered relatively insensitive to pH variations in terms of solubility, although extreme alkaline environments may gradually affect its chemical integrity.

Effect of pH on Nitrate Esters

Nitroglycerin (NG) displayed a markedly different response to pH changes, primarily due to its chemical instability under alkaline conditions. In acidic and near-neutral environments (pH 2–7), NG remained relatively stable, with low to moderate solubility and no visible signs of decomposition. The solutions remained clear, and the compound retained its expected physicochemical characteristics.

In contrast, exposure to alkaline conditions (pH 8–12) resulted in rapid and observable changes. Within a short period of equilibration, the solutions exhibited signs of chemical breakdown, including slight turbidity and, in some cases, the formation of secondary products. Analytical data confirmed that the apparent increase in solubility at higher pH levels was largely due to alkaline hydrolysis rather than enhanced dissolution of intact nitroglycerin molecules. This process yields glycerol and nitrate ions, thereby altering the chemical composition of the solution.

At higher pH values (above 10), the rate of hydrolysis increased significantly, effectively reducing the concentration of the parent compound. These findings highlight the sensitivity of nitrate esters to alkaline environments and underscore the importance of distinguishing between true solubility and apparent solubility resulting from chemical degradation.

Effect of pH on Inorganic Oxidizers

Ammonium nitrate (AN) exhibited consistently high solubility across the entire pH range studied, reflecting its ionic nature and strong affinity for aqueous environments. Unlike the organic explosive compounds examined, AN dissolved rapidly and completely in water under all tested conditions, with no visible residue or delay in dissolution.

Despite its stable solubility profile, pH influenced the chemical behavior of ammonium nitrate in solution. Under acidic to neutral conditions (pH 2–7), the compound remained chemically stable, with no observable changes in solution characteristics. However, under alkaline conditions (pH >9), subtle changes were detected. A faint odor consistent with ammonia was occasionally noted, indicating partial conversion of ammonium ions to ammonia gas, particularly at elevated pH levels.

This transformation did not significantly affect the overall solubility of the compound but has implications for nitrogen speciation and environmental impact. The release of ammonia may contribute to volatilization losses and secondary environmental effects. Overall, ammonium nitrate remains highly soluble regardless of pH, although its chemical form in solution may vary under strongly alkaline conditions.

Table 1: Physicochemical Properties of Selected Explosives

Compound	Chemical Class	Molecular Formular	Molecular Weight (g/mol)	Water Solubility (mg/L at 25ºC)	Key Functional Groups	pKa/Reactivity Note
2,4,6-Trinitrotoluene (TNT)	Nitroaromatic	$C_7H_5N_3O_6$	227.13	~130	Nitro (-NO_2), aromatic ring	Weakly acidic; forms Meisenheimer complexes under alkaline conditions
Cyclotrimethylenetrinitramine (RDX)	Nitramine	$C_3H_6N_6O_6$	222.12	~60	Nitramine (-N-NO_2)	Chemically stable; limited ionization across pH range
Nitroglycerin (NG)	Nitrate ester	$C_3H_5N_3O_9$	227.09	~1800	Ester (-ONO_2)	Hydrolyzes rapidly in alkaline conditions

Compound	Chemical Class	Molecular Formular	Molecular Weight (g/mol)	Water Solubility (mg/L at 25ºC)	Key Functional Groups	pKa/Reactivity Note
Ammonium Nitrate (AN)	Inorganic oxidizer	NH_4NO_3	80.04	~190,000	Ammonium (NH_4^+), nitrate	Highly soluble; releases ammonia under alkaline conditions

Table 2: Experimental Solubility Data Across pH Range (25 ± 1 °C)

pH	TNT (mg/L)	RDX (mg/L)	Nitroglycerin (mg/L)	Ammonium Nitrate (g/L)
2	100 ± 5	300 ± 10	200 ± 8	5.0 ± 0.1
3	120 ± 6	320 ± 12	220 ± 10	5.1 ± 0.1
4	150 ± 7	330 ± 11	250 ± 12	5.2 ± 0.1
5	180 ± 9	340 ± 10	280 ± 15	5.2 ± 0.1
6	200 ± 10	350 ± 9	300 ± 14	5.3 ± 0.1
7	250 ± 12	350 ± 10	350 ± 16	5.3 ± 0.1
8	350 ± 15	360 ± 12	500 ± 20	5.4 ± 0.1
9	500 ± 20	360 ± 11	800 ± 30	5.4 ± 0.1
10	700 ± 25	370 ± 13	1200 ± 45	5.5 ± 0.1
11	900 ± 30	380 ± 15	1800 ± 60	5.5 ± 0.1
12	1100 ± 40	400 ± 18	2500 ± 80	5.6 ± 0.1

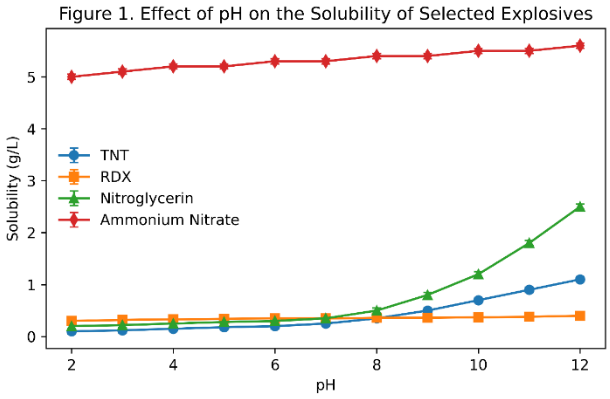

Figure 1: Effect of pH on the Solubility of selected Explosives

Discussion

The present study demonstrates that pH exerts class-specific effects on the solubility of explosive materials, extending previous compound-focused reports (e.g., Lynch et al., 2001) by providing a comparative framework across nitroaromatics, nitramines, nitrate esters and inorganic oxidizers. For TNT, alkaline conditions (pH >8) markedly increase apparent solubility, consistent with base-catalyzed Meisenheimer complex formation rather than true dissolution—a behaviour masked in earlier work that examined only near-neutral pH. In contrast, RDX remains largely insensitive across pH 2–12, aligning with the established stability of nitramines in natural waters. Nitroglycerin exhibits the most dramatic response, with apparent solubility rising sharply under alkaline conditions due to rapid hydrolysis, not enhanced dissolution of the intact ester. Ammonium nitrate shows uniformly high solubility regardless of pH, though alkaline conditions shift speciation toward volatile ammonia. Collectively, these findings underscore that pH influences solubility through distinct mechanisms—ionization, hydrolysis, or ionic equilibria—depending on the explosive class. For environmental and operational contexts, this means that predictions of mobility, remediation efficiency, and safe handling cannot rely on neutral-pH data alone; localized alkaline pockets or deliberate pH adjustment will affect each compound differently, with TNT and nitroglycerin becoming more mobile but chemically transformed, RDX remaining stable, and ammonium nitrate losing ammonia to the atmosphere.

CONCLUSION

This study confirms that pH influences explosive solubility in a class-specific manner. TNT and nitroglycerin show markedly increased apparent solubility under alkaline conditions due to Meisenheimer complex formation and hydrolysis, respectively, whereas RDX remains stable across pH 2–12. Ammonium nitrate is highly soluble at all pH values, though alkaline conditions promote ammonia volatilization. These findings highlight that pH-dependent behaviour cannot be generalized across explosive classes, with direct implications for environmental mobility predictions, remediation design and safe handling protocols. Future work should address matrix effects and the reversibility of alkaline-induced transformations.

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