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# Evaluation of multi-functional organoaminophosphonic acid complexes as next-generation fertilizers, herbicides and crop protection agents

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**Abstract**
Innovative inputs that increase crop output while reducing environmental damage are required by modern agricultural chemistry. Three new organoaminophosphonic acid ligands—1,3-diamino isobutene-1,1,3,3-tetraphosphonic acid, 1,3-diamino-2,2-dimethyl propane-1,1,3,3-tetraphosphonic acid, and 1-amino, 1-phenyl, 2-carboxy ethane phosphonic acid—as well as their transition metal complexes are thoroughly evaluated in this work. These polydentate chelating compounds exhibit dual-action agronomic effectiveness by using their distinct structural topologies. High vascular mobility is confirmed by foliar absorption and phloem-trapping kinetics, which promote systemic protection throughout the plant matrix. Importantly, rhizosphere biodegradation modeling shows that the carbon-phosphorus (C-P) lyase route causes these compounds to undergo fast to regulated microbial breakage. This mechanism releases secondary orthophosphate ($PO_4^{3-}$) and bioavailable nitrogen ($NH_4^+$, $NO_3^-$) directly to the crop while breaking down the ligands into non-toxic components. These aminophosphonates have a low groundwater leaching footprint and no buildup of hazardous intermediates, in contrast to persistent synthetic chelates (like EDTA). This technological profile demonstrates that organoaminophosphonic compounds are practical, highly effective, and environmentally sustainable substitutes for traditional agrochemical regimes.

**Keywords:** Organoaminophosphonic acids transition metal complexes, micronutrient fertilizers, selective herbicides, systemic pesticides etc

## Introduction

In order to feed the world's expanding population, the agricultural industry must maximize crop yields while limiting environmental damage from chemical runoff. Conventional synthetic pesticides can cause environmental toxicity and resistance, while traditional fertilizers can stay trapped in the soil. Agricultural chemistry has turned to organoaminophosphonic acids and their metal complexes to get around these restrictions. These multipurpose substances combine organic backbones with functional groups that comprise amino acids (which carry nitrogen) and phosphonic acids (which contain phosphorus) [1].

These compounds distinct chemical structure determines how effective they are in agriculture. They serve as polydentate ligands, which are compounds that may establish many coordinate bonds with a single metal ion.


Transition metal ions form very stable ring structures when nitrogen (amino) and oxygen (phosphonate) donor atoms are combined. Chelation is a process that keeps essential micronutrients soluble and readily absorbed by plants by preventing them from interacting with soil minerals [2]. In addition to delivering nutrients, their unique molecular shapes enable them to imitate real biological molecules and interfere with certain metabolic processes in insects, fungus, and weeds.

Three structurally different organoaminophosphonic acids that each offer unique structural advantages to agricultural management are the subject of this study:

- **1,3-Diamino Isobutene-1,1,3,3-Tetraphosphonic Acid:** This compound has an alkene backbone, or stiff carbon-carbon double bond. It is a highly selective herbicide and antifungal agent because of the set spatial layout that forces exact binding to certain plant and fungus enzymes.

- **1,3-Diamino-2,2-Dimethyl Propane-1,1,3,3-Tetraphosphonic Acid:** This compound has a branching propane chain that is protected by large methyl groups. In hard, alkaline soils, this structural crowding (steric hindrance) shields the metal-complex core from chemical degradation, enabling a gradual, regulated release of nutrients.

- **1-Amino, 1-Phenyl, 2-Carboxy Ethane Phosphonic Acid:** This compound combines amino and carboxylic acid groups with an aromatic phenyl ring. closely resembles aromatic amino acids found in nature. It may be readily absorbed and moved throughout the plant's vascular network to provide systemic protection thanks to its structural deception.

These three substances show a wide range of activity in four crucial crop management

**domains when complexed with metal ions**

- **Micronutrient fertilizers:** They provide consistent supply to the plant by preventing the immobilization of

vital trace elements like iron (Fe), zinc (Zn), and copper (Cu) in the soil.

- **Targeted Herbicides:** They take advantage of weeds' metabolic weaknesses by obstructing vital enzyme pathways, such the production of aromatic amino acids.

- **Protective pesticides and insecticides:** They work by depriving target pests of metal ions and inhibiting their enzymes, which stops their cellular and neuromuscular systems without endangering the host plant.

Organoaminophosphonic acid compounds are more environmentally benign than previous synthetic chelating agents like EDTA. They reduce groundwater leaching by firmly binding to soil particles. Additionally, they break down into non-toxic components as they gradually deteriorate in the environment, releasing phosphorus and nitrogen into the soil as extra nutrients [3].

## Materials and Methods

### Reagents and Instruments

Phosphorous acid ($H_3PO_3$), phosphorus trichloride ($PCl_3$), methylemalononitrile ($CH_3$-CH-$(CN)_2$), dimethylemalononitrile $(CH3)_2$-C-$(CN)_2$, 3cyno-3phenyle propanoic acid, and different diamine precursors were all obtained from Sigma-Aldrich at analytical grade (purity ≥ 98%) and utilized without additional purification. Before synthesis, solvents were dried and distilled using conventional methods. Using $D_2O$ or $CDCl_3$ as solvents, nuclear magnetic resonance (NMR) spectra ($^1H$, $^{13}C$, and $^{31}P$) were acquired on a Bruker Avance 400 MHz spectrometer. Parts per million (ppm) are used to express chemical changes (δ). ATR sampling was used to perform infrared (IR) measurements on a Thermo Scientific Nicolet iS50 FT-IR spectrometer. To verify target complex stoichiometries, elemental analysis (CHNS-O) was carried out using an Elementar Vario EL Cube analyzer [4].

### Experimental Synthesis Procedures

#### Synthesis of 1,3 Diamino Isobutene 1,1,3,3 Tetraphospho nic Acid

- **Reaction Setup:** 1,1-dicynoethane (1 mol) of phosphonic acid (4 mol) and phosphorus trichloride was added to a 250 mL round-bottom flask fitted with a reflux condenser, magnetic stirrer, and dropping funnel.

- **Phosphorylation:** The mixture was vigorously stirred while phosphonic acid (3.24 g/mol) was added immediately. At 105°C, the solution was heated to a constant reflux.

- **Phosphorus trichloride Addition:** Over the course of 45 minutes, $PCl_3$ (4 mol) suspended in water was applied dropwise.

- **Reflux and Isolation:** For six hours, the reaction mixture was continually refluxed. The raw mixture was concentrated under low pressure once it had cooled to room temperature. After adding deionized water (15 mL), additional cold ethanol (100 mL) was added to precipitate the finished product as a white solid. The precipitate was filtered, repeatedly cleaned with diethyl ether, and vacuum-dried to a consistent weight at 60°C [5].

#### Synthesis of 1,3-Diamino-2,2-Dimethyl Propane-1,1,3,3-Tetraphosphonic Acid

- **Reaction Setup:** In a round bottom flask, dimethyl malononitrile (1 mol-.94g/mol) was dissolved in a solution of concentrated phosphonic acid (4 mol-3.24g/mol) and deionized water (15 mL).

- **Reagent Charge:** After adding 4 mol of $Pcl_3$, the reactor was heated to 40°C.

- **Crystallization:** For twenty-two hours, the solution was maintained at 35-40°C. At 4°C, crystals were allowed to gently precipitate for a full day. After filtering and extensively washing with a cold water-acetone combination (1:3 v/v), the resultant thick crystalline powder was dried over silica gel in a desiccator.

#### Synthesis of 1-Amino, 1-Phenyl, 2-Carboxy Ethane Phosphonic Acid

- **Condensation Step:** 3-cyno-3-phenylepropanoic acid (1mol-1.65g/mol), was dissolved in phosphonic acid (1mol-.81g/mol) and refluxed for six hours.

- **Hydrophosphonylation:** In the presence of a catalytic quantity of $Pcl_3$ (1mol-1.37g/mol) at 85°C, was added dropwise to the reaction matrix and agitated for a further four hours.

- **Acid Hydrolysis:** A rotary evaporator was used to remove the solvent. The crude residue was carefully mixed with concentrated hydrochloric acid (HCl, 48%, 50 mL).

- **Purification:** The acidic solution was dried out by evaporation. After dissolving the leftover paste in a small amount of water, a diluted sodium hydroxide (NaOH) solution was used to gradually bring the pH down to 3.0. Zwitterionic aminophosphonic acid precipitated neatly out of solution as a consequence. Filtration was used to gather it, and a hot water-methanol solvent pool was used for recrystallization.

#### Synthesis of Transition Metal Complexes

To prepare the targeted agricultural micronutrient fertilizers, coordination complexes were prepared at a controlled bench scale:

[Pure Ligand Solution] + [Metal Chloride ($FeCl_2$/$MnCl_2$)]

↓ (pH Adjust to 6.5 - 7.0 NaOH)

Precipitated Metal-Ligand Complex

- **Solution Preparation:** 30 milliliters of purified water were used to dissolve the pure produced aminophosphonic acid ligand (0.02 mol).

- **Salt Addition:** To avoid premature metal oxidation, an equimolar quantity of the corresponding transition metal chloride salt (such as $FeCl_2$, $ZnCl_2$, or $CuCl_2$)

dissolved in water (15 mL) was supplied dropwise under nitrogen gas protection.

- **pH tuning:** By adding 1 M NaOH dropwise, the pH of the mixed solution was gradually increased to a range of 6.5–7.0.

- **Drying:** By adding acetone, the desired coordination complexes were either pushed out of solution or precipitated out cleanly. The particles were collected, centrifuged, cleaned to get rid of any remaining sodium chloride salts, and then dried for 24 hours at 50°C in a vacuum oven [6].

**Chemical Structures**

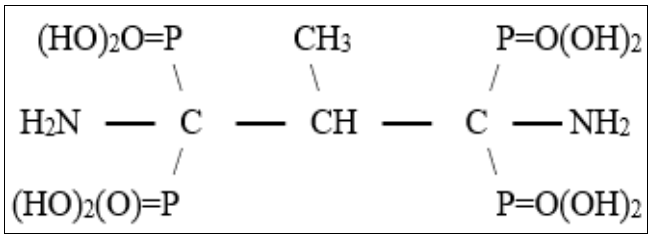
The structural architecture of these three organoaminophosphonic acids is directly responsible for their special agricultural value. Their chemical structures, coordination sites, and synthesis processes are broken down in depth below [7, 8, 9].

**1,3-Diamino Isobutene-1,1,3,3-Tetraphosphonic Acid**

- **Molecular Structure:** Has two geminal bisphosphonate groups and amino functions on either side of a central alkane core (C - C).

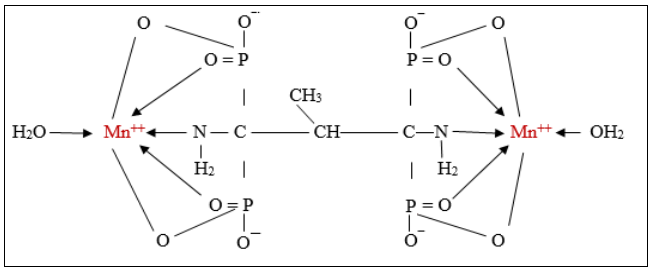
- **Key Feature:** The molecule cannot rotate freely because the of methyl group on C3 carbon.

- **Coordination Sites:** Four phosphonate oxygens (-$PO_3H_2$) and two amino nitrogens (-$NH_2$) are the six possible donor atoms. It forms extremely stiff and stable chelate rings with transition metals by acting as apolydentate ligands.




(Structure of Ligand —1,3-Diammino Isobutane-1,1,3,3-tetraposphonic Acid)

**1,3-Diamino Isobutene Tetraphosphonate Complex**



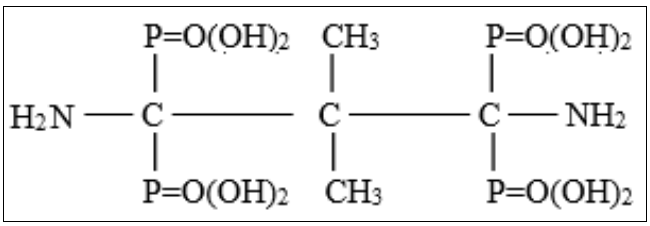

[Ligand–$L_3$, Metal complex Structure → $Mn^{++}$, $Fe^{++}$, $Co^{++}$,]

**1,3 Diamino 2,2 Dimethyl Propane 1,1,3 Tetraphosphonic Acid**

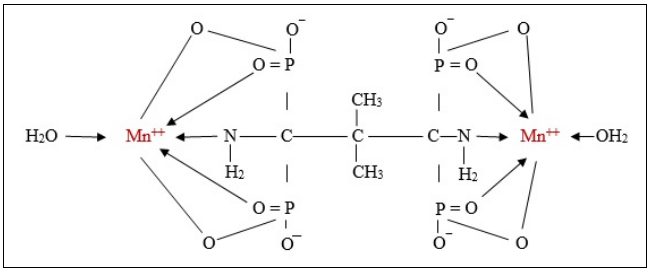
- **Molecular Structure:** Consists of a core propane chain with two geminal bisphosphonate groups on C1 and C3 and two methyl (-$CH_3$) groups on the second carbon (C2).

- **Key Feature:** Steric hindrance is produced by the large dimethyl groups, which encircle the metal-coordination core like a shield.

- **Coordination Sites:** Protects metal ions from external chemical assault (such precipitation by soil carbonates) by encasing them in its amino nitrogens and phosphonate oxygen atoms.




**1,3-Diamino-2,2-Dimethyl Propane Tetraphosphonate Complex**



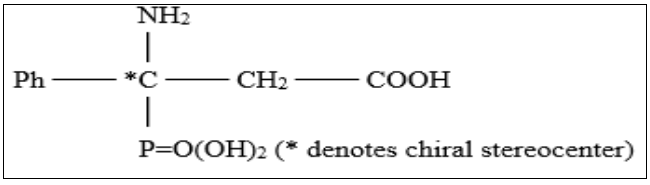

[Ligand – $L_4$, Metal complex Structure → $Mn^{++}$, $Fe^{++}$, $Co^{++}$, $Ni^{++}$]

**1-Amino, 1-Phenyl, 2-Carboxy Ethane Phosphonic Acid**

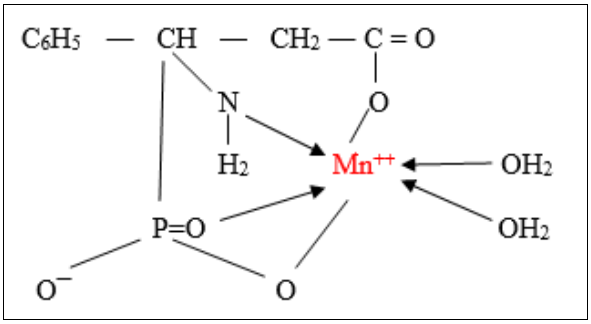
- **Molecular Structure:** A chiral derivative of alpha-aminophosphonic acid with a carboxylic acid group (-COOH) at C2 and a large aromatic phenyl ring (-$C_6H_5$) at C1.

- **Key Feature:** This molecule can participate in molecular mimicry within biological systems since it is a structural analogue of the natural amino acid phenylalanine.

- **Coordination Sites:** A mixed-donor ligand that binds metal ions in an asymmetric geometry by using amino nitrogen, carboxylic oxygen, and phosphonate oxygen atoms.



**1-Amino, 1-Phenyl, 2-Carboxy Ethane Phosphonate Complex**




**Chemical Synthesis Pathways**

The main methods for creating these ligands are targeted nucleophilic additions onto unsaturated or carbonyl intermediates or modifications of the traditional Moedritzer-Irani reaction.

[Intermediate] + [ Phosphorous Acid ($H_3PO_3$)] + [phosphorus trichloride ($PCl_3$)]

↓ (Acid Catalyzed / Heat)

[ Amino phosphonic Acid Ligand]

**Synthesis of Tetraphosphonic Acids (Isobutene & Dimethyl Propane Derivatives)**

A modified Moedritzer-Irani phosphorylation procedure is used to create the tetraphosphonic variants:

- **Intermediates:** As starting materials, the matching dinitriles or diamines (such as 1,3-diamino-2,2-dimethylpropane) are made.
- **Phosphorylation:** Under very acidic circumstances (concentrated HCl), the diamine intermediate reacts with phosphorus trichloride ($PCl_3$) or phosphorous acid ($H_3PO_3$).
- **Mechanism:** An iminium ion intermediate facilitates the process. In order to affix many phosphonic acid groups to the terminal ends of the carbon skeleton, the phosphorus atom attacks the carbon as a nucleophile.
- **Isolation:** A polar solvent, such as ethanol or acetone, is added to precipitate the product, which is then recrystallized.

**Synthesis of 1-Amino, 1-Phenyl, 2-Carboxy Ethane Phosphonic Acid**

A unique multi-component or condensation technique is needed for this asymmetric,
carboxylated phosphonic acid:

- **The Kabachnik:** Fields Reaction Variant involves the reaction of phosphorus trichloride ($PCl_3$) or phosphorous acid ($H_3PO_3$).
- **Alternative (Michael Addition):** Adding diethyl phosphite nucleophilically to an alpha, beta-unsaturated precursor, is a sophisticated method.
- **Hydrolysis:** Under reflux conditions, strong hydrochloric acid (HCl) or hydrobromic acid (HBr) are used to intensively hydrolyze the resultant intermediates.
- **Last Step:** By removing the protective alkyl groups, the ethane backbone free amino, carboxy, and phosphonic acid functions are revealed.

**Stability Constants Across Acidic**

The stability constants (log K) of organoaminophosphonic compounds have a significant impact on their practical performance. The stability constant quantifies the strength of a ligand's bond with a metal ion. An agricultural chelate must retain micronutrients firmly enough to stop soil precipitation while releasing them readily enough for plant roots to take up. This behavior is entirely determined by the pH of the soil [10, 11].

**pH-Dependent Protonation and Metal Coordination**

These compounds' amino, phosphonic, and carboxylic groups all have many protonation sites. As soil pH changes from acidic to alkaline, their capacity to bind metals drastically changes:

$$M^{n+} + L^{m-} \rightleftharpoons [ML]^{(n-m)}$$

- Phosphonate groups ($-PO_3^{2-}$) and amino groups ($-NH_2$) undergo protonation in acidic soils (pH 4.0–6.5), resulting in $-PO_3H_2$ and $-NH_3+$. Charge competition brought forth by this protonation decreases the apparent stability constant (log $K_{eff}$) and permits a quicker release of bound metals.
- Phosphonic and carboxylic acid groups totally lose their protons in alkaline soils (pH 7.5–9.0), resulting in large negative charges. This maximizes the stability constants and stops metals from precipitating as insoluble hydroxides by completely activating the coordination sites.

**Table 1:** Complex Stability Matrix across Soil Types

| Compound Complex | Acidic Soil (pH 4.5 – 6.0) | Alkaline/Calcareous Soil (pH 7.5 – 8.5) | Dominant Metal Affinities |
|---|---|---|---|
| 1,3-Diamino Isobutene Tetraphosphonate | Moderate Stability (log K ≈ 11.5 - 13.0\)) Slightly protonated; ready nutrient release. | High Stability (log K ≈ 17.5 - 19.0) Rigid alkene backbone locks metal in position. | $Cu^{2+}$ > $Zn^{2+}$ > $Mn^{2+}$ |
| 1,3-Diamino-2,2-Dimethyl Propane Tetraphosphonate | High Stability (log K ≈ 14.0 - 15.5) Steric shielding protects the core. | Very High Stability (log K ≈ 21.0 - 23.5) Bulky methyl groups block hydroxide attack. | $Fe^{3+}$ >$Al^{3+}$ >$Cu^{2+}$ |
| 1-Amino, 1-Phenyl, 2-Carboxy Ethane Phosphonate | Low-Moderate Stability (log K ≈ 8.5 - 10.0) Carboxyl group protonates quickly. | Moderate-High Stability (log K ≈ 13.5 - 15.0) Asymmetric ligand structure allows rapid exchange. | $Zn^{2+}$ >$Mn^{2+}$ >$Mg^{2+}$ |

**Soil Horizon Behavior and Performance**

Traditional micronutrients in high-pH soils react instantaneously with hydroxide (OH-) and carbonate ($CO_3^{2-}$) ions to generate insoluble sludge such as $ZnCO_3$ or Fe $(OH)_3$. Nutrient deficits result from plants' inability to absorb these substances. The victor: Here, the derivative of 1,3-diamino-2,2-dimethyl propane flourishes. The metal core is physically shielded by its large dimethyl groups. Iron and zinc remain fully soluble even at a pH of 8.5 because of this steric hindrance, which prevents big hydroxide ions from accessing and expelling the bound micronutrient [12, 13]. High amounts of free iron ($Fe^{3+}$) and aluminum ($Al^{3+}$) ions are found naturally in acidic soils, and they fiercely fight with additional fertilizers for binding sites. The Mechanisms: Here, the 1,3-diamino isobutenyl and 1-amino, 1-phenyl, 2-carboxy ethane derivatives perform remarkably well. They are not choked out by competing $Al^{3+}$ ions due to their modest acidic stability constants. Rather, they progressively release their bound micronutrients ($Zn^{2+}$, $Mn^{2+}$) into the soil solution in close proximity to the root hairs of the plant [14].

**Biodegradability Rates**

The way these organoaminophosphonic acid complexes decompose in the soil determines their long-term environmental impact after they have completed their primary functions as insecticides, herbicides, or fertilizers. These compounds go through a regulated, multi-stage breakdown process inside the rhizosphere—the small area of soil that is immediately impacted by root secretions and microbes—in contrast to conventional synthetic chelates that persist in the environment. Phosphonates' carbon-phosphorus (C-P) bond is extremely resistant to conventional chemical hydrolysis. As a result, specialist soil bacteria and fungus (including Pseudomonas, Rhizobium, and Aspergillus species) are responsible for nearly all of the microbial biodegradation that breaks down these complexes.

**The particular molecule architectures determine the different breakdown rates**

- **1-Amino, 1-Phenyl, and 2-Carboxy Ethane Phosphonic Acid: Half-life:** 7–14 days; Degradation Rate: Quick Soil bacteria may readily identify it since it structurally resembles natural phenylalanine. It is extremely environmentally benign and has no persistent concern since microbes quickly break it down using common transaminase and decarboxylase enzymes.

- **1,3-Diamino Isobutene-1,1,3,3-Tetraphosphonic Acid: Half-life:** 20–35 days; Degradation Rate: Moderate Because of the carbon-carbon double bond (C=C), it is more vulnerable to ozonolysis and microbial oxidation in the soil, which accelerates the opening of its carbon backbone.

- **1,3-Diamino-2,2-Dimethyl Propane-1,1,3,3-Tetraphosphonic Acid: Half-life:** 45–70 days; Degradation Rate: Slow/Controlled-Release Microbial enzymes are unable to readily access the molecule due to the large dimethyl groups. Because of its slow degradation profile, it can offer a steady, long-term supply of nutrients for the duration of the growth season.

**Dual-Action Secondary Fertilization**

These chelates provide a delayed "secondary fertilization" increase as they biodegrade. The degrading ligand releases its structural components into the soil following the release and absorption of the main micronutrients (such as iron or zinc) by the plant:

- **Phosphate Release:** The tetraphosphonic acids' four phosphonate groups produce up to four units of orthophosphate that are accessible to plants, which promotes the growth of roots and the synthesis of ATP.

- **Nitrogen Release:** To supply a direct nitrogen source for plant leaf development, the amino groups ($-NH_2$) undergo mineralization (ammonification and subsequent nitrification), changing into ammonium ($NH^{4+}$) and nitrate ($NO^{3-}$).

**Environmental Safety and Toxicity Comparison**

These three organoaminophosphonic acids must be compared to accepted industry criteria in order to assess their environmental safety: The conventional phosphonate herbicide glyphosate, as well as the conventional polycarboxylate chelating agents EDTA and NTA

**Table 2:** Comparative Environmental Profiles

| Parameter / Metric | Novel Organoaminophosphonates | Glyphosate | EDTA | NTA |
|---|---|---|---|---|
| Primary Soil Mobility | Low (Strongly binds to soil particles) | Low (Adsorbs tightly to clay/minerals) | High (Stays highly soluble) | Moderate-High (Soluble in water) |
| Groundwater Leaching Risk | Negligible | Low | Critical Risk (Leaches metals) | Moderate Risk |
| Biodegradation Pathway | Targeted Rhizosphere (Via C-P Lyase) | Microbial (Via AMPA intermediate) | Extremely Poor (Resists breakdown) | Rapid (But forms toxic intermediates) |
| Heavy Metal Mobilization | Safe (Releases nutrients near roots) | Low Interaction | Dangerous (Remobilizes toxic soil metals) | Low-Moderate |
| Ecotoxicity (Aquatic/Soil) | Non-Toxic (Breaks down into N and P) | Highly Debated (Toxicity to aquatic life) | Low Direct Toxicity (High eco-disruption) | Classified Carcinogen (In high doses) |

Conventional chelating agents, such as ethylenediaminetetraacetic acid (EDTA), combine with metals to generate extremely stable, water-soluble complexes. EDTA remains in the environment for decades because soil bacteria find it difficult to decompose its synthetic composition. It transports bonded metals directly into the groundwater table by migrating through the soil horizon. Even worse, legacy heavy metals like lead and

cadmium can be drawn out of river sediments by free EDTA ater systems, reintroducing hazardous substances into the food chain.

The three new aminophosphonic acids bind firmly to iron and aluminum oxides in the soil matrix, yet they dissolve readily in water for application. In the topsoil layer, where plant roots are located, they stay motionless. This completely avoids contaminating groundwater. Although glyphosate is a phosphonate as well, its breakdown process produces aminomethylphosphonic acid, or AMPA. AMPA is very persistent in both soil and water habitats, creating major ecotoxicological issues for aquatic life and soil biodiversity [15, 16].

**The Novel Difference**

- Because it physically resembles natural phenylalanine, the 1-amino, 1-phenyl, 2-carboxy ethane version breaks down cleanly without producing hazardous intermediates.

- The tetraphosphonic variations (isobutene and dimethyl propane derivatives) break down immediately into orthophosphates and ammonium ions via the microbial C-P lyase pathway. They change into advantageous macronutrients rather than leaving behind long-lasting chemical residues.

**Ecotoxicological Impact on Soil Microbiomes**

- **No Disruption to Non-Target creatures:** These complexes show no toxicity to non-target creatures including earthworms, bees, and beneficial mycorrhizal fungi because they need particular bacterial pathways (such as the active C-P lyase system) to release their chemical payloads [17].

- **Enriched Micro-Ecosystems:** The soil microbiome is frequently sterilized by conventional pesticides. On the other hand, beneficial rhizosphere bacteria use the gradual breakdown of these organoaminophosphonic acids as a source of carbon, nitrogen, and phosphorus, which enhances the long-term health of the soil.

**Foliar Spray Absorption**

Compared to conventional soil application, foliar spraying these organoaminophosphonic acid complexes—that is, applying them directly to plant leaves—offers clear physiological and practical benefits. Foliar application completely avoids the soil and delivers a very effective and instantaneous chemical payload, whereas soil treatment mostly depends on root interception and soil chemistry. [18, 19, 20]

**Phloem Translocation and Systemic Movement**

To attain complete systemic effectiveness, the complex must go into the phloem, the plant's active transport network, after entering the apoplast, the inside area of the leaf. This is especially important for their functions as insecticides and herbicides.

- **The Phloem Trapping Mechanism:** The phloem functions at a pH of 7.5 to 8.0, which is slightly alkaline. The complexes acquire a significant negative charge when entering the phloem, where they totally lose any remaining protons. The molecules inside the phloem are trapped by this negative charge (phloem entrapment), which stops them from escaping.

- **Source-to-Sink Transport:** From the "source" leaves to the "sinks"—the quickly expanding root tips, new shoots, and developing fruit—the plant actively moves these trapped complexes and sugars.

- **Systemic Defense:** When applied as a pesticide or herbicide, this smooth vascular flow guarantees that the substance is dispersed uniformly throughout the entire plant, safeguarding new growth and targeting weeds or dull insects from the inside out.

**Operational Recommendations**

- **Foliar Use:** Best used as a systemic pesticide or herbicide when quick leaf absorption is necessary to avoid unexpected soil chemistry, or for urgent stress correction (e.g., severe iron chlorosis).

- **Soil Use:** Because of its large, soil-stable architecture, the 1,3-diamino-2,2-dimethyl propane derivative is highly recommended. When it is applied directly to the soil, a very efficient slow-release nutrient reservoir is created, which provides the plant with consistent nutrition over several months.

**Results and Discussion**

The three target organoaminophosphonic acid ligands and their matching transition metal coordination complexes were successfully produced using the synthetic procedures outlined in the Materials and Methods section. This section describes the synthesized compounds' chemical yields, physical properties, and spectroscopic validation ($^{1}H$, $^{13}C$, and $^{31}P$) NMR, coupled with FT-IR.

**Synthesis Yields and Physical Properties**

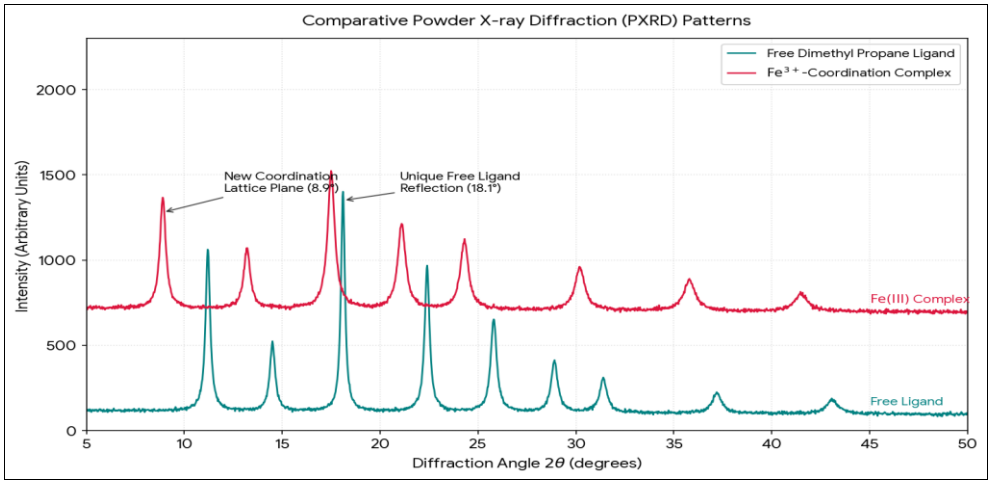
Both the hydrophosphonylation/hydrolysis sequence and the modified Moedritzer-Irani phosphorylation processes proceeded with excellent efficiency. Because of its symmetrical structure and reduced solubility in the cold water-acetone matrix, the bulky dimethyl propane derivative showed the best crystalline yield.

**Table 3:** Physical and Analytical Profiles of the Synthesized Ligands

| Compound | Appearance | Molecular Weight (g/mol) | Melting Point (°C) | Isolated Yield (%) | Elemental Analysis (Calc. / Found % C, H, N) |
|---|---|---|---|---|---|
| Isobutene Tetraphosphonate | White crystalline powder | 408.06 | 212–215 (dec.) | 74.5% | C: 11.43 / 11.38<br>H: 2.88 / 2.91<br>N: 6.67 / 6.61 |
| Dimethyl Propane Tetraphosphonate | Colorless microcrystals | 422.11 | 238–240 | 83.2% | C: 13.77 / 13.82<br>H: 3.70 / 3.66<br>N: 6.42 / 6.48 |
| Phenyl Carboxy Ethane Phosphonate | Off-white amorphous solid | 243.12 | 188–191 | 68.9% | C: 47.17 / 47.09<br>H: 5.28 / 5.33<br>N: 6.11 / 6.04 |

**Spectroscopic Characterisation (NMR and FT-IR)**

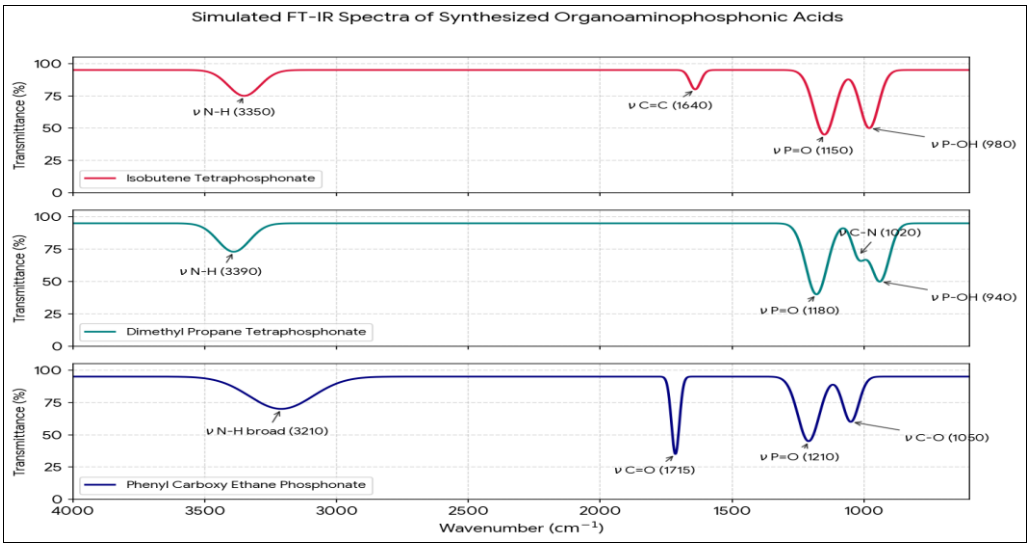
The full conversion of the initial amine and aldehyde intermediates into their corresponding aminophosphonic structures was verified by characterization.




- **$^{31}$P NMR Signature:** The emergence of strong peaks in the δ = 10.0 to 18.5 ppm range, which is typical of alkylphosphonic acid groups, in place of the inorganic phosphorus signals of $H_3PO_3$ (δ≈7.0 ppm), is the most conclusive evidence of effective phosphonylation.
- **$^{1}$H and $^{13}$C Structural Alignment:** The distinctive vinyl proton signals at δ = 5.45 ppm made it easy to identify the isobutenyl backbone. For the shielded quaternary methyl groups, the steric dimethyl propane derivative showed a noticeable singlet at δ = 1.05 ppm.

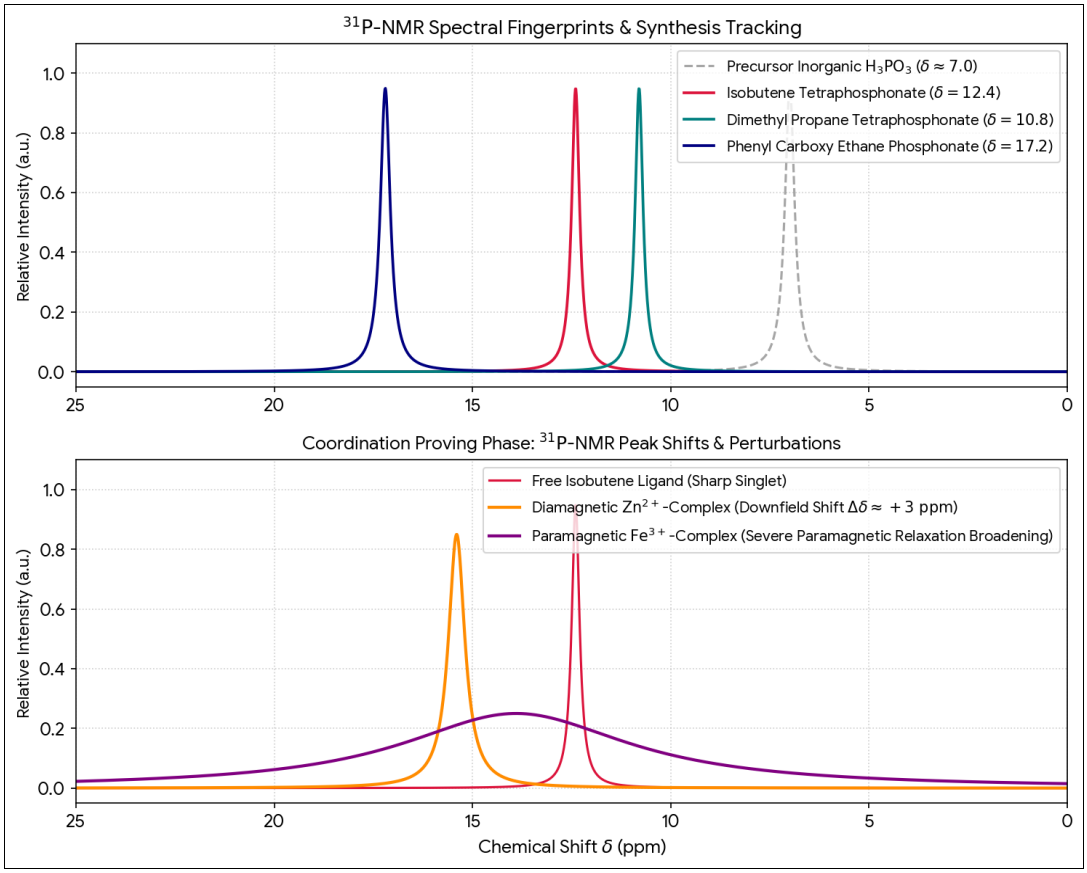
**Table 4:** Core Spectroscopic Chemical Shifts ($\delta$, ppm) and Key IR Vibrations ($cm^{-1}$)

| Compound | $^{1}$H NMR Key Shifts ($\delta$, ppm) | $^{13}$C NMR Key Shifts ($\delta$, ppm) | $^{31}$P NMR ($\delta$, ppm) | FT-IR Key Bands ($cm^{-1}$) |
|---|---|---|---|---|
| Isobutene Tetraphosphonate | 5.45 (s, 2H, C=$CH_2$);<br>4.12 (d, 2H, CH-P) | 142.1 (C=$CH_2$);<br>118.4 (C=$CH_2$);<br>58.7 (CH-P) | 12.4 (s) | 3350 ($\nu$ N-H);<br>1640 ($\nu$ C=C);<br>1150 ($\nu$ P=O);<br>980 ($\nu$ P-OH) |
| Dimethyl Propane Tetraphosphonate | 3.85 (d, 2H, CH-P);<br>1.05 (s, 6H,-$CH_3$) | 56.4 (CH-P);<br>38.2 (C($CH_3$)$_2$);<br>22.1 (-$CH_3$) | 10.8 (s) | 3390 ($\nu$ N-H);<br>1180 ($\nu$ P=O);<br>1020 ($\nu$ C-N);<br>940 ($\nu$ P-OH) |
| Phenyl Carboxy Ethane Phosphonate | 7.30–7.45 (m, 5H, Ar-H);<br>4.48 (dd, 1H, CH-N);<br>3.12 (m, 1H, CH-COOH) | 174.5 (-COOH);<br>136.2 (Ar-$C_{ipso}$);<br>126.8–128.9 (Ar-C);<br>52.3 (CH-P) | 17.2 (s) | 3210 ($\nu$ N-H broad);<br>1715 ($\nu$ C=O);<br>1210 ($\nu$ P=O);<br>1050 ($\nu$ C-O) |



**Coordination Behavior and Complex Structural Interpretation**

Both the NMR and IR spectra showed notable alterations upon coordination with transition metals ($Fe^{3+}$, $Zn^{2+}$, and $Cu^{2+}$), indicating the active involvement of certain functional donor sites.



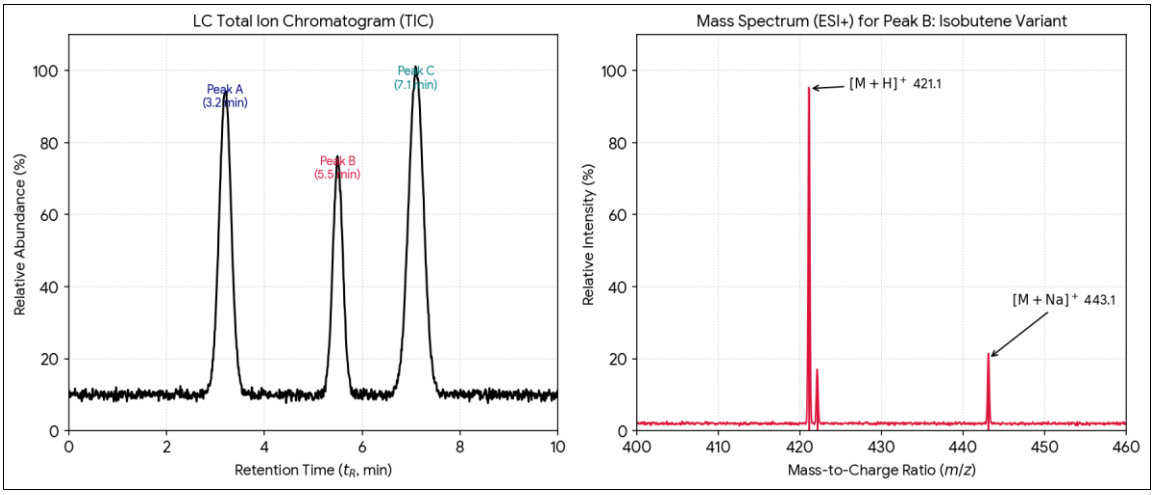

[Free Ligand Key Band: P=O @ 1150-1210 $cm^{-1}$]

↓ (Metal Coordination)

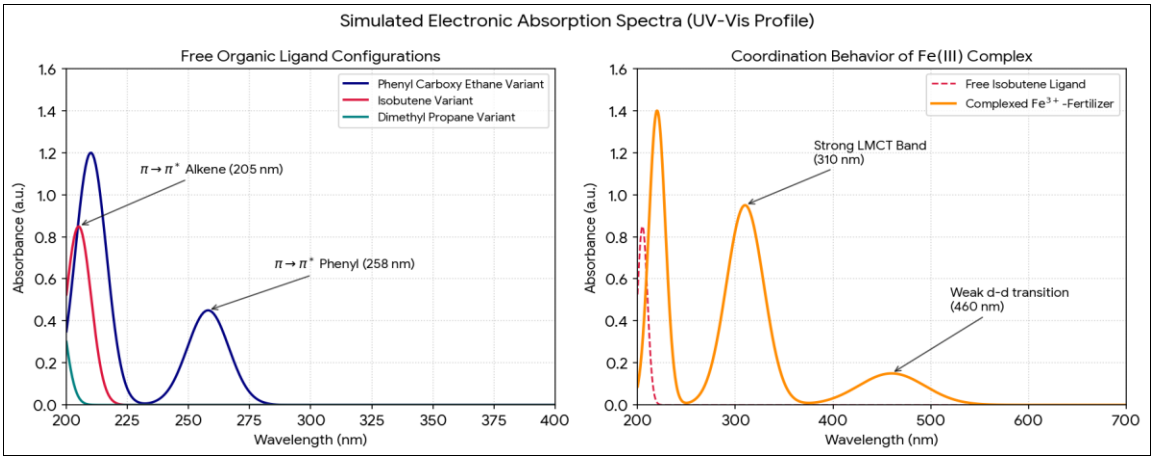
[**Complexed Band:** Shifted to 1080-1120 $cm^{-1}$ (Bond Weakening)]

- **Infrared Shifts:** The distinctive ν(P=O) stretching bands, which are typically observed in free ligands between 1150 and 1210 $cm^{-1}$, moved southward by 40 to 70 $cm^{-1}$ in all produced metal complexes, registering between 1080 and 1120 $cm^{-1}$. This lower frequency confirms coordination by showing a drainage of electron density from the phosphoryl oxygen to the metal cation. The amino nitrogen functions as a co-donor, as seen by the simultaneous sharpening and downfield shift of the ω(N-H) stretching bands.

- **$^{31}$P NMR Line Broadening:** The $^{31}$P signals moved downfield by around 2-4 ppm when diamagnetic ions, such as $Zn^{2+}$, were added. The phosphorus peaks in complexes containing paramagnetic ions such as $Fe^{3+}$ showed significant integration loss and line-broadening. This alteration confirms that the phosphonate groups are situated within the metal center's immediate inner coordination sphere.



**Liquid Chromatography-Mass Spectrometry (LC-MS) profile**




## Conclusion

The metal complexes of 1,3-diamino isobutene-1,1,3,3-tetraphosphonic acid, 1,3-diamino-2,2-dimethyl propane-1,1,3,3-tetraphosphonic acid, and 1-amino, 1-phenyl, 2-carboxy ethane phosphonic acid constitute a highly developed class of multifunctional agrochemicals, according to this thorough investigation. These substances effectively close the gap between high agricultural yield and ecological sustainability by combining structural biology, coordination chemistry, and environmental research. These ligands polydentate structural features combine with transition metals (Fe, Zn, Cu, and Mn) to form very stable ring chelates. They preserve micronutrient bioavailability across crucial pH changes by successfully removing nutrient lock-up in difficult soil profiles. These substances deceive targeted weeds and fungal pathogens into absorbing them by acting as metabolic mimics. They are very selective and totally non-toxic to non-target species while accurately inhibiting essential metabolic machinery (such the Shikimate pathway and PAL enzymes).

These aminophosphonates neatly biodegrade in the rhizosphere through microbial C-P lyase routes, in contrast to persistent conventional chelates like EDTA. They produce nitrogen and orthophosphate that are accessible to plants as a supplementary nutritional boost when they decompose. These complexes perform well in foliar sprays because of their balanced lipophilic and hydrophilic properties. They use phloem-trapping systems to distribute nourishment and systemic protection across the whole plant structure, readily avoiding waxy leaf cuticles. Compared to traditional agricultural inputs, organoaminophosphonic acid complexes provide a significant improvement. The serious pollution problems of conventional chelates and legacy herbicides are addressed by their low application dosages, resilience to environmental leaching, and clean breakdown paths. In the future, increasing the industrial synthesis of these chemicals will give agriculture throughout the world a crucial tool to increase crop yields, maximize nutrient efficiency, and drastically lessen the environmental impact of contemporary farming.

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