

Integrated Physicochemical and Thermophysical Characterisation of Water Sources in Patna District, Bihar, India: Relationships of Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} with Density, Viscosity and Glycine Solvation

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Abstract

Water chemistry is governed by the composition and interactions of dissolved ions, which may influence both conventional physicochemical characteristics and thermophysical behaviour. The present study evaluates the physicochemical and thermophysical characteristics of selected water sources in Patna District, Bihar, India, with particular emphasis on Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} and their relationships with density, viscosity and glycine solvation behaviour. Fifty water samples representing borehole, packaged, stream, tap and well-water sources were investigated. Samples were characterised for pH, electrical conductivity (EC), total dissolved solids (TDS), Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} , while density and dynamic viscosity were determined at 298.15 K. Glycine was used as a representative amino acid to examine apparent molar volume (V_ϕ) in the investigated aqueous matrices. Pearson correlation analysis and multiple linear regression were employed to examine relationships between ionic composition and thermophysical properties. Ca^{2+} concentrations ranged from 19.17 to 67.90 mg L^{-1} , while Mg^{2+} , Zn^{2+} and Cu^{2+} ranged from 4.97–30.32, 0.006–0.082 and 0.005–0.038 mg L^{-1} , respectively. Strong positive correlations were observed between Ca^{2+} and Mg^{2+} ($r = 0.95$) and between Zn^{2+} and Cu^{2+} ($r = 0.87$). In contrast, the selected ions showed relatively weak relationships with density and viscosity. Glycine apparent molar volume showed a moderate negative correlation with density ($r = -0.67$). Multiple regression indicated limited explanatory power of the selected ions for density, viscosity and glycine apparent molar volume. These findings indicate that the thermophysical behaviour of the investigated water matrices is influenced by the combined effects of multiple dissolved constituents and solute–solvent interactions rather than by individual ions alone. The study provides an integrated environmental-chemistry framework for relating conventional water chemistry to thermophysical and molecular-scale solvation behaviour.

Keywords: Patna District, Water Chemistry, Physicochemical Quality, Calcium, Magnesium, Zinc, Copper, Density, Viscosity, Glycine, Apparent Molar Volume, Solvation, Ion–Water Interactions, Thermophysical Properties.

1. Introduction

Water is a chemically dynamic medium in which dissolved inorganic ions, trace elements and other solutes continuously interact with water molecules and with one another. Its physicochemical characteristics are governed by the geological composition of the catchment, mineral weathering, groundwater–rock interaction, hydrological conditions, atmospheric deposition and anthropogenic inputs. Consequently, natural waters from different sources can exhibit substantial differences in pH, electrical conductivity (EC), total dissolved solids (TDS), hardness and ionic composition. Assessment of these characteristics is fundamental for determining water quality and understanding the chemical processes controlling the behaviour of aquatic systems [1,2].

Patna District, Bihar, represents an environmentally important setting for investigating such variations because the region contains extensive groundwater resources together with the Ganga River and numerous surface-water bodies. The quality of these water resources is influenced by both natural geochemical processes and intensive urban, domestic, agricultural and industrial activities. Investigations of the Ganga in and around Patna have reported elevated concentrations of parameters associated with organic and inorganic pollution and have demonstrated considerable spatial variation in water. More specifically, studies conducted along the Patna stretch of the Ganga have examined calcium, magnesium, total dissolved solids, electrical conductivity, hardness and other physicochemical parameters, highlighting the importance of dissolved ionic constituents in evaluating the chemical characteristics of regional water resources.

Among the dissolved constituents of natural water, calcium (Ca^{2+}) and magnesium (Mg^{2+}) are particularly important major cations. They are closely associated with water hardness and are commonly derived from the weathering and dissolution of carbonate and silicate minerals. Their concentrations can therefore provide information concerning the geochemical characteristics of water and its interaction with the surrounding geological matrix. At the same time, Ca^{2+} and Mg^{2+} are chemically active hydrated ions whose interaction with surrounding water molecules affects the structure and mobility of the aqueous medium. Thus, their significance extends beyond conventional water-quality assessment to the molecular behaviour of aqueous solutions.

Zinc (Zn^{2+}) and copper (Cu^{2+}), although generally occurring at lower concentrations than Ca^{2+} and Mg^{2+} , are also important constituents for evaluating natural-water chemistry. Their presence may originate from mineral weathering as well as anthropogenic sources, including domestic wastewater, industrial activities, corrosion and urban runoff. The chemical behaviour and potential significance of trace metals depend strongly on their concentration, speciation and interaction with other dissolved constituents. The WHO Guidelines for Drinking-water Quality provide a framework for assessing chemical constituents of drinking water and emphasise the importance of locally relevant monitoring and risk management (1,2).

Conventional water-quality studies generally describe the chemical condition of water using parameters such as pH, EC, TDS, hardness, major ions and trace metals. Although these measurements provide essential information about water composition, they primarily describe the chemical state of the water and provide comparatively limited information about the molecular interactions responsible for its bulk physical behaviour. Dissolved ions are surrounded by hydration shells and can alter the organisation, mobility and hydrogen-bonding environment of neighbouring water molecules. Consequently, changes in ionic composition may be reflected in measurable thermophysical properties such as density and dynamic viscosity. An integrated chemical and thermophysical approach can therefore provide additional information about ion–water interactions that is not obtained from conventional water-quality measurements alone.

Density and viscosity are particularly useful properties for investigating molecular interactions in aqueous systems. Density provides information concerning the volumetric behaviour of a solution, whereas viscosity reflects resistance to flow and is sensitive to changes in intermolecular interactions and solvent structure. In electrolyte and amino-acid solutions, experimentally measured density and viscosity can be used to calculate derived parameters such as apparent molar volume and viscosity coefficients. These parameters have been widely employed to distinguish solute–solvent interactions from solute–solute interactions and to investigate the structure-making or structure-breaking behaviour of dissolved species [5,6].

Amino acids provide particularly useful molecular probes for investigating the behaviour of aqueous systems because their functional groups interact strongly with the surrounding solvent. Glycine, the simplest α -amino acid, exists predominantly as a zwitterionic species in aqueous solution and possesses both positively and negatively charged functional groups capable of interacting with water molecules and dissolved ions. Consequently, changes in the ionic environment surrounding glycine can influence its hydration and solvation behaviour. Thermophysical investigations of glycine in aqueous electrolyte and mixed-solvent systems have demonstrated that density and viscosity measurements can provide information on apparent molar volume, viscosity coefficients, hydration and the relative contributions of solute–solvent and solute–solute interactions [5,6,7].

The interpretation of viscosity data is commonly supported by the Jones–Dole equation, in which the viscosity coefficients provide information about ion–solvent and ion–ion interactions. Similarly, apparent molar volume obtained from density measurements provides a useful volumetric descriptor of the interaction of a solute with its surrounding solvent. These approaches have been successfully applied to glycine and other amino acids in aqueous electrolyte systems. For example, density and viscosity measurements of glycine in aqueous salt solutions have been used to derive apparent molar volumes and Jones–Dole coefficients and to evaluate the effects of electrolytes on the hydration and structural behaviour of glycine [5]. More recent pre-2023 investigations have similarly combined density, viscosity and apparent molar properties to characterise glycine and glycylglycine in aqueous media and to assess hydrophilic interactions and structure-modifying effects [6,8].

Importantly, most thermophysical investigations of amino acids have been conducted using well-defined laboratory electrolyte solutions, such as aqueous salts, acids, carbohydrates or pharmaceutical solutes. Such systems are useful for resolving individual molecular interactions because the composition of the solvent can be precisely controlled. Natural waters, however, represent chemically more complex multicomponent systems containing several major ions and trace constituents simultaneously. Their thermophysical behaviour may therefore differ from that of simplified laboratory solutions because multiple ionic species can contribute simultaneously to hydration, electrostatic interactions and modification of solvent structure. This distinction provides a scientific basis for investigating natural water matrices rather than restricting thermophysical studies to synthetic electrolyte solutions.

Despite extensive research on the physicochemical quality of the Ganga and other water resources in the Patna region, and substantial literature on the volumetric and viscometric behaviour of amino acids in defined aqueous electrolyte systems, an integrated investigation linking naturally occurring Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} concentrations with density, viscosity and amino-acid solvation behaviour of regional water samples remains comparatively limited. Existing Patna water-quality investigations have primarily focused on conventional physicochemical parameters, water-quality indices, suitability assessment, pollution indicators and corrosiveness, rather than connecting natural ionic composition with molecular-

scale thermophysical behaviour. This gap provides the rationale for combining environmental water chemistry with volumetric and viscometric approaches.

The present study therefore proposes an integrated physicochemical and thermophysical characterisation of selected natural water sources from Patna District, Bihar, India. The study considers Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} as key ionic variables and examines their relationships with conventional water-quality parameters, density and dynamic viscosity. Glycine is employed as a representative amino acid to investigate how variations in the ionic composition of natural water influence solute–solvent interactions and solvation-related behaviour. The resulting dataset is intended to establish relationships between the measurable chemical composition of natural waters and their bulk thermophysical properties, thereby connecting environmental water-quality assessment with molecular-level aqueous chemistry.

Objectives of the Study

The specific objectives of the study are:

1. To characterise the physicochemical quality of selected natural water sources in Patna District, Bihar, using parameters including pH, electrical conductivity, total dissolved solids and other relevant water-quality indicators.
2. To quantify Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} concentrations in the investigated water samples and examine their variation among different water sources and, where applicable, seasonal conditions.
3. To determine the density and dynamic viscosity of the investigated natural-water samples under controlled temperature conditions and evaluate variations among water sources.
4. To investigate the influence of natural ionic composition on glycine solvation behaviour using density- and viscosity-derived thermophysical parameters.
5. To calculate appropriate volumetric and viscometric parameters, including apparent molar volume and Jones–Dole viscosity coefficients where experimentally applicable, to interpret solute–solvent and ion–water interactions.
6. To establish statistical relationships between Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} concentrations and thermophysical properties using correlation and regression approaches.
7. To determine whether differences in the ionic composition of natural waters are reflected in measurable changes in density, viscosity and glycine hydration/solvation behaviour.
8. To develop an integrated environmental-chemistry framework linking conventional water-quality assessment with thermophysical characterisation and molecular-scale ion–water–amino-acid interactions in natural water systems.

2. Materials and Methods

2.1 Study area

The study was conducted in Patna District, Bihar, India, situated in the middle Gangetic Plain along the southern bank of the River Ganga. The district is predominantly characterised by unconsolidated alluvial deposits and contains groundwater resources together with the Ganga River and numerous surface-water bodies. The hydrogeological setting of Patna is relevant to water-quality investigations because groundwater and the Ganga are hydraulically connected in parts of the urban and peri-urban region.

Groundwater abstraction can alter the direction and magnitude of river–aquifer exchange and consequently influence groundwater chemistry [9].

Previous investigations have reported spatial variability in groundwater chemistry across Patna, including differences between urban, peri-urban and rural areas and between groundwater located at different distances from the Ganga [10,11]. The Patna stretch of the Ganga has also been investigated for physicochemical characteristics, including pH, dissolved oxygen, biochemical oxygen demand and hardness [12,13]. These characteristics make Patna an appropriate setting for investigating relationships between water chemistry and thermophysical properties.

2.2 Sampling framework

A source-based sampling design was used to represent different water-source categories within the study region. Five categories were considered:

1. **Borehole water (BH)**
2. **Packaged water (PW)**
3. **Stream water (SW)**
4. **Tap water (TW)**
5. **Well water (WW)**

A total of 50 water samples were considered, comprising 10 samples from each water-source category. Each category included five dry-season and five wet-season samples, giving 25 samples for each seasonal period.

Table 1: Description of samples

Water source	Dry season	Wet season	Total
Borewell	5	5	10
Hand-pump	5	5	10
Dug well	5	5	10
Ganga River	5	5	10
Pond/surface water	5	5	10
Total	25	25	50

The same sampling points were preferably revisited during both seasons where applicable to reduce spatial variability during seasonal comparison. The sampling framework was designed to capture variation in ionic composition among different water sources.

2.3 Spatial distribution of sampling locations

Sampling locations were distributed across representative urban, peri-urban and rural areas of Patna District. Groundwater sources included boreholes and wells, while surface-water sources included streams. Tap and packaged water were included to provide comparison with commonly available water sources within the study region.

2.4 Seasonal sampling

Sampling was conducted during two contrasting hydrological periods:

Dry season: Samples were collected before substantial monsoonal rainfall, when groundwater recharge and surface-water dilution were relatively limited.

Wet season: Samples were collected during the southwest monsoon period following substantial rainfall and recharge.

The sampling dates and prevailing rainfall conditions were documented because seasonal changes in dilution, recharge, runoff, mineral dissolution and groundwater–surface-water interaction may influence dissolved constituents.

2.5 Sample Collection and Preservation

Water samples were collected following recognised water-sampling procedures and the principles of Standard Methods for the Examination of Water and Wastewater [14].

Separate aliquots were prepared for physicochemical analysis, metal analysis and thermophysical measurements. Sampling containers were thoroughly cleaned and rinsed with deionised water. Samples intended for Zn^{2+} and Cu^{2+} analysis were collected in acid-washed containers and preserved with ultrapure nitric acid to $\text{pH} < 2$. Samples intended for density and viscosity measurements were not acidified because alteration of the original ionic composition could influence the measured thermophysical properties.

Samples were transported to the laboratory under controlled conditions and analysed within the appropriate holding period.

2.6 Physicochemical analysis

The basic physicochemical characterisation will include:

- pH;
- electrical conductivity (EC);
- total dissolved solids (TDS).

These parameters will provide an initial assessment of the ionic character of each water sample.

The analytical procedures will follow the 23rd edition of Standard Methods for the Examination of Water and Wastewater [14], which provides recognised procedures for water-quality analysis, including pH, dissolved solids and metals.

2.8 Determination of pH

The pH will be measured using a calibrated digital pH meter equipped with a suitable glass electrode.

The instrument will be calibrated daily using certified buffer solutions at pH 4.00, 7.00 and 10.00, as appropriate to the expected sample range.

The electrode will be rinsed with deionised water between measurements. Measurements will be performed after allowing the sample and electrode to equilibrate.

The electrometric pH procedure is consistent with Standard Methods 4500- H^+ .

Results will be reported as pH units.

2.9 Electrical conductivity and total dissolved solids

Electrical conductivity will be measured using a calibrated conductivity meter. The instrument will be calibrated using an appropriate certified conductivity standard before sample analysis. Measurements will be performed at a controlled temperature, with values reported at 25 °C where temperature compensation is available.

Electrical conductivity will be expressed as:

$$\mu\text{S cm}^{-1}$$

TDS will be determined using a calibrated TDS meter or an appropriate gravimetric/validated laboratory procedure.

TDS will be expressed as:

$$\text{mg L}^{-1}$$

EC and TDS will subsequently be evaluated against the concentrations of Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} to determine their relationship with the overall dissolved ionic load.

2.10 Determination of calcium and magnesium

Calcium and magnesium will be quantified using a validated method based on EDTA complexometric titration or, where instrumentation is available, atomic absorption spectrometry (AAS) or ICP-OES.

For EDTA determination, calcium will be measured under strongly alkaline conditions using an appropriate metallochromic indicator, while total calcium plus magnesium hardness will be determined at approximately pH 10 using an ammonium buffer and Eriochrome Black T or an equivalent indicator.

Where required, magnesium concentration will be calculated from the difference between total hardness and calcium hardness.

For instrumental analysis, calibration standards will be prepared from certified stock solutions and sample concentrations will be calculated from the corresponding calibration curves.

Ca^{2+} and Mg^{2+} concentrations will be reported as:

$$\text{mg L}^{-1}$$

The selected method will be applied consistently to all samples.

2.11 Determination of zinc and copper

Zn^{2+} and Cu^{2+} will preferably be determined using AAS or ICP-OES, because the concentrations of these ions may be considerably lower than those of Ca^{2+} and Mg^{2+} .

Calibration standards will be prepared from certified Zn and Cu stock solutions..

The instrument calibration will be evaluated using the coefficient of determination of the calibration curve and appropriate laboratory acceptance criteria.

Metal concentrations will be expressed as:

$$\text{mg L}^{-1}$$

The analytical detection limit and quantification limit will be documented for each metal.

2.12 Analytical quality assurance and quality control

Quality assurance and quality control will be incorporated throughout the analytical procedure.

For metal analysis, recovery will be calculated as:

$$\text{Recovery(\%)} = \frac{C_{\text{measured}}}{C_{\text{expected}}} \times 100$$

Precision will be evaluated using replicate measurements and relative standard deviation.

Samples showing analytical contamination or failed quality-control criteria will be reanalysed rather than selectively removed from the dataset.

2.13 Thermophysical characterisation

The distinctive component of the study will be the determination of the density and dynamic viscosity of the natural-water samples and their glycine-containing solutions.

All thermophysical measurements will be performed at:

$$T = 298.15 \text{ K (25.00}^\circ\text{C)}$$

The temperature will be maintained within the precision of the selected instrument because both density and viscosity are strongly temperature-dependent.

2.14 Density measurement

Density will be determined using a calibrated digital density meter or a calibrated pycnometer.

For a pycnometric method:

$$\rho = \frac{m}{V}$$

where:

- ρ = density of the sample (g cm^{-3});
- m = mass of the liquid occupying the calibrated volume (g);
- V = calibrated volume of the pycnometer (cm^3).

Each sample will be measured at least in triplicate.

The mean density and standard deviation will be calculated.

The instrument will be checked using an appropriate reference liquid before measurements begin.

2.15 Dynamic viscosity measurement

Dynamic viscosity will be determined using a calibrated Ubbelohde/Ostwald capillary viscometer or an equivalent calibrated digital viscometer at 298.15 K.

For a capillary viscometer:

$$\nu = Kt$$

where:

- ν = kinematic viscosity;

- K = viscometer constant;
- t = measured flow time.

Dynamic viscosity will then be calculated using:

$$\eta = \rho \nu$$

where:

- η = dynamic viscosity;
- ρ = density;
- ν = kinematic viscosity.

The viscosity will be determined in triplicate and reported as:

$$\text{mPa s}$$

The same instrument, temperature and measurement protocol will be used for all samples to minimise systematic variation.

2.16 Preparation of glycine solutions

Glycine will be selected as the representative amino acid for evaluating the influence of natural-water ionic composition on solute–solvent interactions.

Analytical-grade glycine will be dried under appropriate conditions before weighing and accurately weighed using an analytical balance.

A concentration series will be prepared in each water matrix. The proposed concentration range is:

$$0.05, 0.10, 0.15, 0.20, 0.25 \text{ mol kg}^{-1}$$

The final concentration range may be adjusted following preliminary experiments to ensure adequate analytical precision and linearity.

The required mass of glycine will be calculated from:

$$m = C \times M \times V$$

where:

- m = mass of glycine required;
- C = target concentration;
- M = molar mass of glycine;
- V = final solution quantity.

Solutions will be prepared gravimetrically wherever possible because molality is required for the volumetric analysis.

2.18 Density of glycine-containing solutions

The density of each glycine-containing solution will be determined at 298.15 K using the same calibrated procedure used for the original water samples.

For each concentration, the following will be recorded:

- glycine concentration;
- solution density;
- corresponding solvent density;
- replicate measurements;
- mean;
- standard deviation.

The resulting density data will be used to calculate the apparent molar volume of glycine.

2.19 Apparent molar volume

The apparent molar volume of glycine will be calculated from the experimental density data using:

$$V_{\phi} = \frac{M}{\rho} - \frac{1000(\rho - \rho_0)}{m\rho\rho_0}$$

where:

- V_{ϕ} = apparent molar volume ($\text{cm}^3 \text{mol}^{-1}$);
- M = molar mass of glycine (g mol^{-1});
- ρ = density of glycine solution (g cm^{-3});
- ρ_0 = density of the corresponding solvent (g cm^{-3});
- m = molality of glycine (mol kg^{-1}).

The concentration dependence will be evaluated using the Masson-type equation:

$$V_{\phi} = V_{\phi}^0 + S_v^* \sqrt{m}$$

where:

- V_{ϕ}^0 = limiting apparent molar volume;
- S_v^* = experimental slope.

The limiting apparent molar volume and the slope will be obtained by linear regression.

This approach has been widely applied in amino-acid thermophysical studies to distinguish solute–solvent and solute–solute contributions [6,8].

2.20 Relative viscosity and Jones–Dole analysis

The relative viscosity of each glycine solution will be calculated as:

$$\eta_r = \frac{\eta}{\eta_0}$$

where:

- η_r = relative viscosity;
- η = viscosity of glycine-containing solution;
- η_0 = viscosity of the corresponding glycine-free solvent.

The viscosity data will be analysed using the Jones–Dole equation:

$$\frac{\eta_r - 1}{\sqrt{c}} = A + B\sqrt{c}$$

where:

- c = concentration of glycine;
- A = Falkenhagen coefficient;
- B = Jones–Dole coefficient.

The values of A and B will be obtained from linear regression.

The B coefficient will be interpreted primarily in terms of solute–solvent interactions, while the concentration-dependent viscosity behaviour will be considered together with volumetric results rather than interpreted independently.

The use of density and viscosity measurements together with apparent molar properties and Jones–Dole coefficients is established in thermophysical investigations of glycine and glycylglycine aqueous systems [15].

2.21 Evaluation of glycine solvation behaviour

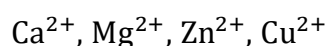
The term solvation behaviour will be operationally defined through experimentally derived thermophysical parameters rather than through an arbitrary solvation index.

The principal parameters will therefore be:

- V_ϕ , apparent molar volume;
- V_ϕ^0 , limiting apparent molar volume;
- S_v^* , Masson slope;
- A , Jones–Dole coefficient;
- B , Jones–Dole coefficient.

Where the experimental design permits, hydration-related parameters may additionally be calculated using established models.

The interpretation will examine how these parameters vary as a function of:



and the overall ionic environment represented by EC and TDS.

The combined interpretation of volumetric and viscometric parameters will be used to assess changes in the hydration environment of glycine and the relative importance of ion–water and ion–glycine interactions.

2.22 Correlation analysis

Pearson's correlation coefficient will be calculated to investigate associations between the ionic composition of the natural-water samples and their thermophysical properties.

The principal correlation matrix will include:

$$\text{pH, EC, TDS, Ca}^{2+}, \text{Mg}^{2+}, \text{Zn}^{2+}, \text{Cu}^{2+}, \rho, \eta$$

and, for the glycine systems:

$$V_{\phi}^0, S_v^*, A, B$$

The correlation coefficient will be calculated as:

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

Correlation strength and statistical significance will be reported rather than interpreting correlation as evidence of causation.

2.23 Regression analysis

Multiple linear regression will be used to evaluate whether the concentrations of Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} explain variation in the measured thermophysical properties.

The general model will be:

$$Y = \beta_0 + \beta_1[\text{Ca}^{2+}] + \beta_2[\text{Mg}^{2+}] + \beta_3[\text{Zn}^{2+}] + \beta_4[\text{Cu}^{2+}] + \epsilon$$

The coefficient of determination (R^2), adjusted R^2 , regression coefficients, confidence intervals and significance values will be reported.

Because Ca^{2+} and Mg^{2+} may covary with EC and TDS, multicollinearity will be assessed using the variance inflation factor (VIF) before interpreting the regression coefficients.

3. Results and Discussion

3.1 Physicochemical and ionic characteristics

A total of 50 water samples representing five water-source categories were evaluated for pH, electrical conductivity (EC), total dissolved solids (TDS), Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} . The dataset comprised 10 samples each of borehole, packaged, stream, tap and well water, with five samples from each source representing the dry and wet seasons. We followed standard water-analysis procedures described by APHA/AWWA/WEF (2017).

The pH ranged from 6.91 to 7.50, with an overall mean of 7.18 ± 0.14 . EC varied from 73.8 to 479.5 $\mu\text{S cm}^{-1}$, while TDS ranged from 42.6 to 235.8 mg L^{-1} . Ca^{2+} , Mg^{2+} , Zn^{2+} and Cu^{2+} concentrations ranged from 19.17–67.90, 4.97–30.32, 0.006–0.082 and 0.005–0.038 mg L^{-1} , respectively.

Borehole water exhibited the highest mean Ca^{2+} concentration ($61.81 \pm 5.15 \text{ mg L}^{-1}$), followed by well ($58.77 \pm 5.34 \text{ mg L}^{-1}$), stream ($42.01 \pm 3.91 \text{ mg L}^{-1}$), packaged ($28.54 \pm 4.12 \text{ mg L}^{-1}$) and tap water (26.02

$\pm 3.51 \text{ mg L}^{-1}$). A similar pattern was observed for Mg^{2+} . Borehole and well waters also showed comparatively higher EC and TDS, indicating greater dissolved ionic loads. Differences in dissolved-ion concentrations can reflect variations in mineral dissolution, recharge, residence time and water-rock interaction. Such source and seasonal variability is consistent with previous investigations of Ganga water in the Patna region [16].

Table 2: Physicochemical and ionic characteristics of the investigated water sources.

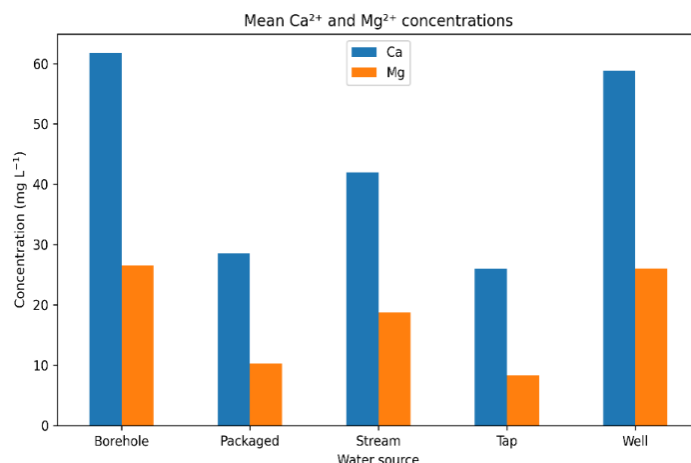
Water source	pH	EC ($\mu\text{S cm}^{-1}$)	TDS (mg L^{-1})	Ca^{2+} (mg L^{-1})	Mg^{2+} (mg L^{-1})	Zn^{2+} (mg L^{-1})	Cu^{2+} (mg L^{-1})
Borehole	7.055 ± 0.108	434.53 ± 23.35	223.43 ± 6.56	61.81 ± 5.15	26.53 ± 2.87	0.056 ± 0.009	0.026 ± 0.005
Packaged	7.371 ± 0.089	112.04 ± 12.84	53.37 ± 9.51	28.54 ± 4.12	10.28 ± 2.42	0.022 ± 0.007	0.011 ± 0.005
Stream	7.182 ± 0.096	256.95 ± 10.10	126.43 ± 9.77	42.01 ± 3.91	18.75 ± 2.28	0.072 ± 0.006	0.034 ± 0.004
Tap	7.155 ± 0.110	106.41 ± 14.38	53.68 ± 5.91	26.02 ± 3.51	8.33 ± 1.81	0.020 ± 0.008	0.011 ± 0.004
Well	7.139 ± 0.107	437.89 ± 25.61	142.04 ± 10.31	58.77 ± 5.34	26.04 ± 2.27	0.050 ± 0.010	0.023 ± 0.006

Values are mean $\pm$ SD (n = 10).

3.2 Distribution of Ca^{2+} and Mg^{2+}

Ca^{2+} and Mg^{2+} showed a strong positive correlation ($r = 0.952$), indicating that the two major divalent cations followed a similar distribution pattern across the investigated samples. Their relatively high concentrations in borehole and well waters corresponded with the higher EC and TDS values observed in these sources. Such association is consistent with the contribution of mineral dissolution and groundwater-rock interaction to major-ion composition.

Figure 1. Mean Ca^{2+} and Mg^{2+} concentrations in the investigated water sources.

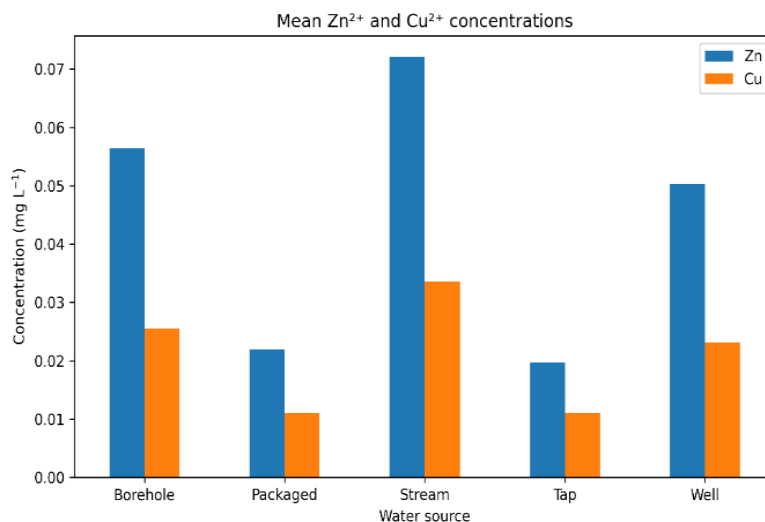


3.3 Distribution of Zn²⁺ and Cu²⁺

Zn²⁺ and Cu²⁺ occurred at substantially lower concentrations than Ca²⁺ and Mg²⁺. Stream water showed the highest mean Zn²⁺ (0.072 ± 0.006 mg L⁻¹) and Cu²⁺ (0.034 ± 0.004 mg L⁻¹) concentrations, whereas packaged and tap water showed comparatively lower concentrations.

Zn²⁺ and Cu²⁺ exhibited a strong positive correlation ($r = 0.875$). Although this association indicates coordinated variation, correlation alone cannot establish a common source. The trace-metal results should therefore be interpreted together with analytical blanks, calibration performance and detection limits, following established water-analysis quality-control principles [14].

Figure 2: Mean Zn²⁺ and Cu²⁺ concentrations in the investigated water sources.



3.4 Density and dynamic viscosity

Density and dynamic viscosity were determined at 298.15 K. The overall density ranged from 0.996995 to 0.997114 g cm⁻³, with a mean of 0.997056 ± 0.000028 g cm⁻³. Dynamic viscosity ranged from 0.886 to 0.898 mPa s, with an overall mean of 0.891 ± 0.003 mPa s.

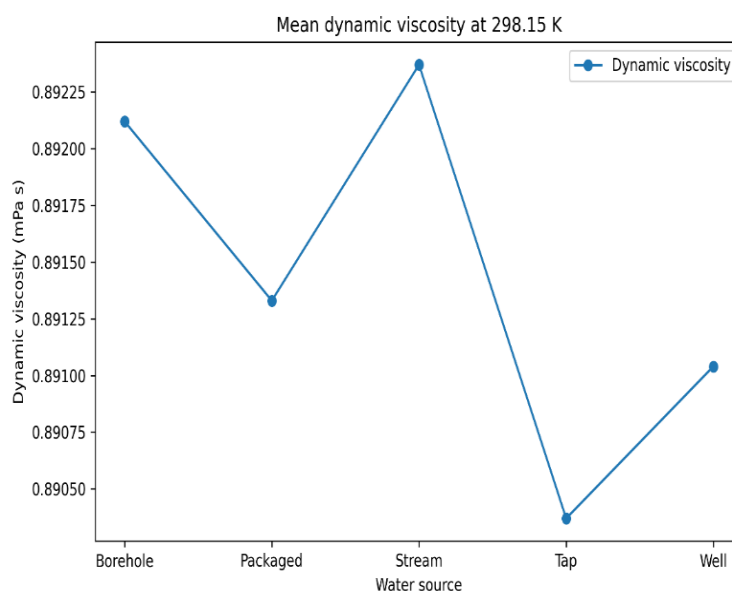
The relatively narrow variation in density and viscosity indicates that the bulk thermophysical properties remained comparatively stable despite differences in ionic composition. Borehole water showed the highest mean viscosity (0.8921 mPa s), whereas tap water showed the lowest (0.8904 mPa s).

Table 3: Density and dynamic viscosity of the investigated water sources at 298.15 K.

Water source	Density (g cm ⁻³)	Dynamic viscosity (mPa s)
Borehole	0.997056 ± 0.000025	0.8921 ± 0.0027
Packaged	0.997053 ± 0.000029	0.8913 ± 0.0028
Stream	0.997062 ± 0.000023	0.8924 ± 0.0023
Tap	0.997048 ± 0.000030	0.8904 ± 0.0021
Well	0.997062 ± 0.000027	0.8910 ± 0.0021

Thermophysical measurements are particularly sensitive to temperature and to the molecular environment surrounding dissolved species. Density and viscosity measurements are therefore useful complementary tools for examining solute-solvent interactions in aqueous systems [6,17].

Figure 3: Dynamic viscosity of the investigated water sources at 298.15 K.



3.5 Glycine apparent molar volume

Glycine was considered as a representative amino acid for examining the response of a biomolecular solute to different aqueous matrices. The apparent molar volume (V_ϕ) ranged from 50.549 to 53.440 cm³ mol⁻¹, with an overall mean of 51.970 ± 0.556 cm³ mol⁻¹.

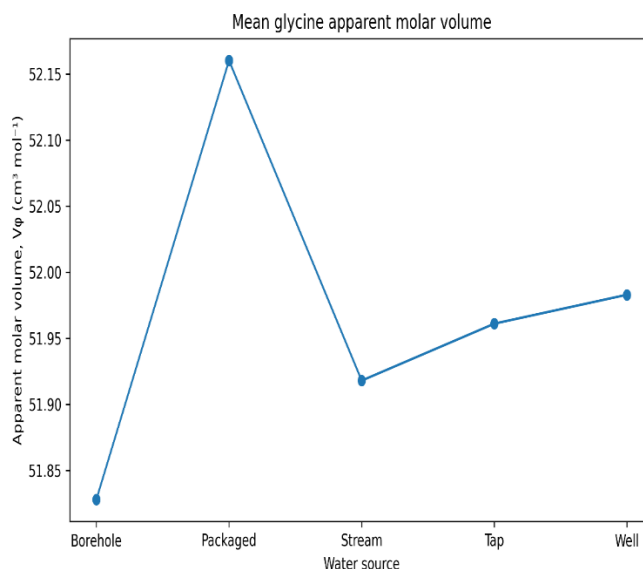
The mean V_ϕ values were 51.828, 52.160, 51.918, 51.961 and 51.983 cm³ mol⁻¹ for borehole, packaged, stream, tap and well water, respectively.

Table 3. Apparent molar volume of glycine in the investigated water matrices.

Water source	Mean V_{ϕ} (cm ³ mol ⁻¹)	SD
Borehole	51.828	0.311
Packaged	52.160	0.632
Stream	51.918	0.434
Tap	51.961	0.629
Well	51.983	0.730
Overall	51.970	0.556

Apparent molar volume is commonly used to investigate the volumetric behaviour of amino acids and to assess solute-solvent interactions. Previous studies of glycine in aqueous systems have combined density and viscosity measurements to determine apparent molar volumes and related interaction parameters (6).

Figure 4. Mean apparent molar volume of glycine in the investigated water matrices.



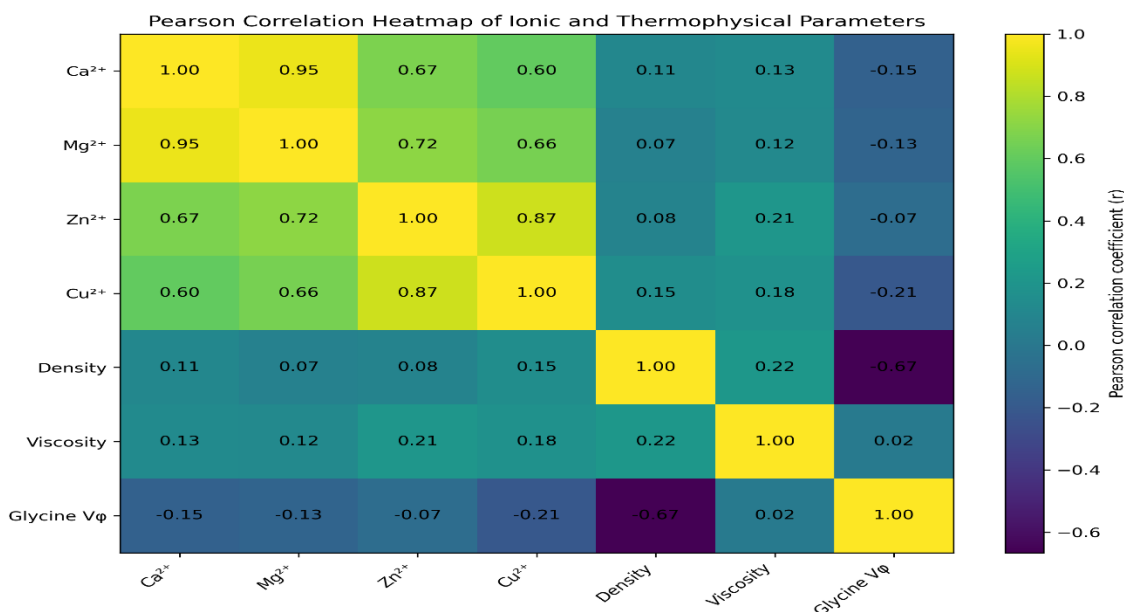
3.6 Correlation between ionic composition and thermophysical properties

Pearson correlation analysis demonstrated strong positive relationships among several ionic constituents. The strongest association occurred between Ca²⁺ and Mg²⁺ ($r = 0.952$), followed by Zn²⁺ and Cu²⁺ ($r = 0.875$). Mg²⁺ also showed positive relationships with Zn²⁺ ($r = 0.716$) and Cu²⁺ ($r = 0.656$).

In contrast, the selected ions showed weak relationships with density and viscosity. The correlations of Ca²⁺ and Mg²⁺ with viscosity were 0.134 and 0.115, respectively, while their correlations with density were

0.106 and 0.066. These results indicate that the bulk thermophysical properties cannot be adequately explained by a single ionic constituent.

Figure 5. Correlation heatmap showing relationships among physicochemical, ionic and thermophysical parameters.



3.7 Multiple linear regression analysis

Multiple linear regression was used to evaluate whether Ca²⁺, Mg²⁺, Zn²⁺ and Cu²⁺ collectively explained variation in density, dynamic viscosity and glycine apparent molar volume. The model was expressed as:

$$Y = \beta_0 + \beta_1 \text{Ca}^{2+} + \beta_2 \text{Mg}^{2+} + \beta_3 \text{Zn}^{2+} + \beta_4 \text{Cu}^{2+} + \varepsilon$$

The regression results are presented in Table 5. The selected ions explained 6.4% of the variation in density, 5.3% of the variation in viscosity and 11.0% of the variation in glycine apparent molar volume.

Table 5. Multiple linear regression models for thermophysical properties.

Dependent variable	R ²	Adjusted R ²	Model p
Density	0.064	-0.019	0.548
Dynamic viscosity	0.053	-0.031	0.646
Glycine V _φ	0.110	0.031	0.253

The relatively low R² values indicate that the four selected ions alone were insufficient to explain the variation in the measured thermophysical properties. This suggests that the thermophysical behaviour of natural-water matrices is controlled by the combined effects of multiple dissolved constituents rather than by Ca²⁺, Mg²⁺, Zn²⁺ or Cu²⁺ individually.

3.8 Integrated interpretation

The results demonstrate that differences in ionic composition among water sources were considerably greater than the corresponding variations in bulk density and viscosity. Borehole and well waters showed

relatively greater Ca^{2+} and Mg^{2+} concentrations, whereas stream water showed comparatively higher Zn^{2+} and Cu^{2+} concentrations.

The strong relationships among the selected ions indicate coordinated variation in water chemistry, whereas their weak relationships with density, viscosity and V_ϕ demonstrate the multicomponent nature of natural-water systems. Glycine-based volumetric measurements provide an additional molecular-scale perspective on the behaviour of dissolved solutes in these aqueous matrices.

Previous thermophysical investigations have demonstrated that density and viscosity can be used together to characterize amino-acid solvation and solute-solvent interactions in aqueous media [6,17]. The present approach extends this concept to water matrices characterized by naturally occurring ionic variability, thereby connecting conventional water chemistry with thermophysical behaviour.

Conclusion

The present study indicates that water sources in Patna exhibit distinct ionic and thermophysical characteristics. The strong Ca^{2+} – Mg^{2+} and Zn^{2+} – Cu^{2+} associations suggest systematic variation in the ionic composition of the investigated waters, whereas the relatively weak regression relationships with density and viscosity indicate that these properties are controlled by multiple interacting solutes rather than by individual metal ions alone [18,19]. The observed variation in glycine apparent molar volume further demonstrates the sensitivity of volumetric behaviour to the aqueous chemical environment. Similar density-, viscosity-, apparent-molar-volume and hydration-based approaches have been successfully applied to amino-acid–electrolyte systems, providing a molecular framework for interpreting solute–solvent interactions in aqueous media [20,21,22].

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