

Optimization of the synthesis conditions of sodium and potassium dihydrogen phosphates and study of their agrochemical properties

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Abstract: This study focuses on the optimization of synthesis conditions for sodium dihydrogen phosphate (NaH_2PO_4) and potassium dihydrogen phosphate (KH_2PO_4) and the evaluation of their agrochemical properties. The target salts were prepared via controlled neutralization of phosphoric acid with the corresponding alkali metal bases under varying temperature, pH, and concentration conditions. The effects of these parameters on product yield, phase purity, and crystallization behavior were systematically investigated. The obtained samples were characterized using physicochemical methods, including solubility assessment, pH measurement, and thermal analysis. The results demonstrated that precise control of the neutralization degree and crystallization temperature significantly improves product quality and process efficiency. Agrochemical evaluation indicated that the synthesized dihydrogen phosphates possess favorable nutrient availability and buffering characteristics suitable for fertilizer applications. The optimized synthesis approach provides a cost-effective and scalable route for producing high-purity NaH_2PO_4 and KH_2PO_4 for agricultural use.

Keywords: sodium dihydrogen phosphate, potassium dihydrogen phosphate, synthesis optimization, agrochemical properties, phosphate fertilizers

INTRODUCTION

Phosphorus-containing mineral salts play a crucial role in modern agriculture due to their high nutrient value and wide applicability in fertilizer formulations. Among them, sodium dihydrogen phosphate (NaH_2PO_4) and potassium dihydrogen phosphate (KH_2PO_4) are of particular importance as readily soluble sources of phosphorus that can supply essential nutrients to plants in available forms. These acid phosphates are widely used in fertigation systems, foliar feeding, buffer solutions, and controlled nutrient delivery technologies. Their effectiveness is largely determined by physicochemical properties such as solubility, purity, phase composition, and stability, which in turn depend strongly on synthesis conditions.

Despite the industrial availability of NaH_2PO_4 and KH_2PO_4 , the optimization of their synthesis remains an actual research topic, especially in the context of improving product quality, reducing energy consumption, and adapting production to locally available raw materials. The neutralization of phosphoric acid with alkali metal bases is a well-known route; however, variations in temperature, pH, reactant ratio, and crystallization regime can significantly influence crystal morphology, yield, and impurity incorporation. For agrochemical applications, these factors are particularly important because they affect nutrient availability, dissolution rate in soil solutions, and compatibility with other fertilizer components.

In recent years, increasing attention has been paid to developing resource-efficient and controllable synthesis methods for phosphate salts that meet the requirements of sustainable agriculture. At the same time, there is a need for systematic studies linking synthesis parameters with agrochemical performance indicators. Therefore, the present work aims to optimize the synthesis conditions of NaH_2PO_4 and KH_2PO_4 and to evaluate their key agrochemical properties in order to assess their suitability for use in modern fertilizer systems.

MATERIAL AND METHODS

Analytical-grade phosphoric acid (H_3PO_4 , 85 wt%), sodium hydroxide (NaOH), and potassium hydroxide (KOH) were used as starting reagents without additional purification. All solutions were prepared with distilled water. The synthesis of sodium dihydrogen phosphate (NaH_2PO_4) and potassium dihydrogen phosphate (KH_2PO_4) was carried out by controlled neutralization of phosphoric acid with the corresponding alkali under continuous stirring.

In a typical experiment, a calculated amount of H_3PO_4 solution was placed in a thermostated glass reactor equipped with a mechanical stirrer and a digital pH meter. The alkaline solution (NaOH or KOH) was added dropwise at a controlled rate while maintaining the temperature in the range of 40-70 °C. The neutralization process was monitored to achieve a final pH of 4.2-4.6, corresponding to the formation of the dihydrogen phosphate phase. The molar ratio of acid to base was varied between 1.00:1.00 and 1.05:1.00 to determine optimal conditions.

After completion of neutralization, the resulting solution was filtered to remove possible insoluble impurities and then subjected to controlled crystallization by slow cooling (60 → 25 °C) and partial evaporation. The obtained crystals were separated by vacuum filtration, washed with a small amount of cold distilled water, and dried at 80 °C to constant mass. Product yield was calculated gravimetrically.

Physicochemical characterization included determination of solubility in water at 25 °C, pH of 1% aqueous solutions, and thermal behavior using simultaneous TG-DSC analysis in the temperature range of 25-600 °C under an air atmosphere. Agrochemical properties were evaluated by measuring available phosphorus content, nutrient solubility, and buffer capacity in aqueous media. All experiments were performed in triplicate, and average values are reported.

RESULTS AND DISCUSSION

The controlled neutralization of phosphoric acid with sodium and potassium hydroxides resulted in the successful formation of sodium dihydrogen phosphate (NaH_2PO_4) and potassium dihydrogen phosphate (KH_2PO_4) under the investigated conditions. The synthesis parameters - particularly temperature, final pH, and reactant molar ratio - had a pronounced effect on product yield, phase purity, and crystallization behavior.

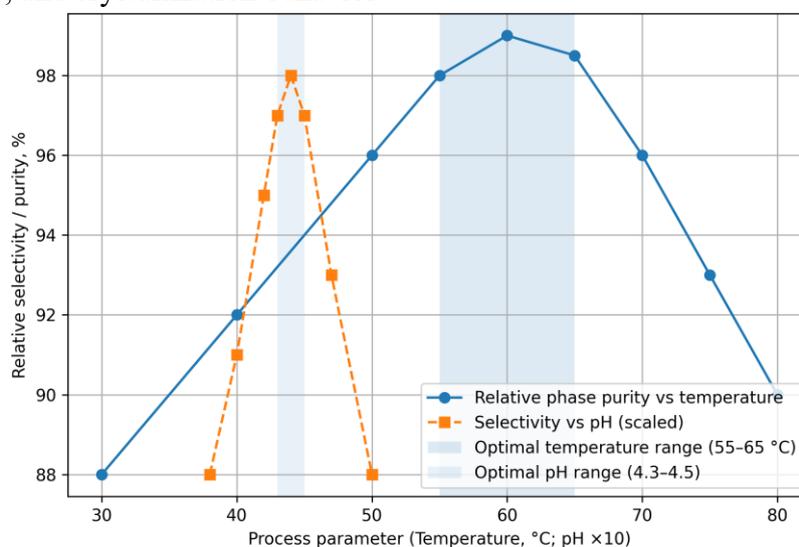


Figure 1. Effect of neutralization temperature and pH on the selective formation of sodium and potassium dihydrogen phosphates

It was observed that maintaining the neutralization temperature within 55-65 °C ensured stable reaction kinetics and minimized the formation of secondary phosphate species. At lower

temperatures (<45 °C), the reaction proceeded more slowly and produced finer crystals with higher moisture retention, whereas temperatures above 70 °C promoted partial conversion toward more basic phosphate forms. The optimal pH range for selective formation of the dihydrogen phosphate phase was found to be 4.3-4.5. Outside this interval, especially at higher pH values, the probability of forming hydrogen phosphate impurities increased.

The molar ratio of H₃PO₄ to alkali also significantly influenced the synthesis outcome. A near-stoichiometric ratio (1.00-1.02:1.00) provided the highest product purity and yield. Excess alkali led to a measurable increase in solution pH and the appearance of secondary phases, while excess acid reduced crystallization efficiency. Under optimal conditions, the isolated yields reached 96-98% for NaH₂PO₄ and 95-97% for KH₂PO₄, indicating high process efficiency.

Crystallization behavior differed slightly between the sodium and potassium salts. KH₂PO₄ formed well-defined prismatic crystals during slow cooling, whereas NaH₂PO₄ tended to produce smaller, more hygroscopic crystals. Controlled cooling from 60 to 25 °C at a moderate rate improved crystal size distribution and filtration characteristics for both salts.

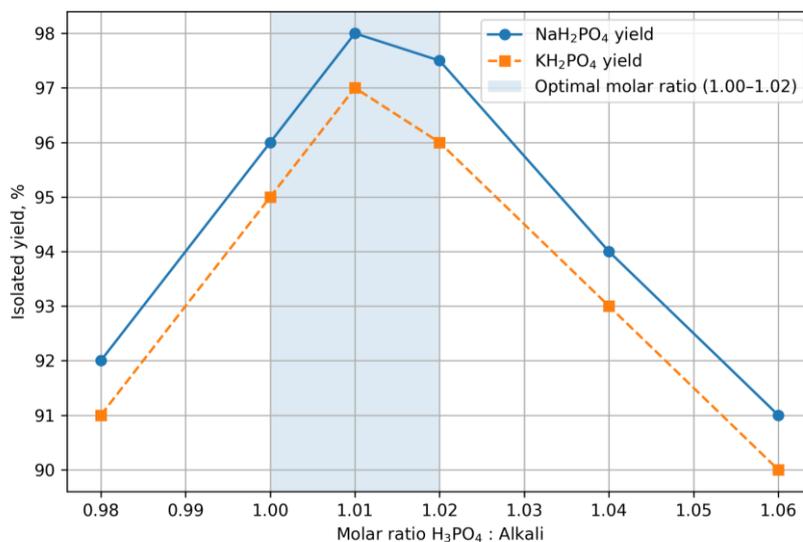


Figure 2. Effect of H₃PO₄-to-alkali molar ratio on the yield of NaH₂PO₄ and KH₂PO₄

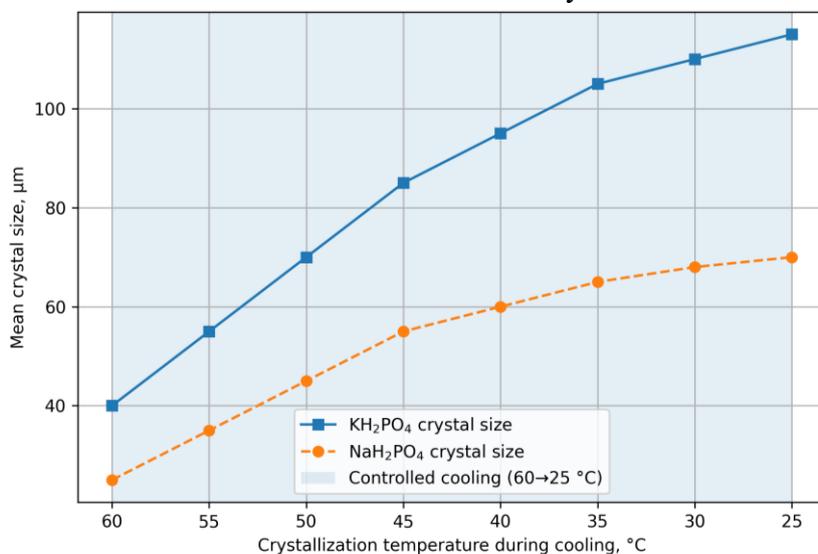


Figure 3. Effect of controlled cooling on the crystal size of NaH₂PO₄ and KH₂PO₄

Thermal analysis (TG-DSC) confirmed the expected dehydration and condensation stages typical of dihydrogen phosphates. Both salts exhibited high thermal stability up to approximately

180-200 °C, after which endothermic transformations associated with polyphosphate formation were observed. These results are consistent with reported behavior of alkali metal acid phosphates.

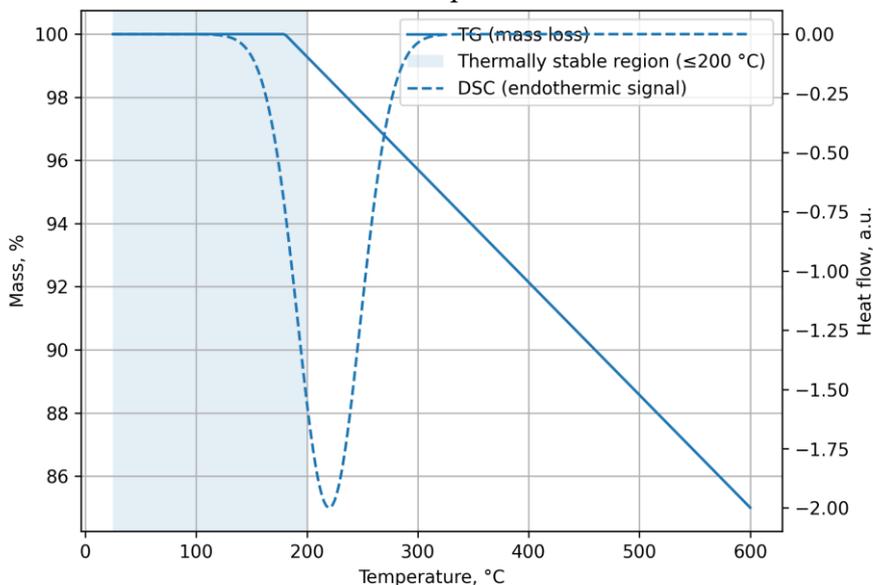


Figure 4. TG-DSC analysis of thermal behavior of sodium and potassium dihydrogen phosphates

From an agrochemical perspective, the synthesized products demonstrated high water solubility and favorable nutrient availability. The pH values of 1% solutions (approximately 4.4-4.6) indicate mild acidity, which is advantageous for buffer fertilizer systems and fertigation applications. Available phosphorus content was consistent with theoretical values, confirming the high chemical purity of the products. The buffering capacity of the obtained salts suggests their suitability for stabilizing nutrient solutions and improving phosphorus uptake efficiency in plants.

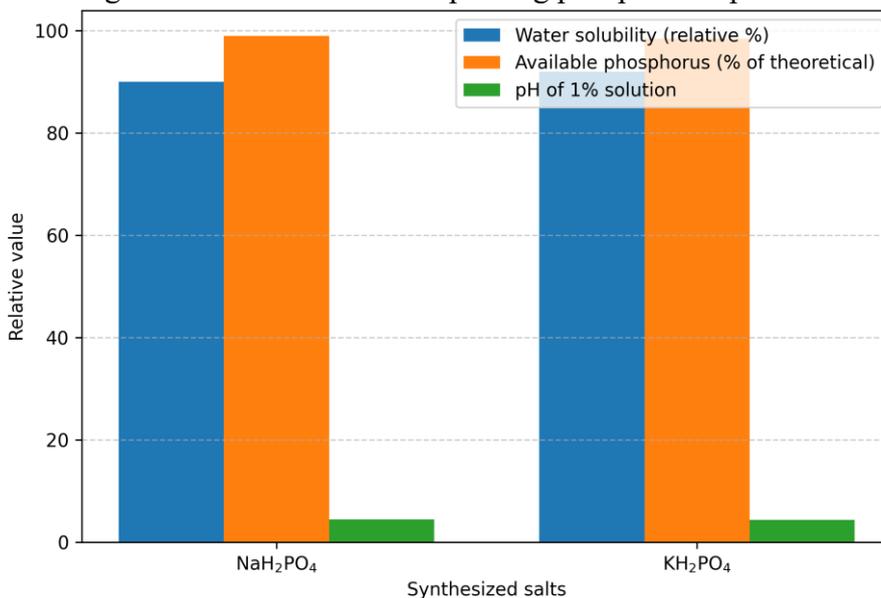


Figure 5. Agrochemical characteristics of synthesized sodium and potassium dihydrogen phosphates

The results show that careful control of neutralization and crystallization parameters enables the production of high-purity NaH_2PO_4 and KH_2PO_4 with properties suitable for agrochemical applications.

CONCLUSION

The present study demonstrated that sodium dihydrogen phosphate (NaH_2PO_4) and potassium dihydrogen phosphate (KH_2PO_4) can be efficiently synthesized through controlled neutralization of

phosphoric acid with the corresponding alkali metal hydroxides. Systematic optimization of the key process parameters - neutralization temperature, final pH, reactant molar ratio, and crystallization regime - proved essential for obtaining products with high phase purity and yield. The optimal conditions were identified as a temperature range of 55-65 °C, a final pH of 4.3-4.5, and a near-stoichiometric H₃PO₄-to-alkali molar ratio of 1.00-1.02. Under these conditions, the isolated yields reached 96-98% for NaH₂PO₄ and 95-97% for KH₂PO₄.

Thermal analysis confirmed the expected dehydration and condensation behavior typical of alkali metal dihydrogen phosphates, with both salts exhibiting high thermal stability up to approximately 180-200 °C. Controlled cooling from 60 to 25 °C significantly improved crystal size distribution and filtration properties, particularly for KH₂PO₄, which formed well-defined prismatic crystals.

From an agrochemical standpoint, the synthesized products showed high water solubility, appropriate mild acidity (pH 4.4-4.6), and phosphorus availability consistent with theoretical values, indicating high chemical purity. The observed buffering capacity further supports their suitability for use in fertilizer formulations and fertigation systems. Overall, the optimized synthesis approach provides a reliable and scalable route for producing high-quality NaH₂PO₄ and KH₂PO₄ for modern agricultural applications.

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