



Scientific Review Report



The future of high-impact publication is here



[Prepared by our Peer Reviewer, Senior Science Editor, and Managing Editor]

Summary



It was a pleasure working on your document. Your study on the synthesis and characterization of acetamidinium salts is expected to draw significant interest from researchers working in the fields of biochemically active compounds and energetic materials. The range of materials investigated and main findings with respect to the hygroscopic properties were clearly described. The present title can be made more specific to the study to pique the reader's interest, and the significance of the study and the implications of its findings can be presented better. I have made recommendations to help you address these focus areas.

Scientific Review Report

(Click on any section label to go to that section)

Peer Reviewer's Comments.....	3
Senior Science Editor's Comments on Language and Paper Structure	6
Senior Science Editor's and Managing Editor's Comments on the Paper's Journal Readiness	8

Peer Reviewer's Comments

Peer Reviewer's Comments.....	3
Senior Science Editor's Comments on Language and Paper Structure	6
Senior Science Editor's and Managing Editor's Comments on the Paper's Journal Readiness.....	8

1. Major issues (likely to be raised by the journal peer reviewer and cause rejection) and corresponding next steps the author should take.

- ◆ Although the methodology was described well, it could be improved by stating a hypothesis and/or clarifying the study design. For example, was it your intention to choose both 2D and 3D structures as you expected them to have different hygroscopic behaviors? Why were these specific compositions chosen?
- ◆ Elemental analysis and mass spectrometry (MS) are listed as characterization methods in the abstract, but there is no mention of either type of analysis in the results and discussion or conclusions section. Please either (a) remove the mention of elemental analysis and MS from the abstract, or (b) add the results of the analyses and your interpretation of them to the results and discussion section and update the conclusions section accordingly
- ◆ To increase the credibility of your data, it is advantageous to briefly discuss the reproducibility of your data and any statistical/data analyses that were performed. I would recommend placing error bars as relevant in the illustrations, discussing the resolution of the measurement techniques, and stating any standards, reference samples, and controls used. For example, the weight increases used to determine the hygroscopy are highly dependent on the resolution of the balance used and the conditions under which the samples were stored. How many samples were measured in each case?
- ◆ The purpose of the Conclusions sections is to highlight the relevance and significance of the study to the field. For example, how is the development of these new salts expected to impact the field? What applications could benefit from these materials? Are there economic, environmental, or policy implications of these findings? Are there any limitations of the study or scope for future work?
- ◆ Please state explicitly how hygroscopicity (%) is calculated. It is difficult to determine how the authors obtained the experimental values from the description given in the text.

2. Minor issues (likely to be raised by the journal peer reviewer for consideration but not cause rejection) and corresponding next steps the author should take.

- ◆ The title could be improved by including some mention of the hygroscopic properties, as this was the main motivation for the work. For example, you could revise the title to “Synthesis and characterization of novel acetamidinium salts with reduced hygroscopy.”
- ◆ As the abstract is well within the recommended word limit, I suggest including some more details to highlight the significance of the study. For example, what advantages do acetamidinium salts with low hygroscopy offer to the field? What specific applications/fields could be benefited? How do the hygroscopic and thermal stabilities of the new salts compare to those of acetamidinium chloride?
- ◆ You have also identified and explained the physicochemical properties that underlie hygroscopicity in these compounds. If any or all the salts you characterized might reduce manufacturing costs, a mention of this would strengthen this section.

3. Does the paper present novel ideas/a novel direction with regard to the field of research?

It is not clear from the manuscript if such acetamidinium salts have been synthesized or characterized previously. Although it is stated that several acetamide salts have been studied so far, it is not clear if those salts could overcome the limitations arising due to their hygroscopic nature. In the absence of this information, the novelty of the study is not clear.

4. Does the paper present novel ideas or build on the research published in the target journal?

Chemical Science publishes findings from across various area of chemical sciences. Articles are expected to present new findings of exceptional significance to their field and be of wider interest to readers working in other areas across the chemical sciences. However, as mentioned before, the novelty of the study is not clear from the manuscript. Please discuss this aspect to highlight the novelty of the study. The journal does not seem to have recently published articles exploring the synthesis of acetamidinium salts with altered hygroscopic properties.

5. Is the research rationale sound? (is the reason for conducting the research explained clearly in the paper?)

In the introduction, the authors discussed the motivation for the study and highlighted the gap in knowledge that the study is trying to fill. As mentioned previously, it would be a good idea to talk about specific applications/fields that could benefit from these salts with altered hygroscopic properties to showcase the importance of the study and its potential impact.

6. Is the literature review complete and which other papers can the author cite?

The uses and limitations of acetamidinium salts have been described well in the background. The results were discussed well in reference to previous studies. I am, however, unable to comment on the appropriateness of the cited papers or the completeness of the literature review since the complete list of references has not been provided. Please ensure that all relevant studies have been cited and that your own previous studies are only cited if they are highly relevant to this study. While it is common

to cite old seminal papers, it is preferable for most of the references to be recent to indicate that the topic is currently relevant and interesting to the field. In addition, please ensure that you cite a balance of papers from different research groups/countries.

7. Are the research implications clearly mentioned? If they are mentioned, are they are sound? If they are not mentioned, what tips should the author follow?

The key finding of the study is the drastically different hygroscopic properties of the 2D and 3D layered structures. However, it is unclear how the development of these new salts is expected to impact the field. What applications could benefit from these materials? Are there economic, environmental, or policy implications of these findings? The answers to these questions will strengthen the presentation of the study's implications.

8. Are the concluding statements clear, and do they mention the contributions, limitations, and next steps for other researchers in the field?

As mentioned above, the concluding statements need to highlight the relevance and significance of the study to the field and the scope for future work.

9. Is the research design appropriate? What are the gaps, and what should be done to fill the gaps?

A wide range of acetamidinium salts were investigated, with both 2D and 3D structures, which enabled the comparison of a range of hygroscopic properties. The study design could be clarified further. You could elaborate on the rationale underlying the selection of both 2D and 3D structures and the compositions chosen for the study.

10. Is the research methodology sound and relevant to the field?

The chosen methods for evaluating the properties of the salts were appropriate as they are well-known and accepted in the field. The specific methodologies and experimental techniques were not presented (which is acceptable in such a short paper) but were referenced appropriately. Any known limitations of the methods used should be briefly stated.

11. Does the data appear accurate, and has it been interpreted appropriately? Flag cases of insufficient or insignificant data with the author.

The results were discussed well in reference to the illustrations and logical conclusions were drawn. The results were compared well with previous studies and there were no obvious inconsistencies. As mentioned previously, you should discuss the reproducibility of your data, and any statistical/data analyses that were performed.

12. Should the author get their data verified by a statistician or submit analyzed datasets to the journal?

The data presented in this paper seem statistically sound, and the analyzed datasets can be submitted to the journal.

13. Does the journal accept this article type?

Chemical Science publishes all original research in one format: Edge articles. There are no page limits for Edge articles, but the journal specifies that lengthy introductions and discussion, extensive data, and excessive experimental details and non-experiment-based conjecture should not be included. The manuscript meets this requirement.

14. Does the research in this article lie within the target journal's scope?

Chemical Science is a multi-disciplinary journal and publishes findings from across the breadth of the chemical sciences. It requires articles to present new findings of exceptional significance to their field and be of wider interest to readers working in other areas across the chemical sciences. As mentioned before, the relevance, significance, and novelty of the study should be highlighted more clearly to pique the journal's interest.

Senior Science Editor's Comments on Language and Paper Structure

Peer Reviewer's Comments.....	3
Senior Science Editor's Comments on Language and Paper Structure	6
Senior Science Editor's and Managing Editor's Comments on the Paper's Journal Readiness.....	8

1. How was the paper's overall language quality prior to editing?

The manuscript needed several revisions to make it submission-ready. The revisions have addressed issues with grammar, word choice, and sentence construction and have ensured the use of formal language in the text.

2. What were the top 3 recurring grammar and language issues found and edited for native tone?

1. Wordiness: The use of too many words to convey one idea can muddle the message and divert the reader's attention.

Example: (a) "Chemical substances" can be concisely written as "chemicals."

(b) "The formation of the free base in *methanol by the use of sodium* methoxide produces sodium chloride" can be written as "The formation of the free base in *methanol by using sodium methoxide* produces sodium chloride"

2. Incorrect word choice: Example: “list” is relevant when referring to a table (which contains values etc.). When referring to figures, “show,” “display,” and “demonstrate” are more suitable alternatives. Thus, the correct sentence would be “Here we describe the synthesis, crystal structure, hygroscopicity, and thermal stability of several of the acetamidinium salts *shown* in Fig. 1.” rather than “...listed in Fig. 1”

3. Sentence construction: Sentences were revised to better convey your intended meaning. For example, “The difference is the higher carbon content of acetamidinium salts compared to the analogous guanidinium ones (replacement of the amino group in guanidines by a methylgroup)” was changed to “The acetamidinium salts have a higher carbon content than their guanidinium analogs, as an amino group in guanidine is replaced by a methyl group in acetamidine.”

3. Does the paper adhere to the target journal's language preference?

The journal guidelines specify that standard British and American spellings are allowed, but they recommend being consistent in the choice of language preference. We have used American spelling, as per your preference. The journal also asks authors to keep the writing clear and concise, avoiding repetition or embellishment. The manuscript meets this requirement.

4. Do the main ideas in the paper flow well? Was the flow of ideas/the main argument natural?

Overall, the introduction is organized well, and it provides adequate context for the reader to understand the need for alternatives to acetamidinium chloride. Please check with the journal on the need for a clearly defined Methods section. Several articles published in *Chemical Science* do not contain a materials and methods section. Rather, the experimental work is discussed more generally in the results and discussion section. The results of the study are clearly stated both in the results and discussion section and the abstract. The importance of the study's findings is not explicitly stated, and the conclusion is quite brief. I have added comments in the manuscript to help you address these issues.

5. What types of changes were made for improvements to paper flow and how has the paper's readability improved because of these?

As mentioned previously, the flow of the ideas in the manuscript was appropriate, but some essential information pertaining to the study's novelty, the implications of its findings, and its limitations is lacking.

6. Does the target journal have a word count limit, and does the paper adhere to this limit after editing?

The journal does not have a word limit, but the guidelines specify that lengthy introductions and discussion, extensive data, and excessive experimental details and non-experiment-based conjecture should not be included. The manuscript meets this requirement.

7. List out all the author preferences and instructions that could not be followed and why.

All author preferences and instructions have been followed.

8. What were the major formatting requirements of the journal for this paper, and what changes have been made to meet these requirements?

The manuscript has been formatted for submission to *Chemical Science* using the template from the journal's website. The in-text citations have been formatted per the journal's requirements. The reference list was not included with the original manuscript, so I was not able to format this section. The tables and figures were not included, so I was not able to comment on these either. I have, however, added placeholders for table titles and figure captions.

Recommendations:

- ◆ Some of the in-text citations and figure references were written in purple font. I have not changed font color for these, so please make sure that font color is consistent in each section prior to submitting the manuscript.
- ◆ The added placeholders will need to be updated with the relevant titles, captions, and in-text descriptions.
- ◆ Please check with the journal regarding the maximum number of figures allowed. Some of the figures could be consolidated to reduce the overall count. Places where this may be possible are indicated with comments in the text.

Senior Science Editor's and Managing Editor's Comments on the Paper's Journal Readiness

Peer Reviewer's Comments.....	3
Senior Science Editor's Comments on Language and Paper Structure	6
Senior Science Editor's and Managing Editor's Comments on the Paper's Journal Readiness.....	8

1. What details or documents are missing in the paper submission package based on the target journal's formatting and submission requirements?

Details of supporting information (if any), the conflict of interest statement, references, and acknowledgements/funding details are missing in the current manuscript.

2. Does the paper need to be split for submission?

The paper does not need to be split for submission.

3. Does the paper need to be blinded for review, and has it been blinded?

The manuscript does not need to be blinded for review.

4. Have all the formatting guidelines, including the right file format for submission, been addressed? Mention any that have not and why they have not been addressed.

The formatting guidelines have been adhered to for the sections made available for edit. The target journal's template has been applied, and the formatted manuscript is in the .docx format, as required. Some sections in the manuscript are incomplete (mentioned below). Please ensure that the necessary details are provided before submission.

5. Have ethical and financial declarations been provided? If not, alert the author to do so and explain why.

This information has not been provided in the manuscript. Please include the funding details in the manuscript before submission.

6. Is a conflict of interest statement provided? If not, alert the author to do so and explain why.

The conflict of interest statement has not been provided in the manuscript. Please ensure that this information is included before submission.

7. Has a data availability statement been provided? If not, alert the author to do so and explain why.

A data availability statement has not been provided. Please provide it before submission.

8. Has the corresponding author been identified for journal interaction?

Yes, the corresponding author has been identified in the manuscript, and the necessary contact details have been provided.

9. Are all the references, tables, and figures present?

The reference list was not included with the original manuscript, so I was not able to format the section. The tables and figures were not included, so I was not able to edit them or comment on the data presentation. Please ensure that these are added before manuscript submission.

10. Are the references in the right format and the figures and tables labelled appropriately?

The journal requires authors to use the Vancouver style of referencing. The manuscript had the in-text citations in this style, but a few changes were required to meet the journal's requirements. These changes have been made. I have not checked the format of the reference list, since it was not provided for editing.

Some of the in-text citations and figure references were written in purple font. I have not changed font color for these, so please make sure that font color is consistent in each section prior to manuscript submission. I included placeholders for table titles and figure captions; however, the titles, captions, and in-text descriptions will need to be updated prior to submission.