

Dear David:

Thanks for the final draft of the Working Group's report. I am happy to vote for its acceptance with the following mostly minor changes:

1. All references in the report to the IUPAC Chemical Identifier or to IChI should be replaced by the IUPAC-NIST Chemical Identifier or INChI, as Brian suggested. I have received confirmation of this change from the chair of IUPAC's Chemical Nomenclature and Structure Representation Division Committee, the committee responsible for INChI. Incidentally, Alan McNaught writes "We plan to issue the final beta test version in a week or so, leave it open for comment for a couple of months, and then issue version 1.0 in the autumn."
2. No CCN report uses the form "first name, given name" for its authors as used in the present list of members of the Working Group. All CCN reports use initials followed by the given name of each author. We should follow CCN's form.
3. In the SUMMARY, the meaning of the word "flag" may well be ambiguous to many readers. Why not replace the sentence in which it appears by: "These layers consist of the chemical formula, an indicator of the state of matter, the space group number and the Wyckoff sequence."
4. In the INTRODUCTION, the .txt format converted the letter "é" in "Tolédano" into "e," and should be corrected. Other examples of this conversion are in the REFERENCES.
5. The problem with the "first name, given name" form noted in #2 above applies equally to the MEMBERSHIP section and should also be corrected.
6. The section GENERAL CONSIDERATIONS is very clear about well-characterised materials. It gives no guidance in the case of ill- characterised materials. We should add a final paragraph to this section with appropriate advice.
7. Section 5.1 may require revision after the final beta test version is out in a week or so. Perhaps we should consider holding this report until INChI v.1.0 is issued?
In the same section, use of the word "main" as in "SC:m/" is not immediately clear and should be clarified.
8. Section 7 largely repeats portions of Section 6. It would be advisable either to clarify the purpose of the repetition in the opening sentence or else amalgamate the two sections.
9. Footnote to Section 8.1 should be replaced by:
<http://www.iucr.org/iucr-top/index.html>.
Item 3 should read "The Hermann-Mauguin symbol and number of the space group. When incomplete crystallographic information is available, these data may be replaced

by specifying the point group (e.g. $4mm$) or the crystal system (e.g. tetragonal)", using the wording given in the original recommendations.

Regarding Steve Heller's article, I thought his major point was the need to provide maximum multimedia services to all electronic publications in order to remain competitive in the long run. Our current html services are clearly of value with the links provided despite references outside the IUCr family being mostly inaccessible. Other facilities that could be immensely helpful to the reader are just around the corner. Steve emphasizes the importance of not resting on our laurels, an attitude I would expect IUCr to endorse with enthusiasm.

With best wishes

Sidney