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Interactive comment on “Analysis of COSIMA spectra: Bayesian approach” by H. J. Lehto et al.

H. J. Lehto et al.

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We would like to thank the anonymous referee #1 for the report. We have changed all the technical notes as recommended, except for figure 4, where a change of the mass difference was recommended to be changed to 0.027u, but as we have two lines and they were offset by 0.027u and 0.017u from the possible identification, and because we have no prior knowledge which one is "more correct" we took an average, and hence retained the original 0.022u.

We have explained the reasons for not showing the full spectrum, as it would have not brought really new information, and refer on several occasions to the excellent paper Paper of Stephan T., 2001. We have added comparison of points relevant to

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our paper. We have made serious efforts in clarifying all the other points raised by the referee including restructuring of the chapters and proofreading by several persons. We attached a pdf file indicating our changes.

===== detailed reply specifying the major changes made in response to Ref #1

Our replies have been marked with a *.

Reply to Referee #1 specifying indicating the pages and lines where these changes show up in the updated version of the manuscript "Analysis of COSIMA spectra: Bayesian approach" by H. J. Lehto et al. Anonymous Referee #1 Received and published: 1 March 2015 General comments: The subject of the manuscript is very interesting because it leads the way to a possible automatic evaluation of mass spectra. This would be very useful for all TOFSIMS users because data evaluation can often take a lot longer than acquiring the data and is a major time sink. The introduction to the subject is detailed and informative but the result section seems rather a bit short and in some points misleading. The manuscript is mainly concerned about single/double peak evaluation despite promising "the whole spectrum" in the abstract and this is where the manuscript falls short in my eyes. From the abstract I expected to see a full spectrum analysis

*Page: Abstract, page 2 lines 2-3

and comparison with traditional methods like in Stephan T. (2001, TOF-SIMS in cosmochemistry. Planet. Space Sci. 49, 859–906) for better judgment if this approach is actually worth it. Stephan also describes a peak fitting routine (although only for isotope ratios but this could be extended to elemental ratios) which seems as promising as the Bayesian approach to me. Therefore a comparison of these two approaches would be helpful.

*Page: p15, The last three lines in the 1st par of ch 4.5 References to Stefan added,

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unfortunately it is difficult to make a detailed comparison as the mathematics is not explained by Stephan (2001).

Specific Comments:

Section 4.3 is entitled Simulated Data but actually seems to mix simulations and real data and is therefore confusing. It would be better to keep the real data and simulated spectra separate in the result section. The discussion of the two line case in section 4.3 fits better into 4.4.

*Page: p14- We renamed the chapters in section 4 to make a clearer separation of the different types of calculations.

The discussion also falls a bit short as only total ion counts are discussed as being close to the starting point when counts for individual peaks are actually far off. The Bayesian method doesn't seem to work any better than a traditional approach marking peak limits and backgrounds. A better comparison with a traditional approach might be helpful here.

*p15, The last three lines in the 1st par of ch 4.5 is rewritten to crystallize the important properties of the Bayesian analysis compared to conventional methods.

578, lines 5-6: Surely the b term is determined by the mass resolution and not the mass resolution by the b term. And yes, every instrument/mass spectrum yields better results if the mass resolution is higher but you can't just increase the b term to achieve this.

*p15, lines 5-6, we have corrected the wording.

Section 6: I'm not sure why the authors assume that in conventional analysis the background is ignored. Yes, some people might have done so and therefore skewed their results but by not ignoring the background, it's possible to gain good results using conventional methods, so it's not clear to me why the Bayesian approach has any advantage here?

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*This is unfortunately what we see in manuals, textbooks and happening in practice, although it is clear that it is not the correct thing to do. *p15, The last three lines in the 1st par of ch 4.5 is rewritten to crystallize the important properties of the Bayesian analysis compared to conventional methods.

Technical Notes: The manuscript could do with some proof-reading. Some paragraphs especially in the introduction seem well written in contrast to some in the result section which have most of the typos.

*We have redone the proof reading and corrected many grammatical and typographical errors.

I listed the ones I found below but this list is probably far from complete. There are also some very minor specific comments in here. Page 567, line 12; recorded Page 576, line 13: AMD Page 576, line 19: "line parameters line" doesn't make any sense Page 577, line 1: shown Page 577, line 6: of or in Page 577, line 12: 5775 Page 578, line 1: such as Page 580, line 23: observed Page 581, line 1: I guess these are the mass calibration parameters a and b. Not sure why they are just called scaling parameters which seems rather confusing. Page 581, line 20: 13C+ Page 581, line 20-23: This sentence needs extending. It's not really understandable in its current form. Page 582, line 2: its Page 582, line 5: of Figure 3: That should be a separation of 6 bins and 4 bins respectively, not 6 and 6.

*Pages: All these have been corrected

Figure 4: The mass difference of these given masses is 0.027u.

*fig caption 4 see comments in the main reply.

Interactive comment on Geosci. Instrum. Method. Data Syst. Discuss., 4, 563, 2014.