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Interactive comment on "Analysis of functional groups in atmospheric aerosols by infrared spectroscopy: sparse methods for statistical selection of relevant absorption bands" *by* S. Takahama et al.

Anonymous Referee #1

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In this paper the authors present a very detailed and thorough anlysis of sparse methods for selection of relevant absorption bands in IR. The paper is well presented and the analysis is very detailed. I only have a few general comments regarding the general accuracy of methods according to reliability of the sampled data.

Page 2 line 24 onwards. Is the justification for sparse methods, in this sense, more with regards the end-point accuracy or prohibitive cost of other methods?

In section 2.1.1 the laboratory and ambient samples are discussed. It would be nice to see a brief consideration of instrument variability and how this might impact of the

performance of your evaluation. For example, is there an underlying assumption that there is no 'drift' in instrument response function across all datasets used? I wonder whether this might lead to the variability discussed in section 3.2 onwards? Perhaps I have misunderstood this, but is agreement between instruments proven?.

Towards the end of page 6 the authors discuss the rationale for choice of variable selection method. In section 2.3.1, how is the test fair in the sense of being able to cover a broad range of functionality expected in amboent samples? In other words, would it be possible to visualise where your test and training set 'sit' on a general 2D basis sets or even simple Ven Krevelen diagrams? Does this even matter?

On this point, there seems to be complicating factors in sample collection from ambient campaigns that might degrade the performance of any 'tuned' method. For example, could it be that whether any semi-volatile loss, for example, occured during sample preparation might lead to a functional group dependency of variable selection?. It might be prudent to assess such effects with a consideration of other factors such as RH, Temp, provenance of sample. Based on the high mass loadings displayed in figure 3, this might not yet be apparent but its worthwhile considering. I guess I'm wondering whether, aside from variable selection refining a fixed instrument response, the algorithms are also picking up 'noise' from external factors.

Minor comments:

Page 8, line 18: I think an 'if' is missing after 'examining' I would recommend expanding acronyms in all figure captions for ease of reading.