

Reviewer report on “Application of fuzzy c-means clustering for analysis of chemical ionization mass spectra: insights into the gas-phase chemistry of NO₃-initiated oxidation of isoprene” by Wu et al.

In this manuscript, Wu et al. show how fuzzy c-means clustering (FCM) can be applied to mass spectrometric data. The FCM method is highly suitable for such data types where one variable/object may represent multiple different compounds (here isomers) or formation processes and thus should not be forced to belong to only a single cluster. The combination with gamma kinetics parametrisation links the clustering results to the chemical pathways and provides further insights into the reaction mechanisms relevant in the atmosphere.

The authors provide a good balance between the more technical investigation of the method to show its validity for this type of data and the scientific content with the application of the method to a case study.

The topic is highly relevant for the atmospheric science community as it provides an alternative dimension reduction technique for mass spectrometry and similar data. I recommend publication in this journal after my comments listed below are addressed.

Major comments

- 1) It is not clear how the authors treated the presence of nitrogen (N) when interpreting the elemental composition and oxidation state.

For the interpretation of the scientific meaning of the clustering results, the authors use the average elemental composition (H:C and O:C) and the oxidation state of carbon (OS_C). These are indeed important proxies for the composition of organic compounds. But in their case study, the authors use an experiment where a considerable amount of nitrogen containing compounds are formed. The presence of N in sum formulas complicates the interpretation of the elemental compositions as the O atoms can be bound either to C or to N. E.g., the two ions C₅H₁₀O₃ and C₅H₁₁NO₃ both have a O:C ratio of 0.6. For the second ion, it is reasonable to assume that there is a NO₃ group, i.e., none of the O atoms is bound to a C. Thus, the formal value of O:C=0.6 becomes meaningless for the comparison of the degree of oxidation or the interpretation of trends in van-Krevelen diagrams between these two ions. Further, N does not necessarily occur as a nitrate (NO₃) group. The authors do not clarify how they handled the presence of N when calculating OS_C. Did they use Eq. 1 in Kroll et al. (2011)? What oxidation state did they assume for N? Priestley et al. (2021) encountered the same issue and suggested an algorithm to estimate the effect of N on OS_C (Eq. 3 in this reference). The authors need to clarify how they handled the presence of N when calculating OS_C and carefully check if their interpretations of the O:C trends are really valid when N is present in some of the ions.

- 2) It is not clear how the different distance metrics were used in reference to the investigated clustering validity index (CVI) metrics and how that impacts the conclusion about the usability of the different metrics.

It is commendable that the authors investigated multiple distance metrics for their investigation (Eq. 4 - 7). But I could not derive how these different methods of determining the distance between clusters was then incorporated when using the CVIs, especially when determining which metric is the most meaningful. Eq. S1 - S4 seem to use the Euclidian distance ($\|x_j - v_j\|^2$). For Eq. S10, “a” and “b” are described as intra- and inter-cluster difference without stating how these are calculated. If the clustering algorithm applies any other than the Euclidian distance metric to assign the clusters, how can a CVI calculated with the Euclidian distance metric truly evaluate the quality of the clustering

result? Is the conclusion that the Euclidian metric is most suitable in FCM driven by the fact that the CVIs are calculated with that method and will then only give the “best” result if the clustering was performed using the same distance method?

The scaling of the input data was also selected to be beneficial for the Euclidean distance method. Could this have an effect of the concluded suitability of the other distance metric methods?

The authors need to clarify which distance metric was used when calculating the CVI values and how/if that impacts their conclusions.

- 3) The manuscript needs some reorganisation/rewriting for the methods part to make it more reader friendly.
 - Equations must appear when they are first brought up. It is extremely tedious to keep scrolling back and forth between the descriptive text and the equations at the end of the section (e.g., in section 2.3.2).
 - Equations cannot simply be dumped as a block like Eq. 1-3. They need introductory sentences identifying what these equations are about and linkage between them.
 - In other places, the reader has to wait for several sections before getting information that is only hinted about. E.g., it is mentioned multiple times that multiple runs were conducted (first in section 2.3.1). Why that was necessary, why sometimes 50 then 100, what was the difference between the runs, and how are these runs will be treated in the interpretation? Part of that information is presented much later, buried at the end of the “other parameter” section which at least for me was not an intuitive place to look for this information. The least that is needed here is a link/pointer to the section where this information will be provided.
 - Splitting section 3.3.1 and 3.3.3 feels forced. For me, the flow would make more sense to have the paragraph 875-889 with Fig 10 as part of 3.3.1. The rest would go to the end of 3.3.2

Minor comments

These comments are present in the order they appear in the text not by relevance.

- 1) The authors claim that FCM classifies the ions by their kinetic properties (e.g., in the abstract). But it is the fitting with the GKP approach that provides this classification. The authors need to emphasize that it is the combination of FCM with GKP that reveals the chemical pathway information. As an example, if there are fast 1st generation reactions and slow 1st generation reactions, the slow 1st generation reaction cluster could not be distinguished from a 2nd generation cluster by its time trace alone. Only the fit with GKP approach and the $m > 1$ value allows that distinction and the mechanistical interpretation of the cluster results. The authors need to rephrase the related part in the manuscript to emphasize the combined effect of FCM and GKP.
- 2) “m” is used in Equations to mean the fuzzifier (e.g., Eq. 1) and the oxidation generation (Eq 12). The authors should consider renaming one of these parameters to avoid confusion.
- 3) Line 72f and 123f: The cluster or factor identification usually uses some type of analysis of the correlation of the variables. These correlations are not necessarily caused by physical or chemical reasons. We interpret them as such.

In the studied case, the clusters represent typical chemical processes because of your measurement setup where the main reason for correlation/similarity is the chemical pathway. For ambient measurements, this may not be true. There, the source and not the reactions in the atmosphere may be the predominant driver of correlation.
- 4) line 88ff and 116f: Defining the “right” error matrix can indeed be a problem and cause for bias. But the error matrix intentionally added to the method to account for the uncertainty in measurements

(e.g., reduce the impact of outliers or less reliable data points). Thus, it can also be seen as an “advantage” of PMF over NMF. Also note that (Buchholz et al., 2020) is showing the error matrix bias for a specifically challenging data set (FIGAERO thermal desorption data). It is yet to be seen if the same issues can occur for “easier” time series data sets.

- 5) Line 76ff: I recommend splitting this paragraph into two: one for factorisation methods and one for clustering (starting at line 91).
- 6) Line 113ff: To put the “fuzziness” property of FCM into context, it would be helpful to specify which of the other mentioned methods allow variables/objects to participate in multiple factors/clusters /components.
- 7) The introduction does not contain any information about the studied VOC/SOA system. A brief paragraph about its relevance and the expected processes may be beneficial.
- 8) Line 336ff: The selected scaling method will shift the emphasis of the signals (maybe even as much as the error matrix can for PMF?). I guess that scaling would enhance the importance of signals with lower intensities. Is there any work how different scaling methods impact cluster identification?
- 9) Section 165 – 181: This section was more confusing than helpful to me. These are the questions I was left with. Most of them are not really relevant for the study as no UMR data was used (but that is not clear at that part of the manuscript yet).
 - The “500 peaks” (line 165) does not refer to the HR analysis result? I guess the authors mean UMR “peaks” in the first sentence? Why is that relevant if the study is about HR data? Rather than the “500 peaks” information, the authors should provide how many HR ions were identified (and how many were considered “product” ions).
 - Why were the UMR (?) peaks screened if they contain product ions? Shouldn’t the FCM group the precursor/educt ions into separate cluster? Running FCM with all ions would then result in a higher number of clusters but the educt clusters should be distinct from the product ones. It would be yet another advantage of FCM if FCM indeed easily separates the educt ions as it would eliminate a step in the data cleaning process.
 - what is meant with pronounced changes in line 172? Increase/ decrease of signal intensity? How much would the change have to be to be pronounced?
 - Starting the sentence in line 175 with “Therefore” implies that the HR fitting was only applied because there was some uncertainty in separating the product ions when using the UMR data. What would have been the benefit to run FCM with UMR data?

This section should be rewritten, omitting the UMR parts and only focusing on introducing and describing the HR data analysis.

- 10) Line 184f: What is “reasonable chemical meaning “ in this context?
- 11) Line 189f: Is this normalisation now the same thing that is called “scaling” in lines 336-344?
- 12) Line 192ff: The Jenkin reference is for the Master Chemical Mechanism (MCM). Is there a reference for the actual box model? Is it the Carlsson et al 2022 reference at the end of the paragraph? If the model was “build” by the authors, should the code be made available?
- 13) Line 264: It is not clear what “with improvements” refers to in this sentence. Do the CVIs still need to be improved? Or they have been improved? But what is that improvement?
- 14) Line 369ff: This section is very difficult to follow. This is one of the examples where improvement is needed as pointed out in Major Comment 3.

The sentence implies that J_m is defined in Eq. 8 and H_m is given in Eq 9. While J_m is surely the Variable defined in Eq. 1, H_m seem to not have a definition equation. Further, the text speaks of G and C while the equations are defining μ_G and μ_C . The equations are given as a block instead of interlacing them with the relevant text. What are the alpha and beta constants in Eq 8 & 9?

- 15) Line 386ff: How does increasing the maximum number of iterations solve the issue of converging to early on a local minimum? The algorithm stops when the convergence criterium is reached. If that happens for a local minimum, increasing the maximum number of iterations should not have an effect because the criterium is already fulfilled at a low number of iterations. Increasing the number of iterations should only change the outcome if no convergence is reached within the number of allowed iterations.
- 16) Line 397ff: How frequent are invalid solutions? For one value of c (and m), how many of the 50 runs were disqualified. Also, was there a trend in number of invalid solutions? E.g., more valid solutions close to the "optimal" cluster number?
- 17) Section 2.3.4 The title "Other parameter" is misleading for this section. This section does not deal with other parameters used in FCM, but rather with the constraints and methods to improve the quality/reliability of the solutions.
- 18) Line 447: The authors went to the trouble of running ensembles of 50 or 100 runs. But now only one "representative" run is shown. Why not provide the average with standard deviation or interquartile range? Or using a heatmap of the distributions?
How small are considered "small variations"? E.g. compared to the dip for Vkwon and VXB for $c=5$.
- 19) Line 481: VBWS was shown to worked well for largely overlapping clusters: Is the investigated data set such a case where large overlap is expected?
- 20) Figure 1: I found it challenging to keep all the mentioned numbers for optimal cluster number for each CVI in my head while looking at Fig 1. It would be helpful to mark the optimal cluster number for each CVI in each panel (red circle for selected value, blue square for optimal number based on this CVI)
- 21) line 516f: why does this suggest that the cosine metric is more suited? Is there an assumption that the shape of VBWS should be smooth as a function of c ?
- 22) Line 514: is it really true that the impact on clustering output is neglectable? Or isn't it rather that this metric is not sensitive to the differences? These metrics only tell us how well the solution was separated. But it does not tell us about the shape of the clusters. I.e., with the same degree of separation, the actual clusters might look different.
- 23) Why are the curves in Fig 1 not matching any of the lines in Fig 2?
- 24) Section 3.1.3 My take on what was described in this section: With small cluster number, we have too few clusters. Hence, we need to allow more overlap for variables. When we allow more clusters, we can be stricter with assigning the objects (m^* gets smaller). As the solutions may be more "specific" we are now more sensitive to "local" minima. As those are driven by the starting point, we get more sensitive to the U0.
- 25) Section 3.1.3 How much does a difference of 0.1 in m really change the clustering results? I.e., how sensitive is the actual result to a slightly different m value? ~ 1.5 seems much closer to 1 (=non fuzzy) than to 9 (upper limited in this study)
- 26) Line 565ff: Do the authors have any idea why the 5 cluster case was super stable, but the 3, 4, and higher ones varied more? Could this be an indicator for the "perfect number of clusters"? Or just coincidence?
- 27) Line 592f "Part of the species from the former cluster 1 is separated out as a new cluster 2, dominated by molecule(s) from a very narrow mass range, where mass profile 1 also has its Maximum" – I do not understand this sentence.
However that sentence is meant, while the mass spectra of C1 and C2 may look similar, the time series are not. C2 is not directly linked to the injections (peak is later). Or are the authors implying that the C1 of the 3cluster solution had some reaction products grouped in which are now taken out?

- 28) Line 635ff: Could it also be that compounds which would retain the nC and get more functionalised are too low volatile to remain in the gas phase? Where particles formed in these experiments? If not, could low volatility compounds be lost to the chamber walls?
- 29) Fig 6: Cluster 1 has the most “outliers” while the other clusters seem to have the grey lines closer together. Do the authors have any explanation for this higher “spread” of members in Cluster 1?
- 30) Line 713f & 717f: These sentences seem contradictory. The first sentence says that C1 and C2 differ in their formation & production rate. Second sentence says that formation rate of C2 resembles that of C1. Are they different or similar?
- 31) Figure 5 & S5: The meaning of the grey circles is not clearly explained when the Figure is first mentioned. What are the “individual species”? What does their marker size refer to? Is it the average mass spectrum over the full experiment? Who do the size of the grey markers relate to the size of the cluster markers?
- 32) Line 750: The fact that the cluster markers cover a smaller space than the original data: 1) that is a logical consequence when doing clustering. The result will not be on the edge of the distribution. 2) this graph is not comparing the range of OSc vs nC for the clusters. Only the average of the cluster is given. But to check the range, one would have to see the position of all species contributing to each factor and evaluate those.
- 33) Line 766: assuming that the clusters are sorted by their oxidative “age”, the statement is only partially true. 1 – 2 – 3 follow the trend. 4 is on the “line” but has higher nC than 3. Cluster 5 is off the line.
- 34) line 777: It is not the measurements that are fitted to the function, but the function is fitted to the data points. But which parameters in Eq 12 are “free fit”? k and m? Also a?
- 35) How are products of auto-oxidation classified in the GKP approach? The intermediate stage of one oxidation step with NO₃ (=first generation) can lead to a range of products with varying number of autooxidation steps. Are such products still classified as “first generation”? How will varying degree of autooxidation affect the “m” parameter?
- 36) Line 784f “chemically realistic time patters” what is meant by that? That the time series looks like it could be from a combination of realist reactions? What is meant by chemical properties here?
- 37) Line 784f: What is the issue with Cluster 5? That it is so low intensity? Or that it is so noisy? Or is it the “unusual” shape? Are the authors not trust this “unchemical” shape?
- 38) isomer theory. If one ion represents isomers from different steps, shouldn’t those isomers than be assigned to different clusters? I.e. the ion should show up in a first and second gen cluster
The example C₅H₉NO₅ shows exactly that. It has a considerable contribution to C1 and to C2 (but there it falls under the 0.5 mark)
- 39) Fig 11: The position of the red star feels odd. The position seems to be at a “too low” m value. The 5 individual highest signals all have much higher m values. For the other clusters, the star falls more in the middle of the point distribution. If the position of the red star is correct, it should mean that the m and k values of the red cluster are not represented well by the high affiliation species but rather dominated by the species with lower affiliation.
- 40) The existence of C₅ N₁ monomers (e.g. C₅H₇NO₆) as second-generation products confirms the importance of H abstraction by NO₃ radicals as oxidation mechanism. Or are the authors suggesting a different mechanism that does not result in addition of the NO₃ radical to the molecule? Anyhow, the reaction scheme in Scheme S1 does not consider any such products, only dual NO₃ addition products are listed.
- 41) Line 986 & Scheme S2: In my book, there are two pathways to form C₄H₇NO₅: one via 1,4 h shift and one via +RO₂ reaction. The split ratio will depend on the RO₂ conc. But for the formation kinetics, the rate limiting step is relevant. Since that is most likely the first NO₃ addition, no differentiation between the two paths is possible (i.e., it is impossible to determine the split ratio). This shows the limitation of this approach. If a product is formed through different pathways, but the rate limiting

- step is common, FCM coupled with GKP will only provide the sum over those paths. This comment also relates to the claim in Line 970 that those compounds are formed by a single pathway.
- 42) SI section (1) What is meant by the “knee”? How is it determined? Is it the turning point of the curve? In Fig 1 a) $c=5$ is chosen? But why? What is the math behind that? If it is “by eye” I could also take $c=6$ as “knee” or elbow or other bent body part.
 - 43) SI section (2) The equation of V_{FS} is of the shape $V_{FS} = A-B$. A smaller value of V_{FS} would only indicate that A and B become more similar. That means that a bad compactness value (high A) could be compensated by a larger difference between the clusters (high B)
 - 44) Equation S2 would be much easier to read if they introduce a variable for cluster compactness and separation of cluster. Especially since these variables are used again for V_{XB} and later. The similarities/differences between the CVIs will be much easier to see using variables instead of the lengthy double sums.
 - 45) SI section (2): What are recommended values to identify a good solution for this CVI? From Fig 1b, V_{FS} seems to always go down with cluster number until reaching a minimum at ~ 8 . If smaller is better, why is $c=5$ chosen?
 - 46) SI section (3): “the smaller the numerator...” this sentence is talking about the individual clusters. But the formula is summing over all clusters. I think this should be changed to plural. So, the more compact the clusters are. The more the clusters are separated.
 - 47) SI section (4): Eq S4 will become much more readable if the “punishing function” is defined in its own equation.
 - 48) SI section (4): If c approaches n , the key point about using a clustering algorithm (dimension reduction) is not achieved. Why is a metric needed that works at c approaching n ? In Fig 1 c and d are identical in shape. What is the added values? To enhance clarity of the already complicated manuscript V_{kwon} or V_{XB} should be omitted.
 - 49) SI section (5) This section implies that overlapping clusters are not treated well with all previous metrics. Is that indeed the intention?
 - 50) Higher V_{BWS} values indicate a better solution. Fig 1e looks like there is a “maximum” in the curve. Is that a feature of this CVI?
 - 51) SI section (6) “The average cluster silhouette score can tell if the cluster is appropriately configured or not. “ Isn’t it a problem if there are an equal number of bad assigned and well assigned ones? Because the positive and negative cancel each other out?
 - 52) how are a and b calculated for equation S10? Section 2.3.2 introduces 4 ways of calculating the difference. Which one is used here?

Language and technical comments

General: The authors should carefully check their manuscript for adverbial constructions/inserts at the start of a sentence and decide if they follow the recommendation of separating them by a comma from the main clause. E.g., the sentence in line 57ff (“Benefitting from this it has....”) should have a comma after “this”. Personally, I like using the comma for this grammatical structure as it enhances readability.

Line 26: “an approach by using FCM” -> omit the “by”

Line 32 “system investigated” -> investigated system

Line 32ff “chemical properties were characterised... “: characterised and parameterised can be used in this sentence, but the term “described” may be better in this context.

Line 44: "...and convert to condensable vapors" Not all products of atmospheric VOC oxidation are condensable. In most cases, the majority will be still too volatile. -> rephrase

Line 46: add comma before "and thereby" to indicate that that is referring to both condensation and nucleation.

Line 47: SOA was already introduced in the sentence before.

Line 55: "propagation": is that the right word here?

Line 67: "nonwithstanding the apparatus of high resolution": this insert is not clear. What is the apparatus of high resolution? Do the authors mean an instrument with high resolution?

line 73f: "thus simplify the chemistry of the investigated system" what is meant by that? Clearly, the actual chemistry does not change? It is just our representation of the chemical processes that is simplified?

Line 77f: "best-known approach": in my opinion "most commonly used approach" seems more appropriate here.

Line 74 and later: (Buchholz et al., 2019) is the wrong reference. The authors most likely mean (Buchholz et al., 2020)

Line 148: "the injection was repeated...": Using the term "injection" can be easily misunderstood in this sentence. The previous sentence only calls the addition of isoprene an injection and nothing about the delivery of NO₂ and O₃. -> rephrase

Line 154: "particle-phase" no hyphen in this case as it is a noun (but gas- needs the hyphen)

Line 169 "related to ion source" -> related to the ion source

Line 273: "There're" -> there are

Line 278: "...among all the alternatives following..." -> alternatives the following

Line 322: "are called as distance" -> omit "as"

Line 331: "Since it is difficult..." sentence: comma after "data"

Line 379: "Where b a constant that is usually set to be 10 in practice": The grammar of this sentence seems broken.

Line 393: "The clustering results of FCM is..." -> "The results are..."

Line 409: "produce target compound" -> produce the target(ed) compound

Line 409: "The kinetic information..." sentence: comma after "species" to close the insert

Line 411: "involve" should be include

Line 485 "Crisp Silhouette (C)": in the next sentences CS is used as an abbreviation

Line 533 "is dependent" should be "depends"

Line 599: Which one is meant by "new " cluster? C5 (yellow)?

Line 630f "Even clusters with similar generation number [...] are grouped into different clusters due to their different chemical properties." I do not understand this sentence. Clusters are grouped into clusters?

Line 668f: What is meant by "screened out"? Do you mean identified? Selected?

Line 685f: The trend description in this sentence (for the model data) may be easier to understand if presented with in the opposite way. I.e., speaking of the less pronounced increase of OSc and decrease of nC with increasing chemical age of the clusters.

Line 698: “information underlying in the mass spectrometric data.”: this sounds incorrect. It probably should be “underlying information in the mass spectrometric data”

Line 744: Is “attribution” the correct word here or should it be “contribution”?

Line 726f “it is indeed mainly the former cluster 2 in the five-cluster solution is further split into new clusters 2 and 3” -> it is indeed ... which is further split...”

Line 826 “larger N:C values as expected” the “as expected” sounds a bit weird in this context. Using a comma to indicate the “as expected” as a grammatical insert will help. Or putting the “as expected” at the start of the sentence.

Line 856f “resulting products” -> omit resulting

Line 875 “fuzziness of FCM in belongingness of cluster members”: the term “belongingness” does not work here. Maybe change to “assignment of cluster members”

Line 895 “gamma kinetic parametrisation” was already introduced -> use GKP here

Line 951 & 962 Using the comma separated values for oxygen in the sum formulas confused me at first. (C5H9NO4,5). Since there are only two cases where this nomenclature is used, consider writing both formulas out.

Line 963: “preferably occupied by cluster 3” this sounds incorrect. I am not sure what is meant by occupied in this context

Line 1001: the acronym “HAC” was not introduced

Figure 2a has a y scale up to +/-600? FS value is -2 - -8 in Fig 1f -> reduce scale in Fig 2a

Fig S1: left y axis labels are cut off

What is Table S1 for? I did not notice any reference to this table in the main manuscript or the SI.

SI paragraph (6) “...was first proposed by Rousseeuw (1987), which can be used... “ it is not clear where the “which” is pointing to. Better link the two parts with “and” -> “...was first proposed by Rousseeuw (1987) and can be used... “

SI paragraph (6) “With different cluster number...” sentence is difficult to understand. -> consider rephrasing

Fig S7: it was difficult for me to line up the markers for, e.g., cluster 1 with the names on the x axis. For me, some vertical grid lines every X ions would help to make this figure more readable.

Fig7 and S7: What is the sorting criterium for the species in these figures? Ion mass? Consider if that is the optimal way of presenting the data or if another order (e.g. by C number) would be beneficial.

References

Buchholz, A., Lambe, A. T., Ylisirniö, A., Li, Z., Tikkanen, O.-P., Faiola, C., Kari, E., Hao, L., Luoma, O., Huang, W., Mohr, C., Worsnop, D. R., Nizkorodov, S. A., Yli-Juuti, T., Schobesberger, S., and Virtanen, A.: Insights into the O:C dependent mechanisms controlling the evaporation of a-pinene secondary organic aerosol

particles, *Atmos. Chem. Phys. Discuss.*, 1–21, <https://doi.org/10.5194/acp-2018-1305>, 2019.

Buchholz, A., Ylisirniö, A., Huang, W., Mohr, C., Canagaratna, M., Worsnop, D. R., Schobesberger, S., and Virtanen, A.: Deconvolution of FIGAERO–CIMS thermal desorption profiles using positive matrix factorisation to identify chemical and physical processes during particle evaporation, *Atmos. Chem. Phys.*, 20, 7693–7716, <https://doi.org/10.5194/acp-20-7693-2020>, 2020.

Kroll, J. H., Donahue, N. M., Jimenez, J. L., Kessler, S. H., Canagaratna, M. R., Wilson, K. R., Altieri, K. E., Mazzoleni, L. R., Wozniak, A. S., Bluhm, H., Mysak, E. R., Smith, J. D., Kolb, C. E., and Worsnop, D. R.: Carbon oxidation state as a metric for describing the chemistry of atmospheric organic aerosol, *Nat. Chem.*, 3, 133–139, <https://doi.org/10.1038/nchem.948>, 2011.

Priestley, M., Bannan, T. J., Le Breton, M., Worrall, S. D., Kang, S., Pullinen, I., Schmitt, S., Tillmann, R., Kleist, E., Zhao, D., Wildt, J., Garmash, O., Mehra, A., Bacak, A., Shallcross, D. E., Kiendler-Scharr, A., Hallquist, Å. M., Ehn, M., Coe, H., Percival, C. J., Hallquist, M., Mentel, T. F., and McFiggans, G.: Chemical characterisation of benzene oxidation products under high- And low-NO_x conditions using chemical ionisation mass spectrometry, *Atmos. Chem. Phys.*, 21, 3473–3490, <https://doi.org/10.5194/acp-21-3473-2021>, 2021.