Reply to Reviewer #2

We thank the Reviewer for carefully reviewing our manuscript and providing insightful comments. Below we address each comment point by point. For clarity we mark the reviewer comment in **blue**, our answers in **black**, and changes to the manuscript in **red**. Page and line numbers in our replies refer to the revised manuscript.

Summary:

The authors performed positive matrix factorisation on FIGAERO-CIMS data of SOA before and after isothermal evaporation, under both low and high humidity. They provide a detailed description of their methods including two ways of estimating PMF errors, which is useful and interesting. However, I found some of their interpretations to be a bit unconvincing or not completely evaluated. A lot of the analysis revolves around the highOC case under wet conditions, but I have several questions as to the quality of their PMF solutions for that case, and whether the aerosol in that case is even representative of anything that would be present in the atmosphere. The authors also haven't convinced me that PMF of thermograms could provide more information than one could get from single ion thermograms, so more discussion is needed to show how they're actually advancing the field. I think this work could be suitable for publication in ACP if these major revisions can be addressed. I include several major comments as general comments, followed by some more specific and technical comments.

General Comments:

1: Looking at Fig S7, what jumped out at me was that typically all of the factors are decreasing in absolute magnitude after 4 h compared to 0.25 h of evaporation. My first thought was that I would have expected the lower volatility factors to remain more constant, and just the higher volatility factors would evaporate. However, I think you could explain that all factors should lose at least some absolute mass because the total amount of OA will be decreasing, and that will change the equilibrium partitioning causing even the lower volatility compounds to evaporate. I think it could be really interesting if you would calculate how much of each factor you expect to evaporate, using their estimated volatility from the FIGAERO combined with the change in OA mass measured after evaporation, and compare this with how much you measured to evaporate. Do they match? This might be outside the scope of your manuscript, but it wouldn't take too much effort and would add value to the paper if you decide try it. It would give the reader more information with which to judge how well PMF actually is able to separate compounds of different volatilities.

This investigation would be indeed interesting and a good way to verify our interpretation. But this is not possible with the experimental setup that was used for this data set. First, the difference between the total mass collected for t_{evap}=0.25h and 4h does not depend only on the aerosol mass lost in the RTC. The t_{evap}=0.25h sample was collected directly after the size selection unit (and not from the RTC at 0.25h). The total amount collected on the FIGAERO filter depended on the collection time and the particle concentration in the sample flow. This concentration was 4 – 10 times higher than reached in the RTC after filling. For the t_{evap}=4h samples, the collected mass depended on the aerosol mass filled into the RTC (which was different for the different aerosol types) and how much was lost due to evaporation, wall losses and sampling from the RTC before collection. Second note that there is no equilibrium partitioning inside the RTC as the stainless-steel walls, in practice, act as perfect sinks for the evaporating compounds. This ensures that there is no build-up of organic vapours in the gas phase that would limit the particle evaporation. These experiments were designed to provide optimal input data for process modelling. For future investigations we will consider designing experiments to obtain the data needed to directly investigate the particle mass losses as the reviewer suggests.

2: Following up on my previous comment, one piece of information you've given the reader with which to judge the ability of PMF to separate compounds of different volatilities is table 2, the T_max values for each factor for each experiment. In addition, you've described in the abstract page 1 line 29 how "Thus, the factors identified with PMF could be interpreted as volatility classes." However, I would expect that if PMF is truly separating compounds of similar volatilities into each factor, that the factor would maintain roughly constant T_max (and roughly constant desorption shape) for each of the dry and wet experiments at both evaporation times. I would say that your factors for the lowOC and mediumOC cases maintain roughly the same T_max and shape across all wet/dry and 0.25,4 h cases. The only thing that changes is the magnitudes of the factors. This appears to be supporting evidence of the argument that PMF is separating compounds successfully by volatility. But for the highOC case, it doesn't appear to be successfully separating the volatility factors. The T_max for most of the factors changes substantially between dry and wet cases and after evaporation. This suggests to me that the factors are somewhat blended together. Another thing that leads me to that conclusion is that a lot of the mass gets shifted to the background HB1 factor during the wet,4h case, whereas the HB1 factor was much lower during other highOC cases. A background factor shouldn't change like that from case to case. I don't doubt that it is likely to be aqueous chemistry causing these changes in the PMF factors, but you haven't convinced me that PMF is giving you real and useful information about the process, particularly for the highOC/wet case which you're using as evidence of aqueous chemical changes. Maybe you need to revisit your PMF methods and see if you can find a 'better' solution, otherwise please explain your interpretation of the chosen factors in context of the points I've raised here.

The fact that the T_{max} values are changing together with the appearance of a "new" factor (HWET) is the strongest argument that there are additional processes at work apart from simple isothermal evaporation. Each V-type factor consists of a large number of compounds with similar (but not identical) volatility. In the low- and mediumOC cases, the volatility of the compounds in each V-type factor are similar enough that most of them are affected in a similar fashion by the isothermal evaporation. I.e., a similar fraction of all constituents of a volatile V-type factor evaporate, thus not changing the overall shape and T_{max} value of the factor. (If the grouping of a factor would be too wide (i.e., covering a too broad C* range), isothermal evaporation would result in a change in shape and T_{max} as the more volatile compounds in a factor would have evaporate more than the less volatile ones.) In the highOC case, not all compounds in the volatile factors participate in aqueous phase chemical processes. This will contribute to changes in the shape of the factor profiles of v-type factors and possibly their T_{max} values. It seems that slightly more volatile compounds in each V-type factor (those at slightly lower T_{desorp}) are affected more by the aqueous phase.

Regarding the apparent strong increase of HB1 in the wet, t_{evap} = 4h we need to correct the perception of the reviewer. The change in y-axis scaling in Figure 7 is mainly causing this. We have added a note about the different y-axis scaling to the figure description of Figures 5-7 in the main manuscript and S 4 - S 6 and SI material to prevent this misconcenption to happen to future readers.

In Figure R2_1 below, we show the temperature profiles of HB1 for all highOC samples and the blank measurement. The absolute values for all samples are within the same range. This suggests that the “source” for this factor is the instrument itself as the amounts of particular mass collected on the filter in these 5 cases were very different. There is a decrease of the profile between ~50 and 120 °C which is not there for the wet, t_{evap} = 4h and the blank sample. This can be interpreted as part of the background not being separated from the main signal (or factors “blended together”). This is most likely caused by the main factors being so much stronger than the background in that part of the data. Similar behaviour (a dip in the B factor) was also observed some of the in the low- and mediumOC case, but there the effect was not as pronounced has in the highOC case. This can be interpreted as short coming of the PMF method. Some adjusting of the error matrix may help with this. With the used CNerror scheme a relatively higher importance was assigned to strong signals in their peaks.

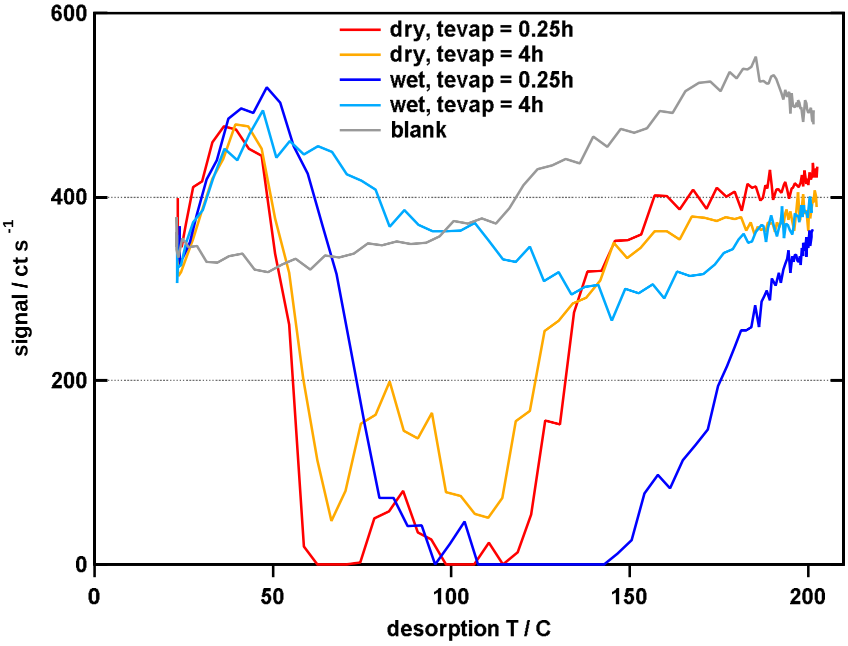

Figure R2_1: Factor profile of HB1 for all highOC samples.

3: You have demonstrated that PMF can be useful for pulling out background/contamination signals from thermograms, and also that higher volatility factors evaporate preferentially over lower volatility factors (though you could also say the same using just T_max of total signal). But, I'm not sure I see much discussion of which scientific insights you're gaining by doing PMF on thermograms. E.g., PMF on aerosol mass spectrometer (AMS) data can be used for general source apportionment. All of your aerosol comes from the same source in this particular experiment, but is there any information gained through PMF that could indicate anything about the aerosol formation/evaporation process? Are there factors that can be used as tracers for aqueous chemistry, that could be searched for in ambient datasets? Please expand on how you are making specific scientific advances using thermogram PMF that we can't get using other non-PMF methods.

Thermal decomposition in FIGAERO is one of the major problems of the method when the aim is to identify the detailed composition or volatility of the compounds. One major output of the PMF analysis which is not accessible from simple analysis of the thermograms is the contribution of thermal decomposition to the overall signal. Without PMF, we can only speculate that a broader peak, a shoulder, or a tail is caused by thermal decomposition of larger compounds. Especially broadening may also be cause by instrument artefacts. Schobesberger et al. (2018) use a modelling approach to capture the contribution of "reversible oligomers" (i.e. thermally decomposing compounds) on an ion by ion basis. But there estimates for several physical parameters (e.g. enthalpy of evaporation) are needed for each ion. PMF does not need any such assumptions to identify that fraction of a single ion thermogram that stems most likely from thermal decomposition. Knowing about the thermal decomposition is extremely important when using data from FIGAERO-CIMS (or any other instrument involving treatment at elevated temperatures) with sum formula based parametrisation (e.g. DeRieux et al., 2018; Li et al., 2016) or for modelling applications. The companion paper (Tikkanen et al., 2019) shows an example of how the output of this type of PMF analysis can be combined with detailed process modelling.

We cannot provide a simple tracer for aqueous phase chemistry in the atmosphere as this dataset was limited to a-pinene SOA formed under specific conditions. But the PMF analysis directly revealed the presence of aqueous phase chemistry in the highOC case and identified the ions affected by the process. In the original analysis of the data (Buchholz et al., 2019), we had to combine multiple features in the dataset that just "did not add up" (e.g. very little change in apparent volatility from isothermal evaporation but a strong change in the thermograms) and then manually inspect hundreds of single ion thermograms to realise that besides the simple isothermal evaporation there was a different process dominating the composition changes in the high OC case.

The next step with this method is clearly the application to ambient datasets. First, preliminary results are suggesting that the PMF analysis does separate different ambient sources for the SOA and provides valuable insights into the volatility of those sources.

We expanded the discussion in the conclusion part including more information on how the presented method improves the interpretation of FIGAERO-CIMS measurements and thus increases our understanding of the aerosol composition.

To maintain the context of these additions, we provide here the full paragraph from the Conclusion section highlighting the additions in **bold.**

PMF was able to separate the measured signal of each ion into instrument background, contamination, and collected aerosol mass. This separation worked even if no filter blank data was added to the datasets. However, adding filter blank measurements to the dataset simplified the identification of background factors. Identifying background factors in this way instead of simply subtracting periodically taken filter blank measurements is especially helpful, if an insufficient number of filter blank measurements were collected or if the background changed between filter blank samples. **Being able to determine the actual contribution of background compounds becomes even more important for low concentration measurements (i.e., low collected sample mass on the FIGAERO filter). The shape of the combined thermogram of the background may significantly alter the overall shape of the thermogram (e.g., shift the T_{max} value) and thus change the interpretation of the volatility of the collected aerosol.**

The collected aerosol mass signal part was separated into (mostly) direct desorption factors (i.e., volatility classes) and thermal decomposition factors. Thermal decomposition became the dominant process for many low M_w ions observed at temperatures above 120 °C. Then the observed "desorption" temperatures are actually the decomposition temperatures and thus give an upper limit for the true volatility of the parent compounds. This shows again that FIGAERO-CIMS measurements may overestimate the volatility of aerosol particles based on parameterisation of the overall composition but also on desorption temperatures as described by some previous studies (Lopez-Hilfiker et al., 2016; Schobesberger et al., 2018; Stark et al., 2017). **The knowledge about the contribution of thermal decomposition to a thermogram measurement obtained with the PMF method presented here can be used e.g. to improve the input into process models. An example for such an application is presented in Tikkanen et al. (2019).**

For each SOA type (i.e., α-pinene SOA of different oxidative age) 5 main volatility classes were identified in the chosen PMF solution. Isothermal evaporation prior to sampling with FIGAERO-CIMS systematically removed the more volatile factors with T_{max} values corresponding to SVOCs. Low M_w compounds remaining in the particles after evaporation were attributed to low volatility factors indicating that they most likely were products of thermal decomposition above ~100 °C. However, between ~100 and 120 °C thermal decomposition was still a minor process. In the highOC case, the aqueous phase chemistry occurring under wet conditions was captured by introducing a new factor and shifts in T_{max} for other factors. Both the educts and products (or thermal decomposition products of them) could be identified. This highlights how PMF analysis can help with identifying processes in the particle phase.

The highOC SOA in our study may not be representative of ambient SOA of the same OC ratio as it was formed under extremely strong oxidation conditions in an OFR. But the type of compounds affected by aqueous phase chemistry (i.e., organic compounds containing (hydro)peroxides or other functional groups which easily hydrolyse and then continue to react) are not unique to OFR reactors. One formation path of compounds containing several hydroperoxyl or peroxiacid groups is the auto-oxidation of terpenes in the gas-phase leading to highly oxygenated material (HOM) (Bianchi et al., 2019; Ehn et al., 2014). These compounds play an important role in particle growth and detected more and more in ambient measurements (Lee et al., 2018; Mohr et al., 2017). Another compound class which is possibly susceptible to hydrolysis is organo-nitrates (which did not occur in our study due to the experiment design). Thus,

ambient aerosol will probably not show as clear signs of aqueous phase chemistry as our high OC case, but it is very likely that such processes occur to some degree and may be detected with the PMF analysis of FIGAERO thermogram data.

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The example ions shown in Figure 9 highlight how important it is to allow a single ion to contribute to more than one class/factor when analysing FIGAERO-CIMS data. Clustering techniques, as for example described by Koss et al. (2019) or Li et al. (2019), which assign each detected ion/composition to a single cluster, are incapable of capturing such a behaviour, i.e., the shift of T_{max} between two measured thermograms due to the selective removal of some of the isomers/thermal decomposition products. For the investigated dataset, we artificially removed the volatile fraction at a set ion composition with the prior isothermal evaporation. However, as the composition of ambient aerosol changes with time, e.g. by changes in the gas-particle partitioning or due to aging processes, the ratio between different isomers or the educts for thermal decomposition will change causing similar features in single ion thermograms of FIGAERO-CIMS data.

Preliminary tests with a dataset of ambient FIGAERO-CIMS measurements show how PMF immediately separates the data by its ambient sources (i.e., which precursors and/or processes created the aerosol) and/or SOA type (e.g. fresh and aged OA). This information is also accessible with a PMF analysis of the time series of mass spectra integrated for each desorption cycle. However, in addition to this, PMF of the thermal desorption data provides detailed information on the volatility of each of these sources or SOA types while also showing how much of the signal is affected by thermal decomposition. This information on the contribution of thermal decomposition is crucial when the FIGAERO-CIMS data is used to identify the detailed composition or volatility of SOA particles. Details of this investigation will be the content of a future publication.

4: The highOC/wet case that you're using as evidence for aqueous chemistry is a particular case, in that the aerosol you're producing using the OFR is highly oxidized, and that oxidation happened much faster (and possibly through differing chemical pathways) than would happen in the real atmosphere. Thus, the specific molecules that comprise the aerosol are probably not representative of anything you'd get in the atmosphere. So, while the wet cases for lowOC and mediumOC illustrate that the diffusion limitation to evaporation is decreased in aqueous aerosol, you are suggesting that aqueous chemistry doesn't happen much except for the highOC aerosol, which may no longer be relevant for the atmosphere. Can you add some discussion of how your results relate to atmospheric aerosol?

The highOC SOA in our study is definitively an extreme case. We suggested that many of the compounds affected by aqueous phase chemistry could be organic (hydro)peroxides or contain other functional groups which easily hydrolyse and then continue to react (Buchholz et al., 2019). The (hydro)peroxide formation is probably enhanced by the very high HOx levels in the OFR. But such compounds are not unique to OFR reactors. One formation path of compounds containing several hydroperoxyl or peroxiacid groups may be auto-oxidation of terpenes in the gas-phase which leads to highly oxygenated material (HOM) (Bianchi et al., 2019; Ehn et al., 2014). These compounds play an important role in particle growth and are being detected more and more in ambient measurements (Lee et al., 2018; Mohr et al., 2017). Another compound class which is possibly susceptible to hydrolysis is organo-nitrates (which did not occur in our study due to the experiment design). Thus, we conclude that ambient aerosol will probably not show as clear signs of aqueous phase chemistry as the high OC case, but to some degree it is very likely and may be detected with the right measurement and analysis method. We mention how (hydro-)peroxides are most likely responsible for the different behaviour of the highOC samples in section 3.3 and extended the conclusion section with regard to the atmospheric relevance.

First paragraph in section 3.3:

As discussed by Buchholz et al. (2019), the different behaviour of the highOC SOA is most likely due to higher fractions of (hydro-)peroxides in the particles caused by the much higher HO_2 concentrations in the OFR at the highOC oxidation conditions. Most peroxides are sensitive to hydrolysis which will initiate a range of reactions in the aqueous phase. The low volatility products of these reactions thermally decompose to similar fragments as did the peroxide precursor. Thus, the same groups of ions are detected but at a higher T_{desorp}.

Conclusions:

The highOC SOA in our study may not be representative of ambient SOA of the same OC ratio as it was formed under extremely strong oxidation conditions in an OFR. But the type of compounds affected by aqueous phase chemistry (i.e., organic compounds containing (hydro)peroxides or other functional groups which easily hydrolyse and then continue to react) are not unique to OFR reactors. One formation path of compounds containing several hydroperoxyl or peroxiacid groups is the auto-oxidation of terpenes in the gas-phase which leading to highly oxygenated material (HOM) (Bianchi et al., 2019; Ehn et al., 2014). These compounds play an important role in particle growth and are detected more and more in ambient measurements (Lee et al., 2018; Mohr et al., 2017). Another compound class which is possibly susceptible to hydrolysis is organo-nitrates (which did not occur in our study due to the experiment design). Thus, ambient aerosol will probably not show as clear signs of aqueous phase chemistry as the high OC case, but it is very likely that such processes occur to some degree and may be detected with the PMF analysis of FIGAERO thermogram data.

Specific Comments:

Pg. 4 Ln. 9: Which size particles were you selecting in the nano-DMA? Also, it would be useful to mention to flow rates of your sheath and sample flows in the DMA, the ratio of which will determine just how quasi-monodisperse your selected particles become.

The Nano-DMAs were set to select 80 nm particles. The fraction of double charged 120 nm particles was very small (both regarding the total number and mass). Sample flows were always 1.0 lpm and the sheath flows were 10.0 lpm in the dry experiments and 8.0 lpm under wet conditions. The ratio between sheath and sample flow was thus 10 (dry) or 8 (wet) which led to a small increase in broadening in the wet cases.

We have added the information about the particle size in section 2.1 and for the flows in the detailed description in SI section 1.1.

A Nano differential mobility analyser (NanoDMA) was used to select a quasi-monodisperse particle distribution (electromobility diameter 80 nm) …

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The NanoDMA was operated with an open loop sheath flow (10 L min^{-1}, (dry): 8 L min^{-1} (wet)) which together with the extremely short residence time inside the NanoDMA (≤ 0.3 s) limited the diffusion of gaseous compounds into the selected sample flow (1 L min^{-1}).

Pg. 4 Ln. 13: You have already assigned the acronym OFR, so you should avoid writing out the words oxidative flow reactor hereafter.

Changed the text as requested.

Pg. 4 Ln. 17: I assume the 0.25 h evap time for fresh particles is due to the collection time on the filter? Please make this clear, as it may confuse readers unfamiliar with FIGAERO operation, and they may wonder why you didn't sample fresh particles without a 15 min delay.

We point this out in the more detailed description in SI section 1.1. but for clarity we highlight this information also in the main manuscript text (page 4 line 22):

Note that the evaporation time of 0.25 h for the "fresh" sample does not stem from residence in the RTC but rather from time needed to collect sufficient mass on the FIGAERO filter (more details in SI section 1.1).

Pg. 11 Ln. 20: Have you considered summing the LB1, LC1 and LC2 factors together? It could be that PMF is splitting up the background factor before pulling out the last of the V-type factors, so you could just recombine the split background factors.

We agree on that the splitting of LC1 and LC2 is probably artificial. But note that the contamination (LC1 and LC2) only occurred for one sample due to "user interference" (most likely some issues when changing the filter or maintaining FIGAERO). Thus, adding LC1 and LC2 to the general background LB1 stemming from the instrument is not helpful.

Pg. 13 Ln. 1: How have you taken into account the effect of the stainless steel RTC walls on changes in VFR? Could there have been different wall effects during dry vs. wet conditions, i.e., different uptake coefficients to the wall surface? When it's humid enough to have one or several monolayers of water molecules on the walls, they could appear very different to a gas or particle than if it's bare metal.

The reviewer is correct in pointing out that "wetted" walls (RTC RH 80%) will have different uptake properties than dry stainless steel.

We tested the capability of the stainless-steel RTC wall to take up all evaporating vapours under dry conditions for a previous study (Yli-Juuti et al., 2017). An increase in SOA mass inside the RTC by a factor of 20 did not change the observed evaporation behaviour. This means that the particle evaporation was not limited by build-up of compounds in the gas phase, i.e., the dry walls acted as "perfect sinks".

Under wet conditions, the changes of wall losses of gases will depend on their Henry's law constants or, more generally, on if the compounds are hydrophilic or hydrophobic. As most of the compounds evaporating from the studied SOA types should be at least slightly hygroscopic, we can expect an increase in wall uptake under wet conditions. As the stainless-steel walls we already such good sinks in the dry case, this increase will not have an effect on the observed evaporation behaviour and composition changes of the particles.

The particle wall loss increases most probably in the wet case as both the walls and the aerosol particles may be more "sticky". Our study is not based on the overall mass conservation. The particle population is homogeneous so loss to the wall reduces the available particulate mass but not the composition of the population.

We have tried to measure the evaporating gaseous compounds with CIMS during some of the evaporation experiments, but the signals were too low for detection. In addition, we did not observe any accumulation of vapours in the gas phase during the evaporation experiments. This confirms that the stainless RTC walls are indeed efficient sink for the vapours.

Table 2: It would be informative if you present here and discuss elsewhere the estimated volatility of each of your V-type factors (by converting their T-max to volatility).

We deliberately did not show the C* values here as we did not want to go into details of the calibration necessary for this conversion. This manuscript is focusing on the method and general interpretation of the PMF factors with regard to the underlying particle phase processes while the companion paper (Tikkanen et al., 2019) investigates how the C* values assigned with this method compare to those derived with process modelling of isothermal evaporation data for the same SOA particles. Assuming an average molecular weight of 200 g mol^{-1} and applying the same T_{max} -> C* calibration as in Tikkanen et al. (2019), we find that the linear part of the FIGAERO heating ramp from 25 °C to 190 °C corresponds to log10(C*) values of +2 to -12. This covers the majority of SVOC to ULVOC (ultra-low volatility organic compounds, Schervish and Donahue, 2020) that can be expected from α-pinene oxidation. We use these C* values to indicate the desorption temperature ranges for S-, L-, and ELVOC in Figures 5 - 7 and S 4 – S 6 as a rough guideline for the reader.

Figure 9: Could you subtract the background signals from the total, such that the V-type factors will add up to the light blue lines? It could be visually easier to understand then.

We changed the Figure as requested. We noticed a small mistake in panel (c) in the original Figure (the reconstructed signal had been used instead of the measured) and a typo regarding the sum formula in the labels of panels (a) and (b) and the corresponding text ($[C_8\mathbf{H_{12}}O_5+ I]^-$ is shown, not $[C_8\mathbf{H_{10}}O_5 + I]^-$).

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