

FTIR-based structural interpretation of lipid oxidation in potato chips in relation to chemical indices

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Abstract

Fat oxidation is an important factor for the quality and stability of fried products such as potato chips. However, the traditional chemical indices only give a partial characterization, without an explanation of the structural changes associated with this process. The present study was carried out to analyze the structural changes associated with oxidation using Fourier transform infrared spectroscopy (FTIR) and to correlate them with the chemical indices of oxidation in eight samples of potato chips. Spectra were acquired before and after oxidation and FTIR indices were calculated, such as carbonyl index (CI), unsaturation index (UI), phenolic index (PhI), oxidation index (OI), conventional oxidation indices (PV, p-AV, TOTOX) and total phenolic compound content (TPC). Results showed increase of CI and OI totals after oxidation, compared to decrease of UI and PhI, which indicates formation of secondary oxidation products and depletion of unsaturated fatty acids and antioxidant compounds. The CI showed positive and strong correlation with TOTOX ($r = 0.85$) and the UI exhibited negative correlation with p-AV ($r = -0.79$), whereas PhI showed positive and strong correlation with TPC ($r = 0.91$) confirming the ability of FTIR to represent the structural changes associated with oxidation and its defense against oxidation. Samples with faster oxidative behavior showed more pronounced structural change and differences in flavor could be related to differences in oxidative behavior, in accordance with their functional role as oxidation promoters or inhibitors, respectively, in previous work. These results indicate that FTIR is an effective analytical tool to interpret the oxidation pathway at the structural level and can be adopted as a complement to traditional chemical indicators to provide more comprehensive assessment of lipid stability in complex diets.

Keywords: molecular fingerprinting, oxidative deterioration, shelf-life prediction, spectral profiling

Introduction

Lipid oxidation is one of the most important chemical reactions that affect the quality and stability of food products, especially fried foods such as potato chips. In these foods lipids are subjected to conditions of heat and oxygen which trigger a complex series of changes such as formation of hydroperoxides, degradation of these hydroperoxides to secondary compounds including aldehydes and ketones, consumption of unsaturated fatty acids and degradation of antioxidant compounds. These modifications affect not only the sensory characteristics but also the nutritional value and safety of the food product (Jerónimo & Alves, 2022; Rohman & Indrayanto, 2023).

Traditional methods for the determination of lipid oxidation are Peroxide Value, p-Anisidine Value and TOTOX Index and are based on the accumulation of primary and secondary oxidation products. These indices

are important but they provide only a partial view on the oxidation process, as they take into account the specific products and do not reveal the structural changes occurring in the lipid matrix itself. This is especially true in the advanced stages of the oxidation where the reaction pathways overlap and become complex (Jacobsen et al., 2021; Ahmed et al., 2026).

In this respect Fourier transform infrared spectroscopy (FTIR) has emerged as an analytical tool that can provide direct structural information by monitoring changes of functional groups in the lipid system. This technique can detect transformations in specific regions such as the carbonyl group ($\sim 1740\text{ cm}^{-1}$), unsaturated bonds ($\sim 3006\text{ cm}^{-1}$) and aromatic compounds related to phenols, allowing the tracking of oxidation at the molecular level (Jia et al., 2013; Saadi & Ghanim, 2019).

FTIR has been increasingly used to study lipid oxidation, but most of the past studies have focused on

the description of spectral changes or the use of simple relative indexes, without providing a complete analysis relating these structural indexes to conventional chemical indexes within a clear interpretative framework of the oxidation pathway. Moreover, the potential of FTIR to monitor the consumption of antioxidant compounds and its relation to oxidative behavior in complex food matrices such as flavored potato chips is still underexplored (Jamwal et al., 2021; Rohman et al., 2020).

The relevance of this study is therefore based on the goal to go beyond the descriptive application of FTIR technology and take advantage of it as an interpretive tool that has the potential to track structural changes associated with oxidation and relate them to known chemical markers. The current study was therefore conducted to evaluate the structural changes of potato chips prior to and following oxidation using FTIR indices, to assess their correlation with classical oxidation indices (PV, p-AV, TOTOX) and to assess their correlation with the concentration of total phenolic compounds for a more detailed view of the oxidation pathway in these food systems (Siddique, 2024; Alsawaf & Ibraheem, 2023).

Materials and Methods

Study Design

This study is an extension of the structural analysis of potato chip samples, whose oxidative behavior was characterized in our previous study (Mohammed, 2026) by different chemical indicators and kinetic techniques. Previous studies have been directed to the evaluation of the oxidation stability or the effect of flavors, while the present work is directed to the analysis of the structural changes involved in the oxidation process using FTIR spectroscopy and their correlation with chemical indicators.

Samples

The same sample set (F1–F8) representing different flavor compositions of potato chips available in the local market, whose chemical properties and oxidative behavior were characterized in previous studies (Mohammed, 2026), was used.

Sample Preparation

The lipid fraction of the samples was extracted using organic solvent extraction according to standard methods, taking necessary precautions to minimize oxidation during preparation. The lipid extracts were then stored under refrigerated and light-protected conditions until spectroscopic analysis.

FTIR Analysis

The Silverstein and Bassler (1962) method was followed to detect the functional groups present in the studied samples (F1–F8). Fourier transform infrared (FTIR) analysis was performed at the Central Laboratory of the College of Agriculture, University of Mosul, recording the spectrum in the 400–4000 cm^{-1} range.

The focus was on spectral bands associated with structural changes in lipids, including:

- Carbonyl (1743 cm^{-1})
- Unsaturated bonds (3006 cm^{-1})
- Reference band (2922 cm^{-1})
- Phenolic compounds (1600 and 1510 cm^{-1})^{2,5}

Spectral Indices Calculation

The relative FTIR indices were calculated to assess structural changes:

- Carbonyl index (CI)
- Unsaturation index (UI)
- Phenolic index (PhI)
- Oxidation index (OI)

using the ratios of absorption intensity to the reference beam at 2922 cm^{-1} .

Based on the pre/post FTIR data, the relative change in FTIR indices after oxidation was calculated:

$$(\Delta\text{CI}(\%), \Delta\text{UI}(\%), \Delta\text{PhI}(\%), \Delta\text{OI}(\%)): \Delta\% = \frac{(\text{After} - \text{Before})}{\text{Before}} \times 100$$

Chemical indicators

The chemical indicator data for oxidation (PV, p-AV, TOTOX) and total phenolic content (TPC), which were previously determined using standard methods (AOAC, 2019 & AOCS, 2017) were used for the purpose of analytical correlation with FTIR indicators.

Statistical Analysis

The relationship between the studied variables was statistically analyzed by calculating the correlation coefficient to measure the strength and the direction of the relationship between the different traits. Statistical correlations were considered significant when $P \leq 0.05$ (Antar, 2010).

Results and Discussion

Sample FTIR result as received by the device

Figure 1 displays the Fourier transform infrared spectra (FTIR) of the samples before and after oxidation and shows noticeable differences in three functional regions, i.e., carbonyl region ($\sim 1743 \text{ cm}^{-1}$), unsaturated bond region ($\sim 3006 \text{ cm}^{-1}$) and phenolic region (1600 – 1510 cm^{-1})

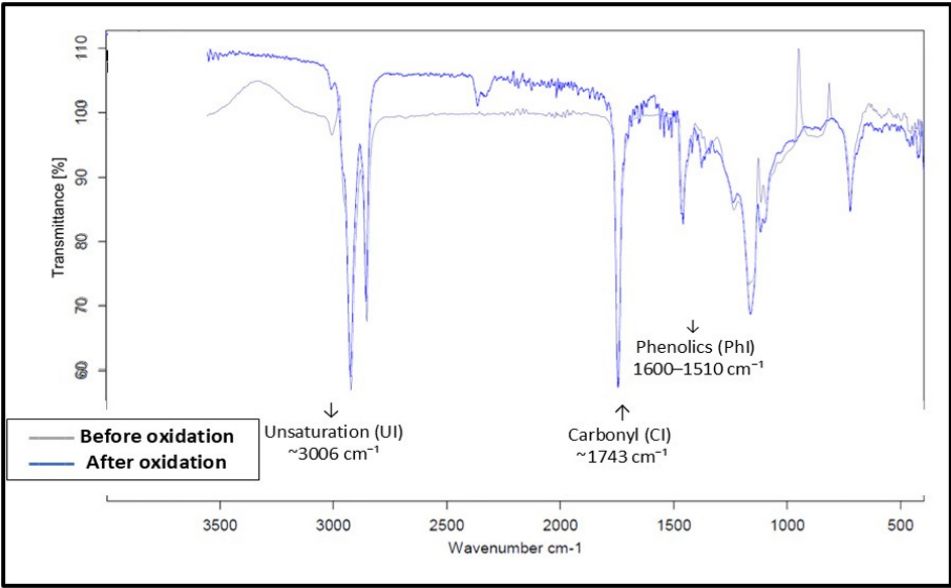


Figure 1. FTIR spectra of a representative potato chip sample before and after oxidation, showing increased carbonyl absorption (~1743 cm⁻¹) and decreased unsaturation (~3006 cm⁻¹) and phenolic regions (1600–1510 cm⁻¹).

Table 1 - FTIR indicators before and after

Sample	CI_b	CI_a	UI_b	UI_a	PhI_b	PhI_a	OI_b	OI_a
F1	1.07	1.118	1.011	0.972	2.08	1.912	1.045	1.132
F2	1.045	1.095	1.005	0.981	2.145	1.955	1.032	1.118
F3	1.05	1.108	1.009	0.975	2.13	1.92	1.038	1.125
F4	1.06	1.12	1.012	0.968	2.115	1.905	1.042	1.14
F5	1.035	1.08	1.015	0.99	2.18	2.02	1.02	1.105
F6	1.055	1.1	1.008	0.978	2.1	1.95	1.035	1.12
F7	1.065	1.13	1.01	0.965	2.095	1.89	1.04	1.145
F8	1.048	1.102	1.007	0.979	2.075	1.94	1.03	1.118

FTIR index values for different samples before and after oxidation (CI, UI, PhI, OI)

The FTIR indices for the different samples (F1–F8) before and after oxidation are shown in **Table 1**. The results showed that the carbonyl index (CI) increased after oxidation in all treatments, with values increasing from the range of (1.035–1.07) before oxidation to (1.08–1.13) after oxidation. Oxidation also resulted in a reduction of unsaturation index (UI) from (1.005–1.015) to (0.965–0.99). Similarly, the phenolic index (PhI) was significantly decreased from the range (2.075–2.18) before oxidation to (1.89–2.02) after oxidation. However, the oxidation index (OI) increased from (1.02–1.045) to (1.105–1.145) after oxidation. The highest value of both CI and OI after oxidation was recorded in treatment F7, while for the PhI index before oxidation the highest value was recorded in treatment F5. The results show clear variations of the spectral indices as a function of oxidation.

Relationship Between FTIR Indices and Traditional Oxidation Parameters

Figure 2 shows significant correlations between

FTIR indices and some conventional oxidation parameters. The section (A) indicates an excellent positive correlation between the carbonyl index (CI) and the TOTOX value, which means that the secondary oxidation products increase with the increase of CI values. As shown in section (B), a strong negative correlation exists between the unsaturation index (UI) and the anisidin value (p-AV), which indicates that the unsaturated bonds are reduced due to the advanced oxidation. In section (C), a positive correlation between the phenolic index (PhI) and the total phenolic content (TPC) was observed, pointing to the ability of phenolic compounds to help maintain the oxidative stability and reduce the degradation of the samples.

Correlation Coefficients Between FTIR Indices and Oxidation Parameters

The results in **Table 2** show different correlation coefficients between the FTIR indices and the studied parameters. The carbonyl index (CI) was significantly correlated with the anisidine (0.82) and TOTOX (0.85) values, and with the total phenolic content before

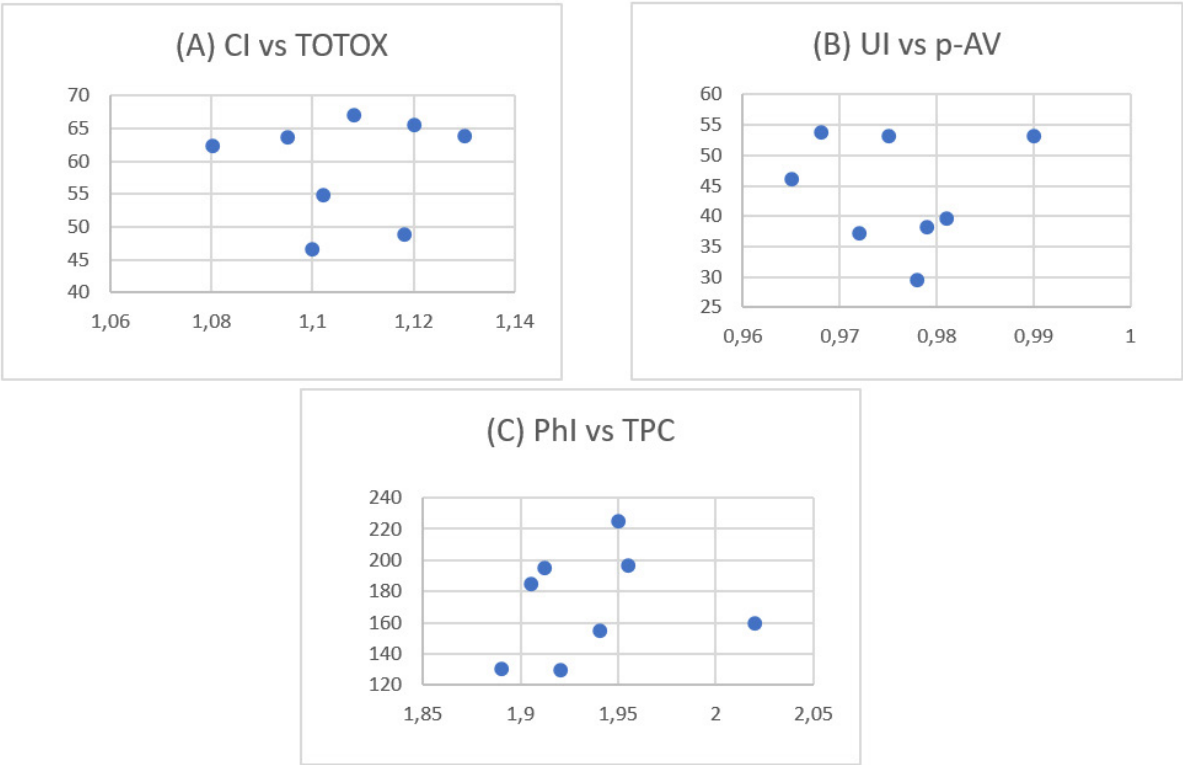


Figure 2. Correlation between FTIR indices and conventional oxidation parameters: (A) CI vs TOTOX, (B) UI vs p-anisidine value, and (C) PhI vs total phenolic conten

Table 2. Correlation coefficients of the studied factors

Variable	CI	UI	PhI	OI
PV_after	-0.21	0.18	0.35	-0.25
p-AV_after	0.82	-0.79	-0.68	0.76
TOTOX_after	0.85	-0.81	-0.72	0.79
TPC_before	-0.65	0.61	0.88	-0.7
TPC_after	-0.72	0.66	0.91	-0.74

Table 3. Relative change in FTIR indices after oxidation

Samples	Δ CI (%)	Δ UI (%)	Δ PhI (%)	Δ OI (%)
F1	4.49	-3.86	-8.08	8.32
F2	4.78	-2.39	-8.86	8.33
F3	5.52	-3.37	-9.86	8.38
F4	5.66	-4.35	-9.93	9.41
F5	4.35	-2.46	-7.34	8.33
F6	4.27	-2.97	-7.14	8.21
F7	6.1	-4.46	-9.78	10.1
F8	5.16	-2.78	-6.51	8.54

and after oxidation (-0.65 and -0.72, respectively). The unsaturation index (UI) showed a negative correlation with p-AV and TOTOX values, and a positive correlation with phenolic content. The phenolic index (PhI) showed the highest positive correlation coefficients with TPC, before and after oxidation, 0.88 and 0.91, respectively, showing the sensitivity of this index to changes in phenolic compounds, The oxidation index (OI) also showed a positive correlation with the oxidation parameters and a negative correlation with the phenolic content.

Relative Change in FTIR Indices After Oxidation

Table (3) shows that all samples had significant changes in FTIR indices after oxidation. The increase in the carbonyl index (Δ CI) was from 4.27% to 6.10%, with the maximum value being in sample F7, indicating an increase in the formation of carbonyl compounds due to oxidation. The unsaturation index (Δ UI) decreased from -2.39% to -4.46% during oxidation, suggesting the consumption of double bonds. Also the phenolic index (Δ PhI) decreased from -6.51% to -9.93% due to a decrease of phenolic compounds. In all samples, the total oxidation index (Δ OI) increased from 8.21% to 10.10%, which means a significant development of oxidation during the treatment.

Oxidation-Related Spectral Changes

Figure 1 The significant increase in the intensity of the carbonyl band after oxidation indicates not only the formation of aldehydes and ketones, but also the transition of the lipid system from the primary stage of oxidation with accumulation of unstable hydroperoxides to advanced stages with accumulation of more stable products of secondary oxidation. On the other hand, the decrease of the intensity of the unsaturated band is indicative of the consumption of the double bonds in unsaturated fatty acids, an important step in the course of oxidative reactions,

On the other hand, the changes in the phenolic region are indicative of real consumption of antioxidant compounds because of their involvement in the inhibition of the radical reactions and not only a transient spectral change. This indicates a dynamic balance between free radical generation and consumption of protective compounds from diet (Rodriguez-Amaya & Shahidi, 2021; Geng et al., 2023).

FTIR Index Analysis: A Structural Reading of the Oxidation Pathway

The FTIR indices (CI, UI, PhI, OI) of Table 1 showed a uniform behavior for the whole set of samples. But their importance is not in the direction of change itself but rather in their capacity to reflect structural transformations within the lipid matrix. The steady increase in carbonyl index (CI), indicates that the formation of carbonyl compounds is the major pathway in the advanced stages of oxidation. However, the diversity of the magnitude of this increase among the samples is indicative of a difference in the susceptibility of the lipid systems to the formation of these compounds, which is associated with the flavor composition and added ingredients, and not only the oxidation conditions (Bastos & Pereira, 2010; Mostfa et al., 2025).

In contrast, the decrease in the unsaturation index (UI) reflects the depletion of double bonds. However, the variation in this decrease among the samples suggests that the rate of consumption of unsaturated fatty acids depends on structural factors, such as the type of oil and the presence of oxidation-promoting or inhibitory compounds within the flavor.

A clear decrease of the phenolic index (PhI) was observed as a reflection of the consumption of phenolic compounds during oxidation. But what is really important is the rate at which this decrease occurs, since it reflects the different antioxidant capacity of the various systems, which is a key factor in determining their oxidative stability. This reading is supported by a high oxidation index (OI) that suggests the accumulation of more complex secondary oxidation products, which demonstrates the variety of oxidation pathways in advanced stages (Franco et al., 2014).

The Relationship Between FTIR and Chemical Indices

Figure (2) illustrates the relationships between FTIR indices and conventional oxidation indices. Quantitative correlation coefficients are presented in Table (2), and the interpretation of these relationships is further supported

by the relative changes in FTIR indices, as shown in Table (3). This provides a comprehensive understanding of the structural and chemical transformations associated with the oxidation process.

Figure (2A) shows a strong positive correlation between the carbonyl index (CI) and the TOTOX value with a high correlation coefficient ($r = 0.85$). A greater CI is correlated with a greater overall oxidation state. This outcome is verified by the values obtained in Table (3) in which the samples with higher relative increase in CI like sample F7 had a higher degree of structural transformations correlated with higher secondary oxidation products.

In contrast, Figure 2B shows an inverse relationship between the unsaturation index (UI) and the anisidin value (p-AV), where a decrease in UI is associated with an increase in p-AV ($r = -0.79$), reflecting the consumption of double bonds and the formation of aldehyde compounds. As can be seen from Table 3, the samples that exhibited the largest relative decrease in UI, such as F7 and F4, also showed higher levels of secondary oxidation products.

The phenolic index (PhI) in Figure 2C correlates strongly and positively with total phenolic content (TPC) ($r = 0.91$), suggesting that FTIR is a reliable reflection of the consumption of antioxidant compounds. This trend is supported by the data in Table 3, where the samples with the greatest relative decrease in PhI, such as F3 and F4, had higher depletion of phenolic compounds, indicating their role in inhibiting oxidation.

However, the results in Table (2) revealed a poor correlation between the carbonyl index and the peroxide value (PV), indicating the limited role of PV in representing the oxidation state in the advanced stages as a result of the decomposition of hydroperoxides, which explains the apparent variation in their values despite the continued progress of oxidation.

Overall, these results demonstrate that combining spectral analysis (Figure 2) and relative variations (Table 3) provides a deeper understanding of the oxidation pathway, where the interpretation extends beyond statistical relationships to encompass the dynamics of structural shifts between different samples. The findings suggest that FTIR is not merely a spectral characterization tool but also provides a comprehensive structural framework for understanding the oxidation pathway in dietary systems (Borba & Gomez-Zavaglia, 2023; Wang et al., 2025).

Classical chemical indices represent the accumulation of oxidation products, whereas FTIR indices

reflect the kinetics of the structural change, with the consumption of the lipid substrate (UI), the formation of by-products (CI, OI), and the depletion of antioxidant compounds (PhI). This integration suggests that the oxidation is not a linear process but a multi-pathway interactive system, directly affected by the composition of the diet and its functional components, particularly the active compounds of added flavours (Rohman, & Che Man, 2020).

Integrating Structural and Kinetic Analysis and the Influence of Flavors

When interpreting the current results within the context of previous studies on the same samples, it becomes clear that FTIR provides a direct structural explanation for the oxidative behavior observed using kinetic and chemical indices.

Results from the oxygen consumption studies suggest that some samples, such as F5 and F1, have higher oxygen consumption rates and shorter half-lives, indicating accelerated oxidative reactions and decreased oxidative stability. This is in agreement with the present findings as these samples showed a higher increase of the carbonyl index (CI) and a larger decrease of the unsaturation index (UI) suggesting that the fast kinetic behavior of oxidation is associated with a strong structural transformation in the lipid matrix.

In contrast, the more kinetically stable samples, such as F2 and F3, showed less pronounced structural changes, reinforcing the idea that the oxidation rate not only reflects the reaction speed but is also related to the degree of structural transformation of the system.

The variation in oxidative behavior, combined with the influence of flavors, clearly reflects the functional role of the chemical composition of the flavor. Garlic and lemon flavors behaved oxidatively, whereas pepper and cheese flavors behaved in an inhibitory manner. This was reflected spectroscopically by the high oxidation indices of the oxidized flavors, in relation to the relative retention of phenolic compounds in the flavors with antioxidant activity.

These results indicate that oxidation in potato chips is a multidimensional phenomenon integrating:

- Kinetic dimension (rate of oxygen consumption)
 - Chemical dimension (accumulation of oxidation products)
 - Structural dimension (molecular changes).
- Thus, FTIR not only serves as a characterization tool but also acts as an explanatory link, elucidating the system's transition from kinetic behavior to structural change and demonstrating how these transformations are reflected in

the measured chemical indices.

Conclusion

This study demonstrated that Fourier transform infrared spectroscopy (FTIR) is an effective analytical tool for interpretation, rather than simply monitoring, the structural changes associated with lipid oxidation in potato chips. The increase in the carbonyl index (CI) and the oxidation index (OI) was associated with the accumulation of secondary oxidation products, while the decrease in the unsaturated index (UI) and the phenolic index (PhI) reflected the consumption of unsaturated fatty acids and antioxidants.

Statistical relationships showed a clear correlation between the FTIR indices and the chemical indices. CI was strongly correlated with the TOTOX index, while its correlation with the peroxide value was weak, confirming the limitations of primary indices in representing advanced stages of oxidation. These results, analyzed in the context of previous studies, demonstrate that oxidation in complex food systems is a multidimensional phenomenon that integrates kinetic, chemical and structural aspects. FTIR thus offers an explanation for the correlation between reaction rate and molecular transformations that take place. The results also indicate that flavor composition is an important factor in the oxidation pathway, as some flavors can act as either promoters or inhibitors depending on their chemical nature and directly influence the oxidative stability of the product.

Therefore, FTIR indices can be adopted as a complementary analytical tool to traditional indices, capable of providing an advanced structural reading of the oxidation pathway. This supports their use in assessing food product stability and developing more efficient strategies for controlling lipid oxidation in fried foods.

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Conflict of Interest Statement: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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