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Content of macro- and trace elements determined by ICP-OES in brews from whole-bean and freeze-dried coffee roasted to different degrees*

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Abstract

Coffee is one of the most widely consumed beverages worldwide, and its mineral composition varies significantly depending on roasting parameters and product form. This study aimed to assess the content of macronutrients (K, Mg, Ca, Na, P) as well as trace and potentially toxic elements (Al, Co, Cr, Fe, Mn, Ni, Sr, Zn) in brews made from coffee beans roasted to five levels (5/10-9/10) and from two variants of freeze-dried instant coffee (5/10 and 6/10). Brews were prepared at a standardized coffee-to-water ratio of 6:100 (m/v), at 92°C for 5 min, digested with HNO₃ and H₂O₂, and then the concentrations of elements were determined by the ICP-OES method. Potassium was the predominant element in all brews, with mean concentrations of 287 mg L⁻¹ in whole bean coffees and 688 mg L⁻¹ in freeze-dried coffees. The concentrations of macronutrients in freeze-dried coffees were 1.51-2.36 times higher than in whole-bean coffee, reflecting the greater content of soluble solids in the instant product. In contrast, iron concentrations were practically identical in both product forms regardless of the degree of roasting, suggesting differences in the physicochemical form in coffee beans. It was demonstrated that roast degree affects element concentrations in a curvilinear manner, with maximum extraction occurring at 7/10-8/10, while intense roasting (9/10) led to a 35-55% reduction in concentrations relative to maximum values. The results indicate that dark-roasted coffee contains lower concentrations of minerals than medium-roasted coffee, which may have nutritional implications for consumers who regularly drink coffee as a source of magnesium and potassium in their diet. Concentrations of arsenic, cadmium, and lead remained below the method's limit of quantification in all samples, confirming the safety of the analysed brews with respect to toxic metal content.

Keywords: coffee mineral profile, degree of roasting, freeze-dried coffee, ICP-OES

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INTRODUCTION

Coffee is one of the most widely consumed beverages in the world, being also an important source of both macronutrients and micronutrients. Its chemical composition depends on many factors: the origin of the raw material, growing conditions, processing method, including the degree of bean roasting, and method of preparation (Cruz et al. 2015, Janda et al. 2020, Febrianto, Zhu 2023, Latief et al. 2025). In recent years, particular attention has been paid to the potential presence of heavy metals in coffee, which may be introduced into the product at various stages of production and processing (Cruz et al. 2015). The degree of coffee bean roasting influences the physicochemical changes in their structure, which can modify both the total content of elements and their extractability into the brew (Tarigan et al. 2022). Coffee roasting, which is conducted at high temp. (160-260°C) can affect the availability and concentration of elements in the final brew (Hernandez et al. 2007). During roasting, a series of physicochemical changes occur in the coffee beans, including intense heat absorption, structural changes observed at temp. around 50°C, protein denaturation, and water evaporation, resulting in mass loss and an increase in the material's porosity, which may modify the efficiency of macro- and micronutrient extraction into the brew (Bicho et al. 2013). Another aspect is the commercial form of coffee. Whole bean coffee and freeze-dried coffee differ fundamentally in their production processes (Al-Ghamdi et al. 2024). Freeze-drying of a pre-brewed liquid extract can affect the concentration and distribution of elements in the final product. By comparing the mineral profiles of brews made from whole bean coffee and instant coffee with similar roast levels, it is possible to evaluate the degree to which the additional processing step influences the beverage's mineral composition (Stelmach et al. 2013). An important aspect of food safety is the presence of heavy metals in coffee, such as lead (Pb), cadmium (Cd), arsenic (As), and chromium (Cr), which can leach into the brew and pose a potential health risk to consumers with regular consumption (Nędzarek et al. 2013).

The aim of this study was to assess the content of selected macroelements (Ca, K, Mg, Na, P) and trace elements (Fe, Mn, Al, Sr), as well as the presence of heavy metals (Pb, Cd, Cr, Ni), in coffee brews of varying roast levels, in the form of beans and freeze-dried coffee.

MATERIALS AND METHODS

Coffee samples

The study examined commercial coffee samples from a single brand consisting of five whole-bean coffee samples with different roast levels and two

varieties of freeze-dried instant coffee. The five whole-bean samples differed in roasting degree (5/10, 6/10, 7/10, 8/10, and 9/10 on the manufacturer's scale). The two additional samples were freeze-dried instant coffees with roasting degrees of 5/10 and 6/10. The whole-bean coffees were ground to medium grind in a DeLonghi KG79 grinder (Italy) immediately before brewing. The grind size was kept consistent across all whole-bean samples. Each of the seven samples was prepared and analysed three times in independent measurements ($n=3$).

Preparation of the infusion

A 15.0 g coffee sample was added to 250 mL of deionized water at 92°C, maintaining a coffee-to-water ratio of 6:100 (m/v). The brewing time was 5 minutes. After brewing, the brew was divided into two fractions. Two fractions were collected, an unfiltered fraction and a filtered one obtained by passing 0.75 mL through a filter immediately after brewing (Figure 1).

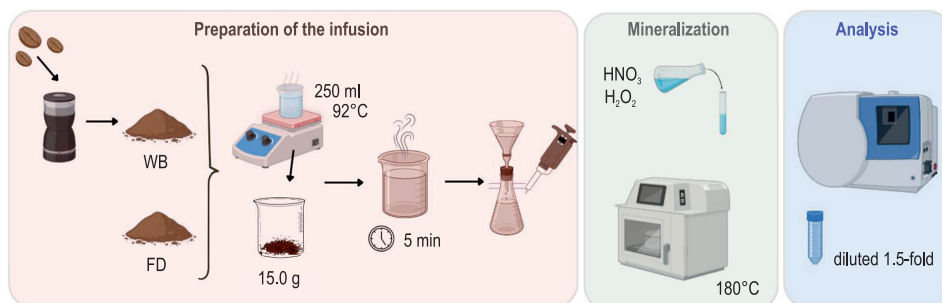


Fig. 1. Schematic diagram of coffee preparation: whole bean coffee (WB) was ground before brewing, while freeze-dried coffee (FD) was used directly. Both forms were brewed under standardized conditions (15.0 g, 250 mL, brewing time 5 min) and filtered. Samples were mineralized and analysed using ICP-OES

Sample digestion

Each 0.75 mL aliquot was transferred into Teflon digestion vessels. Subsequently, 4.0 mL of 65% (v/v) HNO_3 were added. Samples were pre-digested for 30 min at room temperature. Then, 1.0 mL of 30% (v/v) H_2O_2 was added to oxidise organic matter. Microwave-assisted digestion was performed in a closed-vessel system by heating to 180°C for 15 min and holding for 20 min (Anton Paar, Graz, Austria). After digestion, the solutions were quantitatively transferred into polypropylene tubes and diluted to a final volume using deionized water. The entire sample preparation and analytical procedure for each coffee was performed in triplicate, constituting independent analytical replicates of the mineralization and measurement procedure.

Determination of element content

The content of macronutrients (Ca, K, Mg, Na) and trace and minor elements (Al, Co, Cr, Cu, Fe, Mn, Ni, Sr, Pb) in mineralised samples was determined by inductively coupled plasma optical emission spectrometry (ICP-OES) using a Spectroblue spectrometer (AMETEK Inc., Meerbusch, Germany). The elements were quantified in concentrations in mg L^{-1} (ppm), except for Cr, which was reported in $\mu\text{g L}^{-1}$ (ppb) due to its trace-level concentrations. For each sample, three replicates were analysed. Instrument calibration was performed separately for each element using a multi-element standard solution (LGC Standards, Poland) prepared in a HCl/HNO_3 mixed acid matrix. Calibration curves were constructed over the concentration range of 0.5–100 mg L^{-1} . The limits of detection (LOD) were determined individually for each element and were as follows: Al – 0.00077 mg L^{-1} , Ca – 0.00469 mg L^{-1} , Co – 0.00013 mg L^{-1} , Cr – 0.0373 $\mu\text{g L}^{-1}$, Fe – 0.00114 mg L^{-1} , K – 0.00339 mg L^{-1} , Mg – 0.00117 mg L^{-1} , Mn – 0.000353 mg L^{-1} , Na – 0.000906 mg L^{-1} , Ni – 7.89×10^{-5} mg L^{-1} , P – 0.000861 mg L^{-1} , Sr – 7.66×10^{-6} mg L^{-1} . Concentration values below the limit of detection (LOD) were reported as “< LOD” and excluded from statistical analyses. Recovery testing via standard addition was not performed; instead, accuracy was assessed through the consistency of results with published reference data for coffee brews obtained under comparable analytical conditions.

Statistical analysis

Basic descriptive statistics were calculated for all measurements. For each sample, the mean ($\bar{x}$) and standard deviation (SD) were calculated from three independent analytical replicates. The precision of the method was expressed as the relative standard deviation (RSD%), calculated as $\text{RSD\%} = (\text{SD}/\bar{x}) \times 100$.

RESULTS AND DISCUSSION

Characteristics of the elemental composition of coffee brews

An analysis of the elemental composition of the brews under study revealed that potassium was the dominant macroelement among those measured (Table 1).

These values are lower than those reported for pour-over brews by Adler et al. (2019) – 814.67–1323.33 mg L^{-1} and Gogoşa et al. (2016) – 522 mg L^{-1} for powdered coffee. The second most abundant macronutrient was magnesium (Table 1), followed by calcium and sodium. Magnesium concentrations obtained for whole-bean brews are consistent with those reported by Adler et al. (2019), who found a range of 46.00–84.63 mg L^{-1} for pour-over brews,

Table 1

Mean concentrations ($\bar{x}$) and standard deviations (SD) of selected elements in brews prepared from whole-bean (WB) and freeze-dried (FD) coffee

Element	WB $\bar{x}$	WB SD	FD $\bar{x}$	FD SD
Al (mg L ⁻¹)	2.44	0.72	1.80	0.01
Ca (mg L ⁻¹)	53.84	12.41	98.55	2.33
Co (mg L ⁻¹)	2.34	0.15	2.40	0.14
Cr (mg L ⁻¹)	201.38	104.68	16.55	7.99
Fe (mg L ⁻¹)	8.44	0.57	8.55	0.35
K (mg L ⁻¹)	287.30	55.98	687.50	30.41
Mg (mg L ⁻¹)	39.82	9.26	99.55	7.71
Mn (mg L ⁻¹)	39.82	9.26	99.55	7.71
Na (mg L ⁻¹)	68.58	11.97	133.10	5.52
Ni (mg L ⁻¹)	0.26	0.08	0.83	0.20
P (mg L ⁻¹)	26.80	18.63	94.20	6.36
Sr (mg L ⁻¹)	0.45	0.09	0.81	0.01

and 77.15-116.30 mg L⁻¹ depending on a brewing technique (Janda et al. 2020). Calcium concentrations in the literature vary widely with a brewing method, from 10.37 to 18.27 mg L⁻¹ for pour-over (Adler et al. 2019) to 25.71 mg L⁻¹ for espresso (Janda et al. 2020). The calcium concentrations obtained in this study for freeze-dried coffee (Table 1) are relatively high compared to literature data for whole bean coffee, which again indicates the concentration effect characteristic of instant products. Similarly, Grembecka et al. (2007) reported sodium levels of 119 ± 116 mg 100 g⁻¹ wet weight for instant soluble coffee, which is consistent with the higher Na values obtained for freeze-dried coffee in this study. Among the trace elements, iron was predominant and showed virtually identical concentrations in both product forms, while manganese and zinc remained more than an order of magnitude lower. These values are significantly higher than those reported by Gogoasă et al. (2016), who measured Fe at 0.158 mg L⁻¹. The difference may result from a different analytical method, the degree of sample mineralisation used, or the type of coffee used, and requires careful interpretation. Hasan et al. (2026) obtained a similar result for manganese, with an average of 0.612 ppm. Gogoasă et al. (2016) reported values of 0.206 mg L⁻¹ (Mn) and 0.146 mg L⁻¹ (Zn) for these elements, which is broadly consistent with the present study, although direct comparison is complicated by differences in brewing and digestion conditions.

Potentially harmful elements were also identified in the brews. Aluminium was detected at concentrations ranging from 1.30 to 2.60 mg L⁻¹, while nickel was detected at 0.17-0.97 mg L⁻¹. Chromium was detected only in trace concentrations (µg L⁻¹). The Ni concentrations were markedly higher than those reported by Adler et al. (2019) – 0.0078-0.0182 mg L⁻¹. Arsenic,

cadmium, and lead concentrations in all samples remained below the method’s limit of detection (< LOD), consistent with the observations of Grembecka et al. (2007), who did not detect lead or cadmium in ground coffee or in the brews either. The concentrations of potentially toxic elements obtained did not exceed the limits specified in Commission Regulation (EU) No. 2023/915 (European Commission, 2023) on maximum levels for certain contaminants in food, indicating that the analysed brews do not represent a significant source of toxic metal exposure for consumers and can be considered safe in terms of elemental composition.

Differences in the mineral composition of brews from whole bean and freeze-dried coffee

A comparison of macronutrient concentrations in brews from whole bean (WB) and freeze-dried (FD) coffee, prepared under identical conditions, reveals higher concentrations in freeze-dried coffees regardless of the roast level (Figure 2), with FD/WB concentration ratios falling into three functionally distinct groups (Table 2).

Table 2
FD-to-WB concentration ratios for selected elements at roast levels 5/10 and 6/10, with mean values

Element	FD5/WB5	FD6/WB6	Average ratio	Interpretation
Al	0.72	0.69	0.70	lower in CL
Ca	1.88	1.77	1.82	significantly higher in CL (~1.9×)
Co	1.04	1.00	1.02	virtually identical
Cr	0.09	0.04	0.07	significantly lower in CL
Fe	1.00	1.00	1.00	virtually identical
K	2.36	1.98	2.17	highly concentrated in CL (~2×)
Mg	2.36	2.01	2.18	highly concentrated in CL (~2.4×)
Mn	2.33	1.24	1.79	higher in CL (~2.2×)
Na	2.07	1.51	1.79	significantly higher in CL (~2×)
Ni	2.88	3.46	3.17	significantly higher in CL (~3×)
P	5.50	1.82	3.66	significantly higher in CL (~5.5×)
Sr	1.82	1.76	1.79	higher in CL (~1.8×)

The FD/WB ratios cluster into three distinct groups that reflect differences in the physicochemical forms of elements in the brew. The first group, comprising K, Mg, Ca, Na, Mn, and Sr with ratios of 1.51-2.36, shows proportional concentrations during industrial extraction and freeze-drying, consistent with their predominantly ionic speciation in solution (Table 2). The second group (Fe and Co), with ratios of approximately 1.0, shows no concentration effect, suggesting that these elements occur as stable

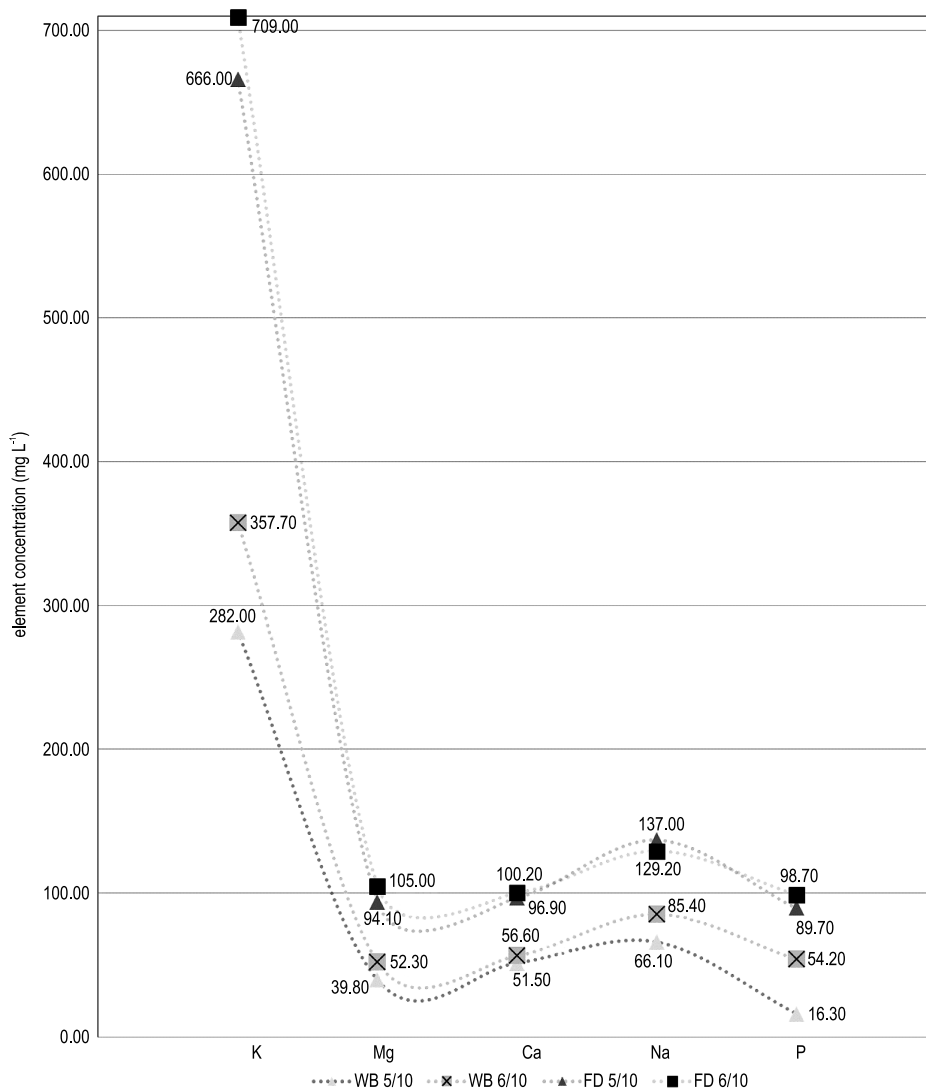


Fig. 2. Comparison of K, Mg, Ca, Na, and P concentrations (mg L^{-1}) in brews prepared from whole-bean (WB) and freeze-dried (FD) coffee with roast levels of 5/10 and 6/10

low-molecular-weight complexes whose extractability is independent of a product form and processing intensity. The third group includes elements with anomalous ratios (P and Ni), which are disproportionately enriched in freeze-dried coffee relative to macronutrients, possibly reflecting selective enrichment during industrial extraction or the presence of particularly soluble chemical species. Lower concentrations of Al and Cr in freeze-dried coffees compared to whole bean coffees suggest that these elements in whole bean coffee occur partly in colloidal forms or bound to organic fractions, which are

not subject to effective industrial extraction. This divergent behaviour highlights that brew mineral concentration is not a simple linear function of dry matter content, and that the product form selectively alters the extractability of individual elements through mechanisms that warrant further investigation.

These results are consistent with the literature data showing higher mineral content in instant coffee brews compared to roasted and ground coffee prepared using conventional methods (Pokorska-Niewiada et al. 2024). With the growing popularity of high-dose instant coffees concentrations, these differences may be clinically significant in the context of daily potassium and magnesium intake (Buda et al. 2025).

Iron is the predominant trace element in all samples, and its concentrations were virtually identical in both product forms (8.80 and 8.30 mg L⁻¹, for roast levels 5/10 and 6/10, respectively) – Figure 3. This indicates that iron is extracted into the brew predominantly in ionic form or as stable low-molecular-weight complexes with a similar degree of extraction regardless of the product form. Aluminium exhibited the opposite trend relative to the other macronutrients, as its concentrations were higher in whole bean coffee (2.50–2.60 mg L⁻¹) than in freeze-dried coffee (1.80 mg L⁻¹ for both roast levels). The absence of a roast-level effect in freeze-dried samples suggests that the Al content in instant products is determined during industrial processing rather than during home brewing. Nickel concentrations are markedly elevated in freeze-dried coffee relative to whole-bean coffee, with the FD/WB ratio reaching 3.46 at roast level 6/10.

The higher mineral concentrations observed in freeze-dried coffee brews do not follow from the intrinsic mineral composition of the beans; instead, they reflect a fundamental difference in the product form, namely freeze-dried coffee consists entirely of pre-extracted, concentrated extract that dissolves completely upon brewing, whereas in whole-bean coffee a substantial proportion of the bean mass including insoluble fibre, waxes, and structural proteins remains in the spent grounds and never enters the liquid phase (Bicho et al. 2013). Since individual elements differ in their physico-chemical forms and the association with soluble versus insoluble bean fractions, the product form selectively alters the extractability of each element rather than uniformly scaling all concentrations. Consequently, a direct comparison of the mineral profile of whole bean coffee and freeze-dried coffee based solely on concentrations in the brew, without considering the chemical form of the elements and the effective mass of the extracted dry matter, may lead to erroneous conclusions regarding nutritional value and food safety.

Elemental content in brews of whole bean coffee with varying degrees of roasting

The results obtained for five degrees of coffee bean roasting (C5/10–C9/10) are summarized in Figure 4. Data analysis indicates that none of the tested macronutrients (Figure 4a) exhibits a linear relationship with the degree of

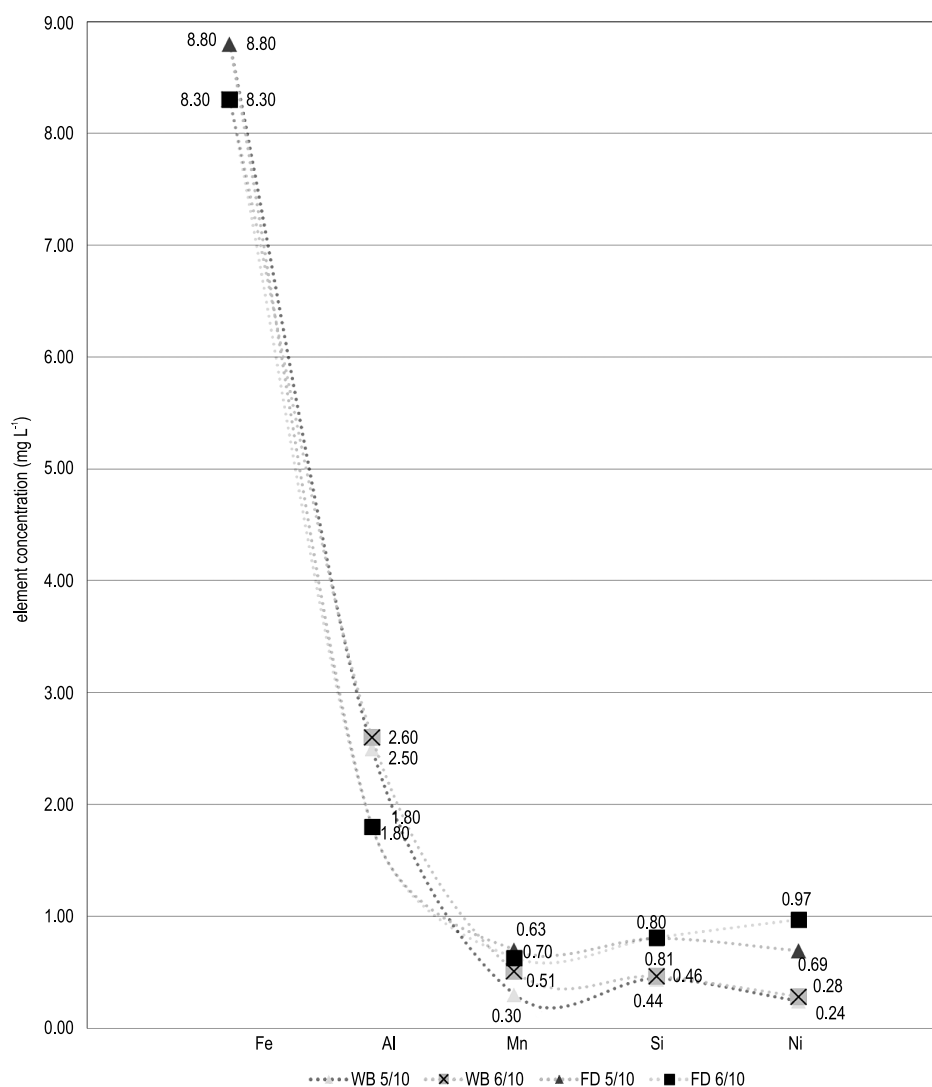


Fig. 3. Comparison of Fe, Al, Mn, Sr, and Ni concentrations (mg L^{-1}) in brews prepared from whole-bean (WB) and freeze-dried (FD) coffee with roast levels of 5/10 and 6/10

roasting. The observed pattern is curvilinear: for most elements, concentrations increased an upward trend from C5/10 to C8/10, followed by a marked decrease at the highest roast level (C9/10).

Potassium reached its highest concentration at C7/10 (357.7 mg L^{-1}) and its lowest at C9/10 (214.7 mg L^{-1}), a difference of 40%. This trend aligns with the mechanism by which moderate roasting increases bean porosity and facilitates the aqueous extraction of K^+ ions, while more intense thermal treatment partially carbonises the organic matrix, thereby reducing the

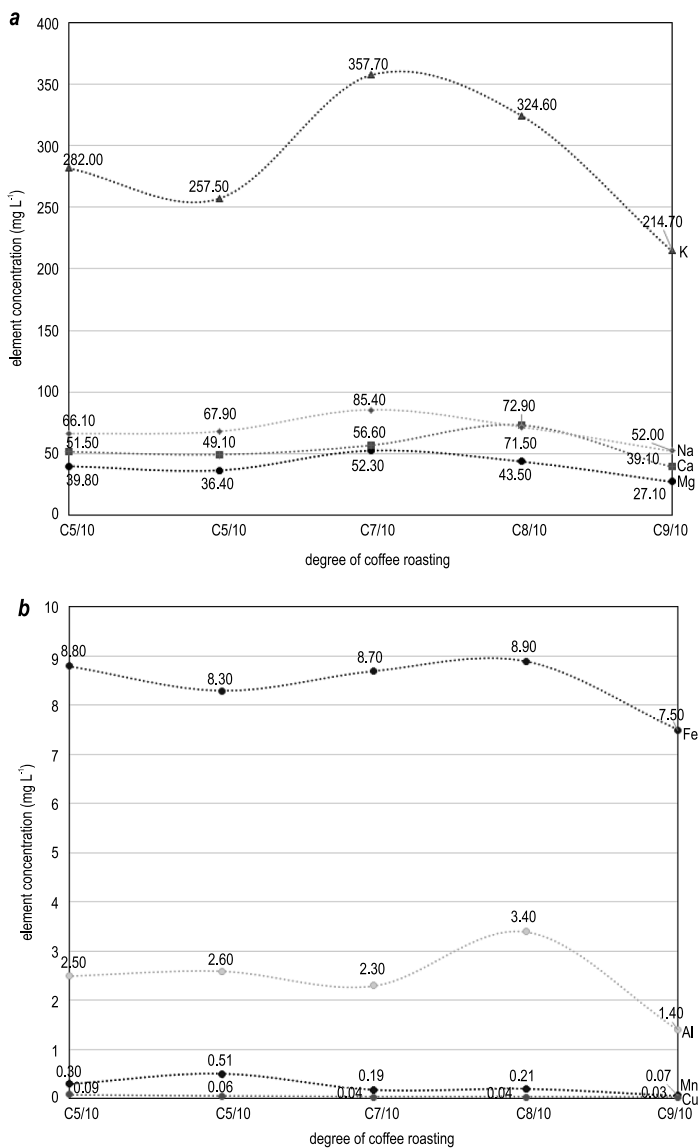


Fig. 4. Concentrations of macronutrients (a) and trace elements (b) in brews prepared from whole-bean coffee as a function of the roast level

extractability of potassium. Magnesium showed its highest value at C7/10 (52.3 mg L⁻¹), decreasing to 27.1 mg L⁻¹ at C9/10 (a 48% decrease). In coffee beans, magnesium is partially bound to chlorogenic acids in a chelated form, the progressive thermal degradation of these releases Mg²⁺ into a more readily extractable form. However, intense pyrolysis at roast level 9/10 results in the entrapment of ions within the carbonised bean matrix. Calcium followed a similar trend, but with a peak at C8/10 (72.9 mg L⁻¹),

dropping to 39.1 mg L⁻¹ at C9/10. Since deionised water was used for all brew preparations, the contribution of water-derived calcium to the measured concentrations was negligible, and the values reported in this study reflect exclusively bean-derived Ca. This is a methodological advantage over studies using tap or mineral water, where water hardness may contribute 10-25 mg L⁻¹ of calcium to a 250 mL brew, complicating the interpretation of roast-dependent trends. The consistent decrease in Ca at C9/10 therefore directly reflects the immobilisation of calcium within the carbonised bean matrix under intense roasting conditions. Sodium reached a maximum at C7/10 (85.4 mg L⁻¹) and a minimum at C9/10 (52.0 mg L⁻¹). In studies using tap or mineral water, sodium concentrations in coffee brews are strongly influenced by the water composition, as Na is naturally present in tap water at concentrations of 10-50 mg L⁻¹ depending on the source, which may represent a substantial proportion of the total sodium measured in the brew and obscure the bean-derived signal (Olechno et al. 2021). The use of deionised water eliminates this confounding effect entirely, meaning that the measured Na concentrations reflect exclusively the extractability of sodium from the bean matrix. The roast-dependent trend observed for Na therefore unambiguously parallels the behaviour of K and Mg, the elements whose brew concentrations are unambiguously bean-derived, and supports the hypothesis that intense roasting at level 9/10 reduces the extractability of all major cations through carbonisation-induced immobilisation of mineral ions within the insoluble carbon matrix of the bean.

Naibaho et al. (2026) demonstrated that both the method of conducting the roasting process and its intensity significantly determine the physico-chemical and functional properties of coffee. The mechanism responsible for the relationships between the macronutrient content in the brew may depend on several processes. In the bean roasting range from 5/10 to 8/10, there is progressive thermal degradation of chlorogenic acids, proteins, and polysaccharides, leading to the release of mineral ions (particularly K⁺, Mg²⁺, Ca²⁺, and Na⁺) into forms easily extractable with water, accompanied by an increase in the porosity of the bean structure, which facilitates contact between the extraction medium and the mineral-containing matrix (Dawidowicz, Typek 2017, Han et al. 2025). At a roast level of C9/10, corresponding to intense carbonisation, mineral ions are immobilized within an insoluble carbon matrix, and the highly sintered surface of the bean limits water penetration. The result is a decrease in the concentrations of elements in the brew, resulting in lower mineral concentrations in dark-roasted coffee compared to medium-roasted coffee. Similar relationships were reported by Dippong et al. (2022), who showed that the macronutrient content in coffee varies widely (approximately 22-50%) depending on the variety and roast level, with the highest levels of many minerals found in medium-dark roast beans. Specifically, K, Ca, Mg, and P concentrations increased with roasting intensity, whereas Na, Mn, and Zn were relatively unaffected by the degree of roasting.

Iron exhibits the lowest variability among the four elements present in smaller quantities (Figure 4b). Concentrations range from 7.50 to 8.90 mg L⁻¹, with no clear trend, the only notable decrease occurring at roast level 9/10. This stability suggests that iron in coffee beans is bound in chemical forms resistant to thermal degradation within the range of roasting temperatures studied, likely as complexes with proteins or within crystalline structures (Yashwanth et al. 2025). Aluminium displays a non-monotonic pattern with a distinct maximum at roast level 8/10 (3.40 mg L⁻¹), with all remaining samples falling within 1.40-2.60 mg L⁻¹. Manganese reaches its highest concentration at 6/10, then decreases to 0.07 mg L⁻¹ at roast level 9/10, representing an 86% reduction relative to the maximum value. Manganese is particularly susceptible to oxidation state changes under thermal conditions and readily forms stable complexes with phenolic compounds in coffee, especially with chlorogenic acids (Jaganyi, Madlala 2000). Copper exhibited a monotonically decreasing trend across the full roast range studied.

CONCLUSIONS

Analysis of the elemental composition of coffee brews revealed that the mineral profile is determined by the product form and the degree of bean roasting. Potassium was the dominant element in all brews tested, with concentrations substantially exceeding those of other macronutrients. Higher concentrations of macronutrients in freeze-dried coffee compared to whole bean coffee (up to 1.51-2.36 times higher) reflect the concentrated nature of the instant product. Iron was an exception, showing virtually identical concentrations in both product forms regardless of the degree of roasting, suggesting a distinct physicochemical speciation within the bean matrix. The degree of roasting affects the concentrations of macronutrients in the brew in a curvilinear manner. Maximum extraction of K, Mg, Ca, and Na occurs at roast levels of 6/10 to 8/10, while a dark roast (9/10) leads to a marked decrease in all concentrations by 35-55% relative to the maximum. The results indicate that very dark-roasted coffee is significantly poorer in minerals than medium-roasted coffee, with potential nutritional implications for regular coffee drinkers.

Author contributions

A.D. – conceptualisation, methodology, data curation, visualisation, writing – original draft preparation, I.M. – funding acquisition, supervision, project administration, M.S.-S. – methodology, writing – review & editing.

All authors have read and agreed to the published version of the manuscript.

Conflicts of interest

The authors declare no conflicts of interest.

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