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# Comparative Assessment of Optical Properties of PETG, PU & PETC based Orthodontic Clear Aligners Exposed to a Common Staining Agent: An- InVitro Study

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**KEYWORDS**

Clear aligner, clear aligner material, colour stability, optical properties, PET-C, PET-G, PU.

**ABSTRACT:**

**Introduction:** An increase in non-fixed orthodontic appliance treatment options has been attributed to the growing demand for aesthetic procedures, particularly among adults. As a result, clear aligner therapy was created to treat malocclusion or misaligned teeth. When making aligners, polyurethane (PU) (CA Pro+, Scheu Dental; Iserlohn, Germany) and polyethylene terephthalate glycol (PETG) (Scheu Dental Duran; Iserlohn, Germany) are the most often utilised materials. Recently, a material known as polyethylene terephthalate copolyester (PETC) (Erkodur-al; Pfalzgrafenweiler, Germany) was created. It has great dimensional stability, is viscoelastic, hard, crystal clear, and is break-resistant. To date, no research has been conducted to compare the optical characteristics of PET-C-based materials.

**Aims and Objectives:** The primary objective was to evaluate and compare the optical properties of PETG, PU & PETC-based aligner material exposed to different staining agents in vitro.

**Materials and Methods:** The study was carried out on Polyurethane (PU), Polyethylene terephthalate glycol (PETG) and Polyethylene terephthalate copolyester (PETC) based aligner material. A UV-visible spectrophotometric analysis ($T_0$) of the unexposed aligner samples was taken. They were then exposed to a staining agent (black coffee) (Nescafe/ Nestle/ Switzerland) for up to 7 days. Spectrophotometric analysis was done post 7 days ($T_1$) to exposure of staining agent.

**Results:** After 7 days of immersion, the aligners were washed in an ultrasonic cleaner and measured with a colourimeter. The colour changes (ΔE*) were calculated based on the Commission Internationale de I'Eclairage L*a*b* colour system (CIE L*a*b*), and the results were then converted into National Bureau of Standards (NBS) units. Fourier transformation infrared (FT-IR) spectroscopy and scanning electron microscopy (SEM) were conducted to observe the molecular and morphologic alterations to the aligner surfaces, respectively. The three types of aligners exhibited slight colour changes after 12

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hrs of staining.

**Conclusion:** The evidence amassed from this comprehensive investigation underscores the imperative need for further exploration and understanding of the optical characteristics of PETC-based aligner materials. By elucidating the nuances of how different materials respond to staining agents, this study not only contributes to the existing body of knowledge but also informs clinical practices and material selection in orthodontic treatment. Through continued research and refinement, we can strive towards optimizing the performance and aesthetic appeal of clear aligner therapy, ultimately enhancing patient outcomes and satisfaction.

**Introduction:**

The development of clear aligner therapy as a pleasant and aesthetically pleasing treatment modality was spurred by an increase in adult patients' demand for orthodontic treatment.[1-2] Nowadays, fabrication[4] can be done with a variety of thermoplastic materials,[3] such as polyvinyl chloride,[5] polyurethane (PU),[6] polyethylene terephthalate (PET),[7] and polyethylene terephthalate glycol (PETG).[5,7] Polyethylene terephthalate glycol (PETG) and polyurethane (PU) are the two materials most frequently utilised in the production of aligners.

Recently, a new PETC material was released onto the market. It is extremely transparent, viscoelastic hard, break-resistant, and has excellent dimensional stability.

Clear aligners have been linked to several biomechanical[7,8] and mechanical properties,[9,10] including their manufacturing processes, how well they fit teeth, and, most importantly, the characteristics of the component material. Aligners do, however, have several drawbacks, including poor wear resistance, low strength, and dimensional instability. These problems can be related to the properties of the materials or the production procedures. The material's deterioration during treatment with these aligners may be caused by microcracks, abrasions, localised biofilm deposits, delamination, exposure to heat, humidity, and food particles combined with salivary enzymes in the oral cavity. This alteration in transparency could be a drawback for clear aligners.

Statistics have demonstrated that over 50% of adults drink coffee every day and that their average consumption is 3.2 cups per day.[11] For patients who do not follow the instructions, the pigments in staining agents might accumulate and lead to colour changes in the aligner materials. Thus, clear aligners might become less aesthetically appealing even during the 2- week treatments,[12] and this is a clinical concern. Therefore, there is a need to investigate the colour stabilities of commonly used types of aligners to provide evidence for both patients and orthodontists regarding clinical aesthetic considerations and instructions.

Patients are advised by their orthodontists to wear their aligners all the time, except when eating, drinking anything other than water, and cleaning or flossing their teeth. Patients occasionally fail to follow directions to the letter and eat food items containing colouring agents. This may have an impact on the transparent qualities of the polymer that forms the aligner.

Thus this study seeks to examine and compare the colour stability of commercially available PETG, PU and PETC-based clear aligners exposed to a common staining agent, black coffee for up to 7 days in vitro.

**Aims and objectives**:

The primary objective of the study was to determine which aligner material (PET-G/PU/PET- C) has better colour stability when exposed to a staining agent.

**Materials and methods:**

**Staining of the aligners:**

This in-vitro study was carried out in the Department of Orthodontics and Dentofacial Orthopaedics, MGM Dental College & Hospital Kamothe, Navi Mumbai. The study was approved by the Institutional Ethical Committee. The three aligner materials were divided into three groups:

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**Group 1:** Polyethylene terephthalate glycol (PETG) based aligner material (Duran,Scheu; Iserlohn, Germany)[5,7]

**Group 2**: Polyurethane (PU) based aligner material (CA Pro+,Scheu; Iserlohn, Germany)[6]

**Group 3**: Polyethyelene terephthalate copolyester (PETC) based aligner material (Erkodur- Al; Pfalzgrafenweiler, Germany)

The sample size was calculated using the formula

$N = \frac{2(\$\alpha\&\$\beta)^2[s]^2}{d^2}$ and substituting the values a sample size of **30 per group** was determined.

Because black coffee has been reported to cause more severe stains than other beverages,[13] the present study used these liquids as staining agents and distilled water as a control.[14] The coffee (Nescafe; Nestle, Switzerland) solution was prepared according to the methods used in previous studies.[15] The concentrations were 3 g of coffee powder per 100 mL boiling distilled water[15] The aligners were immersed in each solution in a water bath at 37 °C for 12 h or 7 days. The solutions were refreshed every day. A pre-exposure UV-visible spectrophotometric analysis was performed to determine the baseline of the aligners.

**Colour change evaluations:**

The colour changes were characterised according to the Commission Internationale de I'Eclairage L*a*b* colour system (CIE L*a*b*).[16] The colour parameter L* represents lightness (+ bright, − dark), a* represents the red (+) to green (− ) colour scale, and b* indicates the yellow (+) to blue ( − ) colour scale.[17] The colour parameters L*, a*, and b* (t = 0, 1, 2) of aligners were measured with a standard VITA Easyshade Compact[18] colourimeter (Vita Zahnfabrik, Bad Sackingen, Germany) before staining (T0) and 7 days (T2) of staining. All measurements were conducted in the same ambient light environment with standardized illumination. The total colour change (ΔE*) value was calculated according to the equation ΔE* = [(ΔL*)2 +(Δa*)2 +(Δb*)2]1/2, which represents the colour difference before and after staining.[19]

**Colour change rating:**

The Natonal Bureau of Standards (NBS) system was used to describe levels of perceptible colour change upon visual inspection (Table 1). [20,21] The ΔE* values were converted into NBS units with the equation NBS = ΔE* ×0.92 to relate the colour changes to a clinical standard.[22,23,24]

| National bureau of standards units | Descriptions of colour changes |
|---|---|
| 0.0-0.5 | Trace: extremely slight change |
| 0.5-1.5 | Slight: slight change |
| 1.5-3.0 | Noticeable: perceivable |
| 3.0-6.0 | Appreciable: marked change |
| 6.0-12.0 | Much: extremely marked change |
| 12.0 or more | Very much: change to other colour |

**Table 1:** National Bureau of Standards ratings

**Statistics analysis:**

The normality of each group was analysed via the Shapiro-Wilk test.

Tukey's multiple comparison tests were conducted to investigate the effects of each solution on the materials' ΔE* values. The ΔE* values of each group at 7 days were analysed via two-way analyses of variance (ANOVAs), and one-way ANOVAs (Ad Hoc test). Tukey's multiple comparison tests were conducted to investigate the effects of each solution on the materials' ΔE* values.

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**Results**

**Colour change evaluations:**

Images demonstrating how the aligners colour changed before and after being submerged in coffee and distilled water. Upon visual inspection, aligners for PU, PETG, and PETC showed enhanced colour changes.

**Figure 1:** Before staining PET-G Aligner sheet

**Figure 2:** Before staining PU Aligner sheet

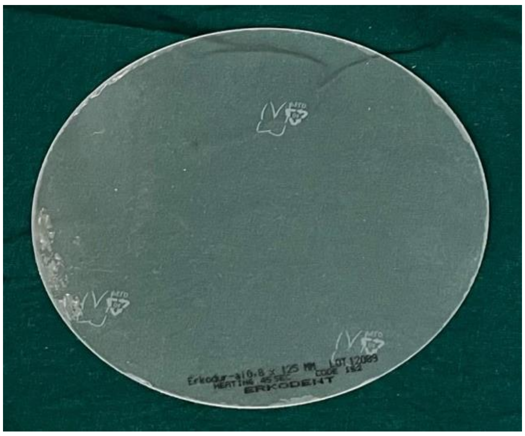

**Figure 3:** Before staining PET-C Aligner sheet

**Figure 4:** 3D printed block specimen

The table below presents the results of the analysis conducted on three different materials used in clear aligners: PETG (Polyethylene terephthalate glycol). PU (Polyurethane), PETC (Polyethylene terephthalate copolyester), and The table provides measurements and statistical values for various parameters related to colour and distribution characteristics of each material.

I. **PETG MATERIAL ,PU MATERIAL, PETC MATERIAL,**: These headings

indicate the three different materials being analyzed.

II. *L, a,* b***: These columns represent color space coordinates based on the CIELAB color model.

- **L***: Indicates lightness from black (0) to white (100).
- **a***: Represents the position on the red-green axis, with negative values indicating green and positive values indicating red.
- **b***: Represents the position on the yellow-blue axis, with negative values indicating blue and positive values indicating yellow.

III. **Mean, Median, Standard Deviation, Skewness, Kurtosis, K-S statistics, p-value**: These statistical parameters provide information about the distribution and characteristics of the color data for each material.

- **Mean**: Average value for each color parameter.
- **Median**: Middle value of the dataset.
- **Standard Deviation**: Measure of the dispersion or spread of the data.
- **Skewness**: Measure of the asymmetry of the data

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distribution.

- **Kurtosis**: Measure of the "tailedness" of the data distribution.
- **K-S statistics**: Kolmogorov-Smirnov statistic, which measures the proximity of the distribution of data points to an ideal normal distribution.
- **p-value**: Indicates the significance level of the K-S test.

IV. **Normally distributed**: Indicates whether the color data for each material follows a normal distribution. Overall, these table provides a comprehensive overview of the color characteristics and distribution properties of the three different materials used in clear aligners, helping to analyze their suitability and performance in orthodontic applications.

| | **PET-G MATERIAL** | | | **PU MATERIAL** | | | **PETC MATERIAL** | | |
|---|---|---|---|---|---|---|---|---|---|
| | **L*** | **a*** | **b*** | **L*** | **a*** | **b*** | **L*** | **a*** | **b*** |
| **Mean** | 100.53267 | 0.381 | 0.9743 | 100.128 | 0.31167 | 0.89233 | 99.523 | 0.241 | 0.66833 |
| **median** | 100.535 | 0.39 | 0.915 | 100.21 | 0.31 | 0.875 | 99.52 | 0.22 | 0.665 |
| **Standard Deviation** | 0.157084 | 0.049921 | 0.202236 | 0.383283 | 0.063359 | 0.130851 | 0.2314 | 0.084091 | 0.093701 |
| **Skewness** | 0.271945 | -0.106271 | 3.117358 | -0.278063 | 0.18459 | 0.947462 | 0.080259 | 0.21732 | 0.076355 |
| **Kurtosis** | -1.096638 | -1.009055 | 12.800265 | -0.882831 | -0.823499 | 0.508927 | -0.886673 | -0.983232 | -0.968182 |
| **K-S statistics** | 0.1371 | 0.13941 | 0.22747 | 0.11685 | 0.10268 | 0.11486 | 0.11384 | 0.13358 | 0.07336 |
| **p-value** | 0.57843 | 0.55737 | 0.07592 | 0.76444 | 0.87811 | 0.78178 | 0.79063 | 0.61075 | 0.99319 |
| | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed |

**Table 2:** Before staining

| | **PET-G MATERIAL** | | | **PU MATERIAL** | | | **PETC MATERIAL** | | |
|---|---|---|---|---|---|---|---|---|---|
| | **L*** | **a*** | **b*** | **L*** | **a*** | **b*** | **L*** | **a*** | **b*** |
| **Mean** | 98.66533 | 0.401 | 2.81033 | 95.67167 | 0.261 | 2.51367 | 96.22867 | 0.36533 | 2.85167 |
| **Median** | 96.7 | 0.395 | 2.855 | 95.676 | 0.26 | 2.535 | 96.225 | 0.36 | 2.88 |
| **Standard deviation** | 0.225323 | 0.053521 | 0.262855 | 0.21343 | 0.08083 | 0.271439 | 0.248883 | 0.052767 | 0.127781 |
| **Skewness** | -1.063969 | -0.202488 | -0.964803 | -0.383944 | -0.05467 | -0.039345 | -0.255099 | 0.0386 | -0.460081 |
| **Kurtosis** | 1.565408 | -1.286288 | 0.19733 | -0.944262 | -0.753805 | -1.214267 | -0.968338 | -0.865475 | -0.32701 |
| **K-S test** | 0.11482 | 0.14255 | 0.16615 | 0.11527 | 0.07324 | 0.12073 | 0.104 | 0.0937 | 0.12289 |
| **p-value** | 0.78217 | 0.5292 | 0.34067 | 0.77822 | 0.99332 | 0.72961 | 0.86874 | 0.93266 | 0.70985 |
| | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed | Normally distributed |

**Table 3**: After staining

The results presented in Tables 2 and 3 show the color and distribution characteristics of three different materials used in clear aligners (PU, PETC, and PETG) before and after staining with a staining agent (black coffee). Herein below we have analyzed the differences in the results before and after staining for each material:

I. **PETG material**:

- Before Staining: PETG material exhibits slightly higher L* values compared to PU and PETC, indicating a lighter color. The values of a* and b* are positive, indicating a slight reddish and yellowish tint.

- After Staining: After staining, there is a decrease in the L* value, indicating darkening, and an increase in the values of a* and b*, suggesting an increase in red and yellow components. The skewness and kurtosis values also show changes in distribution shape post-staining.

II. **PU Material**:

- Before Staining: The mean values for L*, a*, and b* indicate a relatively light color with slightly positive values for a* and b*, suggesting a slight reddish and yellowish tint. The standard deviation is relatively low, indicating consistency in color distribution.

- After Staining: There is a noticeable decrease in the L* value, indicating darkening of the material after staining. The values of a* and b* also increase, indicating an increase in red and yellow components. The skewness and kurtosis values show changes in the distribution shape after staining.

III. **PETC MATERIAL**:

- Before Staining: Similar to PU material, PETC also exhibits relatively light color characteristics with positive values for a* and b*. The standard deviation is low, indicating uniform color distribution.

- After Staining: After staining, there is a decrease in the L* value, indicating darkening, and an increase in the values of a* and b*, suggesting an increase in red and yellow components. The skewness and kurtosis values indicate changes in distribution shape post-staining.

In summary, all three materials show similar trends in color changes after staining, with a decrease in lightness (L*) and an increase in redness (a*) and yellowness (b*). However, there are slight variations in the magnitude of these changes among the materials, as indicated by differences in mean values and standard deviations. These findings provide valuable insights into the color stability and performance of the materials in orthodontic applications.

The table below displays the results of Tukey's multiple comparison tests, which are utilized to determine significant differences between the means of multiple groups. Let's break down the information provided:

- **PU Material, PETC Material, PETG Material**: These columns represent the different materials being compared.

- *L, a,* b***: These are color space coordinates representing lightness (L*), green-red (a*), and blue-yellow (b*) components of the color.

- **t-value**: The t-value measures the magnitude of the difference between the means of two groups, considering the variability within the groups. Higher absolute t-values indicate larger differences between the means.

- **p-value**: The p-value is the probability of observing a t-value as extreme as the one calculated from the data, assuming that there is no significant difference between the means of the groups. Smaller p-values indicate stronger evidence against the null hypothesis (no difference).

- **Interpretation**:

- For PU Material, the p-value is 0.175769, indicating that there is no significant difference in color properties between PU and PETC materials.

- For PETC Material and PETG Material, the p-value is less than 0.05 (0.000368 and 0.069941, respectively), suggesting significant differences in color properties between PETC and PETG materials compared to PU material.

**Conclusion**: Based on these results, there are tatistically significant differences in color properties between PETC and PETG materials compared to PU material.

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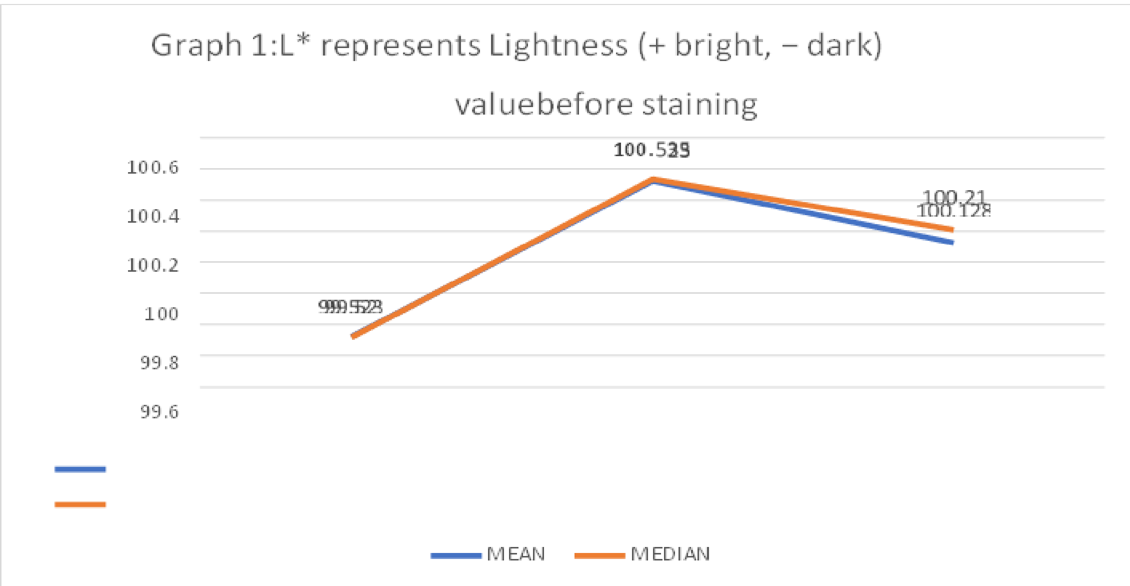
However, there is no significant difference between PU and PETC materials.

- **Significance**: The table also cant or not. In summary, Tukey's multiple comparison tests help identify which materials exhibit significant differences in color properties, providing valuable insights for the evaluation and selection of materials in various applications. provides a summary of the significance of the results, indicating whether each comparison is statistically signifi

| | **PET-G MATERIAL** | | | **PU MATERIAL** | | | **PETC MATERIAL** | | |
|---|---|---|---|---|---|---|---|---|---|
| | **L*** | **a*** | **b*** | **L*** | **a*** | **b*** | **L*** | **a*** | **b*** |
| **t- value** | 77.11772 | -1.49675 | -30.386 | 67.0120 | -0.93917 | -35.19786 | 46.74418 | -3.56493 | -58.78953 |
| | p-value is greater than 0.00001 | p-value is 0.069941 | p-value is greater than 0.00001 | p-value is greater than 0.00001 | p-value is 0.175769 | p-value is greater than 0.00001 | p-value is greater than 0.00001 | p-value is 0.000368 | p-value is greater than 0.00001 |
| | Significant result | Not significant result | Significant result | significa ntresult | not significant result | Significant result | Significant result | Significant result | Significant result |

**Table 4:** Tukey's multiple comparison tests




| | PU | PETG | PETC |
|---|---|---|---|
| MEAN | 99.523 | 100.523 | 100.128 |
| MEDIAN | 99.52 | 100.535 | 100.21 |

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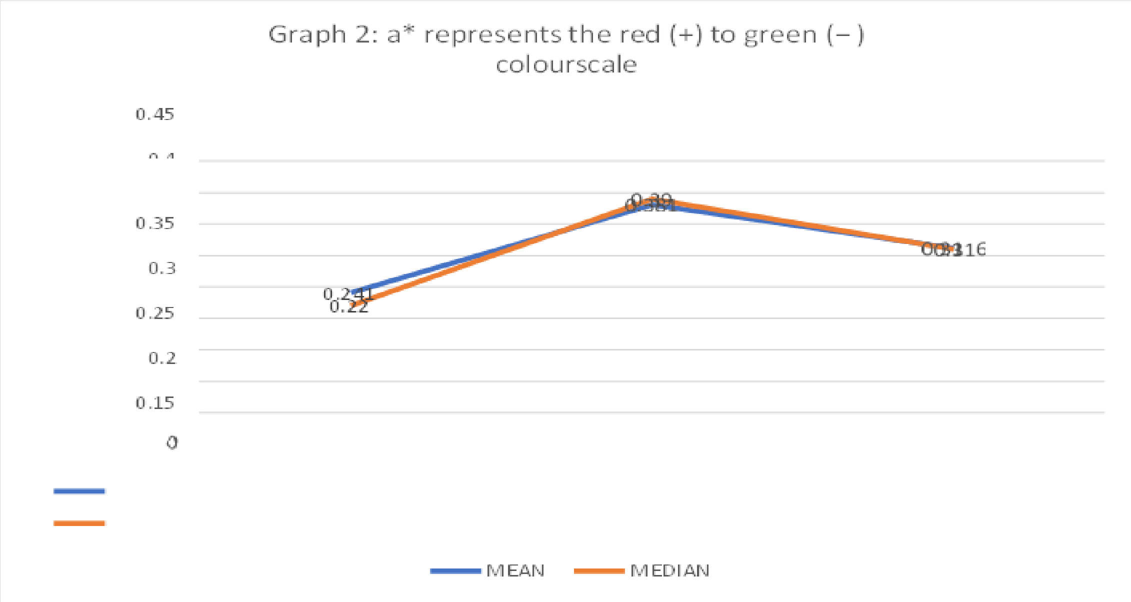
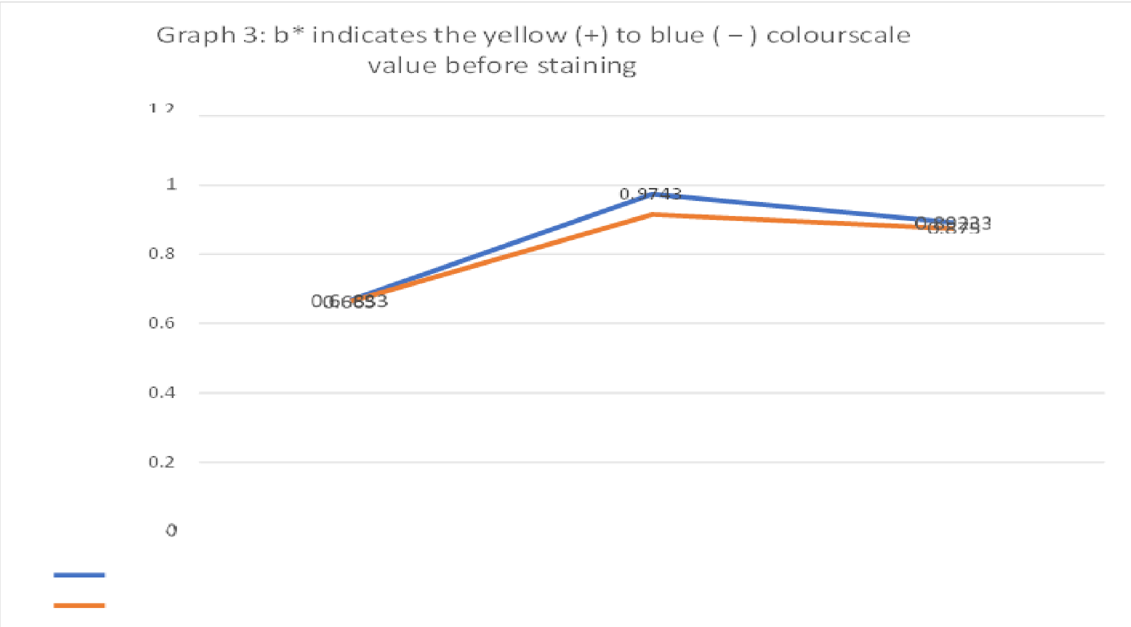



| | PU | PETG | PETC |
|---|---|---|---|
| MEAN | 0.241 | 0.381 | 0.3116 |
| MEDIAN | 0.22 | 0.39 | 0.31 |




| | PU | PETG | PETC |
|---|---|---|---|
| MEAN | 0.66833 | 0.9743 | 0.89233 |
| MEDIAN | 0.665 | 0.915 | 0.875 |

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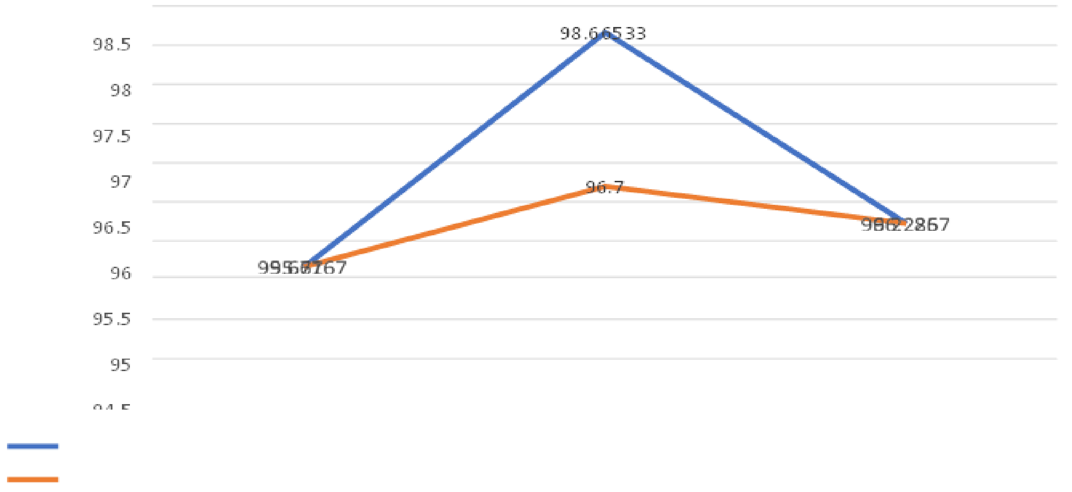
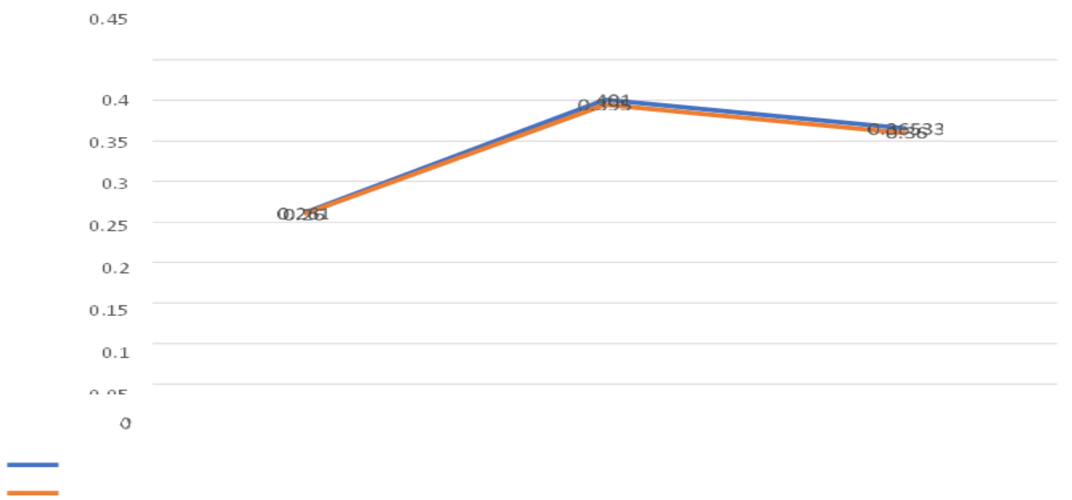
Graph 4:L* represents Lightness (+ bright, – dark) valueafter staining




| | PU | PETG | PETC |
|---|---|---|---|
| MEAN | 95.67167 | 98.66533 | 96.22867 |
| MEDIAN | 95.676 | 96.7 | 96.225 |

Graph 5: a* represents the red (+) to green (– ) colourscale




| | PU | PETG | PETC |
|---|---|---|---|
| MEAN | 0.261 | 0.401 | 0.36533 |
| MEDIAN | 0.26 | 0.395 | 0.36 |

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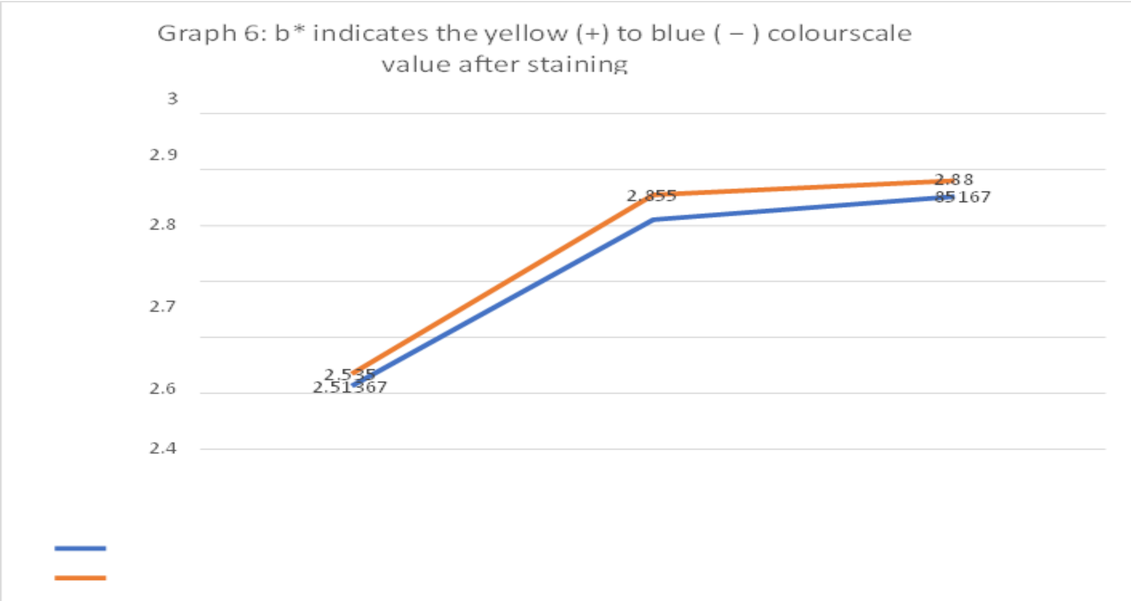

Graph 6: b* indicates the yellow (+) to blue ( − ) colourscale value after staining

| | PU | PETG | PETC |
|---|---|---|---|
| MEAN | 2.51367 | 2.81033 | 2.85167 |
| MEDIAN | 2.535 | 2.855 | 2.88 |

**Discussion:**

The comparative assessment of the optical properties of PETG, PU, and PETC-based orthodontic clear aligners exposed to a common staining agent, black coffee, has provided valuable insights into the color stability and material characteristics of these aligners. The study revealed that all three aligner materials exhibited relatively slight color changes after immersion in the staining solution for 7 days. PETG, known for its durability, transparency, and biocompatibility, demonstrated minimal color alteration, highlighting its suitability for aesthetic orthodontic treatments. PU aligners, while offering flexibility and comfort, showed a slightly higher susceptibility to color change, possibly due to the pigment adsorption associated with its surface chemistry.

The introduction of PETC-based aligners presents a promising alternative Despite its recent introduction to the market, PETC aligners exhibited comparable color stability to PETG, suggesting their potential as a viable option in clear aligner therapy. However, further research is warranted to explore and optimize the mechanical and chemicophysical properties of PETC-BASED alignersfor broader clinical applications.

These findings highlight the importance of patient compliance and clinician guidance in maintaining the aesthetic integrity of clear aligners during treatment. Education regarding dietary restrictions and proper aligner care protocols can mitigate the risk of staining and ensure optimal treatment outcomes. Additionally, ongoing advancements in material science and manufacturing techniques offer promising avenues for enhancing the color stability and performance of orthodontic aligners. The findings of this study shed light on the optical properties and color stability of three common materials used in the fabrication of clear orthodontic aligners: Polyurethane (PU), polyethylene terephthalate copolyester (PETC), and polyethylene terephthalate glycol (PETG).

**Polyethylene Terephthalate Glycol (PETG):** PETG, derived from PET by adding glycol during polymerization, offers transparency and durability. Its flexibility and hardness allow for effective orthodontic alignment. PETG aligners exhibited slight color changes after staining, but less pronounced compared to PU aligners. The observed color changes in PU aligners

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may be attributed to their susceptibility to pigment adsorption, likely due to the presence of '-NHCOO-' groups, which form hydrogen bonds with hydrophilic pigments. In contrast, PETC and PETG aligners, with less polar surface groups, exhibited greater color stability

**Polyurethane (PU):** PU, a flexible polymer, offers tailored treatment options due to its varied degrees of elasticity. Its endurance ensures the aligners maintain their shape throughout treatment, contributing to patient comfort. PU aligners, when appropriately manufactured, are resistant to staining, which preserves their aesthetic appeal. Despite its advantages, PU may exhibit slight color changes when exposed to staining agents, potentially affecting its long-term visual appeal.

**Polyethylene Terephthalate Copolyester (PETC):** PETC, a newer material, boasts dimensional stability, excellent clarity, and durability. These qualities make it an attractive choice for clear aligner fabrication. In this study, PETC-based aligners demonstrated minimal color changes after exposure to staining agents, indicating their robust color stability and suitability for orthodontic treatment.These results highlight the importance of patient compliance with orthodontist recommendations, particularly regarding aligner removal before eating or drinking, especially for those who consume staining agents like various foods and beverages.

The procedure was as follows:

The materials selected were polyethene Terephthalate Glycol (PETG), Polyurethane (PU), and Polyethylene Terephthalate Copolyester (PETC) for aligner fabrication. The unexposed aligner samples were then subjected to UV-visible spectrophotometric analysis to establish baseline optical properties. Once that was established, aligner samples were immersed in a staining agent (black coffee) for 7 days to simulate exposure to common staining agents. After 7 days, aligner samples were washed and subjected to UV-visible spectrophotometric analysis to assess color changes. Color changes ($\Delta E^*$) were calculated using the CIE L*ab** color system and converted into National Bureau of Standards (NBS) units. Fourier Transformation Infrared (FT-IR) spectroscopy and scanning electron microscopy (SEM) were conducted to observe molecular and morphological alterations on the aligner surfaces. Statistical tests, including t-tests and Tukey's multiple comparison tests, were performed to determine significant differences in color properties between materials. Results were interpreted in the context of material properties and implications for orthodontic treatment. Conclusions were drawn regarding the suitability of each material for clear aligner fabrication, along with recommendations for future research directions.

**future research directions:**

Enhancing the color stability and mechanical properties of aligner materials remains an ongoing area of research. Surface modifications, such as creating superhydrophobic surfaces using low surface energy materials or fluorinated compounds, hold promise for improving color stability. Blending modification approaches, such as combining PETG with other polymers like polycarbonate (PC) or thermoplastic PU, may yield aligner materials with superior mechanical properties and color stability.

In conclusion, while all three materials offer unique advantages, PETC emerges as a promising option for clear aligner fabrication due to its excellent color stability and mechanical properties. However, continued research and innovation are necessary to address the aesthetic and practical requirements of orthodontic aligner materials, ensuring optimal patient outcomes.

**Conclusions:**

In summary, this study contributes to the growing body of knowledge concerning the optical properties and clinical implications of clear aligner materials. By elucidating the factors influencing color stability and material behaviour, clinicians can make informed decisions when selecting aligner materials and advising patients on treatment experience and expectations. Ultimately, the pursuit of aesthetic excellence in orthodontic therapy must be balanced with considerations of functionality, durability, and patient satisfaction to achieve successful outcomes in modernorthodontic practice.

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**Abbreviations:**

PU – Polyurethane

PETG – Polyethylene terephthalate glycol PETC – Polyethylene terephthalate copolyester

CIE L*a*b* - Commission Internationale de I'Eclairage L*a*b* colour system NBS – National Bureau of Standards

FT-IR - Fourier transformation infrared SEM – Scanning electron microscopy