

# Assessment of some physical and chemical properties of orthodontic composite after incorporating nano theobromine

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## ABSTRACT

**Objectives.** The study aimed to assess the shear bond strength, changes in FTIR, and degree of conversion for the primer of orthodontic composite after incorporating nano theobromine powder.

**Materials and methods.** Transbond <sup>XT</sup> light cure adhesive Resin was modified by incorporation of theobromine nanoparticle powder in 10% and 15% concentrations. Twenty-four metal brackets attached to premolar teeth were used to test the shear bond

strength, with eight samples for each group. Fifteen samples from the control and the experimental groups were prepared to measure FTIR and the degree of conversion of the primer from monomer to polymer. The differences among groups were analyzed using the ANOVA test at  $p < 0.05$ .

**Results.** The shear bond strength was higher in the group modified with 15% nano theobromine (20.13 Mega Pascal) than in the other groups. On the other hand, the experimental nano theobromine groups yielded no significant change in the degree of conversion when compared to the control. Fourier-transformed infrared spectroscopy also showed no specifically determined chemical changes after nano theobromine powder incorporation.

**Conclusion.** From the current study, it could be concluded that the experimental composite particularly 15% nano theobromine has good physical and chemical properties, which makes it recommendable for successful use in dental practice.

**Keywords:** Degree of conversion, Nano, Shear bond, Theobromine

## INTRODUCTION

The bonding of orthodontic brackets to the enamel of the tooth surface has been an important issue since the introduction of direct bonding in orthodontics. Many bonding agents have been developed such as composite resins with different mixing and polymerization mechanisms [1,2]. Primer is usually an unfilled resin that is employed as part of the bonding process, particularly with light-cured composites. Its main goal is to penetrate the enamel surface and improve the final bond's efficacy [3].

Due to limited accessibility to clean tooth surfaces during treatment, bacterial adhesion, colonization, and proliferation around orthodontic brackets specifically *Streptococcus mutans* increase. The products of these bacteria lead to demineralization of enamel and increase the risk of dental caries [4,5]. Modern preventive dentistry aims to stop the progress of dental caries around orthodontic brackets using non-invasive methods such as antibacterial and/or remineralization toothpaste or mouthwashes [6,7].

One of these promising aspects is the orthodontic bonding that contains potential remineralization materials that prevent enamel demineralization around orthodontic brackets [8]. Previous studies have focused on incorporating fluoride which plays a significant role in the reduction of dental caries [9–11]. Shortcomings of fluoride incorporation in the composite is represented by the majority of fluoride released during the setting process, with a minor quantity of long-term release [12,13]. Moreover, some studies suggested that fluoride may reduce the shear bond strength of the orthodontic brackets [14,15].

Other agents, such as silver, titanium oxide, and quaternary ammonium, have also been incorporated into bonding systems. However, some of these agents impaired the mechanical properties of the materials [16]. Besides this, these agents reduced the degree of conversion and surface roughness, which may affect bacterial adhesion [17].

A new class of bonding agents is the nano-composites, which contain nano-fillers within its constituents. The included filler enhances the mechanical properties, such as shear and compressive strength by reducing polymerization shrinkage due to the reduced particle dimensions and wide size distribution. Additionally, it may reduce surface roughness, which is one of the major contributing factors to bacterial adhesion [18,19].

The use of compounds derived from natural resources has been extremely successful in the development of new medications. One of these products is theobromine derived from Theobroma Cacao. In the calcium and phosphate-rich medium, theobromine forms larger hydroxyapatite crystallites, and the enamel is reinforced and becomes less susceptible to acid attacks of bacterial products and consequently dental caries [20,21]. Moreover, theobromine improves crystallinity by causing less net dissolution of the different minerals from the exposed enamel surface [22,23].

There have been recent attempts to replace fluoride with theobromine as a remineralizing agent and as a potential substitute for fluoride particularly in the mouthwashes and toothpaste [21,24].

Elsherbini, (2020) recorded that following the application of theobromine, the microhardness of the enamel surface increased, potentially indicating that theobromine generally has protective properties for enamel [22].

Limited information is available about the natural products incorporated in orthodontic adhesive, particularly in the primer rather than the composite itself [25]. According to our best knowledge, no study evaluated the effect of adding nano theobromine product into the orthodontic primer.

Thus, this study aims to estimate the effects of incorporating nano theobromine powder with an orthodontic primer on the shear bond strength (SBS) of orthodontic brackets. Assess the effects of this incorporation on chemical properties and degree of conversion of orthodontic primer. The study hypothesis is that there is a significant increase in the shear bond strength of orthodontic adhesive or a change in the chemical properties of orthodontic primer after incorporating nano theobromine.

## 22 MATERIALS AND METHODS

The ethical clearance was obtained from the Research Ethics Committee of the College of Dentistry, University of Mosul in 2023 [UoM.Dent.23/31]. In regards SBS, the samples consisted of 24 extracted human premolars [upper first premolars], which, in general, had normal sizes and shapes. These were taken out of patients between the ages of 16 and 28 in order to be used in orthodontic treatments.

33 The selection criteria for teeth included the absence of hypo-plastic areas, caries, attrition, cracks, severe irregularities, restorations, and any history of prior treatment with orthodontics or endodontia. The labial surface of the teeth was evaluated using a x5 magnifier to ensure the soundness of the chosen teeth. Soft tissue remnants were cleaned up and eliminated. After extraction, the samples were kept at room temperature (about 22 C°) in distilled water. For the remaining research experiments, the water was replaced every week to prevent microbial growth .

## Sample grouping and material

The orthodontic adhesive used in this study was 3M<sup>TM</sup> Transbond XT light cure adhesive (3M ESPE, St. Paul, MN, USA). Theobromine powder purchased from Sigma-Aldrich (Italy), molecular formula [C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>], purity ≥98,0%, and molecular weight 180,16 g/mol. Ball milling is a mechanical milling method to fabricate nanomaterials, one of the most widely used top-down techniques to produce nano-particles is mechanical milling.

The teeth were randomly divided into the following:

The control group consisted of eight teeth subjected to 3M<sup>TM</sup> Transbond XT without any modifications. Experimental (1) consisted of eight teeth subjected to bond mixed with at a concentration of 10%. This was obtained by incorporating 10 % of nano theobromine, by weighing 0.0034g of nano theobromine into the 0.03g primer [0.0034+0.03= 0.0334, 0.0034/ 0.0334= 0.99×100=10% suspension solution]. Experimental (2) consisted of eight teeth subjected to bond mixed with at a concentration of 15%. This was obtained by incorporating 15% of nano theobromine, by weighing a 0.006 g of nano theobromine into 0.034 g primer [0.006+ 0.034= 0.04, 0.006/ 0.04= 0.15×100=15% suspension solution]. This concentration was used in the study, considering the higher concentration of nano theobromine incorporated that maintained the appearance of the surface mixture.

To achieve a uniform color distribution and complete wetting of the nanoparticles within the resinous material, manual mixing with a plastic spatula was conducted for about 60 seconds in a semi-dark environment. The modified orthodontic adhesive was placed inside a sterile disposable dispenser and taped with dark-colored tape.

## Teeth processing and shear measurement

Each tooth was mounted into a plastic ring with 26 mm in height, 18 mm inside diameter, and 20 mm outside diameter<sup>[26]</sup>. The teeth were polished for ten seconds using fluoride-free pumice using a rubber polishing cup and a low-speed handpiece after the cold cure resin had solidified. After giving the enamel surface a thorough 10-second water rinse to get rid of any pumice or debris, the teeth were prepared for use.

Each buccal surface was treated with 37% phosphoric acid for approximately 15 seconds, followed by a 10-second water wash per the manufacturer's instructions. The teeth were then air-dried using a triple syringe, and a chalky look was noticed. Next, standard bracket (Dentaurum, Germany) was hold and a layer of composite adhesive was then applied to the bracket's base. The bracket was centered into the center of the buccal surface of the premolar tooth's crown, about 4.5 mm from the occlusal surface. The excess composite was then removed by a dental explorer prior to curing. The curing process was then started using a hand-held dental curing light (Guilin Woodpecker Medical Instrument Co., Ltd). Using an intensity of  $900 \text{ mW/cm}^2$ , which was determined by using a light-intensity tester. On the occlusal, mesial, distal, and gingival aspects, the curing light was applied for 20 seconds each, with the light curing machine's tip positioned between the bracket margins by about 1-2mm [26].

After bonding, all samples were stored in distilled water at room temperature for 24 hours and subsequently, the universal testing machine was utilized for SBS measurement [27]. The force required to remove the brackets was measured in Newtons (N) at a crosshead speed of 0.5 mm/min. For shear testing, the specimens were secured in the lower jaw of the machine so that the bracket base paralleled the direction of the shear force (Fig.1). Then, an electronic recording of the results of each test was done. The applied force at fracture time was recorded in Newton then it was converted into (MPa) by dividing the debonding force by the surface area of the bracket which is (12.65mm) ( $\text{MPa}=\text{N/mm}^2$ ).

#### **Fourier-Transformed Infrared Spectroscopy (FTIR)**

With a wavelength range of  $400\text{--}4000 \text{ cm}^{-1}$ , the CL alpha-PFTIR spectrophotometer was used to perform Fourier-transformed infrared spectroscopy Alfa Bruker Machine (Bruker, Germany). The infrared spectra bands for non-cured orthodontic adhesive alone, cured orthodontic adhesive alone, non-cured orthodontic adhesive modified with 10% (after mixing) of nano theobromine, cured orthodontic adhesive modified with 10% nano theobromine, non-cured orthodontic adhesive modified with 15% nano theobromine, cured orthodontic adhesive modified with 15% nano theobromine.

#### **Determine the degree of conversion**

The calculation for the percentage of the conversion process from monomer to polymer according to the following:

- 1- The monomer mixtures were photo-cured.
- 2- The percentage of degree of conversion from monomer to polymer for the materials under study was calculated according to the equation: as follows [28]:

$$\text{RDB \%} = 1 - [ R_{\text{cured}} / R_{\text{uncured}} ] \times 100$$

Where R represent the peak absorption of the vinyl group in 3M primer material; aromatic and aliphatic bonds ratio before and after polymerization respectively.

It is important to determine the peaks of the functional groups in the organic compounds before and after the photochemical reaction, where before the light radiation value of carbon-carbon double bonds represents the origin of all double bonds in the compound. The most light-cure dental materials their absorption bands of  $1628\text{--}1640\text{ cm}^{-1}$  and the C-C aromatic absorption band at  $1600\text{--}1612\text{ cm}^{-1}$  which did not contribute in the polymerization reaction [29]. Shape of the most bands before and after the irradiation process is not affected except for the carbon-carbon double bonds, especially the materials used in dental [30].

Double bonds remaining for the behavior of resin compounds were evaluated, where analysis was done using FTIR-ATR for three specimens. it was noticed the change in the shape of the beam where decreased their intensity at  $1637\text{ cm}^{-1}$  and the rest of the packages as expected to appear [31,32], whether for the monomer or the polymer, according to the figures of FTIR analysis.

The number of remaining monomers has been calculated in order to estimate the conversion ratio from monomer to polymer according to the mentioned equation.



## RESULTS

### Shear Bond Strength

The assessment of data normality of distribution has shown that most data along SBS bonded groups followed a normal distribution. The descriptive data for SBS is presented in Table [1]. The analysis of bonded groups revealed that the group modified with 15% nano theobromine had the highest SBS mean value among the groups.

**Tab 1:** The descriptive statistics for the SBS after mixing with nano theobromine

Variable	Mean	SD±	Minimum	Maximum
Control	20.13	6.24	13.54	32.02
Modified with 10% nan theobromine	20.11	8.11	10.85	36.78
Modified with 15% nan theobromine	21.28	6.99	10.83	32.12

Measurement unit is mega Pascal.

A one-way ANOVA was used to evaluate the relationship between nano theobromine concentrations and shear bond strength. The ANOVA was non-significant at the 0.05 level as F value= 0.07,  $p = 0.093$ .

The chemical characteristics of the orthodontic adhesive before and after mixing with nano theobromine of all groups were determined by the FTIR device (Tab. 2). The materials used under study [nana theobromine] showed the expected peaks presented in Figure 1.

**Tab 2:** Description of the chemical bonds in nanothermometer

3149.98 & 3113.32 $\text{cm}^{-1}$	stretching vibration of the -[N-H] group
3016.40 $\text{cm}^{-1}$	stretching vibration of the =[C-H] group
2885.09, 2825.76 $\text{cm}^{-1}$	symmetrical and asymmetrical stretching vibration of the -[CH <sub>3</sub> ] group
1683.09, 1663.50 $\text{cm}^{-1}$	symmetrical and asymmetrical stretching vibration of the [C=O] group
1591 $\text{cm}^{-1}$	stretching vibration of the [C-C]group
1545 $\text{cm}^{-1}$	stretching vibration of the [C=C]group
1485 $\text{cm}^{-1}$	stretching vibration of the [C-N]group

[33,34]

A bond product from a company under the common brand name (Transbond<sup>XT</sup> adhesive primer) under study was used. Its FTIR has been measured as a control specimen (Tab. 2) through the absorption peaks as shown in figures 3, 4, and 5.

**Tab 3:** Shows the description of the chemical bonds in 3M<sup>TM</sup> Transbond XT adhesive primer

3487.97 $\text{cm}^{-1}$	stretching vibration of the -[O-H] group
3106] $\text{cm}^{-1}$	stretching vibration of the =[C-H] aliphatic vinyl group
3085 $\text{cm}^{-1}$	stretching vibration of the =[C-H] aromatic ring group
2958.32, 2928.29 & 2874.20 $\text{cm}^{-1}$	symmetrical and asymmetrical stretching vibration of the -[CH <sub>3</sub> ] group
1714.47 $\text{cm}^{-1}$	stretching vibration of the [C=O] group
1636.50 $\text{cm}^{-1}$	the stretching vibration of the [C=C] aliphatic vinyl group

1608.17 & 1581.82 $\text{cm}^{-1}$	stretching vibration of the [C=C] in aromatic ring group
1509.27 $\text{cm}^{-1}$	stretching vibration of the [C-C] in aromatic ring group
1378.18 $\text{cm}^{-1}$	stretching vibration of the $-\text{CH}_3$ group
1295 $\text{cm}^{-1}$	stretching vibration of the cyclic ether [epoxy]
1040.60 $\text{cm}^{-1}$	stretching vibration of the ether [C-O-C],

[28,35]

Referring to the spectra of the FTIR spectra [after mixing and curing], the control sample [cured orthodontic adhesive] showed a band at wave number  $3488.21 \text{ cm}^{-1}$  that is broad and belongs to the O-H vibration absorption of [Bis-GMA], while the specimens under study for the two concentrations of 10% and 15% showed absorption bands in the range  $3491.85$  and  $3478.34 \text{ cm}^{-1}$ , which are due to the stretching vibration of the hydroxyl group, while distinct absorption bands at  $2964.37 \text{ cm}^{-1}$  in the control,  $2956.12 \text{ cm}^{-1}$  in 10% and  $2954.98 \text{ cm}^{-1}$  in 15% and for saturated C-H stretching of alkanes in [TEGD and Bis-GMA].

The absorption bands at  $1715-1716 \text{ cm}^{-1}$  indicated due to the vibration stretching absorption was due to the carbonyl bond, and no change occurred before and after the polymerization process, while the absorption bands at  $1636 \text{ cm}^{-1}$  were due to the double bond stretching vibration, the intensity of which had decreased significantly after the polymerization process, unlike the band at  $1607 \text{ cm}^{-1}$ . Which is due to the stretching vibration of the single bond, which increases in intensity after the polymerization process due to photo curing along the conjugated system of [Bis-GMA and TEGDMA] [36,37].

The absorption bands at  $1581-1509 \text{ cm}^{-1}$  confirmed the extensions of aromatic C=C bands. Finally, the strong C-OH stretching of the alcoholic group Bis-GMA at  $1038 \text{ cm}^{-1}$  and  $860 \text{ cm}^{-1}$  of the C=C bend is out of the plane of the phenolic ring of [BHT] [36]. When comparing the FTIR spectra of the modified adhesive with nano theobromine with the control group, it was shown that no specifically determined chemical changes after the modification of the orthodontic adhesive as seen in figures 6, 7, and 8.

There is a large overlap between the absorption bands of the additive material and the absorption bands of the binder, due to most of their active groups appearing in approximately the same region of the spectrum, the absorption bands of the binder were dominant on the spectrograph paper. Therefore, when the FTIR measurement was taken before the irradiation process and after the irradiation process we did not notice significant differences in the shape and values of most of the peaks except for the two bonds, which belong to the double bond of the aliphatic vinyl group, which was significantly reduced, in contrast to the single bond which increased [38,39]

The results showed that there is the same behavior, except for the expected difference in the degree of conversion. The degree of conversion from the monomer to the polymer followed up by spectrum, Undoubtedly was the best method [31].

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### Degree of conversion

The descriptive data DC is presented in table (4). Data involved the mean, standard deviation, minimum and maximum values. The analysis of bonded groups revealed that the group modified with 10% nano theobromine had the highest mean value in comparison with the control group. A one-way ANOVA was used to evaluate the relationship between nano theobromine concentrations and DC. The ANOVA was non-significant at the 0.05 level as F value= 1.22,  $p = 0.309$ .

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**Tab 4:** Shows the descriptive analysis of degree of conversion for the study groups

Variable	Mean	SD±	Minimum	Maximum
Control	65.44	0.85	64.00	66.42
Modified with 10% nano theobromine	65.62	0.57	64.67	66.98
Modified with 15% nano theobromine	65.10	1.18	63.04	66.76

## DISCUSSION

During treatment, orthodontic brackets are subjected to various forces. An essential step in evaluating the effectiveness of an adhesive system for use in orthodontics is the shear bond strength. In the current study, we incorporated nanoparticles into the primer rather than composite which could be considered a more applicable approach and beneficial from a clinical viewpoint, since it comes into direct contact with the enamel surface that represents the target area for preventive attempts. Therefore, this is the first study that conducted to investigate the shear bond strength of orthodontic brackets that used primer containing theobromine nanoparticles.

Results of the current study showed an increase in SBS indicating that the modified adhesive had sufficient resistance to shear stress with no adverse effect on the SBS of the tested primers. Generally, this result is comparable with studies that incorporated nanoparticles in Transbond XT adhesive [3M Unitek, USA] such as Toodehzaeim et al. [40], however, disagree with Alkhayat [41] who showed that the addition of AgNPs to Heliosit orthodontic adhesive either alone or mixed with the TiO<sub>2</sub>NPs significantly increases the SBS values.

Comparisons with previous studies that incorporated natural products nanoparticles were contradictory. For example, some studies [37] found that the incorporation of 1%, and 3% cinnamon nanoparticle powder in the orthodontic composite resin resulted in a reduction in SBS with no statistical difference. Whereas, [42] who studied SBS of composites

containing clove nanoparticles found a significant decrease in shear bond strength at 10% concentration compared to the control group. However, shear bond strengths in 2% and 5% clove nanoparticle groups were still in the range of acceptable clinical values. Researches have showed that incorporating 1% chitosan nanoparticles with Transbond™ XT orthodontic adhesive primer increased the orthodontic shear bond strength; however, increasing the percentage of nanoparticles to more than 1% reduced the bond strength [43].

In regards to natural products that used essential oils, the current study disagree with Al-Thiab & Al-Khatib how incorporated zingiber officinale essential oil in 1% and 2% concentrations with orthodontic adhesive [44]. Also, Mohammed who used 1% and 3% lavandula angustifolia and thymus vulgaris essential oil respectively [45]. However, Mohammed found that lavandula anustifolia, particularly 1% non-significantly reduced the shear bond strength [45].

It is important to mention that, the initial increase in SBS of orthodontic adhesive may be attributed to the nanofiller. Because, nanofillers can improve adhesion at the interface between the material and the tooth structure through increasing mechanical strength of the adhesive layer and providing structural reinforcement [46].

The DC is a parameter of principal importance in the light-curing procedure, as it shows the percentage of a resin material that has been polymerized. The DC for light-cured polymers used in orthodontics depends on several factors such as monomer chemical structure, filler size, and polymerization conditions [47].

The high DC is an indicator for better physical properties of the material such as microhardness, resistance to wear, bond strength, and lower degradation over time. It is generally accepted that greater DC is associated with higher hardness [48]. Although minimal values for the DC in clinical orthodontics have not been fully documented yet; in restorative resins the range for the DC is 55–75% [47,49].

The results of the current study have shown no significant change in DC after incorporation of theobromine. It is difficult to compare the results of the current study with those that incorporated different products into the orthodontic adhesive or even dental

composite, however, this result agrees with researchers who assessed the effects of incorporating 1.3% of zinc oxide nanoparticles into the synthesized adhesive and recorded no significant effects on physical and mechanical features including DC [50]. Also, the current results agree with studies that found that the incorporation of 3% TiF<sub>4</sub> degree in dental primer U-Bond orthodontic adhesive might not affect the DC [51].

However, the current results disagree with Degrazia et al. [17] who found that the incorporation of silver nanoparticles with Transbond™ XT primer leads to reduction of DC in higher concentrations of silver nanoparticles.

Due to the nature of theobromine powder, it is expected to get an increase in the viscosity of the primer. A study by de Araujo et al. showed that there is an inverse relationship between the viscosity of the material and it is DC, as the low viscosity resins tend to have higher DC [52]. However, no significant change in DC was observed in the current work. Farzanegan et al. [53] indicated that incorporating chitosan nanoparticles into Transbond<sup>XT</sup> orthodontic adhesive decreases SBS of composite resins and have adverse effects on the DC of composite resins. In addition, they mentioned that nanoparticles may be agglomerated in the form of particles that act as stress-concentrating centers in the polymer matrix.

Although the current study did not aim to assess the relationship between SBS and DC, it is worth mentioning that researchers such as Perković et al. [47] assessed the correlation between SBS and DC in conventional and self-adhesive systems used in orthodontic bonding procedures. They recorded a weak or mild correlation between SBS and DC in conventional adhesives.

Generally, nanofillers can improve adhesive properties mainly at the interface between the composite and enamel surface of the tooth by increasing mechanical strength and interdigitation of the adhesive layers and consequently elevating the structural reinforcement [46].

It is interesting to mention that the quantity and distribution of nanofiller particles are of prime importance as these particles may act as an elastic layer between the adhesive composite and the enamel surface, that in turn be as stress absorbing media [46].

Moreover, inter-particle forces like Van der Waals and magnetic attraction as well as electrostatic forces become stronger, they may alter the enamel surface energy by increasing the minor galvanic current inside the material and/or improve the coefficient of thermal expansion and the dimensional stability [54].

Akhavan et al. [46] recorded that the incorporation of limited concentrations of nanoparticle fillers may not interfere with the polymerization of light-cure composite resin, only higher concentrations of nanoparticles may affect the polymerization reaction. This due to darker shades and the reduction of translucency that produced by some types of the nanoparticles that reduce the ability of light penetration to complete polymerization reaction [40,54].

## CONCLUSION

From the current study, it could be concluded that the incorporation of nano theobromine particularly at 15% concentration may not affect the properties of adhesive primer. For that reason, it can added to the composite to improve the expected remineralization effects.

## CLINICAL IMPLICATIONS

The prevention of dental caries during and even after orthodontic treatment is a major concern for dental clinicians. As the prevalence of white spot lesions is expected to increase around brackets, development of new materials to be incorporated with the orthodontic adhesive is mandatory. Adding nano theobromine which has an expected remineralization activities to the primer rather than composite may increase the susceptibility of the dental composite to reduce the white spot lesions around brackets without any adverse effects on SBS.

## CONFLICT OF INTEREST



The authors declared that there is no conflict of interest regarding this manuscript.

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**Fig. 1:** The SBS testing in a universal testing machine with a knife-edged blade

**Fig. 2:** Chemical structure of nanothermometer

**Fig. 3:** Shows the chemical analysis of the orthodontic primer before polymerization

**Fig. 4:** Shows the chemical analysis of the orthodontic primer with 10% nano theobromine before polymerization

**Fig. 5:** Shows the chemical analysis of the orthodontic primer with 15% nano theobromine before polymerization

**Fig. 6:** Shows the chemical analysis of the orthodontic primer after polymerization

**Fig. 7:** Shows the chemical analysis of the orthodontic primer with 10% nano theobromine after polymerization

**Fig. 8:** Shows the chemical analysis of the orthodontic primer with 15% nano theobromine after polymerization







