ORIGINAL ARTICLE

CHEMICAL CHARACTERIZATION OF SILORANE BY FTIR AND RAMAN SPECTROSCOPY

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ABSTRACT

Background: Silorane, introduced to the dentistry recently. It is named after the functional groups present in the material i.e. Siloxane and Oxirane. It is introduced in the market to overcome the main problems of composite resins i.e. Polymerization shrinkage. Claims are being made that the polymerization shrinkage have been overcome in the material and the material results in less than 1% polymerization shrinkage. The material claims to have properties which may fulfil the criteria of being the ideal restorative materials of all times.

Objective: : To confirm the presence of Siloxane and Oxirane in the chemical structure of the Silorane by Fourier Transform Infra-red (FTIR) and Raman Spectroscopy.

Methods: Solvation of Silorane was done in Tetrahydrofuran (THF) using the magnetic stirrer. After the evaporation of THF, the resultant powder was then evaluated under the FTIR and Raman Spectroscopy.

Results: The FTIR spectrum of Silorane shows some primary reference bands in the spectrum of Silorane and shows the absorption of primary oxirane bands. The peaks indicated the presence of Siloxane bands and CH groups.
Raman spectrum of Silorane confirming the presence of v phase of Siloxane. The peaks show the presence of O-Si-O and C = C group.

Conclusion: The FTIR and Raman spectrums confirms the presence of Siloxane and Oxirane bands which results in low polymerisation shrinkage due to the cationic ring opening mechanism when compared with methacrylates which polymerises via a free radical mechanism.

KEY WORDS: Silorane, Fourier Transform Infra-red, FTIR, Raman Spectroscopy

INTRODUCTION

Silorane has been introduced to the dentistry recently. Claims have been made by the manufacturer that the novel material shows less than 1% of the polymerization shrinkage. It is named after the functional groups presents in the materials, Oxirane and Siloxane. The hydrophobic behaviour of the material is characteristic feature of siloxane which helps in the long term intraoral physical strength of the composites. Moreover, the hydrophobic material tends to absorb very low amount of pigments of daily nutrition resulting in less exogenic staining when compared with hydrophilic material. The polymerisation mechanism of Oxiranes is by a cationic ring opening mechanism which results in low polymerisation shrinkage when compared with methacrylates which polymerises via a free radical mechanism. The polymerisation starts when acidic cation initiates, which opens the oxirane ring and forms a new carbocation, a new acidic centre. After an oxirane monomer has been added, the epoxy ring is opened to form a chain and if there are multifunctional monomers a network is formed. [1, 2] The polymerization reaction is activated by the light source and there is no difference found the transmission of light between Silorane and the conventional composites. [3] Attia et al. used Silorane based restorative material for one year clinical followup and suggested that the materials is found acceptable even after one year of clinical application. [4]

Fourier Transform Infrared (FTIR) Spectroscopy is a type of infrared (IR) spectroscopy. FTIR can be used to recognize the chemical structure and considered a useful tool for recognizing the functional groups. IR rays are passed through a sample which absorbs some rays and some rays are transmitted, which produce a unique wavelength for each molecular structure to form a spectrum. Chemical structure and bonds can be determined by interpreting this spectrum. The spectrum produced for each molecule is so unique that they are called "molecular fingerprint".

FTIR is the qualitative technique widely used for the identification of polymers. [5] There are a few types of FTIR, like FTIR-ATR (Fourier transform infrared attenuated total reflection) spectroscopy, FTIR-PAS (Fourier transform infrared photo acoustic spectroscopy) and FTIR-RAS (Fourier transform infrared reflection-absorption) spectroscopy. FTIR-ART technique can provide data on the process of releasing drugs in formulations and become a usual protocol to study the drug-penetration and drug release in membranes from pharmaceutical products. FTIR-PAS is capable of providing chemical information of transparent to opaque samples. FTIR-RAS is used for the measurement of thin films; up to the depth of 50 µm can be reached by certain ranges by this technique. (6) Fourier transform Raman Spectroscopy is one of the spectroscopic techniques developed with FTIR for the confirmation of the molecules order. It is usually used to characterize the molecular structure of the compound. [6] It characterizes the vibrational, rotational and other low frequencies in a compound.

The objective of the study was to recognize the chemical structure of Silorane by confirming the presence of Siloxane and Oxirane.

METHODS

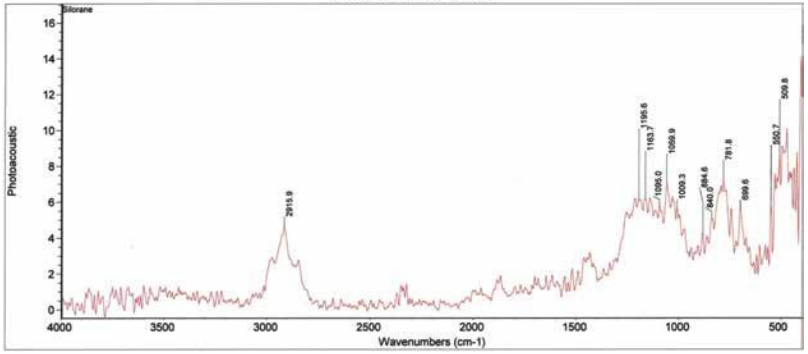
SOLVATION OF SILORANE

Silorane was obtained from 3M ESPE UK, Solvation of Silorane was done in Acetone, N, N dimethyl formamide (DMF) and Tetrahydrofuran (THF) initially. 10 ml of the solvent was taken in the glass beaker and 1 gm of Silorane was added in the beaker. The beaker is then placed on the magnetic stirrer (Model - IKA C-MAG HS 7) with a magnetic stir bar in the beaker. Silorane is then allowed to dissolve in the solvents. After the evaporation of the solvents, samples were analysed by FTIR spectroscopy. FTIR spectrum of Silorane dissolved in THF shows the close resemblance to the Silorane spectrum, showing no chemical changes.

Silorane was dissolved in THF. After the evaporation of THF, the resultant powder was then evaluated under the FTIR and Raman Spectroscopy.

Nicolet Amelga XR dispersive Raman spectrophotometer has been used for Raman spectra. And FTIR spectra were obtained by using a Nicolet 8700 FTIR spectrometer (Thermo Electron Corporation, UK) in combination with a photo acoustic sampling (PAS) cell.

Figure 1: FTIR of Silorane



RESULTS & DISCUSSION

Figure 1 shows the FTIR spectrum of Silorane. The fine structure in 884 – 886 cm^{-1} region shows some primary reference bands in the spectrum of Silorane and shows the absorption of primary oxirane bands. [7] The peak at 2915 cm^{-1} indicated the presence of CH group. Different Siloxane bands can be seen in the region of 770 – 3000 cm^{-1}. Peaks at 781, 848, 1059, 1095, 1195, 1259 and 2915 cm^{-1} indicates the v SiCH3, (SiOSi, CO) and CH3 respectively. [8]