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# ATR-FTIR, SAXS and UV-Vis Studies of Silicone Hydrogel and Bio-Hydrogel Soft Contact Lenses

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#### Authors' contributions

This work was carried out in collaboration among all authors. Author SB designed and directed the study, planned the experiments, contributed to the interpretation of the results. Authors SB, TG, Sİ, and AB performed data collection and data analysis. The first draft of the manuscript was written by authors SB and Sİ. Authors SB and TG reviewed and edited the final version of the manuscript. All authors read and approved the final manuscript.

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## ABSTRACT

**Aims:** This study aimed to evaluate the effect of contact lens materials on the structural properties and to examine ultraviolet (UVA part) and visible (Vis) transmittance with and without UV filters of the commercially available silicone hydrogel (SiHy) and bio-hydrogel (bio-Hy) soft contact lenses (CLs) *in vitro*.

**Place and Duration of Study:** Hacettepe University, Department of Physics, Ankara, Turkey, between May 2018 and May 2021.

**Methodology:**Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectra of CLs were recorded (at removing from its package, after 10 min, 1 h and 1 day at room temperature) in the 4000-650 cm<sup>-1</sup>region to estimate water contents of CLs. Hierarchical Cluster Analysis (HCA) was performed to differentiate chemical structure of CLs based on the spectral differences. Ultraviolet (UVA) and visible light transmittance of (CLs) was measured in the 315 -800 nm region. Small Angle X-ray Scattering (SAXS) analyses were performed to obtain further structural information on nano-scale.

**Results:** One of the key observations in this study is the large influence of lens water content. The HCA analysis grouped all the CLs of same brand in same cluster based on their chemical

similarity. The UVA transmittance results showed that CLs with UV blockers almost met ClassI and ClassII standards. The size (11.8-39.9 nm) and differences in morphologies of the nano globules were determined and correlated with equilibrium water content (EWC). **Conclusion:** This work was designed to explain important characteristics of commercial CLs and results will have implications for future experimental and clinical research regarding hydration/ dehydration experiments with CL polymers.

Keywords: Soft contact lenses; lens polymers; water content; ATR-FTIR spectroscopy; hierarchical cluster analysis; UV-Vis; small angle X-ray scattering.

## 1. INTRODUCTION

Hydrogels (Hy) are commonly used for the manufacture of soft conventional and disposable contact lenses. Soft contact lenses are primarily made from hydrogel or silicone hydrogel material.

The silicone hydrogel lenses (SiHy-CLs) which provides easy adaptability to the eye and allow much more oxygen to pass through to the cornea than previous soft lens materials are the largest proportion of CLs on the market today. They are widely used in an active lifestyle due to their excellent biocompatibility, comfort and optic transparency [1–8].

SiHy-CLs combine silicone based / an extremely plastic flexible hydrophobic/materials and various hydrophilic monomers/polymers such as polyvinylpyrrolidone (PVP), used to increase the surface hydrophilicity of silicone. The bulkiness of the siloxane group and high polymer chain mobility induce the high oxygen permeability of these materials [8-13]. Nowadays, over 12 different SiHy materials are available in the marketplace that are named according to the criteria of the United States Adopted Names Council (USAN). polymerization The conditions/synthesis, manufacturing processes can be altered to produce the same polymer with different properties of CLs such as wear time and comfort [8,14-16].

Water content (WC) in contact lenses is the most important lens characteristics varies depending on the type of lens and effect vision and comfort. In soft CLs, the water content ranges from 38 to 75 % that has been approved by the FDA. The most common ways of measuring WC of soft lenses are by refractometry or gravimetry [17,18]. The contact lenses is strongly influenced by dehydration and this can induce changes in oxygen permeability (Dk), oxygen transmissibility (Dk/t), surface wettability or other lens parameter Differential scanning calorimetry, differential thermal analysis, sorption/desorption experiments Raman Spectroscopy, Near IR and ATR-FTIR spectroscopy have been used to better understand hydration properties of soft contact lenses [19–23].

ATR-FTIR spectroscopy is one of the fast, nondestructive, inexpensive and effective techniques in monomer-polymer analysis. It is also a powerful method to gain structural information on hydrated biological materials. In order to evaluate the differences and similarities among samples, unsupervised techniques such as hierarchical cluster analysis (HCA) can be made statistically based on the infrared spectral data set when the exact chemical components and the amounts of each are unknown in samples [24].

Exposure to UV radiations is the a risk factor and associated with ocular diseases, such as cataracts and macular degeneration [25–31]. The commercial CLs can have UV- protection or some offer limited to no UV-protection. The amount of UV absorbed or transmitted by contact lenses varies markedly between brands depending on manufacturer and lens material. It can even vary within the same manufacturer [5,32–41].

UV radiation spectrum is divided into three regions according to their wavelength called UVC (200-280 nm), UVB and UVA (315-380 nm). According to standard (Z80.20) set by the American National Standards Institute (ANSI), Class I contact lenses block 99% UVB and 90% UVA while Class II contact lenses block 95% UVB and 70% UVA. The spectral transmittance/reflectance properties in the visible region (400-700 nm) are also strongly dependent on the lens material and very important for visual performance.

The refractive index (RI) of a soft contact lens is an important physical parameter that effects the lens design and also indirect measure of its equilibrium water content (EWC) [42–46]. RI index can measure with automated and manual refractometer [46–48]. In the present study RI values of CLs were not measured directly but derived from transmittance/reflectance spectral measurements.

SAXS is a non-destructive and highly popular method to study the nanoscale structure of any type of material, ranging from new composite nano systems to biological macromolecules. The chemical nature of the selected monomers and their compositions of the CLs materials can have effect on the nanoscale structure within the material. A more comprehensive understanding of the relationships between chemical properties and the material structures of CLs needs to be established [49,51].

This study is aiming to investigate the effect of lens materials on water content and examine spectroscopic changes as a function of time using ATR-FTIR spectroscopy and to evaluate of the UVA and visible transmittance characteristics of CLs with and without UV filters of different brands SiHy and bio-Hy CLs.

The shapes (morphologies) of 3D nanoglobules of all CLs of different brands were obtained for the first time investigated by SAXS. The results were used to find associations with some important properties of CLs such as ECW and RI values.

## 2. MATERIALS AND METHODS

Only new, unworn daily wear contact lenses were used in the present study. The commercially available 8 brands spherical SiHy, 2 brands spherical bio-Hy and 3 brands toric SiHy, contact lenses were obtained from the optician shop (6 lenses per box) in Turkey.

The properties of all contact lens studied in this study are detailed in Table 1. An optical lens power of -2.00 and -4 diopters (D) were selected for each spherical lens brand.

## 2.1 ATR-FTIR Spectra

ATR-FTIR spectra were recorded using a Perkin Elmer Spectrum 100 FTIR spectrometer with a Universal diamond ATR accessory. 32 scans were performed for all measurements with a resolution of 4 cm<sup>-1</sup> in the 4000- 650 cm<sup>-1</sup>region. 6 soft contact lenses from each brand were used. Triplicatespectra were acquired for each lens (immediately -removed from package, under airdried after 10 min, 1 h and 1 day) to check the reproducibility of the identical spectra.

All raw spectra are converted from transmittance to absorbance and no ATR baseline correction was applied. The average spectrum was taken for each sample and then was smoothed using a Savitzky-Golay filter (smoothing points: 13) using the OPUS 5.5 software package (Bruker Optics GmbH, Ettlingen, Germany).

The absorbance spectra were then baseline corrected and then normalized with respect to  $CH_2$ - $CH_3$  stretching region (3020-2800 cm<sup>-1</sup>) for visual demonstration of the spectral differences in the spectra of studied CLs. To estimate water content of CLs of different brands the band area under the 3700–3020 cm<sup>-1</sup> region was integrated.

Spectral differentiation of different brand CLs, HCA analysis was performed using OPUS 5.5 software. Vector normalized, second derivative of each spectrum in the range of 4000–650 cm<sup>-1</sup>was used as an input data. Spectra were smoothed using 13-points. The dendrogram was calculated using Ward's method and Euclidean distances.

## 2.2 UV-Vis Measurement

Computer controlled monochromator (CVI Digichrome 240 with a focal length of 20 cm) operating with the spectral range from 315 to 800 nm at 2 nm intervals and a BPW34 photodiode were used for measurements transmittance (T) and reflection (R).

Two measurements were made on each sample to check the reproducibility of the identical spectra.

## 2.3SAXS Measurement

SAXS experiments were performed with Kratky compact HECUS system (Hecus X-ray systems, Graz, Austria) equipped with a linear collimation system and X-ray tube with a Cu target ( $\lambda$ = 1.54Å). The generator was operated at a power of 2 kW (50 kV and 40 mA).

Scattering intensity I(q) is plotted against qmagnitude of the scattering vector. The PDDs were adjusted to be the smallest chi-square (chi2,  $\chi$ 2) value, and 3D morphologies of electron density of CLs were found in the DAMMIN program [52–54].

# Table 1. Properties of conventional soft contact lenses used in this study

Manufacturer	Brand name	Material	Base Monomers and polymer*	EWC	Dk/t	RI	Transmission (%)	
		(USAN)		(%)			Light	UVB/UVA
Cooper Vision	Biofinity	Comfilcon A	NVP, VMA, IBM, TAIC, M3U,	48	160	1.40	>97	
Hamble, UK	PWR :-2/-4	52 %	FM0411M, HOB					
Bausch & Lomb Inc.,	Pure Vision 2	Balafilcon A	NCVE, NVP, PBVC, TPVC	36	130	1.426	95	
Rochester, NY,USA	PWR :-2/-4	64%						
Alkon-USA	Air Optix Aqua	Lotrafilcon B	DMA, TRIS, siloxane macromere	33	138	1.42	96	
Made in Malaysia	PWR :-2/-4	67%					at 610	
Only for sale in Turkey							nm	
Alkon-USA	Air Optix Nigth&Day	Lotrafilcon A	DMA, TRIS, siloxane macromere	24	175	1.43	-	
Made in Indonesia	PWR :-2/-4	76%						
Only for sale in Turkey								
Interojo Inc.	Elegance Comfort	Innofilcon A	-	45	-	-	-	
Gyeonggi-do, Korea	PWR :-2/-4	55%						
Bausch & Lomb Inc.,	Ultra with Moisture Seal	Samfilcon A	TRIS, Ma <sub>2</sub> D <sub>37</sub> , M1-(EDS) <sub>n</sub> -TMS,	46	163	1.41	≥ 95%	
Rochester, NY,USA	PWR :-2/-4	54%	NVP, DMA, HEMA					
Johnson & Johnson	Acuvue Oasys	Senofilcon A	mPDMS, DMA, HEMA, siloxane	38	147	1.42		UVA :less
Vision Care- Ireland	Hydraclear <sup>®</sup> Plus	62%	macromere, PVP, TEGDMA					than 10%
UV Blocking	PWR: -2/-4							
CooperVision	Avaira Vitality	Fanfilcon A	-	55	110	1.398	98% +2/-	10% of
Scottsville,NYUSA	PWR: -2	45 %					5%	UVA
UV Blocking								
WöhlkContaklinsen	Contact Life	Vitafilcon A	-	54	20	-	-	-
GmbH	PWR :-2/-4	46%						
Germany								
UV Blocking								
WohlkContaklinsen	Zeiss Contact Day	Ocufilcon F	-	55	19	-	-	-
GmbH	PWR :-2/-4	45%						
Germany								
UV Blocking								
Toric (for astigmatism) Ler	nses							
CooperVision	Biofinity	Comfilcon A	NVP, VMA, IBM, TAIC, M3U,	48	116		97	
Hamble, UK	SPH -1	52 %	FM0411M, HOB					
	CLY -0,75		·					
	AX 180							
Bausch & Lomb Inc.,	Pure Vision 2	Balafilcon A	NCVE, NVP, PBVC, TPVC	36	91	1.426	≥ 95%	
Rochester, NY,USA	SPH -1	64 %	, , -, -			-		

Manufacturer		Brand name	Material	Base Monomers and polymer*	EWC	Dk/t	RI	Transmis	Transmission (%)	
			(USAN)		(%)			Light	UVB/UVA	
		CLY -0,75								
Johnson &	Johnson	Acuvue	Senofilcon A	mPDMS, DMA, HEMA, siloxane	38	129.3	-		UVA less	
Vision Care		Oasys with	62%	macromere, PVP, TEGDMA					than 10%	
Ireland		HYDRACLEAR <sup>®</sup> PLUS								
		SPH -1								
UV Blocking		CLY -0,75								
		AX 180								

Abbreviations. USAN: United States Adopted Names, RI: Refractive index, EWC : The equilibrium water content, dimethylacrylamide); EGDMA (ethyleneglycoldimethacrylate); FM0411M (2-ethyl [2-[(2-methylprop-2-enoyl)oxy]ethyl]carbamate); HEMA( 2-hydroxyethyl methacrylate); HOB ((2RS)-2-hydroxybutyl 2-methylprop-2-enoate); IBM (Isobornyl methacrylate); M3U (a-[[3-(2-[[2-(methacryloyloxy)ethyl]carbamoyloxy]ethoxy)propyl]dimethylsilyl]-w-[3-(2-[[2-(methacryloyloxy)ethyl] carbamoyloxy]ethoxy)propyl]poly([oxy[(methyl) [3-[w-methylpoly (oxyethylene) oxy]propyl]silylene]/[oxy[(methyl)(3,3,3trifluoropropyl)]silylene]/oxy (dimethylsilylene)])); mPDMS (monofunctional polydimethylsiloxane); M1-(EDS)<sub>n</sub>-TMS (mono ethylenically unsaturated polymerizable group containing polycarbosiloxane monomer); Ma<sub>2</sub>D<sub>37</sub> (silicone bis(meth)acrylamide monomer); NVA (N-vinyl aminobutyric acid); NVP (N-vinyl pyrrolidone); PBVC (poly[dimethysiloxy] di [silylbutanol] bis[vinyl carbamate]); PVP (poly(vinylpyrrolidone)); TAIC (1,3,5-triprop-2-enyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione); TEGDMA (tetraethyleneglycoldimethacrylate); TPVC (tris-(trimethylsiloxysilyl) propylvinyl carbamate); VMA (N-Vinyl-N-methylacetamide); TRIS (3-(methacryloyloxy)propylisiloxy)silane).



Fig. 1. Representative ATR-FTIR spectra of spherical SiHy CLs of Biofinity and Pure Vision 2 brands

#### 3. RESULTS AND DISCUSSION

## 3.1 ATR-FTIR and HCA Analyses

The CL materials used in this study are composed of 10 polymeric materials (Comfilcon A, Balafilcon A, Innofilcon A, Lotrafilcon A, Lotrafilcon B, Samfilcon A, Senofilcon A, Fanfilcon A, Vitafilcon A and Ocufilcon F) with different contents and amounts. The most important factor in these lenses is the amount of carbon, oxygen, nitrogen and silicon (for SiHy). In addition, Lotrafilcon A and Lotrafilcon B contain fluorine, unlike the others. A very small amount (0.61%) of fluorine has reported in Biofinity-Confilcon A [55].

PDMS and /or TRIS macromonemers are the most important components in SiHy CLs. The C-H stretching bands between 2950-2960 cm<sup>-1</sup> and deformation band at around 1260 cm<sup>-1</sup> are characteristics of the Si-CH<sub>3</sub> group of PDMS and TRIS. Si-O-Si and Si-C stretching vibrations usually appear between 1020-1075 cm<sup>-1</sup> and 760-800 cm<sup>-1</sup>, respectively.

Vibrational bands related to O-H, N-H, CH<sub>2</sub>N-C, C=O, C-O and R-CH=CH<sub>2</sub> groups in hydrophilic monomers used for SiHy CLs can also be observed in the infrared spectra.

The ATR-FTIR spectra of -2 and -4 powered lenses appear quite similar. Representative ATR-FTIR spectra with assignments for the main bands for Biofinity contain Comfilcon A and PureVision2 contain Balafilcon A with lens power - 2 are given in Fig. 1.

ATR-FTIR spectra of the toric lenses of 3 brands (Biofinity, Acuvue Oasys and Pure Vision 2 with Comfilcon A, Balafilcon A, and Senofilcon A polymers, respectively) are given in Fig. 2. There is no differences in the ATR-FTIR spectra of spherical and toric lenses of same brand.

The O-H stretching band in the 3700-3050 cm<sup>-1</sup> were associated to general intramolecular and intermolecular hydrogen bonding and to free hydroxyl in lens material. This band is also representative of the contribution of the free or the bound water linked to the substrate. It can be used to describing the hydration process [56–58].The first aim of this study was to compare water content of all studied CLs.

Since the high water content in the packaging solution, a strong broad absorption band exhibit

v (O-H),stretching vibration in the range of 3700-3020 cm<sup>-1</sup>. Fig. 3 shows the average ATR-FTIR spectra of spherical lenses of Biofinity brand (as a representative) immediately removed from package, under air-dried after 10 min, 1 h and 1 day and its packaging solution for comparative purpose.

Band intensities of O-H stretching band decreased and intensities of some band of functional groups of lens material increased due to decrease water content of the lenses, which started to dry.

The intensity of water bands in infrared spectra is actually an indicator of the water content in the lens material. Fig. 4 shows comparative infrared spectra between  $3800-2700 \text{ cm}^{-1}$  after10 min of the spherical CLs from 10 different brands.

The highest and lowest water content were found in the bio-hydrogel CLs of Contact Life /Zeiss Contact Day brands from Wöhlk which are sold for sensitive and dry eyes and in SiHy CLs of Air optic Night& Day / Aqua brands from Alcon, respectively.

The second high water content are for SiHy CLs of Elegance Comfort brand from Interojo and Avaira Vitality brand from Cooper Vision. A close correlation was found between water content found from infrared spectra and claimed by the manufacturers (Table 1).

After 1 day, the wave number of the O-H stretching band shifted towards the high frequency region and the intensities of this band were decreased for all CLs. This observation shows that there is a break between the hydrogen bonds between O-H and other molecules. The intensity of the Si-O-Si stretching band in SiHy CLs found to increase with decrease of water content. The relationship between water content and silicon/fluorine content was examined by Dupre and Benjamin [55] and they found a negative correlation between silicon and lenses with a water content of more than 35%.

It is possible to obtain detailed information on macromolecular structures/composition from the infrared spectra. However, since the exact contents and amounts are not known in the CLs used in the study, analyses were made statistically based on the spectrum difference between the brand and copolymers. The obtained dendrogram based on ATR-FTIR spectra of six lenses from the same box for 3 brands is represented in Fig. 5a. ATR-FTIR spectra of six lenses from the same box from each brand's lens (after 10 min, 1 h and 1 day)

were averaged and subjected to HCA. The obtained dendrogram for spherical CLs of the 10 brands with PWR: -2 and toric CLs (for astigmatism) of the 3 brands is represented in Fig. 5b.



Fig. 2. Average ATR-FTIR spectra of toricSiHy CLs of Biofinity, AcuvueOasys and Pure Vision 2



Fig. 3. Time dependent average ATR-FTIR spectra of spherical SiHy CLs of Biofinity brand and buffered saline as package lens solution



Fig. 4. Comparative normalized average ATR-FTIR spectra after 10 minutes of the ten spherical contact lens brands in 3800-2700 cm<sup>-1</sup> region



#### Fig. 5. Dendrograms of Hierarchical Cluster Analysis performed with ATR-FTIR spectra of a) Three brands ( 6 lenses per box) and b) Averaged ATR-FTIR spectra of ten different brand lenses (PWR: -2, and three toric CLs ) in the 4000 – 650 cm<sup>-1</sup> spectral region

The HCA dendrograms (Figs. 5a and b) showed a good differentiation of CLs with different brands. The classification of spectra depends on molecular composition. The cluster analysis grouped all the CLs of same brand in same cluster. The high heterogeneity between bio-Hy CLs (Zeiss Contact Day/ Contact Life) and Si-HyCLs is caused by large differences between the infrared spectra. The second high heterogeneity between Si-Hy CLs of PureVision2and the other Si-Hy CLs.

#### 3.2 UV-Vis Results

UV-vis transmittance spectra (315 nm - 800 nm) for spherical CLs of 6 brands (UV- blocking

Bayarı et al.; AJACR, 12(1): 1-16, 2022; Article no.AJACR.92382

properties are not claim by the manufacturer), spherical CLs of 4 brands with UV- blocking (claim by the manufacturer) and toric CLs of 3 brands (claim: 1 UV-blocking and two non UVblocking) are presented in Figs. 6 a , b and c, respectively.

Fig. 7a showed that different amounts of UVA were transmitted by non UV- blocking CLs of different brands. PureVision2 brand has the highest UVA protection with approximately 40% blocking among other brand, but Elegance Comfort brand has the lowest value.

Generally, the visible light transmittance of over 90% of CLs satisfied the visual requirements. Visible transmittance values between 400 nm and 800 nm of CLs of different brands except Air Optix Nigth & Day are between 90% and 98%.

Air Optix Nigth& Day Aqua brand (only for sale in Turkey, Alcon -Indonesian) has the lowest visible light transmittance (80 % -85 %). The light transmittance is found over 90 % for Air Optix (Only for sale in Turkey, Alcon- USA). Company' claim value is  $\geq$  96% for these brands.

Company's claim for Acuvue Oasys and Aveira Vitality of 90 % UVA protection (transmittance value 10% Claim; Class II UV-blocking). As can be seen from Fig 7b, UV-A transmittance values for CLs with UV filter of Contact Life, Zeiss Contact Day, Acuvue Oasys and Avaira Vitality brands were found between 8 % and 25 %. These transmittance values higher than the Company' claim. The different findings may due differences in the instrument and methods. These lenses could be claimed as Class II UV protectors.

Acuvue Oasys (toric, Claim; Class I UV-blocking; block 96.1 % of UVA radiation) has the high UV-blocking properties and light transmittance (Fig 7c). Biofinity (toric) and PureVision2 (toric) have low UVA blocking properties but have high visible light transmittance of over 90 % Company claim light transmittance value is  $\geq$  95% for these brands.

## 3.3 Refractive Indices (RI)

In general, RI of lenses are given in the range of 1.40-1.43, depending on the polymeric material and water content. Measurements are made using commercial refractometers (at approximately 590 nm light with a sodium lamp) [17,45,59].

During the measurement, the lens surface water amount affects the RI value [60]. Lens material, ECW and thickness can also alter the properties of a CL [43,61,62].

The refractive index varies with wavelength. In this study, the average RI values were calculated using transmittance/ reflectance spectra in the 500-600 nm and presented in Table 2 with the claimed RI values by manufacturers. Our calculated RI values show good agreement with claimed by the manufacturers except PureVision2 brand. We did not good relationship between EWC and RI values.



Fig 6. Percentage UVA-vis transmittance spectra as a function of wavelength of a) non UVblocking spherical contact lenses b) UV-blocking spherical contact lenses c) Toric lenses

# Table 2. Refractive index (RI) PWR : -2 for spherical lenses

Manufacturer	Brand name	Material (USAN)*	EWC (%)	RI	Mean RI This study
Silicone hydrogel					
Cooper Vision Hamble, UK	Biofinity	Comfilcon A 52 %	48	1.40	1.401
Bausch & Lomb Inc., Rochester, NY,USA	PureVision 2	Balafilcon A64%	36	1.426	1.398
Alkon-USA Made in Malaysia Only for sale in Turkey	Air Optix Aqua	Lotrafilcon B 67 %	33	1.42	1.416
Alkon-USA Made in Indonesia Only for sale in Turkey	Airoptix Nigth&Day	Lotrafilcon A 76%	24	1.43	1.427
InterojoInc Gyeonggi-do, Korea	Elegance Comfort	Innofilcon A 55 %	45	-	1.445
Bausch & Lomb Inc., Rochester, NY,USA	Ultra with Moisture Seal	Samfilcon A 54 %	46	1.41	1.453
Johnson & Johnson Vision Care- Ireland UV Blocking	Acuvue Oasys	SenofilconA 62%	38	1.42	1.436
	Hydraclear <sup>®</sup> Plus				
Cooper Vision Scottsville, NY USA UV Blocking	Avaira Vitality	Fanfilcon A 45 %	55	1.398	1.401
Bio Hydrogel					
Wöhlk Contaklinsen GmbH Germany UV Blocking	Contact Life PWR :-2	Vitafilcon A 46%	54		1.393
WohlkContaklinsen GmbH Germany UV Blocking	Zeiss Contact Day PWR :-2	Ocufilcon F %45	55	-	1.398
Toric (for astigmatism) Lenses					
Cooper Vision Hamble, UK	Biofinity	Comfilcon A 52 %	48		1.402
Bausch & Lomb Inc., Rochester, NY,USA	PureVision 2	Balafilcon A 64 %	36	1.426	1.394
Johnson & Johnson Vision Care Ireland UV Blocking AcuvueOasys		Senofilcon A 62%	38	-	1.436

#### 3.4 SAXS Results

The calculated and measured scattering profiles and the obtained 3D nano- morphologies of all CLs are provided in Fig. S1.

When nano-formations start to show fiber nucleation, the stacking also becomes regular and at the nanoscale, a large hump forms in the middle q (q. scattering vector size) region, which is evidence of nonocrystalline structure.

Aveira Vitality, Elegance Comfort, Pure Vision 2 (toric) and Acuvue Oasys (toric) show that similar to this type of crystalline structure. Average distance varies in the range of 7.7-17.9 nm between nanocrystalline linear lines. The UV blocking properties of these samples (except Elegance Comfort) and the addition of molecules to the polymer may be related to this linear nanostructure arrangement (Fig. S1).

In the CLs of Zeiss Contact Day and Contact Life, the fiber structures show parallel arrays very similar to each other at the nanoscale and resemble the structure of the real eye lens (Fig. S1). According to the manufacturer, sulphobetain is the main component of Vitafilcon A hydrogel material of Contact Life brand. It was developed modelled on the good water-binding components keratan sulphate and chondroitin sulphate found in the human cornea. The material properties are very similar to those of the cornea [63].

Fig. 7 depicts the most importance and evaluated results based on SAXS analyses. The nano nucleation morphologies are variable and similar to the microsize globular aggregations [64–66].

The zipper tooth like morphology and the smallest size of the nano globules (~12 nm) indicate that Bioinfinity (toric, Confilcon A) is very good nanostructured lens.

The equilibrium water content (EWC) varies depending on on the molecular, nanoscopic and microscopic structure of CLs. The volume fraction of selected polymer materials and ECW values were compared with the size of nanoglobules (Fig. 8).



Fig. 7. The correlation between simulated micro and nanoscale structures. Science photo library views were used for microscale simulations and model inspirations [63–65]

As presented in Fig. 8, the EWC and volume fraction of polymer are effected by the size of nanoglobules of the material of CL.



Fig. 8. Nanoscalestructure of contact lenses dependent on ECW/and or lens material

#### 4. CONCLUSION

This work was designed to explain important characteristics of commercial CLs and results would have implications for future experimental and clinical research.

The effect of air drying on the water content in two groups of different brands daily wear soft contact lenses: silicone-hydrogel (lens powers -2 and -4) and bio-hydrogel by means of ATR-FTIR spectroscopy were examined in this paper. The results of ATR-FTIR seems to confirm the water content claimed by the manufacturer (not numerically in values but in order of magnitude).

The results indicate that ATR-FTIR can be successfully used to monitor the water content in soft contact lenses. It was observed that none of the lenses presented any changes depend on the lens power. There is no differences in the ATR-FTIR spectra of spherical and toric lenses of same brand.

The UV-vis transmittance/reflectance spectra of contact lenses with and without UV protection were measured. Average transmittance percentages were calculated for each lens for the UVA and vis portions of the spectrum. Comparison of the results of each lens shows that there are variable amounts of UVA absorbed and transmitted by all the contact lens brands tested. Soft contact lenses with blocking UV should be recommended.

There is not very good agreement between our reflective index (RI) values and those claimed by the manufacturers. One of the limitations of our measurement is that measure transmittance/reflectance on the lens surface and calculated RI with the assumption that the lens materials are homogenous with a uniform RI throughout the lens thickness and diameter. The second limitation: RI is sensitive to surface water contain of lens and water content can be change during measurement. Another potential limitation of our results: most of the previous studies, lens power is selected -3. A wider range of plus and minus lens powers need to be measured to confirm that there is no dependence of transmittance/reflectance/ RI on lens power and correlated center thickness changes.

Nanoscale formations and nucleations aggregate the core of microscale structures. For this reason, nanomorphologies plays a fundamental role in micro-formations and bigger size aggregations. Size and shapes of the nanoglobules are effective on lens parameters.

#### SUPPLEMENTARY MATERIALS

Supplementary materials available in this link: https://journalajacr.com/index.php/AJACR/library Files/downloadPublic/4

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## **COMPETING INTERESTS**

Authors have declared that no competing interests exist.

## REFERENCES

- Alvord L, Court J, Davis T, Morgan CF, Schindhelm K, Vogt J, et al. Oxygen permeability of a new type of high Dk soft contact lens material. Optom Vis Sci.1998;75:30–6. Available:https://doi.org/10.1097/00006324 -199801000-00022.
- Li J, Celiz AD, Yang J, Yang Q, Wamala I, Whyte W, et al. Tough adhesives for diverse wet surfaces. Science. 2017; 357:378–81. Available:https://doi.org/10.1126/science.a

ah6362.

- Zhao Q, Yang X, Ma C, Chen D, Bai H, Li T, et al. A bioinspired reversible snapping hydrogel assembly. Mater Horizons. 2016;3:422–8. Available:https://doi.org/10.1039/C6MH001 67J.
- Maldonado-Codina C. Soft Lens Materials. In: Efron N, Contact Lens Pract. 3rd ed., Elsevier; 2018; p. 45-60.e1. Available:https://doi.org/10.1016/B978-0-7020-6660-3.00004-6.
- Moore L, Ferreira JT. Ultraviolet (UV) transmittance characteristics of daily disposable and silicone hydrogel contact lenses. Contact Lens Anterior Eye. 2006; 29:115–22. Available:https://doi.org/10.1016/j.clae.200 6.03.002.
- Swanson MW. A Cross-Sectional analysis of U.S. contact lens user demographics. Optom Vis Sci. 2021; 89:839–48. Available:https://doi.org/10.1097/OPX.0b0 13e318255da45.

- Moreddu R, Vigolo D, Yetisen AK. Contact Lens Technology: From Fundamentals to Applications. Adv Healthc Mater. 2019; 8:1900368. Available:https://doi.org/10.1002/adhm.201 900368.
- Musgrave CSA, Fang F. Contact Lens Materials: A materials science perspective. Materials (Basel). 2019; 12:261. Available:https://doi.org/10.3390/ma12020 261.
- Nicolson PC, Vogt J. Soft contact lens polymers: an evolution. Biomaterials. 2001; 22:3273–83. Available:https://doi.org/10.1016/S0142-9612(01)00165-X.
- Caló E, Khutoryanskiy V V. Biomedical applications of hydrogels: A review of patents and commercial products. Eur Polym J. 2015; 65:252–67. Available:https://doi.org/10.1016/j.eurpoly mj.2014.11.024.
- 11. Nichols J. Contact Lens Spectrum. PentaVision LLC; Ambler, PA, USA 20– 5;2017.
- Chatterjee S, Upadhyay P, Mishra M, Srividya M, Akshara MR, Kamali N, et al. Advances in chemistry and composition of soft materials for drug releasing contact lenses. RSC Adv. 2020; 10:36751–77. Available:https://doi.org/10.1039/D0RA066 81H.
- Efron N, Morgan PB, Nichols JJ, Walsh K, Willcox MD, Wolffsohn JS, et al. All soft contact lenses are not created equal. Contact Lens Anterior Eye. 2022; 45:101515. Available:https://doi.org/10.1016/j.clae.202 1.101515.
- 14. Iwata J, Hoki T, Ikawa S (2006) Silicone Hydrogel Contact Lens. Patent number: US0063852 A1.
- 15. Santos L, Rodrigues D, Lira M, Oliveira MECDR, Oliveira R, Vilar EY, et al. The influence of surface treatment on hydrophobicity, protein adsorption and microbial colonisation of silicone hydrogel contact lenses. Contact Lens Anterior Eye. 2007

; 30:183–8.

Available:https://doi.org/10.1016/j.clae.200 6.12.007.

 Chalmers R. Overview of factors that affect comfort with modern soft contact lenses. Contact Lens Anterior Eye. 2014;37:65– 76. Available:https://doi.org/10.1016/j.clae.201 3.08.154.

- González-Méijome JM, Lira M, López-Alemany A, Almeida JB, Parafita MA, Refojo MF. Refractive index and equilibrium water content of conventional and silicone hydrogel contact lenses. Ophthalmic Physiol Opt. 2006; 26:57–64. Available:https://doi.org/10.1111/j.1475-1313.2005.00342.x.
- Krysztofiak K, Szyczewski A. Study of dehydration and water states in new and worn soft contact lens materials. Opt Appl. 2014; 44:237–50.
- Available:https://doi.org/10.5277/oa140206
- Mirejovsky D, Patel A, Young G. Water properties of hydrogel contact lens materials: a possible predictive model for corneal desiccation staining. Biomaterials. 1993; 14:1080–8. Available:https://doi.org/10.1016/0142-9612(93)90209-K.
- Roorda W. Do hydrogels contain different classes of water? J Biomater Sci Polym Ed. 1994; 5:381–95. Available:https://doi.org/10.1163/15685629 4X00095.
- Sekine Y, Ikeda-Fukazawa T. Structural changes of water in a hydrogel during dehydration. J Chem Phys. 2009; 130:034501. Available:https://doi.org/10.1063/1.305861 6.
- Munćan J, Mileusnić I, Šakota Rosić J, Vasić-Milovanović A, Matija L. Water properties of soft contact lenses: A comparative near-infrared study of two hydrogel materials. Int J Polym Sci.2016; 2016:1–8. Available:https://doi.org/10.1155/2016/373

7916.

- Lira M, Lourenço C, Silva M, Botelho G. Physicochemical stability of contact lenses materials for biomedical applications. J Optom. 2020; 13:120–7. Available:https://doi.org/10.1016/j.optom.2 019.10.002.
- Maimon O, Rokach L. Data mining and knowledge discovery handbook. Springer, Boston, MA; 2006. Available:https://doi.org/10.5860/CHOICE. 48-5729.
- Tucker MA, Shields JA, Hartge P, Augsburger J, Hoover RN, Fraumeni JF. Sunlight exposure as risk factor for intraocular malignant melanoma. N Engl J Med. 1985; 313:789–92.

Available:https://doi.org/10.1056/NEJM198 509263131305.

- Roberts JE. Ultraviolet radiation as a risk factor for cataract and macular degeneration. Eye Contact Lens Sci Clin Pract. 2011; 37:246–9. Available:https://doi.org/10.1097/ICL.0b01 3e31821cbcc9.
- Delcourt C. Light exposure and the risk of cortical, nuclear, and posterior subcapsular cataracts. Arch Ophthalmol. 2000; 118:385. Available:https://doi.org/10.1001/archopht. 118.3.385.
- 28. Anthony P. UV radiation contact lenses and the ophthalmohelioses. OptomToday. 2005; 1:30–4.
- 29. Tasman W, Edward AJ. Duane's ophthalmology. Philadelphia, Pa.: Lippincott Williams & Wilkins; 2007.
- Yam JCS, Kwok AKH. Ultraviolet light and ocular diseases. Int Ophthalmol. 2014; 34:383–400. Available:https://doi.org/10.1007/s10792-013-9791-x.
- Rahmani S, Nia M, Baghban A, Nazari M, Ghassemi-Broum M. Do UV-blocking soft contact lenses meet ANSI Z80.20 criteria for UV transmittance? J Ophthalmic Vis Res. 2015; 10:441. Available:https://doi.org/10.4103/2008-322X.176890.
- 32. Pitts DG. Ultraviolet-absorbing spectacle lenses, contact lenses, and intraocular lenses. Optom Vis Sci. 1990; 67:435–40. Available:https://doi.org/10.1097/00006324 -199006000-00007.
- Jin I, Tao F, Ho L, Swarbrick HA, Dain SJ. Ultraviolet radiation transmission of soft disposable contact lenses and ISO 18369: claims and compliance. Clin Exp Optom. 2021; 104:579–82. Available:https://doi.org/10.1080/08164622 .2021.1878826.
- Harris MG, Dang M, Garrod S, Wong W. Ultraviolet transmittance of contact lenses. Optom Vis Sci.1994; 71:1–5. Available:https://doi.org/10.1097/00006324 -199401000-00001.
- Lin K-K, Lin Y-C, Lee J-S, Chao A-N, Chen HS-L. Spectral transmission characteristics of spectacle contact, and intraocular lenses. Ann Ophthalmol. 2002; 34:206–15. Available:https://doi.org/10.1007/s12009-002-0025-5.
- 36. Lira M, Dos Santos Castanheira EM, Santos L, Azeredo J, Yebra-Pimentel E,

Real Oliveira MECD. Changes in UVvisible transmittance of silicone-hydrogel contact lenses induced by wear. Optom Vis Sci. 2009; 86:332–9.

Available:https://doi.org/10.1097/OPX.0b0 13e318198d047.

- Osuagwu UL, Ogbuehi KC, AlMubrad TM. Changes in ultraviolet transmittance of hydrogel and silicone-hydrogel contact lenses induced by wear. Eye Contact Lens Sci Clin Pract. 2014;40:28–36. Available:https://doi.org/10.1097/ICL.0000 00000000007.
- Song M, Shin YH, Kwon Y. Synthesis and properties of siloxane-containing hybrid hydrogels: Optical transmittance, oxygen permeability and equilibrium water content. J Nanosci Nanotechnol. 2010; 10:6934–8. Available:https://doi.org/10.1166/jnn.2010. 2984.
- 39. Rahmani S. Mohammadi Nia Μ. Akbarzadeh Baghban A. Nazari MR. Ghassemi-Broumand Μ. Spectral transmittance of UV-blocking soft contact lenses: A comparative study. Contact Lens Anterior Eye. 2014; 37:451-4. Available:https://doi.org/10.1016/j.clae.201 4.07.011.
- Artigas JM, Navea A, García-Domene Mc, Gené A, Artigas C. Light transmission and ultraviolet protection of contact lenses under artificial illumination. Contact Lens Anterior Eye. 2016; 39:141–7. Available:https://doi.org/10.1016/j.clae.201 5.09.008.
- Depry J, Golding R, Szczotka-Flynn L, Dao H, Baron E, Cooper K. UVB-protective properties of contact lenses with intended use in photoresponsive eyelid dermatoses. Photodermatol Photoimmunol Photomed. 2013; 29:253–60. Available:https://doi.org/10.1111/phpp.120

64.
42. Kim E, Ehrmann K. Refractive index of soft contact lens materials measured in packaging solution and standard phosphate buffered saline and the effect on back vertex power calculation. Contact Lens Anterior Eye. 2020; 43:123–9. Available:https://doi.org/10.1016/j.clae.201 9.12.005.

43. González-Méijome JM, López-Alemany A, Lira M, Almeida JB, Oliveira MECDR, Parafita MA. Equivalences between refractive index and equilibrium water content of conventional and silicone hydrogel soft contact lenses from automated and manual refractometry. J Biomed Mater Res Part B Appl Biomater. 2007; 80B:184–91.

Available:https://doi.org/10.1002/jbm.b.305 83.

- Varikooty J, Keir N, Woods CA, Fonn D. Measurement of the refractive index of soft contact lenses during wear. Eye Contact Lens Sci Clin Pract. 2010; 36:2–5. Available:https://doi.org/10.1097/ICL.0b01 3e3181c8135f.
- Lira M, Santos L, Azeredo J, Yebra-Pimentel E, Real Oliveira MECD. The effect of lens wear on refractive index of conventional hydrogel and siliconehydrogel contact lenses: A comparative study. Contact Lens Anterior Eye. 2008; 31:89–94. Available:https://doi.org/10.1016/j.clae.200 7.09.001.
- Young MD, Benjamin WJ. Calibrated oxygen permeability of 35 conventional hydrogel materials and correlation with water content. Eye Contact Lens Sci Clin Pract. 2003; 29:126–33. Available:https://doi.org/10.1097/01.ICL.00 00062463.64717.86.
- 47. Nichols JJ, Berntsen DA. The assessment of automated measures of hydrogel contact lens refractive index. Ophthalmic Physiol Opt. 2003; 23:517–25. Available:https://doi.org/10.1046/j.1475-1313.2003.00147.x.
- Brennan NA. A simple instrument for measuring the water content of hydrogel lenses. Int Contact Lens Clin. 1983; 10:357–61.
- Lee K, Kim K, Yoon H, Kim H. Chemical design of functional polymer structures for biosensors: From nanoscale to macroscale. Polymers (Basel). 2018; 10:551. Available:https://doi.org/10.3390/polym100

Available:https://doi.org/10.3390/polym100 50551.

 Saez-Martinez V, Mann A, Lydon F, Molock F, Layton SA, Toolan DTW, et al. The influence of structure and morphology on ion permeation in commercial silicone hydrogel contact lenses. J Biomed Mater Res Part B Appl Biomater. 2021; 109:137– 48.

Available:https://doi.org/10.1002/jbm.b.346 89.

 Sahabudeen H, Machatschek R, Lendlein A. Multifunctionality as design principle for contact lens materials. Multifunct Mater. 2021; 4 042001. Available:https://iopscience.iop.org/article/ 10.1088/2399-7532/ac1e7d/pdf

- 52. Kline SR. Reduction and analysis of SANS and USANS data using IGOR Pro. J Appl Crystallogr. 2006; 39:895–900. Available:https://doi.org/10.1107/S0021889 806035059.
- 53. Franke D, Svergun DI. DAMMIF, a program for rapid ab-initio shape determination in small-angle scattering. J Appl Crystallogr. 2009; 42:342–6. Available:https://doi.org/10.1107/S0021889 809000338.
- Ilavsky J, Jemian PR. Irena: tool suite for modeling and analysis of small-angle scattering. J Appl Crystallogr. 2009; 42:347–53. Available:https://doi.org/10.1107/S0021889 809002222.
- Dupre TE, Benjamin WJ. Relationship of water content with silicon and fluorine contents of silicone-hydrogel contact lens materials. Eye Contact Lens Sci Clin Pract. 2019; 45:23–7. Available:https://doi.org/10.1097/ICL.0000 00000000527.
- 56. Cotugno S, Mensitieri G, Musto P, Sanguigno L. Molecular interactions in and transport properties of densely cross-linked Networks: A Time-Resolved FT-IR Spectroscopy investigation of the epoxy/H<sub>2</sub> O system. Macromolecules. 2005; 38:801– 11.

Available:https://doi.org/10.1021/ma04000 8j.

- 57. Mantsch HH, Chapman D. Infrared Spectroscopy of Biomolecules. New York : Wiley-Liss; 1996.
- Pastorczak M, Kozanecki M, Ulanski J. Water–Polymer interactions in PVME hydrogels – Raman spectroscopy studies. Polymer (Guildf). 2009; 50:4535–42. Available:https://doi.org/10.1016/j.polymer. 2009.07.048.

- 59. Mousa GY, Callender MG, Sivak JG, Edan DJ. The effects of the hydration characteristics of hydrogel lenses on the refractive index. Int Contact Lens Clin. 1983;10:31–7.
- Millodot M. Dictionary of optometry and visual science. 7th ed. Oxford, UK: Butterworth-Heinemann; 2009. Available:https://doi.org/10.1111/j.1444-0938.2009.00388.x.
- 61. Bennett ES, Weissman BA. Clinical contact lens practice. Philadelphia: Lippincott Williams & Wilkins ; 2005.
- Kollbaum PS, Bradley A, Thibos LN. Comparing the optical Properties of soft contact lenses on and off the eye. Optom Vis Sci. 2013; 90:924–36. Available:https://doi.org/10.1097/01.opx.00 00434275.93435.da.
- 63. Wöhlk Wissen. High performance hydrogel or silicone hydrogel - when to fit which, http://www.vargellini.it/zaccagnini/downloa d/approfondimenti/contattologia/woehlkwissen high performance hydrogel VS SH.pdf; 2022. Accessed 30 May 2022
- 64. Bassnett S, Shi Y, Vrensen GFJM. Biological glass: structural determinants of eye lens transparency. Philos Trans R Soc B Biol Sci. 2011; 366:1250–64. Available:https://doi.org/10.1098/rstb.2010. 0302.
- 65. Science photo library. SEM of the human eye lens showing lens cells, Available:https://www.sciencephoto.com/m edia/308710/view/sem-of-the-human-eye-lens-showing-lens-cells;2022 Accessed 30 May 2022
  66. Science photo library. SEM of the lens of a
- Available:https://www.sciencephoto.com/m edia/308701/view/sem-of-the-lens-of-ahuman-eye; 2022 Accessed 30 May 2022

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