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PII: S1386-1425(17)30600-5
DOI: doi: 10.1016/j.saa.2017.07.037
Reference: SAA 15324

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received date: 11 February 2017
Revised date: 9 July 2017
Accepted date: 20 July 2017

Please cite this article as: Anum Sahar, Shaukat Ali, Tanveer Hussain, Muhammad Irfan, Bertil Eliasson, Javed Iqbal , UV absorbers for cellulosic apparels: A computational and experimental study, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2017), doi: 10.1016/j.saa.2017.07.037

UV absorbers for Cellulosic Apparels : A Computational and Experimental Study

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Abstract

Two triazine based Ultra Violet (UV) absorbers Sulfuric acid mono-(2-{4-[4-chloro-6-(4-{4-chloro - 6 - [4 - (2-sulfooxy - ethanesulfonyl) - phenylamino] - [1,3,5] triazin-2-ylamino-phenylamino)-[1,3,5]triazin-2-ylamino]-benzenesulfonyl}-ethyl) ester (**1a)** and 4-{4-Chloro-6-[4-(2-sulfooxy-ethanesulfonyl)-phenylamino]-[1,3,5] triazin-2-ylamino}-2-[4-chloro-6-(2-sulfooxy-ethanesulfonyl)-[1,3,5]triazin-2-ylamino]-benzenesulfonic acid (**2a**) with different substituents were designed computationally. The influence of different substituents on the electrochemical properties and UV spectra of the absorbers was investigated. The presence of electron deficient unit in **1a** to the molecular core significantly reduces the LUMO levels and energy gap. The designed absorbers were synthesized via condensation reaction and characterized by UV-Vis, FT-IR, MS studies. The performance of synthesized compounds as

UV absorbers and their fastness properties were assessed by finishing the cotton fabric through exhaust method at different concentration and results appeared in good range.

Key Words: Solar Radiations**,** Substituents effect, UV Absorbers, DFT, HOMO-LUMO, Condensation reaction

Introduction

Solar radiations are increasingly valued due to their influence on living and non-living material. Among these solar radiations, UV radiations pose severe threat to human body due to their high energy contents [1-4]. Clothing is a most well-known practice for protection point of view from these radiations and today, cotton fiber is the most used textile fiber which gives 56 percent share for home and apparel but offered low ultraviolet protection due to low weight and high porosity [5]. Subsequently, the global demand for new UV absorbers for cotton fiber is nowadays of great interest as a result of augmented awareness about harmful effects of UV rays [6].

So a serious consideration has been given to synthesize the textile fabrics which can play the role of a shield between humans and unhealthy UV radiations. An effective UV absorber must include; i) effective absorptions of UV rays especially in UV-B (320–400 nm) and UV-A (280–320 nm) regions [7] ii) rapid transformation of UV energy into vibration energy then convert it into heat energy in the surroundings without degradation of fabric and iii) easy application on fabric without addition of colour [5, 8].

For designing the compounds of our interest, quantum mechanical calculations are tremendously potent tools [9, 10] Computational study provides us a great help in theoretical calculations such as wavelength [11-13] and energetic properties [14-16] of chemical systems in general and offer opportunity to mould desirable chemical and physical properties containing molecular systems that reduce the loss of resources [17, 18]. The predicted structures of desirable properties then become a target for synthesis [19]. Moreover, meanwhile in this study our aim was to computationally design new UV absorbers and investigate their electrochemical properties and excited state properties and later on synthesize the molecules with desire properties. After careful assessment of calculated UV properties of designed molecules, two molecules Sulfuric acid mono-(2-{4-[4-chloro-6-(4-{4-chloro - 6 - [4 - (2-sulfooxy-ethanesulfonyl)-phenylamino]-[1,3,5]triazin-2-ylamino}-phenylamino)-[1,3,5]triazin-2-ylamino]-benzenesulfonyl}-ethyl) ester (**1a)** and 4-{4-Chloro-6-[4-(2-sulfooxy-ethanesulfonyl)-phenylamino]-[1,3,5] triazin-2-ylamino}-2-[4-chloro-6-(2-sulfooxy-ethanesulfonyl)-[1,3,5]triazin-2-ylamino]-benzenesulfonic acid (**2a**) were synthesized and their UV property was investigated. Furthermore, ultraviolet protective and fastness properties of these absorbers have been evaluated to define their efficiency.

Computational Methods

In search of the best UV absorber for cotton apparels and to authenticate the most suitable computational methodology to tailor such compounds computational approach was employed by using DFT and TD-DFT level of theory [17]. Primarily, the 3D structure of UV absorbers were created with the Gauss view [16] and executed initial conformational analysis, optimization of geometries were carried out without any structural or symmetry restrictions using DFT theory with three functionals CAM-B3LYP [20], WB97XD [21], B3LYP [22] and the basis set 6-31G(d,p) [23, 24] was implemented in the Gaussian 09 package [25]. Geometry optimization generated different conformers that were submitted to frequency calculations in order to detect the absence of imaginary frequencies, ensuring that the obtained conformation is an energetic minimum of the simulated compound.

Then, excited sates of the molecules were calculated by employing TD-DFT level of theory from the ground states of the optimized geometries with above said functional aiming to calculate the UV-Vis spectra. All calculations were performed employing the implicit solvation model IEFPCM [26] with water as solvent because it is used as solvent for finishing of cotton. From DFT and TD-DFT calculations, several structural and electronic properties were calculated, such as molecular orbital energies as well as its contribution to electronic transition.

Experimental

Materials and Apparatus

Bleached mercerized 100% cotton fabric with plain weave weighing 97.8 g/m^2 was used throughout this work. All chemicals as well as solvents were procured from sigma Aldrich, Merk and Fluka. Solvents were of analytical grade used without further purification. Thin layer chromatography (TLC) was performed on Merk Cellulose F_{254} plate. Spectroscopic measurements of synthesized UV absorbers in UV-Vis range, FT-IR studies and Mass spectra were taken on Perkin Elmer (CE-7200) spectrophotometer, Perkin Elmer (U-2001) and MALDI (matrix assisted laser desorption ionization) technique respectively. Application tests on fabric were carried out on a HD-12E exhaust machine by general procedure for monochlorotriazine reactive dyes. The UV transmittance measurement through fabric was carried out with spectrophotometer (Beckman DK-2A). Whiteness Index of treated fabrics was taken on Gretag Macbeth SpectroEye spectrophotometer. Light fastness tests were carried out with the use of Xenotest (XF-15N Shimadzu).

Synthesis: Heterofunctional two new reactive triazine based UV absorbers **1a** and **2a** were synthesized by following a condensation method as shown in scheme 1 [6].

Synthesis of UV absorber (1a) : For UV absorber (**1a**), solution of 1, 3-phenylendiamine-4 sulfonic (m-PDA) acid (1 mole) was added in cyanuric chloride suspension (2 mole, dispersed in ice water) slowly with constant stirring (Temp. 0-5°C, pH 3-3.5) and completion of first condensation was confirmed through thin layer chromatography (Merk Cellulose F_{254} plate). To the above filtrate 4-(β-hydroxyethyl)sulphonylaniline solution (2 moles, 10% Na_2CO_3, Temp. 40-45°C, pH 6-6.5) was added and second condensation was considered as completed after the vanishing of free amine tested with Ehrlich reagent. Finally synthesized compound was isolated by salting out (KCl), filtered, stabilized (phosphate buffer pH 7.0) and dried at 40˚C.

Synthesis of UV absorber (2a): 2a was prepared by following the above mentioned procedure but *p*-phenylenediamine was used instead of 1, 3-phenylendiamine-4 sulfonic (m-PDA) acid.

Finishing Procedure : Finishing of cotton fiber with reactive UV absorbers was carried out with general procedure of exhaust dyeing of cotton at liquor-fabric ratio of 30:1 as in the case of monochlorotriazine reactive dyes cited in literature [6]. The application bath exhaustion% was measured by using UV/Vis spectrophotometer (CE-7200) at λ_{max} with 1cm quartz cells for all UV absorbers. UV absorber exhaustion percentage was calculated from equation (1).

$$\%E = \left[1 - \left(\frac{C_2}{C_1}\right)\right] \times 100 \qquad (1)$$

Where C_1 is the concentration of the application bath before and C_2 is the concentration of the application bath after finishing [27].

Determination of Ultraviolet Protection Factor (UPF) and Fastness Properties: Ultraviolet protective property of finished cotton fabrics was evaluated using AATCC TM 183 test method. Durability of finished applied on fabric under laundry conditions is extremely important and fastness properties have to be assessed. The finished fabric was tested according to ISO standard methods. Whiteness of all treated samples was measured after introducing UV absorbers and after their exposure to UV radiations by Xenotest apparatus.

Results and discussion

Frontier Molecular Orbital : Geometries of UV absorbers **1a** and **2a** were optimized without imposing any constraint. The geometry optimization shows that both the UV absorbers demonstrate structural similarities, since they possess the same triazine and vinyl sulphone paraester moieties. The structural difference results from different substituent attached with bridging moiety. Afterwards, molecular orbital calculations were carried out. Table 1 shows the HOMO-LUMO and HOMO-1-LUMO+1 energy levels and energy gaps of these absorbers **1a** and **2a** respectively with CAM-B3LYP, B3LYP and WB97XD at 6-31G (d,p) basis set employed in Gaussian 09 program. Comparison of the calculated HOMO-LUMO and HOMO-1 to LUMO+1 energy gaps reveals that the ΔE increases as follows: **1a<2a**, in all the three approaches, showing that the SO_3H unit produce opposite effects on the energy gap when compared with –H unit due to electron withdrawing nature of SO_3H unit.

The calculated energy gap between HOMO and LUMO for **1a** is 7.43, 4.91 and 8.71 eV with CAM-B3LYP, B3LYP and WB97XD respectively and same for **2a** is 7.77, 5.06 and 8.77eV (Table 1). Due to high values of the calculated energy gap, it is anticipated that these molecules will absorb in the shorter region of the UV-Vis spectrum. As **2a** shows greater energy gap values with respect to **1a**, so **2a** will absorb in lower region of spectrum as compared with **1a** which is consistent with experimental results. Moreover due to high levels of the HOMO's and low levels of LUMO's, it is predicted that most of the excitations are from the HOMO to LUMO or HOMO to LUMO+1. The energy values of HOMO, HOMO-1 and HOMO-2 are relatively very close therefore they appear in the same energetic region. HOMO and LUMO sketches of **1a** and **2a** are shown in Fig. 1.

HOMO and LUMO distribution pattern of **1a** and **2a** is almost same with little difference due to presence of substituent on benzene ring. It is clear from the distribution pattern from Fig. 1 that HOMO of **1a** is mostly localized over two triazine rings and phenylendiamine sulphonic acid ring while HOMO-1 is spread over one triazine ring and aniline ring. The LUMO of **1a** is spread over one triazine ring, aniline ring and little bit on phenylendiamine sulphonic acid ring while LUMO+1 is mostly localized over two triazine rings, phenylendiamine sulphonic acid ring and aniline ring. The HOMO of **2a** is present on a triazine ring, phenylendiamine group and slightly on second triazine ring while HOMO-1 is spread over a triazine ring, aniline ring and slightly on sulphonyl group. LUMO and LUMO+1 of **2a** are distributed over a triazine ring, aniline ring with little contribution on sulphonyl group of other/opposite side chain.

Density of States (DOS): Density of the states (DOS) of the molecule **1a** and **2a** were also calculated with CAM-B3LYP/ 6-31G (d,p) and shown in Fig. 2. The results of density of state contribution supported the facts demonstrated by the frontier molecular orbital. Further evaluation of FMOs regarding percentage composition in addition to DOS around HOMOs as well as LUMOs also confirmed that components with different electron withdrawing or donating intensities may change the distribution of electron on molecular orbitals. Similarly, the DOS demonstrates the energies of all the occupied as well as unoccupied MOs of these UV absorbers.

Synthesis : The designed target UV absorbers (**1a** and **2a**) were prepared and their structure elucidated by spectroscopic techniques. The first step comprises the nucleophilic substitution of first Cl-atom of *s*-triazine by NH_2 of diamine through first condensation reaction to yield (**I** and **II** respectively) with an efficient yield. The second Cl-atom is substituted by NH_2 of 4-(β-hydroxyethyl)sulphonylaniline through second condensation reaction to give final products which were further characterized by UV-Vis., FT-IR and ESI-MS studies.

UV absorber (1a)

Colour: colourless, Yield: 75%; Molecular formula; $C_{28}H_{23}Cl_2N_{10}Na_3O_{16}S_5$, UV/Vis. spectra in water (λ_{max}): 292 nm, IR (KBr cm^{-1}):3433 (N-H), 3007(N-H), 1408 (C-N in aromatic amine), 1135(C-S), 840(C_3N_3-*s*-triazine), 736(C-Cl); ESI-MS: *m/z* 994[M (Na, K salt)]$^-$, *m/z* 972[M-Na]$^-$, *m/z* 323[M-2Na-K/3]$^-$ were detected.

UV absorber (2a)

Colour: colourless, Yield: 81%; Molecular formula; $C_{28}H_{24}Cl_2N_{10}Na_2O_{12}S_4$, UV/Vis. spectra in water (λ_{max}): 282 nm, IR (KBr cm^{-1}):3417 (N-H), 3007(N-H), 1442 (C-N in aromatic amine), 1116(C-S), 831(C_3N_3-*s*-triazine), 736(C-Cl); ESI-MS: *m/z* 913[M-Na]$^-$, *m/z* 445[M-2Na/2]$^-$ were detected.

Optical Properties

Comparison of experimental and theoretically measured UV-Vis spectra of **1a** and **2a** with B3LYP, CAM-B3LYP and WB97XD at 6-31G (d,p) is shown in Fig. 3. The UV-Vis spectrum of **1a** consists of two absorption band, one absorption band in low energy region 260 nm to 300 nm and other in higher energy region below 255 nm for the CAM-B3LYP and WB97XD. The higher energy band for B3LYP is ranging from 250 nm to 290 nm and lower energy absorption band is above 290 nm. The low energy electronic transition is due to HOMO to LUMO and HOMO to LUMO+1 overlapping (Table 2). The relatively high oscillator strength (*f*) values of **1a** are due to π-π* electronic transitions and these peaks show relatively strong molecular orbital overlapping. The larger oscillator strengths are due to better overlapping of HOMO to LUMO+1 transition. As HOMO of **1a** is mostly localized over two triazine rings and phenylendiamine sulphonic acid ring while the LUMO of **1a** is spread over one triazine ring, aniline ring and little bit on phenylendiamine sulphonic acid ring while LUMO+1 is mostly localized over two triazine rings, phenylendiamine sulphonic acid goup and aniline ringwhich describe the strong overlapping of the triazine and phenylendiamine sulphonic acid rings.

The UV-Vis spectrum of **2a** consists of one absorption band in low energy region ranging from 250 nm to 320 nm. Absorber **2a** shows low oscillator strength which is due to weak overlapping of molecular orbital in electronic transition. The low molecular orbital transition is due to HOMO of **2a** is present on a triazine ring and, phenylendiamine ring while LUMO and LUMO+1 of **2a** are distributed over a triazine ring, aniline ring with little contribution on sulphonyl group of opposite side chain.

It is important to control the substitution effect on molecular levels which can be best achieved by TD-DFT simulations. Low energy bands are mainly affected by substitution patterns which may change the HOMO levels of the compounds. In case of **2a** the Cl-atoms are present on two triazine rings which extend the π-delocalization on triazine rings. Cl-atoms stabilize the HOMO than LUMO due to its inductive effect (-I), which results in greater HOMO-LUMO energy gap. A blue shift observed and **2a** have λ_{max} at 282 nm. Introducing the –SO3H group on phenylendiamine ring in **1a** changes the π-delocalization and can change the HOMO levels which results in bathochromic shift of this absorber. The absorber **1a** shows λ_{max} at 292 nm.

Ultraviolet Protective Factor and Fastness Properties

Both the synthesized UV absorber absorbs light in the UV-range of 280-400 nm that is specific for UV absorbers. Substantivity of these absorbers was measured during testing on cotton fabric and exhaustion % values of absorbers (**1a-2a**) and commercially available absorber (Rayson C Liquid) are enlisted in Fig 4. It can be seen that exhaustion %age decreases as the concentration of the UV absorber increases and it is above 72% in all the concentrations applied in this study. Maximum exhaustion on fabric is shown at 1%

concentration of the UV absorber. It is clear from the results shown in Fig. 4 that synthesized UV absorbers (**1a-2a**) have good and comparable exhaustion properties on fabric with commercially available absorbers in market.

According to Australian standard [2], ultraviolet protective factor (UPF) ranges are depicted in Table 3. Results of UPF of treated fabric with UV absorber (**1a-2a**) and commercially available absorber (Rayson C Liquid) and un-treated fabric are graphically presented in Fig. 5. The treated fabric fall in very good UPF range at 3% concentration of UV absorber (**1a-2a**) when compared to untreated cotton fabric but have low value of UPF than commercially available UV absorber which fall in excellent range at same concentration. It is crystal clear from results that both the UV absorbers increased the UPF of fabric as the % concentration increase but they impart slightly yellowish colour at 5% on white fabric. In the case of absorber **(1a),** which absorb UV light more and give good improvement in protecting properties as compared to absorber (**2a**) but less than commercially available absorber “Rayosan C Liquid” for cellulosic fibers. This behaviour may be due to high exhaustion of absorber **(1a)** than absorber (**2a).**

UPF of treated fabric was also measured after several washes. The UPF was measured after each washing and repeated it ten times. Treated fabric with UV absorbers (**1a-2a**) remains in good range of UPF for **1a** and for **2a** it is in very good range of UPF. It is also clear from the Fig. 6 that the UPF factor is almost remain same after ten washes (little bit reduction in UPF) for **1a** and **2a**. Both UV absorbers are also in fairly good agreement in terms of UPF with the commercially available absorbers in market after ten washings as shown in Fig 6. This study revealed that designed UV absorber **1a** and **2a** have very good washing fastness properties.

Xenotest was also employed to test the light fastness of absorbers Fig 7. The treated fabric with UV absorber (**1a-2a**) and commercially available absorber (Rayson C Liquid) was subjected to xenotest for 12 hours. After exposition, UV absorber (**1a-2a**) and standard produced reduction in its UPF properties little bit but it was almost same for designed and commercially available UV absorber. The results of UV absorber (**1a-2a**) are very close to the commercially available absorber (Rayson C Liquid) Fig 7.

It is clear that one of the most important characteristic of white cotton fabric is retaining of their white colour during use. The synthesized UV absorbers did not decrease the whiteness of fabric as much at 3% concentration but after exposition to light fastness testing decrease its whiteness little bit as compared to standard but remain in good agreement with the commercially available UV absorbers as shown in Fig 8. This behaviour may be due to photo-destruction of residues of triazine.

It is clear from above discussion that both designed UV absorbers **1a** and **2a** have very good light and washing fastness properties. We have compared their UPF properties with commercially available UV absorbers and found that these can be used to enhance the UV protection of cellulosic fabrics along with commercially available ones.

Conclusion

In search of viable UV protecting cotton fabric, two UV absorbers molecules (**1a, 2a**) are designed and synthesized. Initially, electronic and optical properties of the designed molecules are studied theoretically by employing density functional theory (DFT) and time dependent density functional theory (TD-DFT). Theoretical determinations revealed that both designed UV absorber molecules (**1a, 2a**) show absorption in UV region that is specific for UV protectors. On the basis of these confirmations, these molecules were synthesized and applied on the cellulosic fabric. The application of absorbers on cellulosic fabric indicated that these compounds retained the good ultraviolet protective factor (UPF) which is comparable with commercially available absorbers in market. Current study opened a new prospect for search of such molecules that will be persistent after laundry action and can be utilized commercially.

Acknowledgements

This work is supported by department of Chemistry, University of Agriculture, Faisalabad, Pakistan. The computations/simulations/[SIMILAR] were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at Umeå University, 901 87, Umeå, Sweden.

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Scheme and Figure Captions

Scheme 1: Synthetic route for UV absorbers (**1a-2a**)

Fig. 1: Schematic view of the HOMO, LUMO, HOMO-1 and LUMO+1 of absorber **1a** and **2a** at CAM-B3LYP/6-31G (d,p).

Fig. 2: Density of the state of the UV absorber **1a** and **2a** calculated with CAM-B3LYP/6-31G (d,p).

Fig. 3: Experimental and theoretically calculated UV/Vis spectra of **1a** and **2a** with B3LYP, CAM-B3LYP and WB97XD at 6-31G (d,p)

Fig. 4: Exhaustion % of absorbers (**1a-2a**) and rayosan C liquid on cotton fabric at different % concentration

Fig. 5 Ultraviolet Protection Factor (UPF) of un-treated, treated fabric with **1a, 2a** and rayosan C liquid at different % concentration

Fig.6: Ultraviolet Protection Factor (UPF) of treated fabric (at 3% concentration) by absorber (**1a-2a)** and rayosan C liquid after laundry action (10 times)

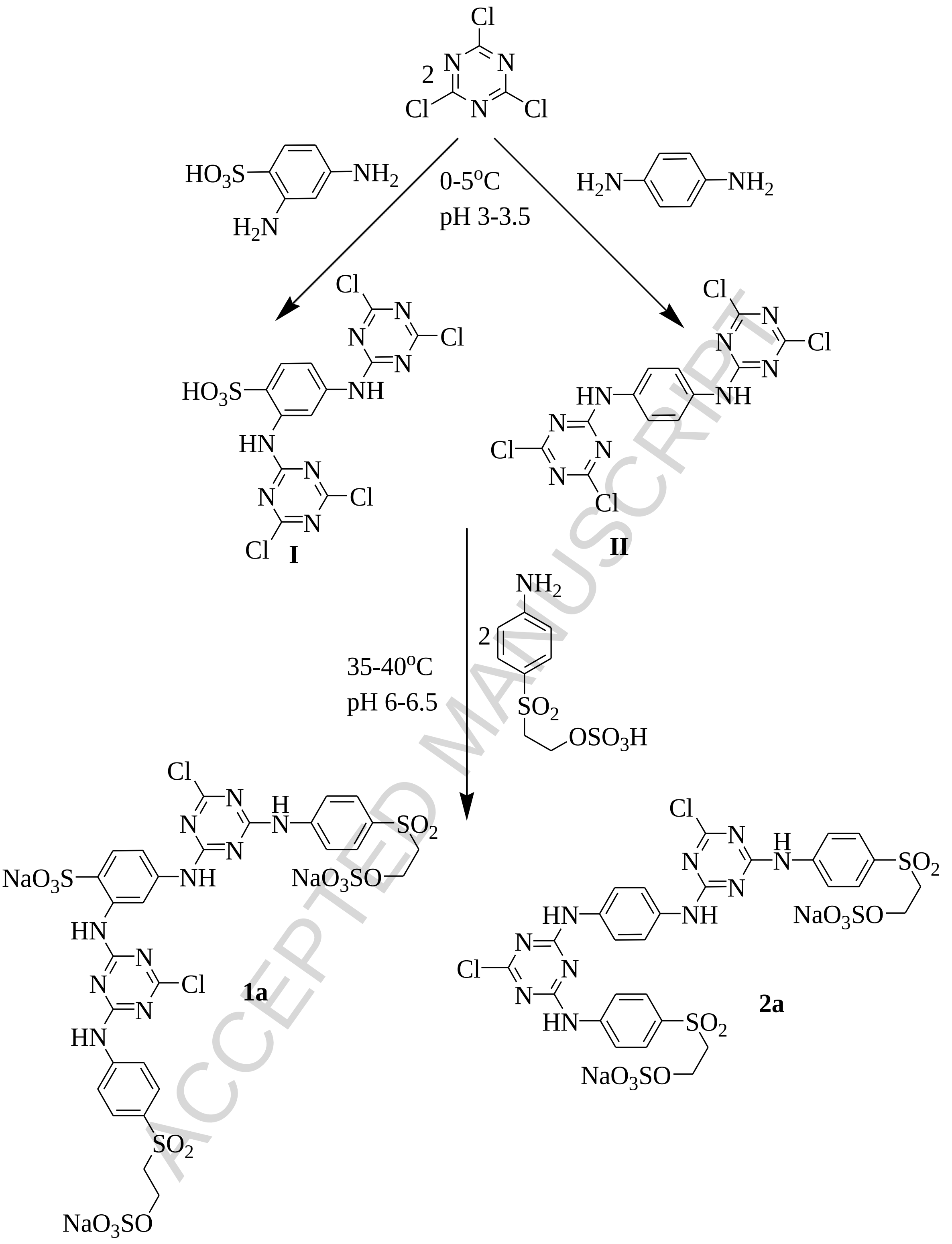
Fig. 7: UPF before and after 12 h exposure to Xenotest at 3% concentration of **1a, 2a** and rayosan C liquid.

Fig. 8: Whiteness Index (%) of un-treated, treated cotton fabric with **1a, 2a** and rayosan C liquid after UV light exposure at 3% concentration

Table 1: Theoretically calculated HOMO, LUMO, HOMO-1, LUMO+1 levels and energy gaps for the absorber (**1a** and **2a)** at 6-31G (d,p) basis set.

Table 2: The experimental and calculated λ_{max}, excitation energies (ΔE), oscillator strength (f) and electronic transition contribution calculated at 6-31G (d,p) basis set.

Table 3: Ultraviolet protection categories



Scheme 1: Synthetic route for UV absorbers (**1a-2a**)

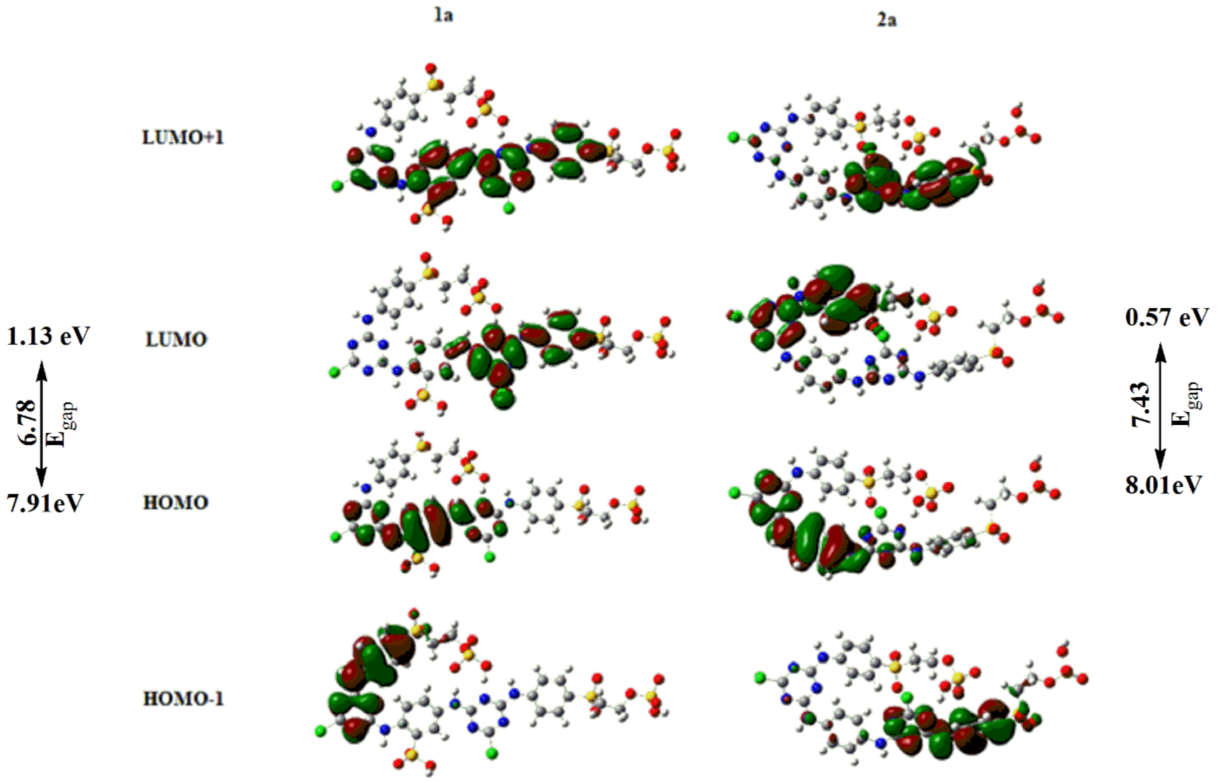


Fig. 1: Schematic view of the HOMO, LUMO, HOMO-1 and LUMO+1 of absorber **1a** and **2a** at CAM-B3LYP/6-31G (d,p).

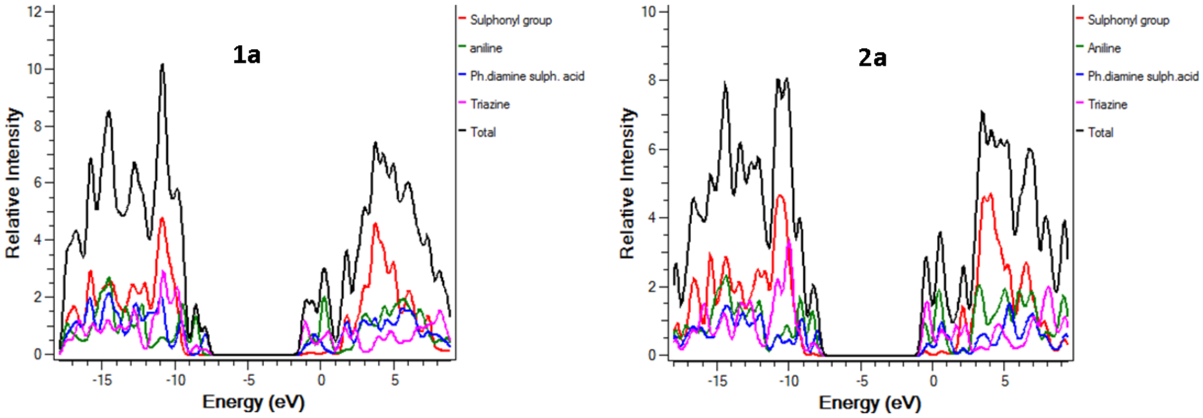


Fig. 2: Density of the state of the UV absorber **1a** and **2a** calculated with CAM-B3LYP/6-31G (d,p).

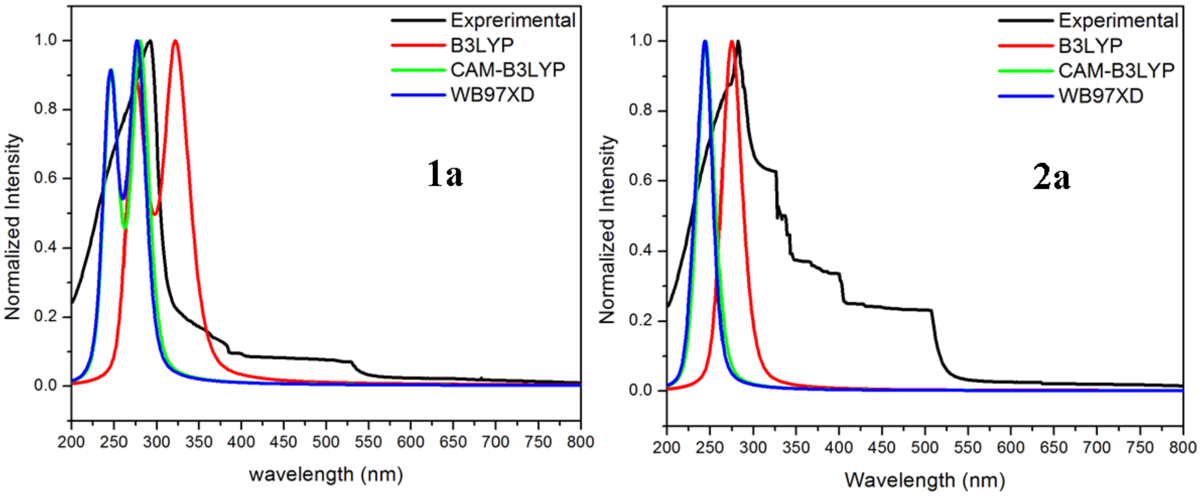


Fig. 3: Experimental and theoretically calculated UV/Vis spectra of **1a** and **2a** with B3LYP, CAM-B3LYP and WB97XD at 6-31G (d,p)

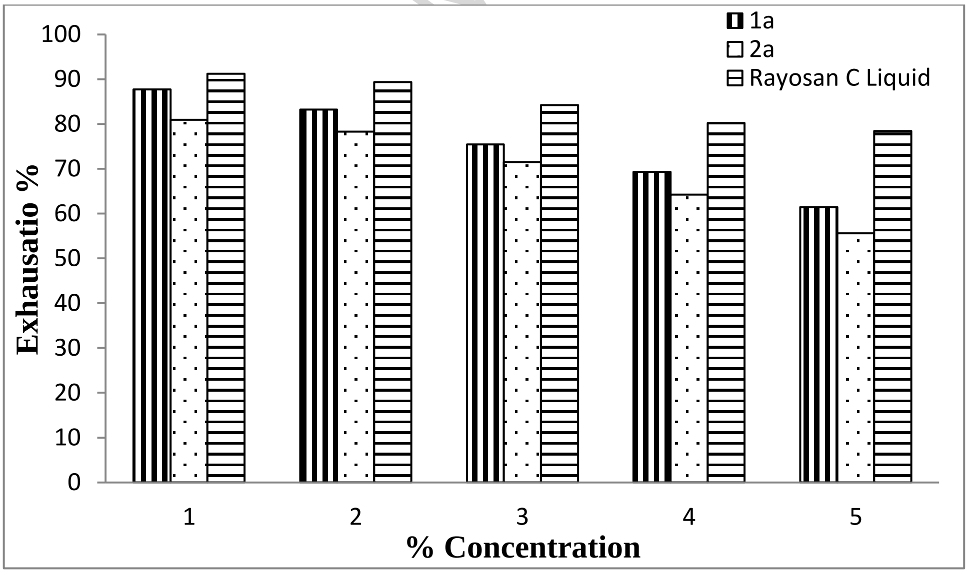


Fig. 4: Exhaustion % of absorbers (**1a-2a**) and rayosan C liquid on cotton fabric at different % concentration

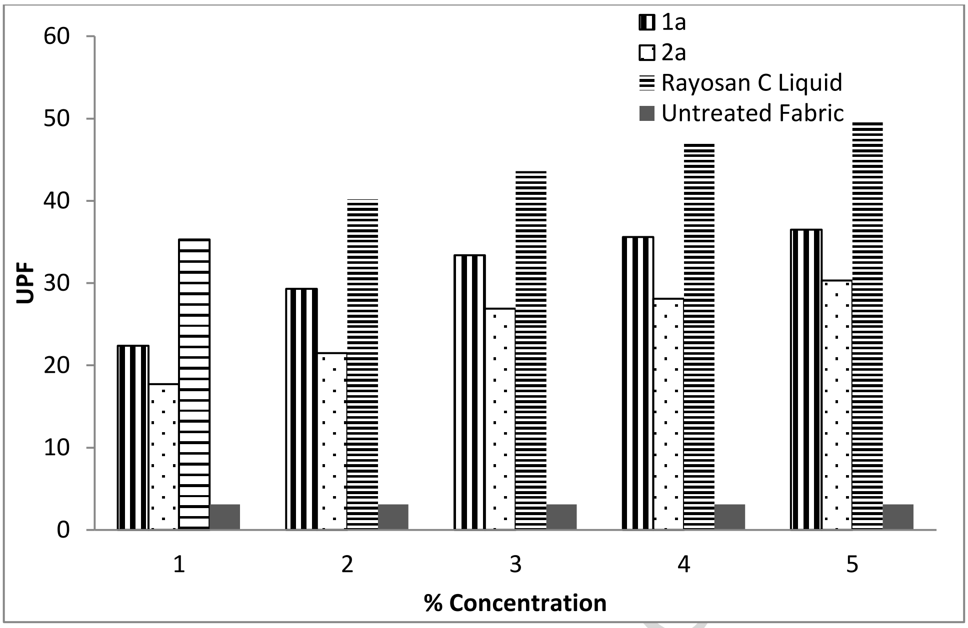


Fig. 5 Ultraviolet Protection Factor (UPF) of un-treated, treated fabric with **1a, 2a** and rayosan C liquid at different % concentration

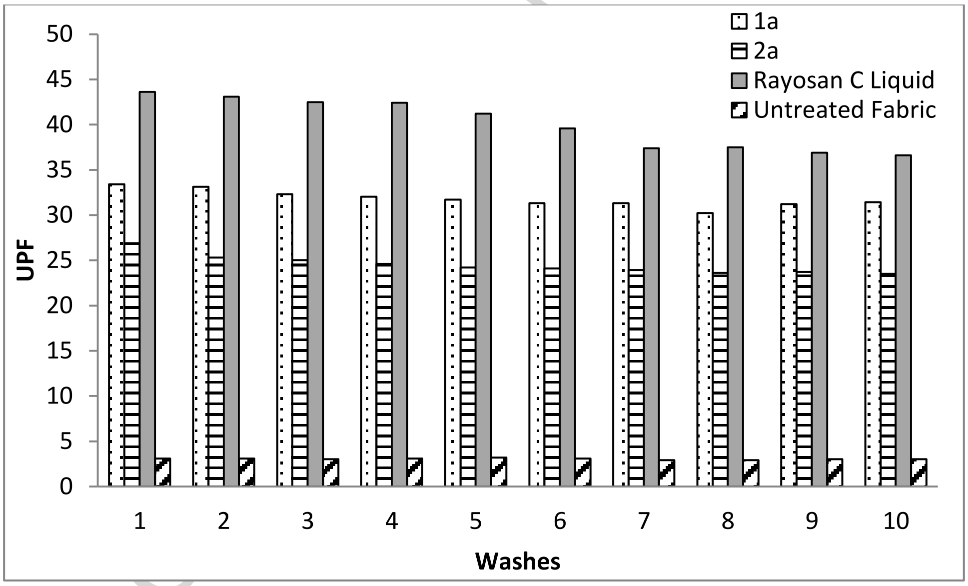


Fig.6: Ultraviolet Protection Factor (UPF) of treated fabric (at 3% concentration) by absorber (**1a-2a)** and rayosan C liquid after laundry action (10 times)

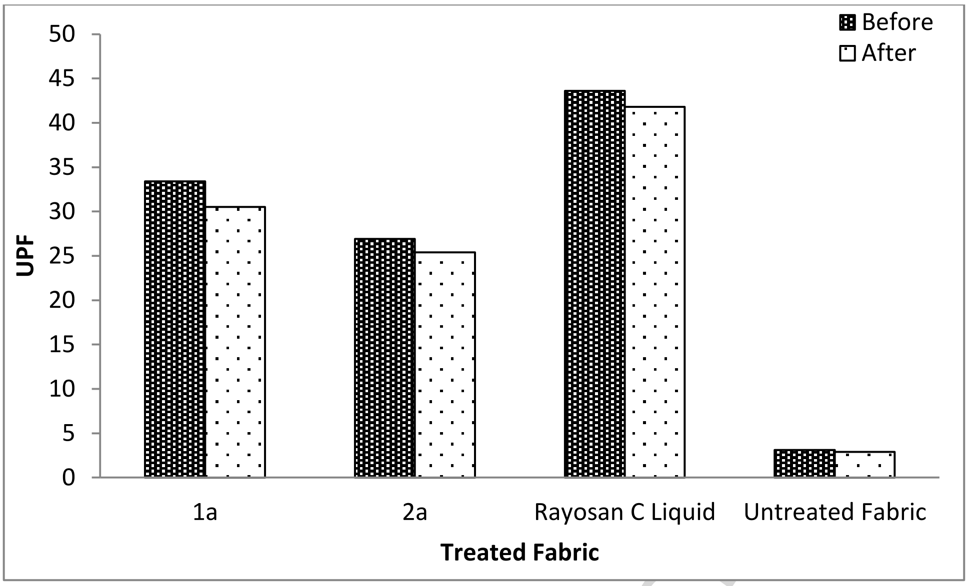


Fig. 7: UPF before and after 12 h exposure to Xenotest at 3% concentration of **1a, 2a** and rayosan C liquid.

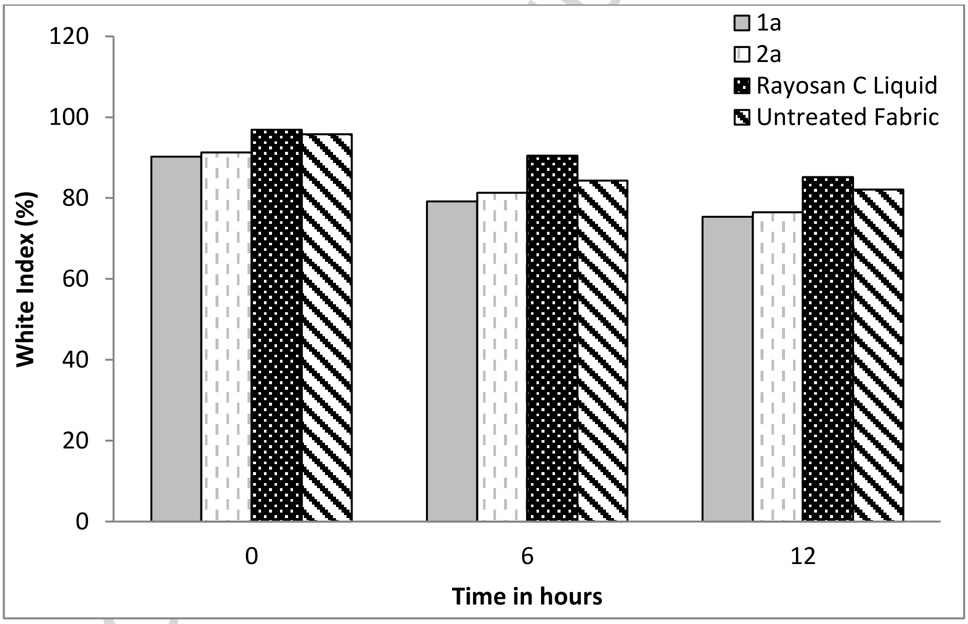


Fig. 8: Whiteness Index (%) of un-treated, treated cotton fabric with **1a, 2a** and rayosan C liquid after UV light exposure at 3% concentration

Table 1: Theoretically calculated HOMO, LUMO, HOMO-1, LUMO+1 levels and energy gaps for the absorber (**1a** and **2a)** at 6-31G (d,p) basis set.

Functional	Absorber	HOMO (eV)	LUMO (eV)	E. Gap (eV)	HOMO-1 (eV)	LUMO+1 (eV)	E.Gap (eV)
CAM-B3LYP	**1a**	7.91	1.13	**6.78**	8.48	0.98	**7.49**
B3LYP		6.60	2.47	**4.12**	7.06	2.25	**4.80**
WB97XD		8.52	0.57	**7.95**	9.06	0.45	**8.61**
CAM-B3LYP	**2a**	8.01	0.57	**7.43**	8.25	0.48	**7.77**
B3LYP		6.81	1.90	**4.91**	6.89	1.83	**5.06**
WB97XD		8.73	0.02	**8.71**	8.84	0.07	**8.77**

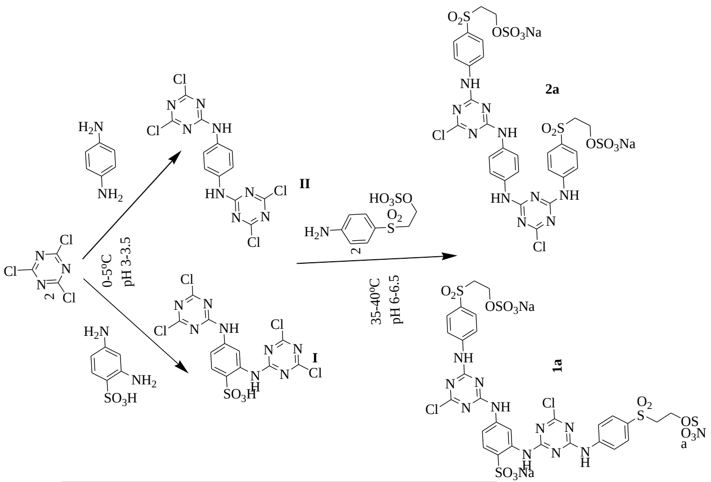
Table 2: The experimental and calculated λ_{max}, excitation energies (ΔE), oscillator strength (f) and electronic transition contribution calculated at 6-31G (d,p) basis set.

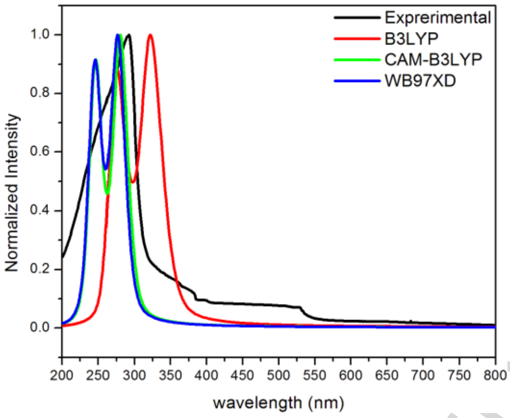
Absorber	**Functional**	**$\lambda_{max}^{Calc.}$ (nm)**	**ΔE (eV)**	**Oscillator strength (f)**	**Electronic Transition Contribution**	**$\lambda_{max}^{Exp.}$ (nm)**
1a	B3LYP	335.8	3.69	0.257	H-0->L+0(+95%)	292
	CAM-B3LYP	280.4	4.42	1.7936	H-0->L+1(+61%)	292
	WB97XD	277	4.48	1.741	H-0->L+1(+63%)	292
2a	B3LYP	295.6	4.2	0.0218	H-0->L+1(+89%)	282
	CAM-B3LYP	256.3	4.84	0.4287	H-0->L+2(+31%) H-1->L+1(+24%)	282
	WB97XD	252.2	4.92	0.2218	H-2->L+1(+27%) H-0->L+2(+19%)	282

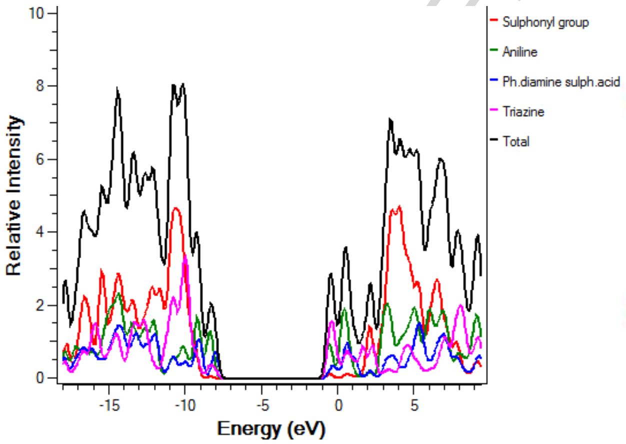
Table 3: Ultraviolet protection categories

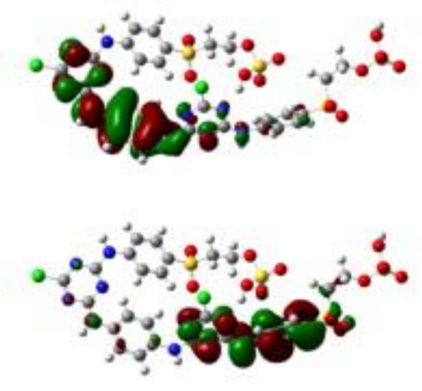
Sr. No	**UPF Range**	**Protection Category**
1	40-50, 50 +	Excellent
2	25-39	Very Good
3	15-24	Good

Graphical abstract









Two triazine based Ultra Violet (UV) absorbers (**1a, 2a**) with different substituents were designed and synthesized. The performance of synthesized compounds as UV absorbers and their fastness properties were assessed by finishing the cotton fabric through exhaust method at different concentration and results appeared in good range.

Highlights:

- Two triazine based Ultra Violet (UV) absorbers with different substituents have been designed computationally and synthesized.
- The application of absorbers on cellulosic fabric indicated that these compounds retained the good ultraviolet protective factor (UPF) which is comparable with commercially available absorbers in market.
- These molecules are anticipated to be persistent after laundry action and can be utilized commercially.