#### act cut clap multipl



acciperet. Lercio ne de filias fuas atbenas vocaret. Doete vero bicút neptunú z minerua atbenas codidif fe. Sed ci ze nomis impolítice inter cos fieret diffenfio. Bijs relide pñtibus fit inter cos couentio. ví d p cuffa terra laudabilioze "pduceret effectú vrbi nome imponeret. Theptun? aŭt tridete fuo pcuffa terra. Equí pdurit belli omen. Et minerua bafta piecta oliuá pdurit pacis arboze. Que qmvtilioz eou iudico vifa fu it .er fuo nomie atbenas birit. Tiá minerua atbene grece bicit .æ d lucan? libzo ferto ait. Brim? ab corea p

#### <u>Content</u>

RS Theory: intro **RS** Pros and Cons Comparison with other spectroscopic methods **Understanding Gorgias:** main components spectrometer radiation source (the lamp) reflectance probe specs software Practicing: **Pigments Checker** white pigments blue pigments Identifying the pigments: Database Applications: woodcut prints statues Notes: dyes and lakes paint layers, example 1, 2, 3 paint mixtures, example 1, 2 paint thickness, example 1 varnishes and binders measure lamps radiation Spectragryph



A Reflectance spectrum shows for each wavelength the percentage of radiation that is reflected (reflectance (%)). The reflectance spectra can provide information useful for the identification of pigments since the radiation that is not reflected is absorbed or transmitted **depending on the chemical composition of the material tested.** 

### **RS** Theory: intro



chsopensource.org

Cultural eritage

cience

pen ource

S

A reflectance spectrum shows Reflectance as a percentage and wavelength as nm. The features of a reflectance spectrum are described as "absorption band", "inflection point" and "maxima". This graph shows the spectra of 3 white pigments. Lithopone's spectrum is characterized by a structured absorption band between 650 nm and 750 nm. This large structured absorption band is made of smaller absorption bands (indicated by the arrows).

### **RS** Theory: intro





"Inflection point" is the other feature to describe a reflectance spectrum. The graph above shows the reflectance spectra of 3 yellow pigments. They are all characterized by a sharp curve representing the increase in reflectance. The inflection point is roughly the middle of this curve and we want to define its position as a specific wavelength.

To be precise, it is the point where the curve goes from concave to convex. Mathematically it can be calculated and spectra editing software generally do this operation. Still a visual inspection is sufficient.

#### chsopensource.org







"Maxima" are the last feature to describe a reflectance spectrum. The graph above shows the maxima for 2 green pigments. A maximum is the result of 2 contingent absorption bands. We have this impression of a "peak" but it is actually the result of the action of the 2 absorption bands.

chsopensource.org



**RS** Theory: Pros and Cons

RS is a first non-invasive
step of a multi-technique
analytical strategy for
identification of pigments
and dye stuffs in art object

- Affordable
- Non-invasive
- Portable
- Light weight and small

ultural

cience

pen

RS Theory: comparison with other spectroscopic methods

### Spectroscopic methods for Art Examination

### **REFLECTANCE SPECTROSCOPY**

UV, VIS and IR regions of the electromagnetic spectrum gives information related to the <u>electronic transitions</u> of the materials.

### VIBRATIONAL SPECTROSCOPY

Raman and FT-IR spectroscopy provide information on molecular vibrations

### ELEMENTAL SPECTROSCOPY

X-Ray fluorescence spectroscopy provides information on the chemical elements



chsopensource.org

Cultural eritage

> pen ource

cience

S

RS Theory: comparison with other spectroscopic methods

# Why to use Reflectance Spectroscopy and/or

### Raman spectroscopy

	Raman	Reflectance
Identification accuracy	High	Medium
Success rate for real samples	Low	High
Easy of use	Low	High
Equipment cost	High	Low

#### chsopensource.org

Cultural Heritage Science

> pen ource

### **Understanding Gorgias: main components**



#### chsopensource.org

#### Cultural Heritage Science Open Source

### **Understanding Gorgias: spectrometer**



There are 2 main kind of Reflectance spectrometers. Their main feature is the spectral range covered by their detector. Gorgias covers the range 300 nm (UV) until 1000 nm (IR). UV, VIS and IR are electromagnetic **radiation bands** with different wavelengths. "**Light**" is the VIS part of the electromagnetic spectrum. The other class of spectrometers cover up to 2500 nm but they use a much more expensive detector.

### Understanding Gorgias: spectrometer



Quantum efficiency (QE) is a measure of how well a specific CCD responds to different wavelengths of light. The higher the QE, the more sensitive a CCD will be at a particular wavelength. The CCD detector inside Gorgias has a high QE in the visible region decreasing QE in the UV and far IR.

This is on of the 2 reasons why we have more noise in our spectra in the UV and far IR regions. The other reason is that the halogen lamp has little UV component.

NOTE: The cap on the spectrometer entrance is a cosine corrector adapter, made with optical Teflon with flat transmission in the spectral region 200-2900nm. A cosine corrector is used to enhance the collection of input radiation.



chsopensource.org

#### chsopensource.org



### **Understanding Gorgias: radiation source**



The radiation source for Gorgias is a 10W halogen lamp. We provide 3 other replacement lamps. It's easy to replace the lamp. Just open the case and remove the burnt lamp from its socket.

The illustration above shows that the halogen lamp is rich in visible radiation and IR but still have sufficient near UV from 300 nm.

#### chsopensource.org

Cultural eritage Science

pen

### Understanding Gorgias: reflectance probe



The reflectance probe is composed of 3 outputs. One goes into the spectrometer, one into the radiation source and the last one is used to make the actual measurements. This probe is a bundle of 7 Thorlabs FT600UMT fiber-optics (core diameter 600 microns). 6 of them are used to collect the radiation from the lamp and one is the used to send the reflectance signal from the sample to the spectrometer. In the illustration above, the fiber in the middle of bundle is the one that collect the signal for the spectrometer. These fibers can cover the range 300-2200nm and have a metal jacket for better mechanical strength.

#### chsopensource.org

### Understanding Gorgias: reflectance probe





We can do the measure with the bare probe or we can add the probe cover. This cover is useful if we are working within an environment with strong light. This cover block out all the external light so we can have a precise measure. The only issue about this method is that we do not see exactly where the probe is measuring. So, generally we use the cover for large color area but definitely we cannot use it for small details.

#### chsopensource.org

DAMMAR

SAMMAR

DAMMAR





Gorgias use a probe with the lamp and the spectrometer fibers bundled together, so we are lighting the sample and collecting radiation from the same direction. This is the best approach to avoid the specular reflection. The illustration above shows that if the observer is on the other side of the lamp, the observer gets most of the specular reflection which is useless for Reflectance spectroscopy because the light does not interact with the material but it is just bounced off, without carrying chemical information. We see the "real" colors if the observer is on top of better on the same side of the lamp, as in Gorgias.

#### chsopensource.org



### **Understanding Gorgias: reflectance probe**



Included with Gorgias kit is our **PLASTIC PROTECTIVE SHEET**. You can apply this plastic film over your artwork if you are concerned of any damage done using the probe. This plastic film is transparent to the range 300-1000 nm so it is not affecting the spectra.

#### chsopensource.org



### Understanding Gorgias: reflectance probe



Two example of spectra collected with and without our PLASTIC PROTECTIVE SHEET. The sheet just reduces the overall high of the spectra, because absorbs and reflects a part of the radiation from the lamp. Though, the shape of the spectra is preserved.

**Understanding Gorgias: specs** 

### **Technical Specifics**

Detector: Toshiba TCD1304DG linear array Detector spectral range: 300 – 1000 nm (100 microns slit) Pixels: 3648

#### **Other Technical Specifics**

Weight: 430 grams Dimensions: 102 mm x 84 mm x 59 mm Pixel size: 8 um x 200 um Pixel well depth: 100,000 electrons Signal-to-noise ratio: 400:1 (10000:1 with averaging) A/D resolution: 16 bit Fiber optic connector: SMA 905 to 0.22 NA single-strand optical fiber. Diffraction order sorting filter: included CCD reading time: 14 ms Power consumption: 100mA @ 5V from USB interface Onboard memory capacity: 64 spectra Data transfer speed: 200 ms / 100 ms (2 points binding) Computer interface: USB 2.0, HID 2.0 Operational system: Windows 10 /Windows 8 / Windows 7 / Vista / XP; 32/64b Software: application software, driver, Hardware: USB cable



**Understanding Gorgias: software** 

## No need for installation No licence



The spectrometer is recognized by Windows operational system as standard HID device. That is why there is no need to install any special drivers to use Gorgias spectrometer. Just start the software from a portable device connected to any computer, such as a USB key. You can also copy the software folder in your hard drive and from there launch gorgias.exe. As simple as that!

Also the software does not have any licence required so you can use it on as many computers you need. Following are some slides for the common operations on the software. Watch the video lessons for further info.

chsopensource.org



#### chsopensource.org

Cultural Heritage Science

pen

### **Understanding Gorgias: software**



Once the spectrometer USB cable is plugged on your PC, launch gorgias.exe. The main window of the software will show up. If the system is correctly recognized by your PC, you will be able to check the "RUN" box. The system will start to acquire spectra, continuously.



We need to setup few parameters.

BOXCAR. This is a smoothing function by averaging the values of adjacent pixels together. Boxcar is useful when the spectrum is relatively flat and little variation is expected between adjacent pixels, as in reflectance spectroscopy. We want input "10".

SCANS. We can have an average of more measures (scans). For Reflectance Spectroscopy, we can just have "1" EXPOSURE. This depends on your actual system and you have to setup. See video "Setup and calibration" in Lessons "Installation and setup"



A background spectrum can be subtracted. For reflectance spectroscopy this is not strictly necessary and we will not do this procedure. Since the exposure time is very short, we do have very little electronic noise which will not affect our spectrum. This software is also used for Raman spectroscopy, that why we have the background subtraction which is important in this case because of the much longer exposure required in this case.



See video "Setup and calibration" in Lessons "Installation and setup" for more info.

We need now to calibrate the system, we put the probe at 45 degree in contact with the white standard and we click the button indicated above. A calibration file has been created (no confirmation comes from the software, no pop up window or beep).



See video "Setup and calibration" in Lessons "Installation and setup" for more info.

The spectrometer can do different kind of spectroscopic measures. We need to check the "spectra/Ref" box in order to have actual Reflectance spectra. This is the main method we will use but we could be interested to other once.



It is possible to add a color bar to our spectra. This feature could be useful for beginners not familiar with the wavelenght values of the UV, VIS and IR spectral ranges.

#### chsopensource.org

### Practising: pigments checker





We recommend to use our Pigments Checker to start practising with your Reflectance Spectrometer.

Pigments Checker is a very useful tool to practice Reflectance Spectroscopy, as well as other imaging and spectroscopy methods.

Pigments Checker is a collection of the most important pigments in art history. Among all the pigments and their varieties ever used in art, this collection selects the most used from antiquity to early 1950'. Pigments Checker is a standard tool designed for Art professionals, scientists, students and conservators to evaluate and practice non-invasive techniques for pigments identification.

**Pigments Checker Timeline** provides a simplified representation of the use of the pigments across ages. Pigments' history is actually quite complex and depends on a number of factors; The kind of artifacts. A pigment can be used on wall paintings while becoming obsolete in easel paintings. Geography. As an example, natural cinnabar is found in Almaden (Spain) and Murillo used it since it was close to him, rather than the artificial form, vermilion, much more diffused elsewhere.

> CLICK HERE Pigments checker webpage



#### chsopensource.org



### Practising: pigments checker

BLACKS	BROWNS	GREENS	BLUES	REDS	YELLOWS	WHITES
ivory black	burnt sienna	chrome oxide green	azurite	naphthol red	cadmium yellow	lead white
vine black	burnt umber	cobalt titanate green	blue bice	cadmium red	cobalt yellow	zinc white
bone black	van dyke brown	green earth	cobalt cerulean blue	red lead	lead tin yellow I	lithopone
lamp black	raw sienna	malachite	egyptian blue	red ochre	lead tin yellow II	titanium white
iron gall ink	raw umber	phthalo green	indigo	vermilion (natural)	massicot	gypsum
	bitumen	verdigris	maya blue	madder lake	naples yellow	chalk
	sepia	viridian	prussian blue	lac dye	orpiment	
		cadmium green	smalt	carmine lake	curcuma	
			ultramarine (natural)	realgar	yellow ochre	
			phthalo blue	vermilion (artificial)	yellow lake Reseda	
			cobalt violet	alizarin	gamboge	
			cobalt blue		chrome yellow	
			cobalt chromite blue		arylide yellow 5GX	
			manganese violet		stil de grain	
			vivianite		saffron	
			han blue			

ultramarine (artificial)

On the pigments checker webpage, you can find chemical and various information on each pigment. You can also download and view their Reflectance, Raman and XRF spectra.

CLICK HERE Pigments checker webpage

### Practising: pigments checker

#### **Pigments** Checker

egyptian blue

The first synthetic pigment used from the early dynasties in Egypt until the end of the Roman period in Europe.

Manufacturer / product code: Kremer / 10060 Chemical description: artificial copper calcium silicate. Kremer PDF Color: blue Color Index: PB31 More info: Pigments Through The Ages

#### Raman spectroscopy



Pigments thoroughly characterized by Reflectance, Raman and XRF spectroscopy

chsopensource.org

Cultural eritage S cience pen S ource

Practising: white pigments

## White pigments



We start practising our Gorgias on the white pigments. Pigments Checker has 4 white pigments: lead white, zinc white , titanium white and lithopone. There are also gypsum and chalk, which are mostly used as grounds. These 4 whites have different reflectance spectra and can be distinguished using Gorgias.



chsopensource.org



The graph shows the spectra of 3 whites. The bar below gives an indication of the 3 main spectral band covered by Gorgias. We can tell immediately that the 3 pigments show very different spectra. Lithopone is characterized by a strong absorption in the near infrared region. Titanium white absorbs strongly in the UV region and, eventually, lead white has high and flat reflectance across all the 3 spectral regions.

#### chsopensource.org



#### Practising: blue pigments



The same can be done with other pigments. Let's try 3 of the most used blues: azurite, ultramarine blue and cobalt chromite blue. Let's start comparing azurite with ultramarine. Both the pigments have a maximum in the blue spectra region. This is what we expect since we are testing "blue" pigments, so we must see strong reflectance in the "blue" region around 450 nm. The different feature between the 2 spectra is in the infrared region. Here we observe that the reflectance of azurite is low and that of ultramarine is high! To be precise, ultramarine becomes transparent in the infrared region, so the high reflectance comes from the white cardboard used as a support for the pigment.



#### Practising: blue pigments



This spectrum shows cobalt chromite blue. This is an example of spectrum rich in features. The pigment has a large absorption band between 500 and 700 nm, but also it has a number of small absorption bands that are very characterizing for the pigment.

#### chsopensource.org

### Identifying pigments: database



We discussed so far how to acquire a reflectance spectrum of a pigment. For its identification we use a database, a simple collection of spectra acquired from known pigments, such as in Pigments Checker. The example above shows the reflectance spectrum of the red point 2 (green line) on this wall painting, compared with the spectrum of red ochre in Pigments checker (black line). Pigments' identification involves a spectral database to compare the spectral features of the investigated unknown spectrum with the ones available in the database.

Cultural Heritage Science Open Source
chsopensource.org



### Applications: woodcut prints

### Sheet with woodcuts from Schedel's World Chronicle (1493)

Courtesy of CHSOS collection

### When were the woodcut prints hand-colored?

Watch lesson "Applications". We have a video "woodcut prints".

#### Lercia etas mundi

Srom Anno mundi.3 4 95. Dimo a natiuitate Haac anno apud argos in Zbeffalia pzim<sup>9</sup> regnare ce pit. Id vero regnū duranit anni 3. 5 4 4. Lecrops aŭt egipti<sup>9</sup> geto z nonagefi mo iudaice fuitur ano regno arguoz relicto pm<sup>9</sup> atbemefib<sup>9</sup> regnit anis. 50.



A Ébene ciuitas fuit pelarifima in attica regiõe. Lui<sup>o</sup> pauca veftigia quedă manêt. Ibăc pzimo ab alabábo coditas dirit Licero libzo tercio te natur raceon. Plato vero în Limeo dirit. Amafim regem eşipti ci<sup>o</sup> vzbis coditozê fuifle. Láçs vocabulo egi ptio cognomiafle. 98 ligua greca atbenă fonat. Elij Lecropem illă odidifle dicut. Et eă fubita apparitio ne arbozis oline mineruă cognoiafle. quă ea arboz d figna<sup>\*</sup>. 7 ligua greca atbena dr. Elena apo illos, p cea colebat. Et ei nomie Dur auguftin °ce ciurtate cer

libro tectimooctauo varia feribit aucite varronis. Lecrope atbenau vrbé inflaurame fubito aquio in loco erupiti Ét alto repta olea arboz. fuper qbus, pdigijs fetfetta? apollo telpbicus qd intelligedus. qdue faciedus fozet refpodifie fertur Do olea mineruā. Equa vo neprinu fignificare ambo cofobrini . Embo oij et cotempozanei. Effetos in cou ciutu arbitrio, vi ex alteri? Duou teou nomie ciut tas vocaref . Logregatis oibus viruifos fer? viri adbeferut neprino. Apulieres vero albinerue. Que v obtinuerut vi ex minerue nomie ciuitas appellaref . Et fic atbenā grece vzbē cognomiaueit qd latine albineruā bicim?. Eo op mulierus voces vna virou numeu fuperarint. Quadobzem irat? neptim? dbarinis effuăți

bus vndis athemenfiù terras populat' eft. Que cues placare voletes triplici fupplicio multeres affecere . "Primo vt decetero nullis publicis intereffent cofultatioid". Scoo vt null' nafcetum cognome maternus acciperet. L'ercio ne de filias fuas athenas vocaret. Poete vero dicut neptună z minerua athenas codidif fe. Sed că de nomis impofitice inter cos fieret diffențio. Dijs relids pfitibus fit inter cos conentio. vt d p cufla terra laudabilicie, pduceret effectă vrbi nome imponeret. Theptun" aŭ tridete fuo pcufla terra. Equa pdurit belli omen. Et minerua bafta, piecta oliuă, pdurit pacis arboze. Que qfiivilice con indico vifa fu it. ex fuo nomie athenas dirit. Thă minerua athene grece dicit. Ce q lucar<sup>0</sup> libro ferto ait. Prim<sup>o</sup> ab cerea p cuflus cuffice faris. Ebeflalic<sup>0</sup> fonipes bellis feralib<sup>0</sup> omen Erilit. Et virgili<sup>0</sup> georgicon pmo. Luca o cui







Reflectance spectra of some brown pigments in *Pigments Checker* 





The best "match" for the brown color of the branch is "raw sienna"



was painted with "raw sienna", available at any historical age





Reflectance spectra of some red pigments in *Pigments Checker* 





The best "match" for the red color of the beard is "red lead"

### Pigments Checker timeline









Reflectance spectra of some blue pigments in *Pigments Checker* 



Albaio The best "match" for the blue color of the vest is "cobalt blue"







Reflectance spectra of some yellow pigments in *Pigments Checker* 









Reflectance spectra of some green pigments in *Pigments Checker* 





### When were the woodcut prints hand-colored?

## After 1862



Srom Anno mundi.3 4 95. Eram vero anno mdi.3 5 4 4. Dicozif regnu argunozi vbi Inach? occani z terre(vt atūt)filius feragefimoa natiuitate Ifaac anno apud argos in Zbeflalia pzim? regnare ce pit. Id vero regnu duranit annis. 5 4 4. Lecrops aŭt egipti? gztoz nonageli mo iudatee butut ano regno arguoz relicto pm? atbeniclib? regnit anis. 50.



A Ébene ciuitas fuit pelarifima in attica regiõe. ab alabábo cöditas birit Étero libzo tercio de natura raceon. Plato vero in Limeo birit. Amafim regeni cajiptu el vero in Limeo birit. Anafim regeni cajiptu el vero in Limeo birit. Anafim regeni ptio cognomiafie. qd ligua greca atbenă fonat. Aliji Lecropem illă odidifie bicut. Et eă fubita apparitio ne arbozis oliue mineruă cognoiafie. quă ea arboz d figna : t ligua greca atbena or. Clen alij ab eo no co dită fiftaurată putăt. 9 tipe Atbena apo illos p cea colebat. De el nomie Diul auguftin ce cinitate cei

libro tecimooctauo varia feribit aucte varronis. L'ecrope athenan vrbé inftaurante fubito aquno in loco erupit: Et alto repta olea arboz. fuper qbus. pdigijs feifeitar? apollo telpbicus qd intelligedus. qdue factedus fozet refpodifie fertur 20 olea mineruă. Aqua vo neptunu fignificare ambo cofobrini. Ambo bij et cotemporanet. Effeteg in con ciutu arbitrio, vt ex alteri? Duon teon nomie ciut tas vocaret. E ogregatis olbus virungs fer? viri adbeferut neptuno. Abulteres vero abinerue. Que t obtinuerut vt ex minerue nomie ciuitas appellaret. Ac fic athena grece vzbé cognomiaueit qo latine abineruă bicim?. Eo op mulierus voces vna viroz numer fuperarint. Quaobzem irat? neptun? Abarinis efluăn



Efrom

bus vndis athemenfiù terras populat? eft. Que cines placare voletes triplici fupplicio multeres affecere. Primo vt decetero nullis publicis intereffent cofultatioid?. Scoo vt null? nafcetum cognome maternus acciperet. Tercio ne de filias fuas athenas vocaret. Poete vero dicti neptunti z minerua athenas codidit? fe. Sed ci ce nomis impositioe inter cos fieret diffensio. Dijs relide pfittbus fit inter cos conentio. vt q p cuffia terra laudabilicie, pduceret effecti vrbi nome imponeret. Theptun? aŭt tridete fuo pcuffa terra. Equi pducit belli omen. Et minerua baffa, piecta oliuă, pdurit pacis arboze. Que qinvilioz eou indico vifa fu it. er fuo nomie athenas dirit. Thă minerua athene grece dicte. ce q lucar? libzo ferto att. Petin? ab cărea p cuffus enfrite farts. Theffalte? fonipes bellis feralib? omen Erilit. Et virgili? georgico2 pmo. Tuqo cui

### Applications: statues



chsopensource.org





Reflectance Spectroscopy is a valid tool for conservators. This statue was extensively gilded but a good part of it has been lost and replaced with yellow ochre. Even in some areas, the bolo (red ochre) preparation is still visible. Reflectance spectroscopy can tell the original gilding from those areas that have been replaced with yellow ochre paint from their different spectra.

#### chsopensource.org



### Notes: dyes and lakes

Reflectance Spectroscopy is a valid tool for mineral pigments. The pigment has always the same chemical formula and so we do not expect changes in the reflectance spectrum. On the other hand, dyes and lakes, made from organic origin, have been realized with different recipes in order to obtain specific tones. This create different reflectance spectra. Let's take the case of madder lake.

We tested 9 madder lake recipes. They were made with same madder root but different mordant and procedures such as for boiling also different reflectance spectra. The madder lakes are all characterized by the increased reflectance in the infrared but the inflection point has a large variability.

Reflectance [%]



### Notes: paint layers, example 1

chsopensource.org





When we tested our Gorgias on the Pigments Checker we tested one pigment at a time. This is the most simple situation. One pure pigment laid on a white ground. Now we have other questions, because in the real cases we have layers of paints and mixture. This example illustrates with a medieval painting technique mock-up. Azurite was painted on the white ground and the was partially covered with ultramarine. This was a technique to enhance the ultramarine color. What happens when we take a reflectance spectrum from the area where ultramarine is painted over azurite?

#### chsopensource.org

Cultural eritage

cience

pen

S

### Notes: paint layers, example 1



This graph shows the spectra of the 3 areas. What happens is that the spectrum of "ultramarine over azurite" is like the one of standard ultramarine but in the infrared region we see much less reflectance. Ultramarine is mostly transparent in the infrared region, so the infrared radiation from the lamp goes through ultramarine and reaches azurite. The bottom layer of azurite absorbs this infrared and we have the resulting spectrum, ultramarine with much less reflectance in the infrared region.

### Notes: paint layers, example 2





This example discusses 2 blue pigments over a white ground preparation made of titanium white, such we can find in art after 1920' when titanium white becomes available as a commercial white paint.

#### chsopensource.org





First we discuss azurite. This pigments reflects blue light but then it absorbs all the other spectral ranges. Consequently, we see that the spectrum of azurite over titanium white is not affected at all.

#### chsopensource.org

#### G Cultural Heritage Science Open Source





Now we discuss smalt. Let's look at the UV region. The reflection of smalt in the UV region is much less when it is painted over titanium white. This is because smalt is a partially transparent in the UV and the UV radiation from the lamp is now absorbed by the titanium white. In the infrared region we see increased reflectance. This is because titanium white is reflecting better than the cardboard used to make the standard in Pigments Checker. Bottom line, the spectrum of smalt over a preparation layer painted with titanium white shows less reflectance in the UV and much reflectance in the IR region. If we understand these processes, we can use these modified spectra to actually figure out the layering of the paints. So a spectrum of smalt with less reflectance in the UV is likely to be smalt over titanium white.

#### chsopensource.org

### Notes: paint layers, example 3





In the previous example we saw pigments over a white pigment. We discuss now pigments over a black paint, lamp black. This would be the same for any other of the black pigments based on carbon, which absorbs on all the spectral regions.

#### chsopensource.org

Cultural Heritage

cience

pen

S

#### Notes: paint layers, example 3

![](_page_61_Figure_3.jpeg)

Let's start discussing smalt. We also have here an infrared photo of the same mock-up. Notice that the spectral range of the Gorgias and our modified digital camera for Technical Photography is the same. Both can see in the range 300-1000 nm. The infrared photo shows that smalt is partially transparent to the infrared and, indeed, the reflectance spectrum shows less reflectance in the infrared region when smalt is over lamp black, since this last one absorbs the infrared.

![](_page_62_Figure_1.jpeg)

Cultural eritage

pen

cience

S

### Notes: paint layers, example 3

![](_page_62_Figure_3.jpeg)

We look now at indigo. The IR photo shows that this pigment is very transparent to the infrared. Consequently, its reflectance spectrum shows much less reflectance in the IR, because infrared is absorbed by the bottom layer of lamp black.

![](_page_63_Figure_0.jpeg)

Eventually, let's discuss cobalt blue. The IR photo shows that this pigment is totally opaque to the infrared. All the infrared is bounced off and we cannot tell the lamp black layer behind it. Consequently, the spectrum of cobalt blue is not affected by the lamp black bottom layer.

#### chsopensource.org

#### Notes: paint mixtures, example 1

![](_page_64_Picture_3.jpeg)

![](_page_64_Picture_4.jpeg)

We prepared a mock-up paint using cobalt blue and titanium white. We painted them pure and 5 mixtures where we progressively added a bit more titanium white. What is the resulting spectrum of the mixtures?

![](_page_65_Figure_0.jpeg)

When we mix pigments, the resulting spectrum is the additive result of the absorption bands from the pigments in the mixture. So, in this case we see that moving from mix 1 (almost pure cobalt blue with a pinch of titanium white) to mix 5, the resulting spectra show a decrease of reflectance in the UV region. This is due to titanium white which has the strong absorption band in the UV region. So, when we collect from a light blue color, a spectrum resembling that of cobalt blue but with much less reflectance in the UV region, we can guess that it is a mixture of cobalt blue plus titanium white.

### Notes: paint mixtures, example 2

![](_page_66_Picture_2.jpeg)

![](_page_66_Picture_3.jpeg)

![](_page_66_Picture_4.jpeg)

We discuss now a common historical mixture to obtain green, indigo plus orpiment. We made 3 mixtures adding more and more indigo to a pure orpiment.

#### chsopensource.org

Cultural Heritage Science

pen

ource

S

### Notes: paint mixtures, example 2

![](_page_67_Figure_3.jpeg)

We show here all the spectra, both pure pigments and the mixtures. We also added the spectrum collected from a green paint on a historical map which matches the mixture 4 spectrum.

![](_page_67_Picture_5.jpeg)

![](_page_67_Picture_6.jpeg)

#### chsopensource.org

![](_page_68_Picture_2.jpeg)

### Notes: paint thickness, example 1

![](_page_68_Figure_4.jpeg)

The thickness of the paint can play a role in the final spectrum We made this mock-up painting smalt as a very thick layer and also very thin. The spectrum of the thick paint shows less characterizing features than the thin one. This happens because the thinner paint allows much more radiation to go through and being reflected back from the support. So, the effect of the absorption bands become more apparent.

### Notes: varnish and binders

chsopensource.org

![](_page_69_Picture_3.jpeg)

![](_page_69_Picture_4.jpeg)

Varnishes and binders have flat reflectance spectra, they are basically just transparent in the range 300-1000 nm. So they do not affect the reflectance spectra of the pigments. As in the example above, the spectra from the varnished and unvarnished paints would be the same.

#### chsopensource.org

#### Cultural eritage cience pen Source

#### Notes: measure lamps radiation

![](_page_70_Figure_4.jpeg)

Gorgias can be used to measure the output radiation from a lamp, such as a UV lamp, and halogen lamps, and an LED. In this case we do not need to check the "Spectra / Ref" box, because we do not need a reflectance spectrum, but just a simple intensity spectrum. Be aware, that this is just a qualitative measure. We can easily get a shape of the emission radiation but the actual intensity would be not correct because we did not calibrated the spectrometer for this measure. Though, it is still useful! For example you can check if your UV lamp is emitting pure UV or also has VIS radiation and / or IR. Also you can check the emission of LEDs.

#### chsopensource.org

![](_page_71_Picture_2.jpeg)

### Spectragryph

![](_page_71_Picture_4.jpeg)

# Spectragryph

The Gorgias software is a simple tool to operate the spectrometer and collect spectra. In order to edit the spectra for publication or their interpretation we need a spectra editor software. Our recommended one is Spectragryph. This is a free software that you can download and use on as many PC you need. It has all the features to properly edit and analyze your spectra.

Spectragryph functions are organized into tabs of the main software window.

The tab "File" is where you can find functions to save the plot as a proprietary Spectragryph format so that you can upload it again when you want to make changes. You can also export the plot as an image format ready to be load in your publicatons. The tab "Plot/View" groups all the functions related to editing the aspect of your graph, like axis labels, typo size, the grid

dimension.

In the tab "Spectra" you find the functions to edit the spectra, such as: their color, the width of their line, and delete them from the plot. These two tabs would be the one you will use most. The other tabs have more advance functions for processing the spectra.

![](_page_71_Picture_11.jpeg)
### chsopensource.org

### Spectragryph: open one or more spectra

1. Drag and drop one or more spectra into the software window.



2. You are presented with this pop-up window asking what kind of spectra are you loading. Choose wavelength (nm) and Reflectance ()0-100%)





#### chsopensource.org

### Spectragryph: edit axes labels and boundaries

1. You can edit everything in your spectra, axes, types, legend, grids, colors. Spectragryph is very versatile. Let's edit the axes labels. Double click on them and pop-up window will show where you can input the new labels.



2. Remember to click on "Custom titles" to actually see your customs labels, otherwise the software keeps using the default ones.

entify	Acqu	ire			😸 set custom axis boundaries		x
nes s	Verda	ana ▼ ← Flip x axis	8 2nd axis	Verdan # Tra	x axis range from:	to: 800 nm	
	•	Show Titles	Custom Titles	📑 E Fic	use for all views	~	×
		Axes	1ai			Apply	Close

3. In the same AXES sub-tab you can also edit the X and Y boundaries of the spectra. Click on the axes line in the graph and the pop-up window will show up asking for your new selection. Remember to click on "Custom boundaries" to actually use your new selection, otherwise the software will use all the spectral range of the file you loaded.

Cultural Heritage Science Open Source

4

#### chsopensource.org



### Spectragryph: edit legend



In Spectragryph we can thoroughly edit the aspect and content of the legend in the plot. Access to the legend properties depends on the tab we are selecting. Let's start selecting the PLOT tab. We click then on the MENU sub-tub and we find here the "legend" menu from which we can arrange the appearance of the legend window in the plot. Then we select the SPECTRA tab and we go again in the MENU sub-tab from where we select "edit legend text" to do all the changes to text and typos.

#### chsopensource.org

Cultural eritage

cience

pen ource

S

### Spectragryph: edit spectra / zooming and panning

VS	SPECTRA	PROCESS	TRANSFORM	ANALYZE	FLUORESC		NOMATE IDEN		
					3720	2			<ul> <li>▲</li> </ul>
а					- 🎤 L	ine Color 👻	filename:37	202.txt	
	Last Spect	rum Select.	. All Spectra	prop ty	/ Line	Type: solid	▪ Line Width:	normal 🝷	
	F	lemove Spect	ira 🕞		D	isplay Propertie	es & Data Propert	ies	
Þ	Zoom Hi	story	• 🛌 • 🛍	• 🗮	#E   🖡	i i i	r 👌	Ē 🕤	
	1			1	1	1	1	1	1

In Spectragryph we can thoroughly edit the aspect of each spectrum in the plot. Select the SPECTRA tab and under the sub-tab "Display Properties & Data Properties" we have plenty of options. Remember to select the spectrum to edit from the drop-down menu in the same sub-tab.

We saw that we can select the boundaries of our plot, we can also dynamically explore the spectral range of the plot using the mouse and the zooming and panning options. These are the main mouse functions:

Clicked mouse scroll button: panning

Left button clicked: select area to magnify

Click the right button: going back to original view

chsopensource.org

#### Cultural eritage Cience Open Source

### Spectragryph: multicursor (vertical line)



We can add a vertical line on our plot. This is useful to indicate the location of inflection points, absorption bands, and maxima.

### chsopensource.org

Cultural Heritage Science

> pen ource

### Spectragryph: hide selected spectra (already loaded)

🤕 i 🖾	ra 🔓 🛛 🛛	Ì 📑 🖻	🖻 📲 🏨 📫 📫	<b>=</b> ∰   <del>=</del>								_	
FILE	PLOT/VIEWS	SPECTR	A PROCESS TRA	NSFORM ANALYZ	E FLUORES	CENC	E/EEM	AUTOMATE ID	ENTIF	ACQUIRE			
Menu	New view	Close View	Multi Cursor Peak Labels   Spectroscope	Stack Spectra	Show Grid Canvas Color	Hic	de ctra	Lines thicker	•≣ <sup>st</sup> &	andard Lines Colours Color Palette	Verdana L¥ ▼ ↓↔	F	
	Create/ Cl	ose	Enhance	Plot		該	Show	all				_	
🕅 Spec	tra2 🙁					睑	Hide a	all					
0	ত হা 🗴	Zoom	History 🛛 🙀 👻 💺	- 🏨 -   🏨		×	Remo	ve hidden spectra		5			
	74 72 70												
50 48 46 44 42 40 38 38 36 36					2 2 2 2		cadm cadm coba	ium green ium yellow It cerulean b					

We have this convenient option to hide spectra that are already loaded in the plot. This is very useful when we are comparing the spectrum of the sample with spectra in the database to check which once better matches. We can load all the possible candidates but then we can decide to just show that one the is a best match. This can be done very conveniently directly on the legend, using the checkbox.

### chsopensource.org

Cultural Heritage Science

> pen ource

## Spectragryph: save formatting settings

💷 i 🖾 🐻 🖬 🕄	😼 📑 🖷 💼	• 🖩 🎟 📫 📫 📫 🗧	Spectragryph version 1.1.1	– 🗆 X
File Plot/Views	Spectra Proc	ess Transform Analyze Fluorescence/EEM E	valuate Automate Identify Acquire	۵
Open/Import Data Save/Export Data	Apply	Apply chosen options Only for this session. Changed settings get lost after closing.	General Application Look & Feel app style: Office 2013 White  Start maximized	
Save/ Export Plot Recent Files New View		Keep options permanently Write your options & settings to registry. Keep them forever, until forced change or reset.	app color:     Color       File       Open, Save	
Print	Write Registry	Restore default settings	Default directory OPEN B Default directory SAVE C:\Program Files (x86)\Spectragryph 1.1\ Save as ASCII (*.dat): x axis stepwidth	
About	Reset	Bring back the initial settings. All user-defined settings get lost. No undo available.	Image: Second	
EXIL			Correction file: Excitation Intensity C:\Program Files (x86)\Spectragryph 1.1\	
			Plot, Views, Spectra	<b>A</b>
			Layout         ✓ Show legend       ✓ Show x axis title       custom axis titles       Background Color •         ✓ Floating legend       ✓ Show y axis title       x:	4

We have this useful function which enable us to save time. For example, we want to always open the spectra on a specific spectral range, instead of using all the spectral range of the spectrum. We open the Files tab / Options / Plot,View, Spectra: there you can configure the most of formatting settings. After pressing the "Keep options permanently", these will be taken for the current and all future plots. Remember to press "custom boundaries" and "custom titles" in the "Plot/View" menu.

### chsopensource.org

#### Cultural eritage Cience Open Source

## Spectragryph: inflection point /derivative



We discussed the meaning of "inflection point" and we said that its position is roughly the middle of the sharp curve. Though, it can be calculated precisely, as the maximum of the derivative of the spectrum. The graph above show a reflectance spectrum and the curve of its derivative. We can see there is a maximum where we expect the inflection point. Spectragryph can calculate and plot the derivative of a spectrum and give the position of its maximum. Just load the spectrum and in the TRANSFORM tab, click on the Derivative button.

chsopensource.org



### Spectragryph: find peak position



Once we have the derivative curve we can calculate automatically the position of the peak, using the "find peal position" function.

#### chsopensource.org



### Spectragryph: add peak label



We can then automatically add the label. Click the button in the "Plot/Views" ribbon to activate peak labeling