

EOMT

## **Óscar's wonderful end of master's thesis**

Óscar Iglesias González

March 25, 2020

Óscar's Room Editions

EOMT

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**Colophon**

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**Publisher**

First printed in May 2019 by Óscar's Room Editions

The harmony of the world is made manifest in Form and  
Number, and the heart and soul and all the poetry of  
Natural Philosophy are embodied in the concept of  
mathematical beauty.

– D'Arcy Wentworth Thompson



# Preface

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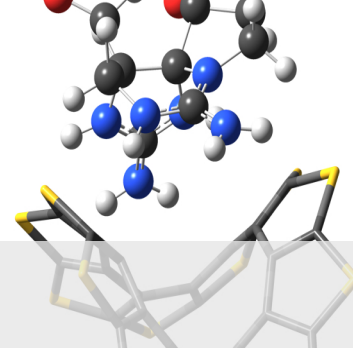
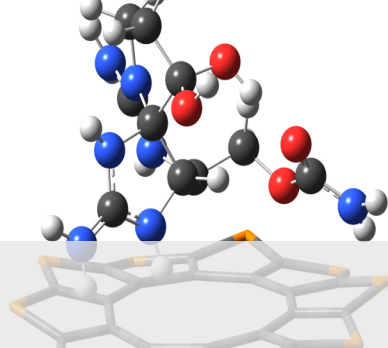
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## 1.2 The work up until now

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## 1.3 Pushing onwards

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the original language. There is no need for special content, but the length of words should match the language.



## 2 Computational methods and specifications

### 2.1 General techniques

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Table 2.1: Computational techniques

Calculation	Technique	Spec.	Functional	Basis set
Geometry optimizations	DFT		M06-2X	def2TZVPP
NICS calculations	DFT	GIAO	b3lyp	base

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### 2.2 Software

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### 2.3 Hardware

All of the calculations were performed using either the Centro de Supercomputación de Galicia’s (CESGA) infrastructures, or the proprietary cluster of the S3 research group.

S3’s cluster is composed of nodes that include 16 Intel®Xeon®CPU E5-2630 v3 2.40GHz cores and 60 GB of RAM.

CESGA’s





## 3 The sunflower molecules

### 3.1 Introduction and origin

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

Despite most people complain at the sight of a book full of equations, mathematics is an important part of many books. Here, we shall illustrate some of the possibilities. We believe that theorems, definitions, remarks and examples should be emphasised with a shaded background; however, the colour should not be to heavy on the eyes, so we have chosen a sort of light yellow.<sup>1</sup>

### 3.2 Study of gometry

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### 3.3 Study of aromaticity

#### Nucleus-Independent Chemical Shift (NICS)

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of

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1: The boxes are all of the same colour here, because we did not want our document to look like [Harlequin](#).

the original language. There is no need for special content, but the length of words should match the language.

### **The basics of NICS**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### **A custom solution for non-planar molecules**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

## **AICD**

### **The basics of AICD**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### **Application and comparison of results**

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the original language. There is no need for special content, but the length of words should match the language.

## 3.4 Spectroscopic characterization

### Vibrational spectroscopy

#### Raman spectra

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#### Decomposition of key modes

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#### VEDA

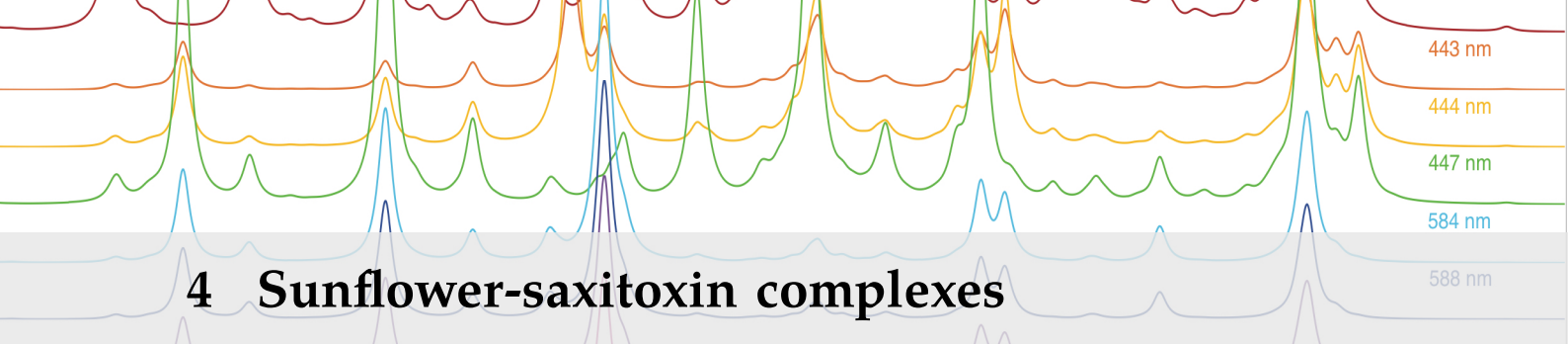
Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### Electronic spectroscopy

#### UV spectra

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference

between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.



## 4 Sunflower-saxitoxin complexes

Having obtained a general characterization of the sunflower-type molecules, it's time to get back to the problem at hand and start looking into how they can be applied. Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### 4.1 Study of adsorption

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

#### Sampling and optimization

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#### Maxwell-Boltzmann statistics

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### **Basis Set Superposition Error correction**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

## **4.2 Study of non-covalent interactions**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

## **4.3 Study of UV behavior**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### **General UV spectroscopy**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like "Huardest gefburn"? Kjift – not at all! A blind text like this gives you information about the selected

font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### **Charge transfer analysis**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

## **4.4 Resonance Raman**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.

### **Generation and comparison of spectra**

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### **Combined resonance graphs**

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of

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### **Final selection**

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# APPENDIX





## A Some more blindtext

Hello, here is some text without a meaning. This text should show what a printed text will look like at this place. If you read this text, you will get no information. Really? Is there no information? Is there a difference between this text and some nonsense like “Huardest gefburn”? Kjift – not at all! A blind text like this gives you information about the selected font, how the letters are written and an impression of the look. This text should contain all letters of the alphabet and it should be written in of the original language. There is no need for special content, but the length of words should match the language.



# Notation

The next list describes several symbols that will be later used within the body of the document.

- $c$       Speed of light in a vacuum inertial frame
- $h$       Planck constant

## Greek Letters with Pronunciation

Character	Name	Character	Name
$\alpha$	alpha <i>AL-fuh</i>	$\nu$	nu <i>NEW</i>
$\beta$	beta <i>BAY-tuh</i>	$\xi, \Xi$	xi <i>KSIGH</i>
$\gamma, \Gamma$	gamma <i>GAM-muh</i>	$\omicron$	omicron <i>OM-uh-CRON</i>
$\delta, \Delta$	delta <i>DEL-tuh</i>	$\pi, \Pi$	pi <i>PIE</i>
$\epsilon$	epsilon <i>EP-suh-lon</i>	$\rho$	rho <i>ROW</i>
$\zeta$	zeta <i>ZAY-tuh</i>	$\sigma, \Sigma$	sigma <i>SIG-muh</i>
$\eta$	eta <i>AY-tuh</i>	$\tau$	tau <i>TOW (as in cow)</i>
$\theta, \Theta$	theta <i>THAY-tuh</i>	$\upsilon, \Upsilon$	upsilon <i>OOP-suh-LON</i>
$\iota$	iota <i>eye-OH-tuh</i>	$\phi, \Phi$	phi <i>FEE, or FI (as in hi)</i>
$\kappa$	kappa <i>KAP-uh</i>	$\chi$	chi <i>KI (as in hi)</i>
$\lambda, \Lambda$	lambda <i>LAM-duh</i>	$\psi, \Psi$	psi <i>SIGH, or PSIGH</i>
$\mu$	mu <i>MEW</i>	$\omega, \Omega$	omega <i>oh-MAY-guh</i>

Capitals shown are the ones that differ from Roman capitals.

