université de BORDEAUX

THÈSE PRÉSENTÉE

POUR OBTENIR LE GRADE DE

DOCTEUR DE

L'UNIVERSITÉ DE BORDEAUX

ÉCOLE DOCTORALE DES SCIENCES PHYSIQUES ET DE L'INGÉNIEUR (SP1)

LASERS, MATIÈRE ET NANOSCIENCES

Nom Prénom

Thesis name enter here in english

Thesis name enter here in french

Sous la direction de : Dr. Director. First

(co-directeur : Dr. Director. Second)

Soutenue le : 1 avril 2015

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Abstract: English abstract

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Unité de recherche

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Dedicated to mankind...:)

Preface

Ce que nous connaissons est **peu de chose**, ce que nous ignorons est **immense**.

French mathematician and astronomer,
Pierre-Simon de Laplace (1749–1827)

Il piacere della vita è imparare.

Italian scholar and poet, Francesco Petrarca
(1304–1374)

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placerat. Ut imperdiet, enim sed gravida sollicitudin, felis odio placerat quam, ac pulvinar elit purus eget enim. Nunc vitae tortor. Proin tempus nibh sit amet nisl. Vivamus quis tortor vitae risus porta vehicula.

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Acknowledgments

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Résumé en français

1 Introduction

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Chapter 1

How to use thesis template

L'art c'est **moi** – la science c'est **nous**.

---

french physiologist, Claude Bernard (1813–1878)

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1.1 General Description

This thesis template was done in 2013-2015 according to the rules of Université de Bordeaux. It can be compiled with two different chains:

1. xelatex – beamer – makeglossaries – xelatex – xelatex
2. lualatex – beamer – makeglossaries – lualatex – lualatex

I as author recommend to use **MiKTeX** or **TeX Live** as a LaTeXdistributions, and from my opinion best editors for general purposes are TeXStudio or TeXMaker.

1.1.1 Organization

Thesis is divided in several part:

1. Settings
2. Front Matter (Title Page, Dedication, etc., contents, list of tables and figures)
3. Main Matter (Chapters, Appendixes)
4. Back Matter (Bibliography, Acronyms)

The thesis is divided in to chapters, but not in parts.

The settings of thesis is mainly kept inside of thesis class *thesis-bordeax.cls*. Settings for bibliography could be found in *settings/Bib.tex*, for fonts *settings/Fonts.tex*.

1.1.2 ARARA

I highly recommend to use **Arara**[1]. To add Arara command to TEXMaker this nice *post* could be used: http://tex.stackexchange.com/a/107995/43831

1.2 Floats

1.2.1 Figures/Images/Drawings

I recommend to use *TikZ+pgfplots* packages to built graphs. All presented graphs in this manual are made using this two packages (see *figures* folder for corresponding *tex* file).

There are several ways to insert figures in thesis:

— Standard way

```
\begin{figure}
\centering
%\includegraphics[width=6cm]{Name-of-file}
\caption{Caption.}
\label{fig:firstFig}
\end{figure}
```

— Using \inputfigure command:
\inputfigure[scale 0 to 1]{File Name}[Caption][Label][type of file pdf, png], example: \FloatBarrier
\inputfigure[.5]{Chapter1/ streak-cameraTIKZ}[Principle scheme of a conventional streak camera][streak-camera][pdf] \FloatBarrier

1. Automation of LaTeXcompilation

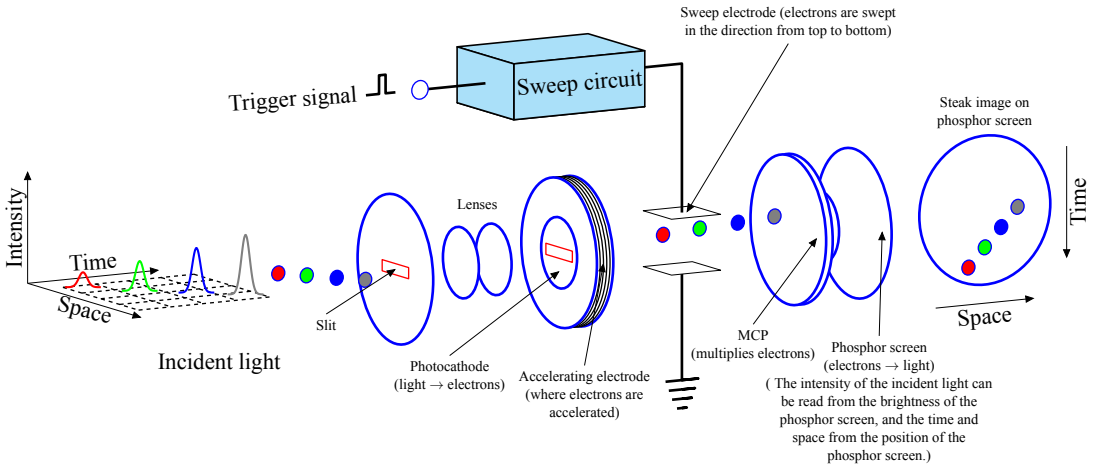

Figure 1.1. Principle scheme of a conventional streak camera.

To get an idea hot *TikZ* package works see *figures/Chapter1/streak-cameraTIKZ.tex*:

— Using \inputfiguresH }[scale]{Name1}{Name2}[Caption1][Caprtion2][Label1][Label2][Height 1][Height 1] command:

```
\FloatBarrier
\inputfiguresH[1]{Chapter1/RuII-GS-bleaching.pdf}{Chapter1/RuII-anth-3growth.pdf}[\acrshort{TRABS} kinetics of ground state bleaching changes for \textbf{2} at $485$\,nm in \acetonitrile ($\lambda_{exc}=465$\,nm)][\acrshort{TRABS} kinetics of anthracene triplet grow-in for \textbf{2} at $430$\,nm in \acetonitrile ($\lambda_{exc}=465$\,nm)][RuII-GS-bleaching][RuII-anth-3growth][5][5]
\FloatBarrier
```

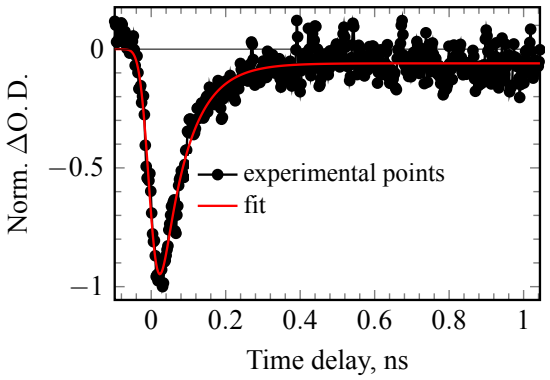

Figure 1.2. TRABS kinetics of ground state bleaching changes for **2** at 485 nm in CH_3CN (λ_{exc} = 465 nm).

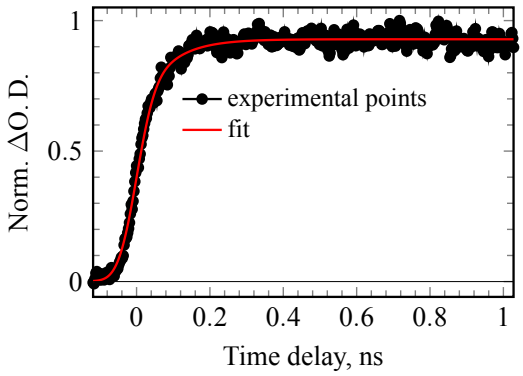

Figure 1.3. TRABS kinetics of anthracene triplet grow-in for **2** at 430 nm in CH_3CN (λ_{exc}=465 nm).

1.2.2 Tables

```
\begin{table}[h!]
\addtocounter{totaltables}{1}
\caption{Characteristic time, distance and energy ranges for chemistry and physics.}
\label{table:Ranges}
\centering
\begin{tabular}{|x{2cm}|>{\centering\arraybackslash}x{2.5cm}|>{\centering\arraybackslash}x{3.7cm}|>{\centering\arraybackslash}x{3.1cm}|}
```

```
\hline
&  Time range, s&  Size range, m&  Energy range, eV\\
\hline
Chemistry&  $\rm 10^{-15} - ^*$& $\rm 10^{-10} -10^{1}$  (11~orders) & $\rm
    10^{-4} -10^{0}$ (4~orders) \\

\hline

Physics&  $\rm 10^{-44} -10^{18}$ ($\rm >50$~orders)& $\rm
   10^{-35}-10^{-18} -10^{26}$ ($\rm >40$~orders) & up to $\rm 10^{70}$ \\

\hline
\end{tabular}
\end{table}
```

Table 1.1. Characteristic time, distance and energy ranges for chemistry and physics.

	Time range, s	Size range, m	Energy range, eV
Chemistry	$10^{-15}-^*$	$10^{-10}-10^{1}$ (11 orders)	$10^{-4}-10^{0}$ (4 orders)
Physics	$10^{-44}-10^{18}$ (>50 orders)	$10^{-35}-10^{-18}-10^{26}$ (>40 orders)	up to 10^{70}

Table 1.2. Photophysical properties of Ru(II) complexes in CH_3CN.

complex	$\lambda_{em.max}$, nm[a]	Φ_{air}[b]	Φ_{degas}[c]	τ, μs[d]	K_{eq}[f]
1	686	2.2×10^{-3}	1.3×10^{-2}	2.7 ± 0.3	–
2	686	4×10^{-4}	9.5×1.3^{-2}	75×10^{-6}[e]; 42 ± 2	15.2 ± 2

[a] Recorded on streak camera and uncorrected.
[b] Luminescence QY in air-equilibrated CH_3CN solution *cf.* $[Ru(bpy)_3]^{2+}$ in H_2O (bpy = 2,2'–bipyridine).
[c] Luminescence QY in degassed CH_3CN solution *cf.* $[Ru(bpy)_3]^{2+}$ in H_2O.
[d] MLCT luminescence lifetime in dilute degassed CH_3CN.
[e] Determined *via* transient absorption spectroscopy in degassed CH_3CN.
[f] Excited-state equilibrium constant.

1.3 Bibliography, Citations and Author Index

The bibliography print commands are located in *backmatter.tex* file:

```
\addcontentsline{toc}{chapter}{\bibname}
\begingroup
\setstretch{1}
\setlength\bibitemsep{0pt}
\renewcommand*{\bibfont}{\small}
\sloppy %Line breaking
\printbibliography
\endgroup
```

The settings are located in *settings/Bib.tex* file. The library itself is stored in *bibliography.thesis-bib.bib* file:

```
@phdthesis{Ducrot-thesis,
author = {Ducrot, A.},
school = {Universit\'{e} Bordeaux 1},
```

```
title = {{Synthèses et études de systèmes supramoléculaires
    photocommutables : récepteurs à ion et molécules entrelacées}},
year=2012,
}

@article{Haas-1971,
author = {Haas, Y. and Stein, G.},
journal = {J. Phys. Chem.},
number = {24},
title = {{Pathways of radiative and radiationless transitions in europium(
    III) solutions. Role of solvents and anions}},
volume = {75},
year = {1971}
}
```

To cite any item from the library the citation command should be used \cite{label} for example \cite{Berlman1971} which gives: [1].

The authors from the article automatically added to *author index* by this code located in *settings/Bib.tex*:

```
\usepackage{imakeidx}
\makeindex[intoc,name=cite,title=Author Index,columns=2]
\indexsetup{level=\chapter*,toclevel=chapter,noclearpage}

%Include authors from bibliography to author index.
\DeclareIndexNameFormat{default}{%
\usebibmacro{index:name}{\index[cite]}{#1}{#3}{#5}{#7}}

\DeclareIndexNameFormat{nondefault}{%
\usebibmacro{index:name}{\nocite[cite]}{#1}{#3}{#5}{#7}}
```

1.4 Abbreviations

The acronyms are kept in the file *Settings/abbr.tex*, which you can find inside of *Bib.tex* file:

```
%Glossaries
\usepackage[nonumberlist,acronym,toc,nomain,nopostdot,nogroupskip]{
    glossaries}
\input{Settings/abbr}
\makeglossaries
```

To set up new acronym this code should be used \newacronym{CSS}{CSS}{Charge Separated State }.

There are tree ways to use acronym in the text:

1. short \acrshort{CSS} – CSS
2. long \acrlong{CSS} – Charge Separated State
3. full \acrfull{CSS} – Charge Separated State (CSS)

At the of thesis the full list of acronyms will be printed:

```
%Glossary
\glsaddall
\renewcommand*{\glsgroupskip}{}
\printglossary[title=Abbreviations, toctitle=Abbreviations, type=\
    acronymtype, style=list]
```

1.5 Indexes

In the thesis two indexes are created in *settings/Bib.tex* file:

```
\usepackage{imakeidx}
\makeindex[intoc,name=pms,title=General,columns=2]
\makeindex[intoc,name=cite,title=Author Index,columns=2]
\indexsetup{level=\chapter*,toclevel=chapter,noclearpage}
```

The *cite* index is used to store cited authors, \cite{} command automatically adds author in author index. To add manually this command should be used \index[cite]{Bernard, C.}

The indexes are printed in the of thesis:

```
%INDEXES
\printindex[cite]
%\printindex[pms]
```

1.6 References

The package *hyperref* is used to create references in the thesis. To create a reference this commands are used:

— reference to chapter, section, etc. \ref{label}, for example reference to chapter *How to use thesis template* \ref{ch:how-to-use} will give 1, or figure....

— reference to chapter, section, figure, table etc. page p.~\pageref{ch:how-to-use} – p. 1.

Chapter 2

Chapter Example

Some very clever idea

Very clever man

2.1 Molecules 8
2.2 Data 8
2.3 Conclusion 11
2.4 First section 12
2.5 Second section 13
2.5.1 New subsection 13
2.6 Third section 14

In this chapter (Chapter 2) will be presented unrelated data...I'm really sorry for that.

2.1 Molecules

Please find structures of molecules [1] which were used in the study (see Fig. 2.1). The data is presented in section 2.2 on p. 9.

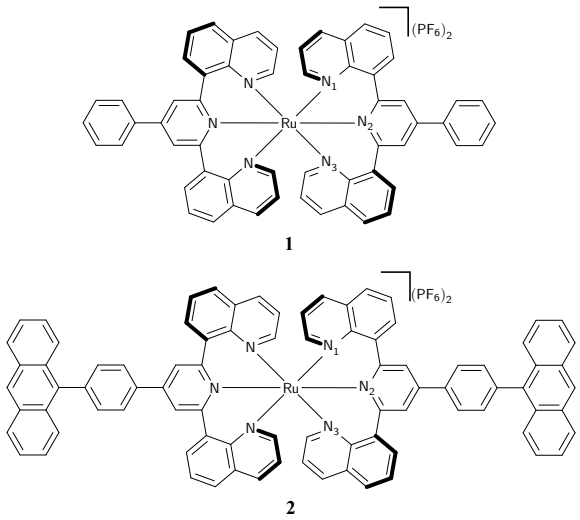

Figure 2.1. Studied molecules.

2.2 Data

We discussed earlier that systems studied in this work are photo-activated (RET, REET, PET, Photoisomerization). It simply means that system should be excited from its ground state to some electronic excited state, because only upon being in the excited state the system could be active from the point of displaying useful property. At room temperature thermal energy is not adequate to significantly populate electronically excited states.

Here we would like to spent some time to discuss such terms as *state* and the term *excited state*.

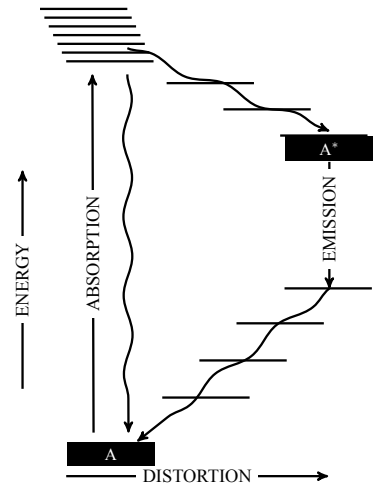

Figure 2.2. Energy versus distortion diagram [2].

The work of Adamson[2] we will helpful in the discussion.

The word *state* has two different usages in science. To the spectroscopist, the state of a molecule is defined by quantum numbers. He will use term designations and thus speak of the $^2P_{1/2}$ state of the sodium atom or the $^3\Sigma_g^-$ state of O_2. In the case of coordination compounds, examples would be the $^4T_{2g}$ and ^2E_g ligand field states of Cr(III). When we assign the various absorption maxima in the UV-vis spectrum of a coordination compound, we are proposing specific state-to-state electronic transitions. Thus the first major absorption band for $Cr(NH_3)_6^{3+}$ is assigned as the $^4A_{2g} \rightarrow ^2T_{2g}$ transition. To the spectroscopist, then, an

1. Made in LaTeX as well.

excited state has different electronic (and rotational and vibrational) quantum numbers than does the ground state.[2]

The word *state* has a rather different meaning in thermodynamics. When we speak of, say, HCl gas at standard conditions, we mean a collection of molecules with a certain average molar energy, entropy, free energy, etc. This is not a single spectroscopic state. Rather, we have a Boltzmann distribution of quantum states. This collection or ensemble has average properties the above thermodynamic ones, and many others, such as density, index of refraction, absorption spectrum, etc. The usual standard state of aqueous $Cr(NH_3)_6^{3+}$ refers to a condition of unit activity under 1 atm pressure and at 25°C. A collection of ions in this state has certain average bond lengths and angles; it has thermodynamic properties; it has chemical reactivity described by one or more rate constants, each having temperature dependence and corresponding activation energy.[2]

Excited states could have different meaning in case of molecular and supramolecular systems. Let take spectroscopic ground state A, and a first electronic excited state A^*, illustrated in Figure 2.2. A^* will, usually, have different bond lengths and angles than system in state A.

When light is absorbed by species A, a population of A^* states is produced, and we expect the transition to be a "vertical" one, that is, electronic rearrangement occurs but no appreciable nuclear motion. Transitions occur in about 10^{-15} s, [2] a time too short for significant displacement of nuclei. The consequence is that A^* molecules are not produced in their equilibrium geometry and should therefore be highly vibrationally excited. This collections of molecules is called Franck-Condon collection or Franck-Condon state (A^*_{FC}).[2]

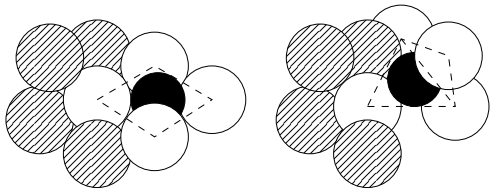

Figure 2.3. Solvent cage effect in excited state thermal equilibration [2].

Assuming that complex A has a square planar geometry, while the equilibrium geometry of A^* is tetrahedral. A newly formed A^* complex cannot immediately relax to tetrahedral geometry, solvent molecules have to rearrange themselves around (Figure 2.3); new solvation sphere must be established. As an estimate, it should take roughly about 200 vibrational periods or about 1 ps for a solvent molecule to make diffusional jump from one position to another. The A^* complex is formed in the ground state geometry in a solvent cage that delays its relaxation to the equilibrium geometry. One could expect the collection of molecules A^*_{FC} to make a succession of configurational adjustments before settling down into an equilibrium Boltzmann distribution of vibrational states. The whole process may take about 10 ps. Thermally equilibrated A^* is a thermodynamic state; it represents an ensemble of A^* molecules that is at ambient temperature with respect to vibrations (a solvated molecule really does not have translation or free rotation).[2]

A representation of molecular electronic state energy levels, with singlet and triplet states in separate columns, is referred to as the Perrin-Jablonski diagram (Figure 2.4). Often, vibrational sublevels are shown schematically as well. Radiative transitions from one level to another are indicated by straight arrows and non-radiative ones by wavy arrows. Most often, the levels correspond to vibrationally relaxed electronic states, i. e. to an equilibrium geometry of each individual state. Sometimes, an effort is made to show the state energies at two or more geometries, and as this representation becomes more elaborate, the diagram gradually turns into a drawing of a slice through potential energy surfaces (Figure 2.5).

$$\frac{dN_1(t)}{dt} = \sigma I(t) - k_1 N_1(t) \tag{2.1}$$

2. The velocity of an electron making one complete circuit in a Bohr orbit is $\sim 10^{16}$ Å/sec. Thus, an electron may move on the order of 10 Å in 10^{-15} sec. Since 10 Å is the order if size of many commonly encountered groups of atoms (chromophores) responsible for absorption of light, we deduce that the timescales of photon interaction and electron are of the same order of magnitude.[3]

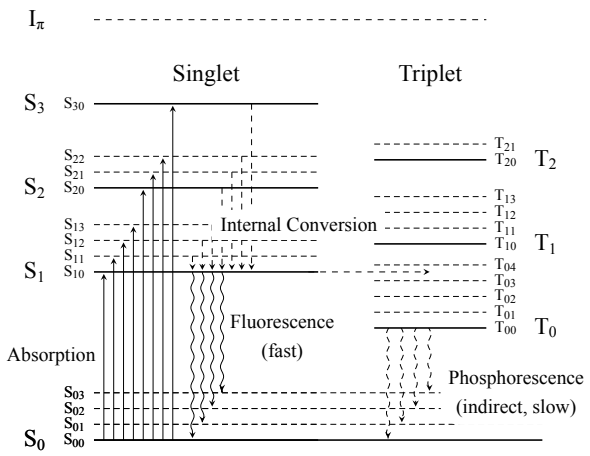

Figure 2.4. One possible form of a Perrin-Jablonski diagram, where I_π – ionisation level, T – triplet and S – singlet state.

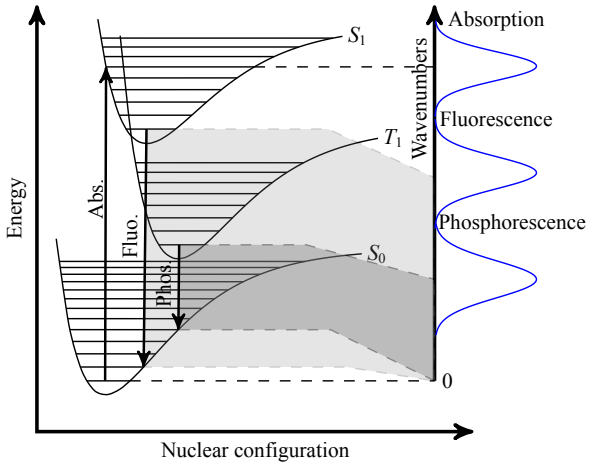

Figure 2.5. The relationship of observed radiative transitions to potential energy curves (schematic) [4].

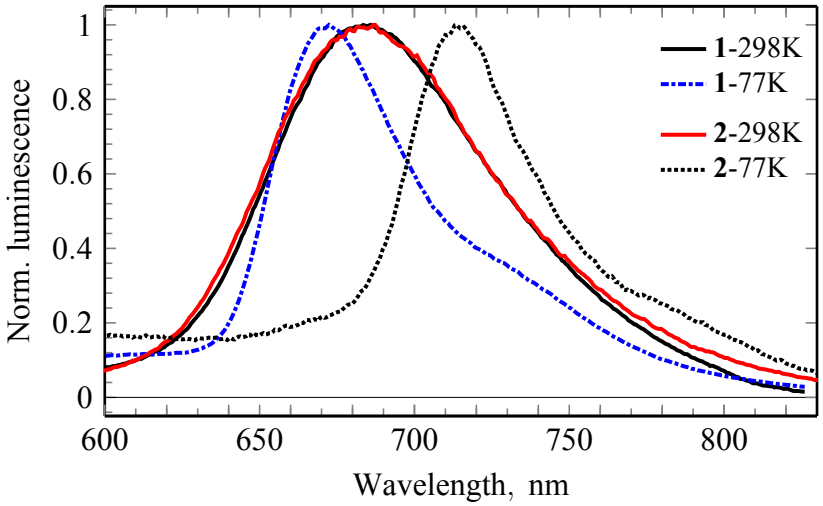

Figure 2.6. Data for molecules presented on Fig. 2.1.

Solution of equation 2.1 is expressed in equation 2.2:

$$N_1(t) = \frac{\sigma\tau_p I_0}{4}\sqrt{\frac{\pi}{\ln 2}\exp\left(\frac{k_1^2\tau_p^2}{16\ln 2}\right)}\left(1+\operatorname{erf}\left(2\sqrt{\ln 2}\frac{t}{\tau_p}-\frac{k_1\tau_p}{4\sqrt{\ln 2}}\right)\right)\exp(-k_1 t) \tag{2.2}$$

To extract deexcitation rate k_1 from such function is a complicated mathematical task. Instead of determining k_1 as an analytical function, we determined it in an iterative manner, by fitting experimental data as following:

$$\frac{N_{i+1}(t)-N_i(t)}{\delta t} = \sigma I(t) - k_1 N_i(t),$$

so:

$$N_{i+1}(t) = (\sigma I(t) - k_1 N_i(t)) \times \delta t + N_i(t),$$

where δt is the time step, equalled to $\frac{\text{time-scale}}{N_{points}}$.

2.3 Conclusion

According to presented data (see Table 1.1) we can make conclusions...(see Fig. 2.7).

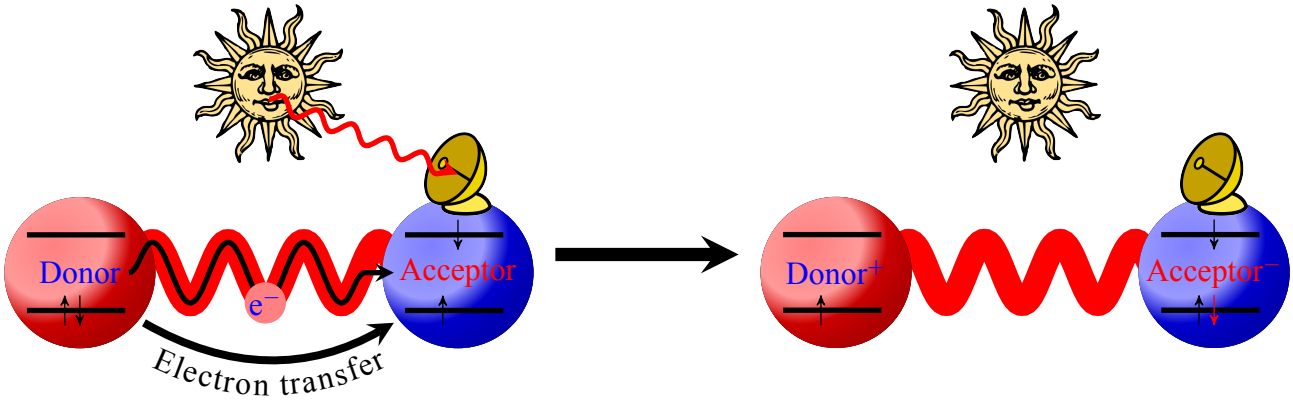

Figure 2.7. Model for PET in foldamers.

The whole published article could included in the thesis, according to the rules of journal where it was published. Here is an example.

1 First section

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Appendix A

Supporting information

1.1 Supporting information

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Abbreviations

CSS Charge Separated State
PCT Photoinduced Charge Transfer
PET Photoinduced Electron Transfer
REET Reversible Electronic Energy Transfer
RET Resonance Energy Transfer
TRABS Transient Absorption Spectroscopy