

# **NEWSLETTER**

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**CONTENTS**

<b>EPA EXECUTIVE COMMITTEE .....</b>	<b>7</b>
<b>EDITORIAL .....</b>	<b>9</b>
President's Letter .....	9
<b>PHOTOCHEMICAL &amp; PHOTOBIOLOGICAL SCIENCES .....</b>	<b>10</b>
<b>PUBLICATIONS .....</b>	<b>11</b>
IUPAC-Project <i>SYNPHO</i> – A Collection of Experimental Standard Procedures in Synthetic Photochemistry .....	11
Photoredox systems in catalysis.....	16
Machine Learning Photodynamics Simulation for Automatic Mechanism Discovery.....	18
<b>Role of the perfluoro effect in the selective photochemical isomerization of hexafluorobenzene .....</b>	<b>21</b>
<b>ABSTRACTS OF THESIS ON PHOTOCHEMISTRY .....</b>	<b>24</b>
Photoremovable protecting groups for carbonyl compounds of biological interest.....	24
<b>OBITUARY .....</b>	<b>29</b>
Professor Doctor Heinz Dürr - A distinguished photochemist ....	29

<b>CONFERENCE REPORT .....</b>	<b>32</b>
Dutch Photochemistry Days on-line, May 10 and 17, 2021.....	32
<b>CONFERENCE ANNOUNCEMENTS .....</b>	<b>34</b>
<b>BOOKS .....</b>	<b>35</b>
G. Knör, Artificial Photoenzymes – Design, Concepts and Applications .....	35
F. Di Giacomo, Interviews with R. A. Marcus on Electron Transfer Reactions.....	36
F. Di Giacomo, Introduction to the Marcus Theory of Electron Transfer Reactions .....	36
<b>EPA IS ON FACEBOOK AND TWITTER.....</b>	<b>37</b>
<b>MEMBERSHIP APPLICATION FORM .....</b>	<b>38</b>

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## **EDITORIAL**

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### **President's Letter**

Dear EPA Members,

In the last six months the pandemic situation continued to affect the academic activities worldwide. This had consequences for the development of projects, the organization of conferences and other events, and teaching. However, lately one can note reason for increased optimism, which nourishes the expectations of returning to previous activity levels. Unfortunately, it is not this time that such traditional events as the International Conference on Photochemistry (ICP) can be held with the physical presence of the participants. Hopefully next year's IUPAC Symposium on Photochemistry will bring us all together as usual in this time of the year.

Speaking of ICP, at the upcoming virtual edition of the conference the European Photochemistry Association will award its prizes. The organization provided us kindly with a time slot for a dedicated award session. If you plan to attend ICP, please do not miss to connect to the EPA Awards Ceremony.

The last six months were also the first ones of our society journal *Photochemical and Photobiological Sciences* with the Springer-Nature group. To all of you who have made contributions to the journal in this period, I would like to express my special gratitude.

As I informed you recently, a very prominent member of our community and the co-founder of the European Photochemistry Association, Professor Heinz Dürr, sadly passed away last February. In the present Newsletter his main scientific contributions are highlighted by Prof. Henri Bouas-Laurent.

Finally, I wish you all the best for the coming summer months and hope that the current developments of the corona crisis are of sustained nature, so that we can re-take our activities to full extent very soon.

With my best wishes,  
Uwe Pischel

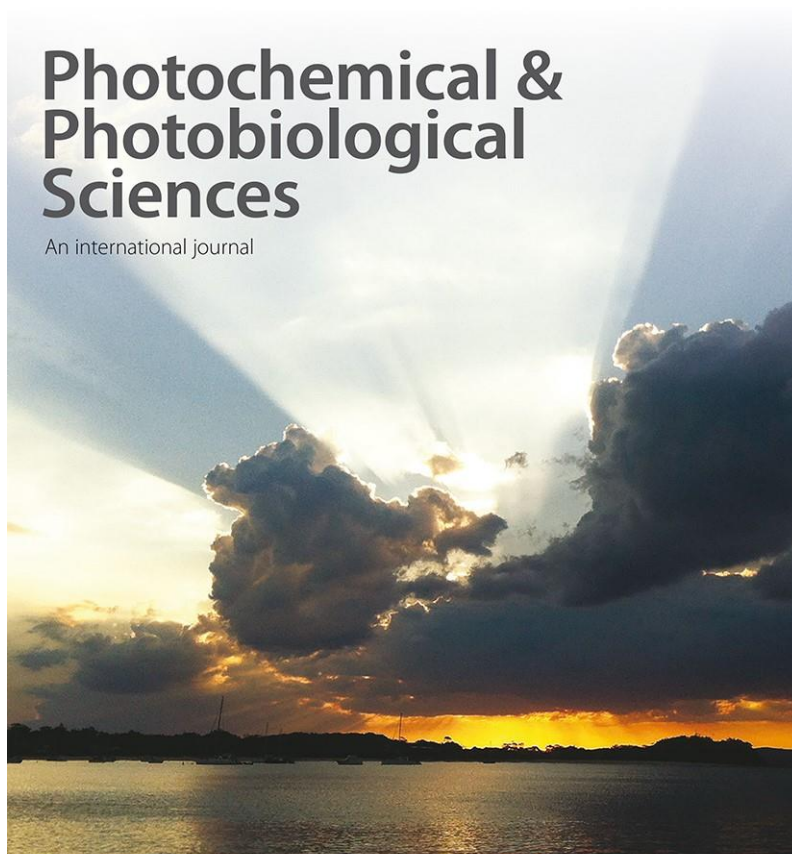
## PHOTOCHEMICAL & PHOTOBIOLOGICAL SCIENCES

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## PUBLICATIONS

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### IUPAC-Project *SYNPHO* – A Collection of Experimental Standard Procedures in Synthetic Photochemistry

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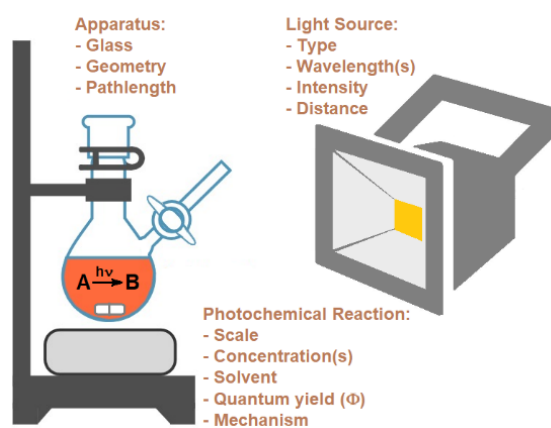
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Photochemistry has seen a remarkable renaissance in synthetic organic chemistry with numerous new methodologies and protocols in the scientific literature. As a result, photons have been declared ‘a 21<sup>st</sup> century reagent’ [1]. Despite this encouraging development, photochemical processes have a longstanding reputation of being complicated, irreproducible or unreliable. Likewise, the determination of photochemical reaction mechanisms is challenging, as for example expressed by Davidson as early as 1957: “*Photochemistry is like a jealous, proud mistress. She demands years of devotion and constant attention of her admirers before she reveals her secrets and bestows her favors.*” [2]. These persistent misconceptions may be linked to the unique experimental requirements of photochemical reactions (reagents, solvents and equipment) and the unconventional underlying photophysical processes involved. These are commonly insufficiently or poorly described in the scientific literature, contributing to the ‘irreproducibility image’ of synthetic photochemistry.

Although several experimental guidelines for conducting photochemical reactions have been developed in the past [3], these have not found widespread implementation in the synthetic community. The need for standardization and mandatory experimental reporting requirements has also been recently expressed by the pharmaceutical industry: “*The critical process understanding on the effect of the light intensity, internal reaction*

*temperature, substrate concentration and reactor geometry is absent, and this is inconsistent with any other area of chemistry when reporting or comparing chemical reactions.*" [4]. Standardization of equipment and 'rational reaction design' approaches have also been proposed for photocatalytic transformations [5,6], where improvised 'home-made' irradiation devices and protocols have been especially widespread.

The IUPAC project '**SynPho**' intends to collect topical experimental procedures in the field of preparative photochemistry with emphases on essential experimental and mechanistic details (**Figure 1**). This collection may become a standard for every new report on synthetic photochemistry, thus guaranteeing a maximum of reproducibility and mechanistic understanding. To achieve this, *SynPho* will gather a large assortment of photochemical reactions and useful synthetic methods that utilize light-initiated and/or light-driven (i.e. photon catalytic or stoichiometric) processes. These will include descriptions of reactor setups (geometries, optics, materials, lamps, filters, wavelengths) and photon-specific information (quantum yields, quantum efficiencies, absorption and emission properties of substrates, intermediates and products).



**Figure 1.** Representative photochemical setup and key-parameters.

Initially, *SynPho* aims to publish 100 examples in a highly condensed (concerning methods and techniques) but also comprehensive (concerning the different photochemical reaction types) collection for *Pure*

*Applied Chemistry*. This will be complemented by an index summarizing relevant information on:

- Reaction type, general process;
- Compound(s) that is (are) electronically excited;
- Excitation mode (direct, sensitized, mediated);
- UV-vis properties of the chromophore(s), absorption and emission;
- Excitation wavelengths and excitation sources used (lamps, filters, optics);
- Irradiation conditions (photoreactor, geometries, pathlengths, light intensity);
- Irradiation time;
- Monitoring parameters (reaction progress determination);
- Quantum yield information (actinometry, direct determination);
- Mechanistic proposal (how the reaction proceeds);
- Workup, product isolation and characterization.

It is envisaged that *SynPho* will ultimately become a ***Standard of Good Practice*** for conducting photochemical reactions, both for publishing (as a guidebook for scientific editors and referees) as well as for conducting these experiments (as a guidebook for experimentalists).

The *SynPho*-project is directed by two established researchers in Germany (*Prof. Axel Griesbeck*, University of Cologne) and Australia (*Assoc.-Prof. Michael Oelgemöller*, James Cook University). Both academic researchers and their groups have longstanding experiences in synthetic organic, mechanistic, technical and applied photochemistry [7,8]. The project is supported by the *International Union of Pure and Applied Chemistry (IUPAC)* and is hosted by its photochemistry subcommittee as part of the Division III. In recent years, several projects were conducted and finalized by publications in *Pure & Applied Chemistry* as glossaries [9,10], technical reports [11-13] or recommendations, e.g. by the former chairwomen of this subcommittee, Prof. Silvia Braslavsky [14].

Selected researchers and fellow colleagues have already been invited to contribute to *SynPho* in order to collect representative 'reaction highlights.

However, any active researchers in the preparative photochemistry community should feel encouraged to pitch their showcase procedure(s) with supporting literature reference(s) to [griesbeck@uni-koeln.de](mailto:griesbeck@uni-koeln.de) or [michael.oelgemoeller@jcu.edu.au](mailto:michael.oelgemoeller@jcu.edu.au) (Subject: SynPho). All contributors will become co-authors of the final *Pure & Applied Chemistry* compilation.

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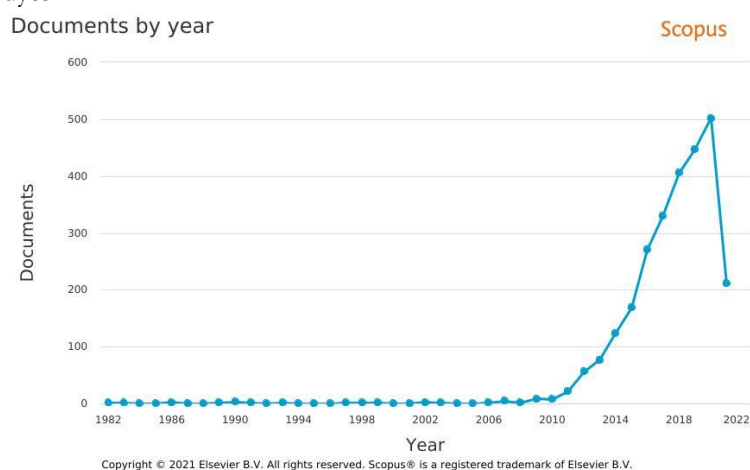
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14. Professor Braslavsky is the first recipient of the *European Photochemistry Association (EPA) Award for Service to the Photochemical Community* in 2020.

## Photoredox systems in catalysis

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Over the past decade, photoredox catalysis has gained a leading role (Fig. 1) in synthetic organic chemistry as an essential tool for the selective activation of small molecules and the formation of chemical bonds. Using visible light instead of heat to drive chemical reactions is attractive not only for solar energy conversion but also for organic synthesis. Currently, photoredox catalysis is at the forefront as an effective bond modification strategy through multi-catalytic strategies and the invention of non-traditional methodologies. It is extremely effective at generating radicals by manipulating their associated transition metal complexes and organic dyes.<sup>1</sup>



**Figure 1.** Increasing scientists interest in photoredox catalysis field (as of 27.05.2021)

Upon excitation, these molecules can engage in single-electron transfer (SET) events with organic (and organometallic) substrates, providing facile access to open-shell reactive species.<sup>2</sup> Irradiation with visible light (at wavelengths where common organic molecules do not absorb) affects selective excitation of the photoredox catalyst. The resultant excited species can act as both a strong oxidant and a strong reductant simultaneously, thereby providing access to a reaction environment that is



unique for organic chemistry. These two synchronizing and rapidly flourishing areas of research in modern synthetic chemistry have recently been merged, and their association was found to be very effective in terms of chemo-, regio-, and stereoselectivity aspects. Over the decades, photoredox catalysis has found widespread application in the fields of water splitting,<sup>3,4</sup> carbon dioxide reduction<sup>5</sup>, and the development of novel solar cell materials,<sup>6</sup> however, only recently has the potential of applying this catalytic platform to organic synthesis begun to be fully realized.

Despite significant advances in the field of organic photoredox catalysis in recent years, there is ample room for further research. When it comes to developing organic photoredox catalysts, there is a clear shortage of strongly reducing catalysts available, and the identification of more durable chromophores is always desirable. Applications of organic photoredox catalysis for the synthesis of natural products are just beginning to emerge. In addition, there is great potential for combining organic photoredoxes with other scientific disciplines such as materials science and biology. All these areas are the field for a large amount of very interesting research

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## Machine Learning Photodynamics Simulation for Automatic Mechanism Discovery

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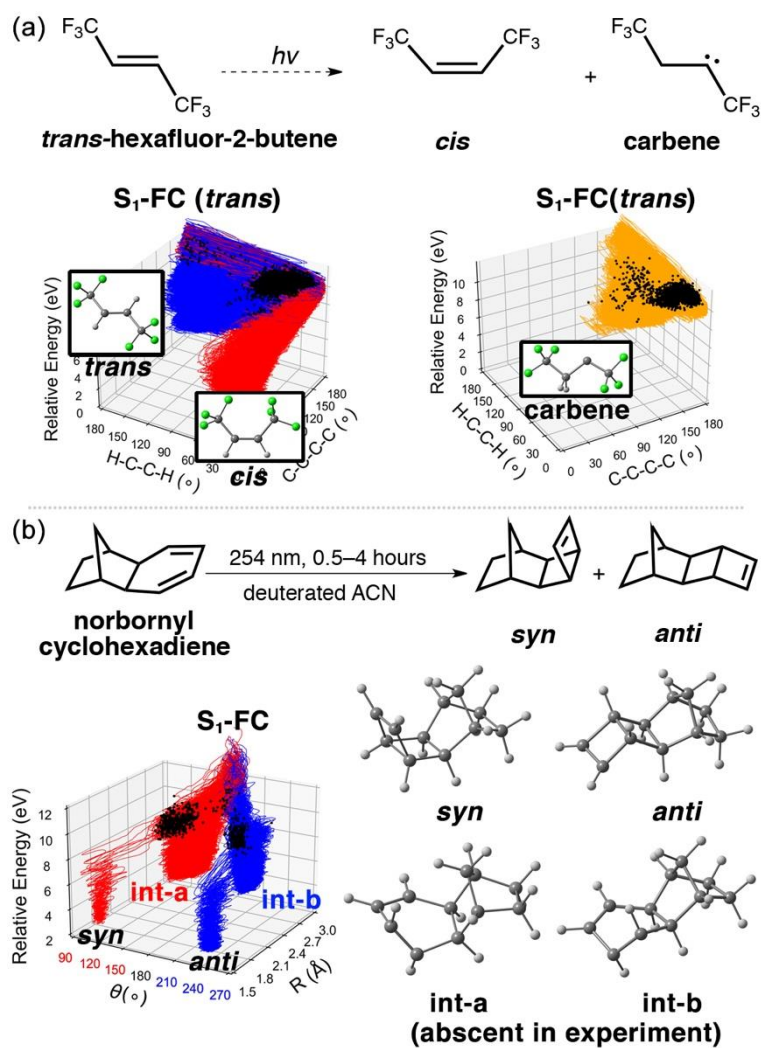
Photodynamics simulation is an emerging technique to disentangle the intricate spectroscopic features and complex reaction mechanisms induced by light. By contrast to a thermal reaction, a photochemical reaction gains high energy from photon absorption without “heating up” the reactant. The reactant is then excited to a higher electronic state, i.e., Franck-Condon point, that triggers ultrafast molecular transformation. The fate of a photochemical reaction goes to a nonradiative process that involves the vibronic relaxation through a state-crossing point, i.e., conical intersection and intersystem crossing. Characterization of state-crossing points is at the central of the mechanism study of photochemical reactions. However, the crossing point determination is not trivial and exhausting because the excited-state potential energy surfaces (PESs) could exhibit multiple crossing points resembling several crossing seams or/and regions.

Photodynamics simulation provides a tool to explore the excited-state PESs with an ensemble of mixed quantum-classically trajectories. The nuclear motions are propagated using Newtonian equations; the electronic energy, forces and state-couplings are solved using quantum mechanics. The electronic transition is stochastically determined by the fewest switches surface hopping algorithm.<sup>1</sup> The crucial ingredient in photodynamics simulation is an electronic structure method that can adequately describe static and dynamics electron correlations, e.g., extended multistate complete active space with second-order perturbation (XMS-CASPT2)<sup>2</sup>, and multiconfigurational pair-density functional theory (MC-PDFI).<sup>3</sup> Due to the computational costs, in our experience, a practical photodynamics simulations are commonly used for moderate-size molecules that must undergo efficient photochemical reactions (FC point→product) within 1 picosecond requiring  $10^1$ – $10^4$  wall-clock hours. Machine learning (ML) is a rapid developing interdisciplinary area in cheminformatics and computational chemistry. In many branches of machine learning algorithms, we are interested in Neural Network (NN) because of its simplicity of implementation, flexibility of learning chemical

properties, and efficiency of training. While the development of NN for ground-state molecular dynamics made tremendous progress on generalized atomistic potential (i.e., high-dimensional neural networks potentials<sup>4</sup> and continuous-filter convolutional neural network, SchNet<sup>5</sup>) for various types of atoms and molecules, the adoption in photodynamics simulation was achieved in 2019 by Marquetand and co-workers. They demonstrated the first ML photodynamics simulation for methylenimmonium cation ( $\text{CH}_2\text{NH}_2^+$ ).<sup>6</sup> Their NN reproduced results of expensive multireference configuration interaction (MRCI) calculations with a negligible cost, thus enabling nanoseconds simulations.

In 2021, our group published a Python-based code, Python Rapid Artificial Intelligence Ab Initio Molecular Dynamics (PyRAI<sup>2</sup>MD) software in *Chemical Science* that further leverages the capability of ML photodynamics method with an improved NN.<sup>7</sup> In the demonstrative example of *cis-trans* isomerization of *trans*-hexafluoro-2-butene, we showed a committee of NNs can automatically discover the out-of-sample structures during active learning. The initial training set only included data relevant to *cis-trans* isomerization assuming a limited prior knowledge of the underlying mechanism. The trained NN not only predicted the *cis-trans* isomerization but also found a side reaction to a carbene intermediate that fully agreed with the reference quantum chemical calculations (Fig 1a). In our second example, we performed the ML photodynamics to study an original photo-torquoselective  $4\pi$ -electrocyclic ring-closing of norbornyl cyclohexadiene. The ML photodynamics simulations reproduced the experimentally observed selectivity of the *syn*- and *anti*-product. Moreover, we found another two unobserved intermediates formed in 1 picosecond. Extending the simulation to 1 nanosecond revealed thermal conversions from the intermediates back to the reactant explaining their absence in the experiment (Fig 1b).

We believe that the ML photodynamics simulation can offer a priori prediction for long-lived excited-states and intermediates, which is not currently possible with multiconfigurational calculations. We anticipate that the PyRAI<sup>2</sup>MD-enabled simulations will pave the way to automatic discovery of photochemical reaction pathways and statistical analyses of currently inaccessible quantum chemical photodynamics simulations



**Figure 1.** (a) The schematics of *cis-trans* isomerization of *trans*-hexafluoro-2-butene and the PyRAI<sup>2</sup>MD predicted reaction pathways. (b) The schematics of 4 $\pi$ -electrocyclic ring-closing of norbornyl cyclohexadiene and the PyRAI<sup>2</sup>MD predicted reaction pathways. The black dots mark the surface hopping points.

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## **Role of the perfluoro effect in the selective photochemical isomerization of hexafluorobenzene**

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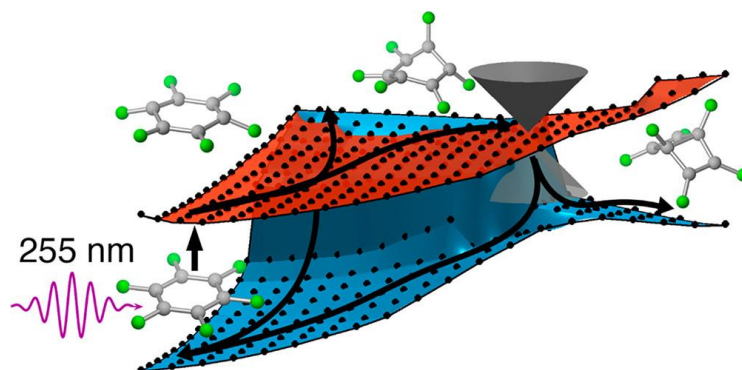
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As early as the 1972, researchers have noticed a puzzling trend in the absorption spectra for the series of fluorinated benzenes.<sup>1,2</sup> Similar absorption spectra are obtained for benzene rings with as many as four fluorine substituents, with observable vibrational fine structure in the lowest-energy absorption peak. However, with five fluorine atoms or the fully-fluorinated hexafluorobenzene (HFB), this vibrational fine structure abruptly vanishes, being replaced by an unstructured absorption peak accompanied by the rise of a new peak, the mysterious “C-band”. Further studies into the light-induced behaviour of benzene and HFB show that the photochemical outcomes in these two systems are also remarkably

different.<sup>3</sup> After excitation to its lowest-energy excited state, benzene predominantly affords its isomer benzvalene as a photochemical product, and only forms the Dewar-benzene isomer in very low (0.6 %) yield when excited to its second excited state.<sup>3</sup> Meanwhile for HFB, no benzvalene-like isomer is formed from the first excited state, and instead the only observed photoproduct is hexafluoro-Dewar-benzene.<sup>4,5</sup>

It is clear that the fluorine substituents in HFB are responsible in some way for the significant differences in behaviour of this molecule compared to its hydrogenated analogue. However, a definitive explanation for this phenomenon remains elusive. Reports in the literature often disagree on the nature of the electronic excited states of HFB, making it difficult to determine the effects these states may have. Research by Brundle *et al.* has demonstrated that the general effect of multiple fluorinations is to selectively stabilize the  $\sigma$ -type orbitals involved in the fluorine bonds<sup>6</sup>, sometimes referred to as the perfluoro effect as it is most prominent in perfluorinated molecules. While reports may come to differing conclusions on the exact mechanism of action, the consensus is that this perfluoro effect stabilized a  $(\pi\sigma^*)$ -type excited state in HFB to near or below the lowest-energy  $(\pi\pi^*)$ -type state.



**Figure 1.** The reaction potential energy surface of hexafluorobenzene showing reaction pathways that lead to reformation of the reactant and photochemical formation of the product, hexafluoro-Dewar-benzene.

A recent study by Steven Lopez and co-workers, published in the *Journal of the American Chemical Society*, developed a unified model of the effects of fluorination on the photophysical properties and photochemical reactions of HFB using a combination of advanced multiconfigurational

computations and static and time-resolved spectroscopic techniques.<sup>7</sup> The lowest-energy excited state is definitively shown to be of ( $\pi\pi^*$ ) nature, the same as it is in benzene. The differences then arise not from evolution on different excited states, but instead from differing topology in the same state. When two electronic states are close in energy, they can interact through molecular vibrations, called vibronic coupling. In cases of strong vibronic coupling, the lower state can become warped by the coupling leading to molecular distortions along the coupled vibrational modes. Lopez and co-workers demonstrate that the perfluoro effect in HFB is so pronounced that it induces strong vibronic coupling between the ( $\pi\pi^*$ ) and ( $\pi\sigma^*$ ) states, which in turn induces molecular vibrations along the appropriate vibrational modes to favour Dewar-benzene formation (Fig 1).

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## ABSTRACTS OF THESIS ON PHOTOCHEMISTRY

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### Photoremovable protecting groups for carbonyl compounds of biological interest

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46022 Valencia, Spain.*

*Supervisors: Prof. Miguel Ángel Miranda and Dr. Virginie Lhiaubet-Vallet.*

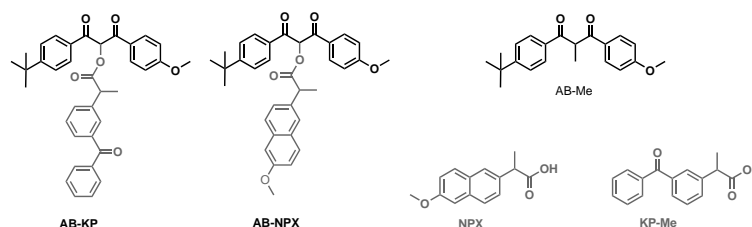
Living organisms are constantly exposed to solar light. From a photobiological point of view, ultraviolet radiation is considered as the most significantly harmful part of the sunlight since it can interact with biomolecules by direct and photosensitized processes.<sup>1</sup> Such interactions result on undesired chemical modifications that might contribute to the development of skin cancer.<sup>2</sup> In this context, the photolesions formed on DNA are of special importance because they can jeopardize the integrity of the genome, and the understanding of the processes responsible for their formation through a direct or photosensitized process is thus of utmost importance.

This doctoral thesis aims not only at deepening the knowledge of the photophysical and photochemical properties of potential photosensitizers but also at developing new photoprotection strategies through the use of photoremovable protecting groups (PPGs). In a first part, new PPGs based on solar filters are studied and designed as new potential photoprotection strategies against xenobiotic-induced photosensitivity. In a second part, the photosensitizing properties of two oxidatively generated DNA damages, namely 5-formyluracil (ForU) and 5-formylcytosine (ForC), are duly analyzed. Additionally, a new synthetic route for the incorporation of ForU into oligonucleotides (ODN) using a PPG is presented. This new alternative facilitates the study of the photosensitizing properties of ForU within the DNA environment.



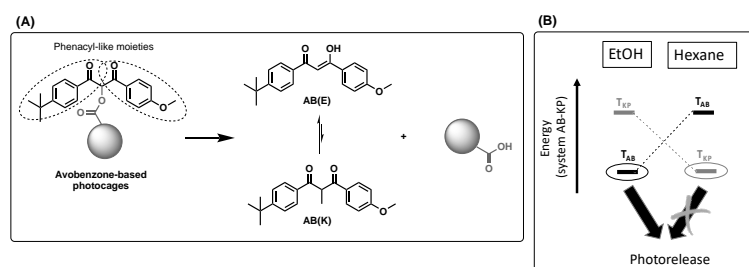
Part I. Development of new sunscreen-based photolabile protecting groups.

In this first part, different systems based on avobenzene and oxybenzone solar filters as photolabile protecting groups have been designed and studied. Concerning the avobenzene-based systems, they contain the phenacyl-like structure, which has been widely developed as PPG for carboxylic acid group.<sup>3</sup> In this context, two dyads (AB-KP and AB-NPX) containing the nonsteroidal anti-inflammatory drugs ketoprofen and naproxen have been analyzed together with their separated components (KP-Me, AB-Me and NPX) (Figure 1).



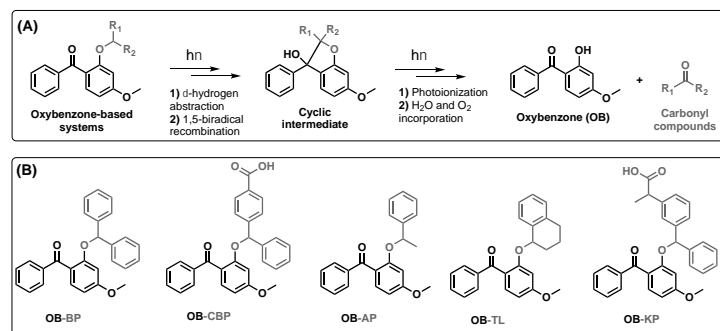
**Figure 1.** Chemical structures of the studied compounds.

Firstly, the photophysical and photochemical properties of the AB-KP system have been assessed in EtOH and hexane using nanosecond laser flash photolysis, femtosecond transient absorption spectroscopy, UV-Vis spectrometry and molecular modeling. The obtained data point toward a dependence on solvent polarity of the relative energy location of the avobenzene triplet state in its diketonic form,  $^3\text{AB}(\text{K})^*$ , with respect to that of its caged compound. Specifically, in hexane the  $^3\text{AB}(\text{K})^*$  is the component of the dyad with the highest energy and an ultrafast intramolecular triplet-triplet energy transfer to KP moiety has been established by transient absorption spectroscopy at femtosecond timescale. Then, since the photorelease occurs from the triplet state of the phenacyl-like moieties of the AB (Figure 2A), the photouncaging process is deactivated in hexane (Figure 2B). In ethanol,  $^3\text{AB}(\text{K})^*$  is the lowest triplet allowing the photorelease.<sup>4</sup> Coherently with these results, this process is deactivated in the AB-NPX system regardless of the solvent polarity due to the low triplet energy of naproxen (NPX), which does not make possible the triplet energy inversion.



**Figure 2.** General representation of the photorelease from the avobenzene-based systems (A) and a schematic representation of the influence of the solvent polarity on the photouncaging process of the AB-KP system (B).

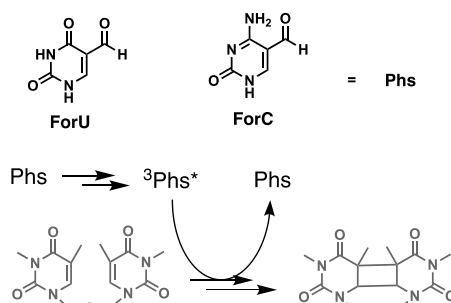
The use of solar filters as PPGs has also been extended to oxybenzone for the photorelease of carbonyl compounds.<sup>5</sup> Here, the photophysical and photochemical properties of OB-BP and OB-CBP have been thoroughly studied through experimental techniques such as laser flash photolysis, HPLC, UV-Vis spectroscopy and mass spectrometry. Based on these results, a photorelease mechanism involving a first  $\delta$ -hydrogen abstraction followed by photoionization and incorporation of oxygen and water has been proposed (Figure 3A). Moreover, the use of OB as a PPG has been applied for the release of other aromatic ketones, *i.e.* ketoprofen (OB-KP), acetophenone (OB-AP) and  $\alpha$ -tetralone (OB-TL).



**Figure 3.** Proposed mechanism for the photorelease of OB and its caged carbonyl compounds from the OB-based systems (A) and the structures of the studied systems (B).

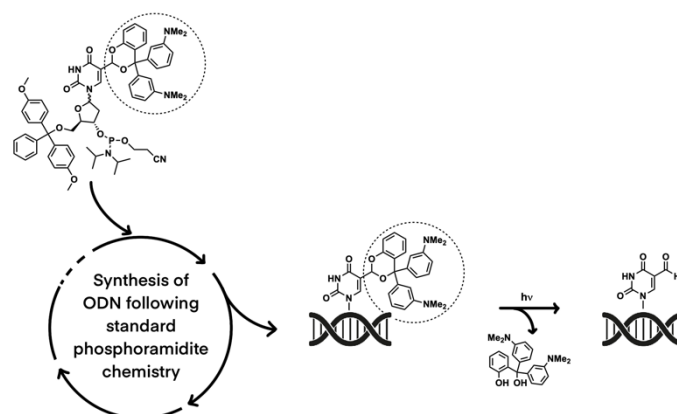
Part II. Study of the photosensitizing properties of two oxidatively generated DNA damages.

In this second part, the photosensitizing properties of two DNA damages, namely 5-formylcytosine (ForC) and 5-formyluracil (ForU), have been studied. Special emphasis has been placed on unraveling their capacity to promote the formation of cyclobutane pyrimidine dimers lesions (CPDs) (Figure 4). These results have shown that both modified nucleobases are able to photoinduced the formation of CPDs, although through different mechanisms and with different efficiencies. In this sense, ForU has been demonstrated to be much more efficient than ForC.<sup>6,7</sup>



**Figure 4.** Photosensitized [2+2] cycloaddition of bipyrimidine model in the presence of 5-formyluracil (ForU) and 5-formylcytosine (ForC).

Thus far, the photosensitizing properties of ForU have only been studied in solution in an intermolecular way. For that reason, it would be very interesting to study how they are affected when ForU is part of the DNA. In this context, the development of new synthetic approaches that facilitate its insertion into oligonucleotides is of great importance. Regarding the incorporation of ForU into ODN, the main challenge is related to the reactivity of its formyl group.<sup>8</sup> To overcome this problem, a new photochemical approach based on the use of a PPG for the protection of the formyl group followed by its selective deprotection using light of wavelength larger than 320 nm is presented (Figure 5).



**Figure 5.** New photochemical alternative for the selective insertion of ForU into oligonucleotides.

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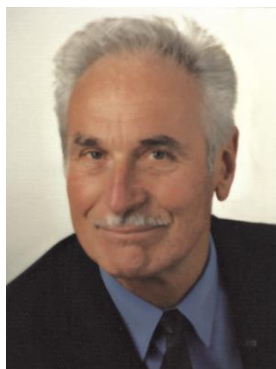
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## OBITUARY

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### Professor Doctor Heinz Dürr - A distinguished photochemist

*Henri Bouas-Laurent*  
*Honorary professor of Chemistry*  
*University of Bordeaux*



Heinz Dürr was born on 14th October 1934 in Pforzheim (Germany, Bade). He passed away on 21<sup>st</sup> February, 2021, in Saarbrücken.

Starting the study of chemistry in Stuttgart, he achieved his diploma in Heidelberg where he obtained a thesis in organic chemistry in 1961 under the supervision of *Georg Wittig* (1897-1987), the winner of a Nobel Prize in 1979.

With his mentor, Dürr studied the reactivity of dienes and *benzynes*, a recently discovered unstable species whose investigations were being intensively developed. During that period, he noticed the renewal of photochemistry, particularly in the USA, and was attracted by the field. This is the reason why he spent a postdoctoral year (1962-1963) in *Howard Zimmerman's* group (Madison, Wisconsin) where he acquired the background knowledge of the discipline.

Back to Europe, he gained a Nato grant to do a second postdoctoral formation with *Guy Ourisson* in Strasbourg (1963-1964) where, inter alia, he became familiar of NMR and French language.

After one year in industry (BASF) to synthesize dyes (and take out a patent), he decided on a career in University and started research for a Habilitation with *B. Eistert* at the University of Saarland. He got his Habilitation in 1969, and an assistant professorship. In 1971 he was appointed full professor in Saarbrücken.

**Professor Dürr's researches can be divided into three main topics.***1- Synthesis and photochemistry of small rings.*

By irradiation, a number of new carbenes were generated. The structures and mechanisms were thoroughly investigated by spectroscopy and semi-empirical calculation (22 articles, ref 1)

*2- Photochromic compounds.*

During an investigation of unsaturated spiroheterocycles, especially dihydroindolizines (DHIs), Dürr discovered the photochromic properties of this new class of molecules (ref 2). Photochromism was well known and an established family, the "spiropyranes" (SPs), had been and were still extensively studied. There is, among others, an important difference between the two families: under U.V. irradiation, SP as well as DHI, are transformed into a thermally unstable coloured form. Whereas for SPs, the latter is neutral, for DHIs the coloured form is zwitterionic. With his coworkers, Dürr synthesized a great number of derivatives and determined their physical properties in view of selecting the more fatigue resistant (i.e. undergoing many photochemical cycles) compounds. He took out some patents (1985-1995).

In 1984, Dürr was contacted by Elsevier to edit a multiauthor book on photochromism. Owing to the blossoming research in the field, it was timely, indeed, to publish a volume following that of George H. Brown (1971), then known as the "Bible". Bouas-Laurent was invited to be the co-editor. The conjugated efforts of 28 authors resulted in a volume of 1040 pages entitled "**Photochromism, Molecules and Systems**" which was published in July 1990 (ref 3a). A comprehensive analysis was reported by H. Görner and H. J. Kuhn in EPA NL (ref 3b). After eight years, the book was out of print. A second, revised, version was released in March 2003.

*3- Photoinduced electron transfer and artificial photosynthesis.*

Dürr was always attracted by fundamental research directed to applications. A very important domain is artificial photosynthesis in order to produce electrical current or dihydrogen etc. In this competitive field, his mark was to design organic ligands to improve the stability of catalysts. In particular, in 1983, he could use a Ru (II) complex of polypyridine to transform CO<sub>2</sub> into CH<sub>4</sub> (ref 4a). In depth mechanistic studies were conducted with *I. Wilner* (4b). His work was frequently presented in international conferences on solar energy.

H. Dürr gave many lectures worldwide (USA, Europe, Canada, Israel, Egypt...) and was invited as plenary lecturer in many symposia. He was the

chairman of the VIII<sup>th</sup> IUPAC Photochemistry Symposium (1980, Seefeld, Austria) and co-chairman of the Workshop on Supramolecular Chemistry and Photochemistry with H.J. Schneider (1989, Saarbrücken).

Of note are his invited various professorships in Nigeria, France, USA (1972-1988). He was awarded the prestigious **Humboldt/Gay-Lussac prize** in 1996.

It should also be emphasized that H. Dürr was a co-founder of EPA in 1974 and served as a co-editor of EPA Newsletter.

Dürr published ca 200 articles in Journals and 10 patents. He supervised more than 70 theses and, remarkably, supported his students until employment.

Professor Dürr will be remembered as an outstanding researcher, internationally praised. Moreover, he was an outgoing, joyful, pleasant fellow, attracting a great sympathy and friendship all over.

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## **CONFERENCE REPORT**

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### **Dutch Photochemistry Days on-line, May 10 and 17, 2021**

*Begüm Demirkurt, Chao Hsu, Maximilian Paradiz  
van 't Hoff Institute for Molecular Sciences, University of  
Amsterdam, The Netherlands*

The Holland Research School for Molecular Chemistry ([www.hrsmc.nl](http://www.hrsmc.nl)) invited the Dutch photochemistry community to two meetings on the afternoons of May 10 and 17 to discuss their research, to network, and to experience new ways to meet online.

The meeting began on May 10 with a keynote lecture from Rachel Crespo-Otero, from the University of London. She explained how modern quantum chemical methods can be used to describe the mechanisms, through which electronically excited molecular crystals dissipate energy as heat. By designing molecules that form crystals in which these dissipation pathways are not accessible, highly luminescent materials can be engineered. The second keynote lecture was given on May 17 by Guillaume Izzet, from Sorbonne Université. He reported on novel Polyoxometalates (POM) - based photosensitizers. By adjusting the moieties between the photosensitizer to POM, the efficiency of the charge injection process is improved and long-lived charge separated states are obtained.

On both days, 12 talks from PhD and postdoc students were scheduled. Jean Paul Menzel (Leiden) discussed the theoretical tools that he uses to predict the electron injection efficiencies of dyes in photoelectrochemical cells. Pedro Miguel M.C. de Melo (Utrecht), on the other hand, explained that long-lived triplet states experimentally detected in dichalcogenides are not predicted theoretically when considering a perfectly pure lattice. It was thus shown that such triplets arise due to the presence of defects.

Along with computational studies, experimental works on photoisomerization, photoswitching, photodegradation mechanisms were also popular topics. Nadja A. Simeth (Groningen) spoke about ways to chemically modify photoswitches to integrate them into complex systems



- such as for the photoreversible control of duplex formation in DNA. Jiayun Fan (Amsterdam) discussed how she spectroscopically studies methyl sinapate's ability to quickly dissipate light energy as heat, with the aim to design better sunscreens. Manee Patanapongpibul (Groningen), hopes that her viscosity responsive photoswitches will allow researchers to study the properties of microscopic environments such as cell membranes. Iris Groeneveld (Amsterdam) showed her photoreactor design. Using low-volume cell and a liquid core waveguide, efficient illumination and simultaneous measurements have been achieved with the aim to study photodegradation of organic compounds. Jorn D. Steen (Groningen) studied electrochemical switching of a spiropyran derivative and discussed that despite being activated by photons, the active form could be reached by using an electrocycle at low temperature. Zoran Ristanović (Leiden), presented his studies on the light-induced changes in organic solids detected by subtle spectral changes at the single-molecule level.

More experimental works from the domain of photocatalysis were presented. Paola Riente (Eindhoven), discussed her study on a commercially available bismuth photocatalyst. With time-dependent UV-Vis Absorption Spectroscopy and molecular simulations, the photocatalytic mechanism has been elucidated as being different from the mechanism of a classical heterogeneous catalyst. Ruben F. Hamans (Amsterdam) discussed mapping fluorogenic reactions catalyzed by the plasmonic fields around gold nanorods. In this regard, he used super-resolution microscopy.

Nicoletta Liguori (Amsterdam) designed a novel time-resolved spectroscopy technique that allows kinetic studies of molecules that respond to pH changes, and Vincenzo Mascoli (Amsterdam) explores ways to extend the energy efficiency of photosynthesis by implementing red-shifted chlorophyll derivatives.

Despite the limitations of the on-line format, the meeting created an interactive environment thanks to the contributions of speakers and participants. There was an active Q&A session after each talk. We highly recommend the 28<sup>th</sup> IUPAC Symposium 2022 in Amsterdam.

## CONFERENCE ANNOUNCEMENTS

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<https://photoiupac2022.amsterdam/>

After the unfortunate cancellation in 2020 due to the COVID-19 pandemic, we hope to welcome the photochemistry community in Amsterdam in July 2022.

The 28th IUPAC Symposium on Photochemistry continues a long tradition of conferences where experts in photochemistry in a broad sense exchange the latest results, and where scientists and engineers who use light in their research or application can pick up new ideas and strengthen their knowledge of the specifics of the interaction of light and matter.

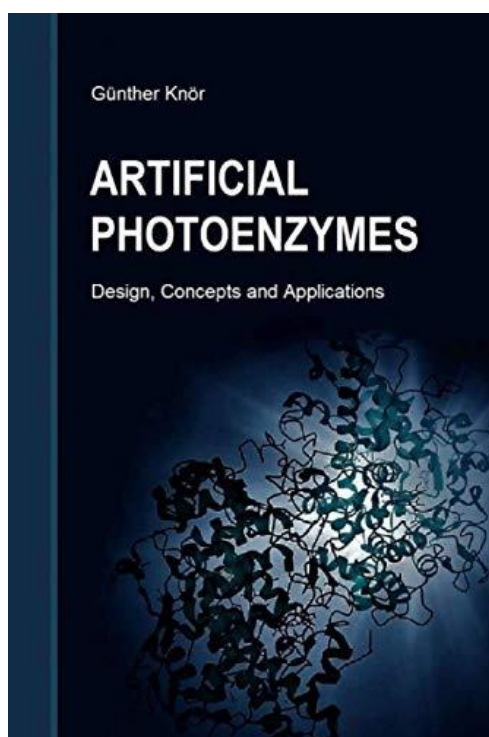
The scientific topics to be covered in the Symposium include areas of unparalleled impact in the world today. These include renewable energy sources, green chemistry, atmospheric photochemistry, single molecule microscopy and super resolution imaging. The latter are key for biosciences and trace analysis of proteins, nucleic acids, and small bioregulators. With more efficient light sources and means to collect solar energy, there is an on-going resurgence in the development of photochemical reactions using flow process, which are beginning to make an impact in an industrial context. This will be an excellent opportunity to engage scientists from pharmaceutical, materials, and other industries. The symposium will also cover advanced spectroscopic methods with increased time and space resolution and methods for analyzing complex samples.

- **Opening of registration:** 15th December 2021
- **Call for abstracts:** 15th December 2021
- **Deadline for submission of oral abstracts:** 15th February 2022
- **End of Early Bird registration:** 20th April 2022
- **Deadline for submission of poster abstracts:** 20th May 2022
- **Symposium dates:** 17th-22nd July 2022

## BOOKS

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### **G. Knör, Artificial Photoenzymes – Design, Concepts and Applications**

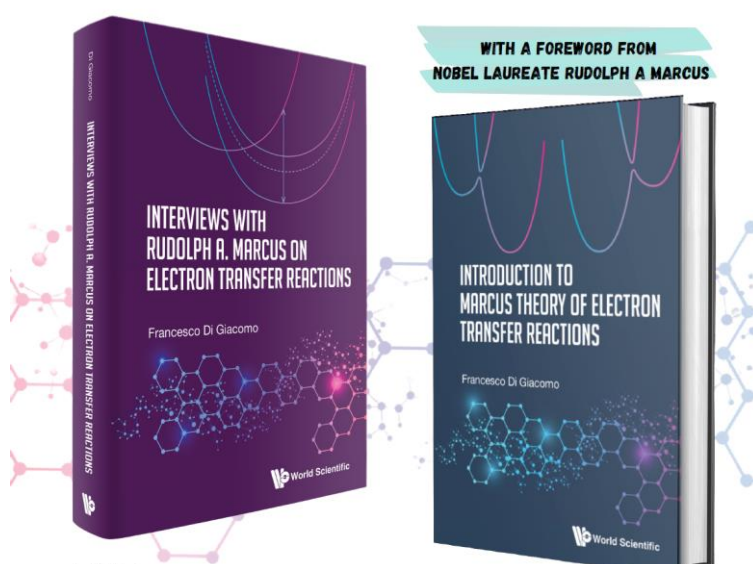


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[alexandre.fuerstenberg@unige.ch](mailto:alexandre.fuerstenberg@unige.ch) or [treasurer@photochemistry.eu](mailto:treasurer@photochemistry.eu))