

N-Allyl-N-ferrocenylmethylamines and ansa-

Biological Evaluation

Ferrocene derivatives functionalized groups have been studied for vario synthetic intermediates, ligands, sens agents.[1] The most seminal example

aminomethylferrocene,[2] the Ugi's an The leading methodology in the de

ompounds of known activity, e.g. tam

ansa-ferrocene hybrids with biologic have appeared as promising anticance

ous studies.<sup>[5]</sup> While mode of their generation of reactive oxygen species. [6

Considerably less is known about a simple ferrocene or ferrocenium deriva nave envisioned the synthesis of seve

structural modifications. Driven by scient

logically active moieties would displa

decided to examine if ferrocenylme

[a] M. Mazur, K. Ziemkiewicz, K. Rawiak, K. Kisie Dr. W. Buchowicz Faculty of Chemistry, Warsaw University of T Noakowskiego 3, 00-664 Warsaw, Poland

Żwirki i Wigury 101, 02-089 Warsaw, Poland Supporting information for this article is Part of the "Ferrocene Chemistry" Special C

Eur. J. Inorg. Chem. 2022, e202101098 (1 of 12

Darek,

**Piotrek** 

crystals

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Light-Induced Transient Species in Molecular Crystals and Selected

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Radek

& Maksio

(with Stasio)

& Krysia

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[b] K. Deresz, Dr. K. N. Jarzembska

Ferrocenylmethylamines: Synthesis, Structure, and

Maria Mazur, [a] Kamil Ziemkiewicz, [a] Karol Rawiak, [a] Kacper Kisiel, [a] Patrycja Wińska, [a] Krystyna Deresz, [b] Katarzyna N. Jarzembska, [b] and Włodzimierz Buchowicz\*[a]

ehyde, and 1,1'-ferrocene-dicarboxaldehyde with The isolated N-allyl ferrocene derivatives were completely

J. Synchrotron Rad. (2020). 27, 405–413

Advances in Diffraction Studies of Light-Induced Transient

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research papers

cesses and structural dynamics in the solid state, putting major emphasis on the X-ray diffraction

erimental possibilities in the field are discussed along with the data processing and analysis approaches, and illustrated with some striking literature examples of the respective successful stud ies. Selected complementary methods, such as ultrafast electron diffraction or time-resolved X-ray

Krystyna A. Deresz † 0, Piotr Łaski † 0, Radosław Kamiński \* 0 and Katarzyna N. Jarzembska \* 0

Species in Molecular Crystals and Selected

**Complementary Techniques** 

The most important include acid-catalysed reactions of ferro-

photocrystallography

ted. In the case of the dialdehyde only one formyl group — structures of four representative compounds were determined ffectively reacted with N-allylmethylamine or N-allylaniline, using single-crystal X-ray diffraction. MTT assays showed that hus providing a simple route to aminomethyl aldehydes and these simple N-allyl ferrocene derivatives display anticance nomethyl alcohol. 2-Aza-ansa[3] ferrocene was also ob- activity (MCF-7, A-549 and PC-3 cell lines) in the micromola

# Structural Dynamics Research Group

## K. N. Jarzembska & R. Kamiński



## Research topics

Photocrystallography - ultra-fast time-resolved and steady-state experiments

Transition-metal complexes and photoactive functional materials

**High-pressure X-ray diffraction** 

Crystallographic software development

Instrumentation design and construction

From left to right: Liliana Siewierska (stud.), Kinga Potempa (stud.), Krystyna Deresz (PhD stud.), Piotr Łaski (PhD stud.), Sylwia Kutniewska (PhD), Patryk Borowski (stud.), Radosław Kamiński (co-PI), Katarzyna Jarzembska (PI, the boss), Jakub Drapała (PhD stud.)

Sylwia

& Piotrek

research papers

9,10-Anthraquinones Disubstituted with Linear Alkoxy Groups: Spectroscopy, Electrochemistry, and Peculiarities of Their 2D and 3D

Agnieszka Maranda-Niedbała, Klaudyna Krzyżewska, Kamil Kotwica, Łukasz Skórka, Jakub Drapała,

Inorganic Chemistry Cite This: Inorg. Chem. 2019, 58, 16712–16721

Sylwia E. Kutniewska, <sup>†©</sup> Radosław Kamiński, <sup>†©</sup> Włodzimierz Buchowicz, <sup>‡©</sup>

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ABSTRACT: A new photoswitchable half-sandwich nitro Ni<sup>II</sup> complex with the

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 $[Ni(\eta^5-C_5H_5)(IMes)(\eta^1-NO_2)]$ 

systems that may find various real-life applications. For instance, they could be utilized in opto(bio)electronics,<sup>2,3</sup> as

inderstand the mechanisms of molecular transformations to

ructure. In such case, structural distortions, as, for example,

asily explored via X-ray diffraction techniques.8-10 The nowledge about structural changes provides information on

Among many photoactive substances transition-metal nitro

mbidentate nitro (i.e., NO2) ligand in their structure and the xibility in designing new molecules of this kind by changing

pordinate to the metal center in various ways, either via the trogen atom, oxygen atoms, or both. <sup>12</sup> Amidst the different ordination modes, the nitro  $(-N(O)_2)$  and nitrito (-ONO)

or adding metal centers and organic ligands, which allows fine

and Katarzyna N. Jarzembska\*,†

Photo- and Thermoswitchable Half-Sandwich Nickel(II) Complex:

further to the more stable endo-nitrito conformation, whereas at temperatures higher than 175 K the crystal converts back to the nermally. Consequently, the highest conversion level (ca. 90%) was achieved after sample irradiation at 145 K. Despite simila

upon irradiation and temperature changes. The photocrystallographic findings and molecular aspects were supplemented b

s generally most stable (i.e., it is the most frequently reported

tabase (CSD); 13,14 it is also the most stable one regarding

cyclic carbene (NHC) moiety. The original  $[Ni(\eta^5\text{-Cp})-(IMes)(NO_3)]$  complex has been synthesized as a part of a

arger project dedicated to finding the optimal catalys

acilitating the C-C bond formation in the polymerization of

DOI: 10.1021/acs.inorgchem.9b02836 Inorg. Chem. 2019, 58, 16712–16721

Theo Woike

& Krysia

Katarzyna N. Jarzembska, Małgorzata Zagórska, Adam Proń, and Robert Nowakowski

Seed-skewness algorithm for X-ray diffraction signal

Dariusz Szarejko, Radosław Kamiński, Piotr Łaski and Katarzyna N. Jarzembska

A one-dimensional seed-skewness algorithm adapted for X-ray diffraction

signal detection is presented and discussed. The method, primarily designed for

ne-dimensional data vectors as well as the capability to determine small ample to laser light. Otherwise, the procedure is objective, and relies only on

skewness computation and its subsequent minimization. The new algorithm was proved to vield comparable results to the Kruskal-Wallis test method

Supramolecular Organizations

III Metrics & More

bathochromic shift of the least energetic band from 325 nm in the case of unsubstituted anthraquinone to ca. 350 nm for the studied

Cite This: Langmuir 2020, 36, 15048-15063

radical anion and spinless anions, res was affected by electron-donating pro

potential being shifted to ca. -1.5 V mV as compared to the case of unsul corresponded to a decrease of IEAI fro

experimental spectroscopic and electroalkoxy substituent improved solution

supramolecular 2D aggregation on Ho carried out on single crystals and mono the resulting supramolecular organizat arrangement in crystals: increasing su

second effect, observed in monolay structures with increasing substitue

increasing correlation of the molecule graphite substrate. As a result, their 2

Redox, optical, and structural pro

 ${
m D}^{1-3}$  and  ${
m 2D}^{4-7}$  supramolecular agg nportance for their use in organ

oppropriate alignment of the energy

organized in thin layers or monolaye

ACS Publications

Instrument-model refinement in normalized

reciprocal-vector space for X-ray Laue diffraction

adosław Kamiński,<sup>a</sup>\* Dariusz Szarejko,<sup>a</sup> Martin N. Pedersen,<sup>b</sup> Lauren E Hatcher, c,d Piotr Łaski, Paul R. Raithby, Michael Wulffe and Katarzyna N

iffraction data is presented and discussed. The method is based on least quares minimization of differences between respective normalized (i.e. unit

ollected for small-molecule single-crystal samples. The method has been shown to work well on both simulated and experimental data. Tests performed on

alidity of the proposed instrument-model refinement approach. Finally

Krzysztof Woźniak,[b] and Sergiusz Luliński\*[a]

fraction. Specifically, biphenyl-based systems show dynam

systems,[1] are currently a subject of their interesting properties and v

hydrolytic cleavage, which can be high

chemistry. In fact, various benzoxa

been recognized as biologically activ

silicon analogues, i.e., benzosiloxi

1-ol<sup>[4,5]</sup> (Scheme 1c) as well as a comp

[b] P. H. Marek-Urban, Dr. hab. K. N. Jarzemb

**Expedient Synthesis of Oxaboracyclic Compounds Based on** 

iphenyl backbones was developed. The key synthetic step tained compounds varies very strongly (pK, ranges from 3.1

ted electrophiles (CO<sub>2</sub>, DMF, Me<sub>2</sub>Si(H)Cl) and hydrolytic luminescent complexes with 8-hydroxyquinoline. A stron tained by an additional reduction step with LiAlH $_{ extsf{4}}$  or  $\;$  527 nm) and photoluminescence quantum yield (10–95 %

aBH<sub>4</sub>. The obtained boracyclic compounds were character- was observed, which was rationalized in terms of specific

research papers

CHEMISTRY CRYSTEN

CCDC references: 1975196; 1975197; 1975198; 1975199; 1975200; 1975201;

1975202; 1975732; 1975733; 1975734;

**IUCrJ** 

Naphthalene and Biphenyl Backbone and Phase-

ed in detail by NMR spectroscopy and single-crystal X-ray aggregation effects.

**Dependent Luminescence of their Chelate Complexes** Krzysztof Durka, [a] Paulina H. Marek-Urban, [a, b] Krzysztof Nowicki, [a] Jakub Drapała, [a

Katarzyna N. Jarzembska, [b] Piotr Łaski, [b] Aleksandra Grzelak, [a] Marek Dąbrowski, [a]

■ INTRODUCTION

LANGMUIR

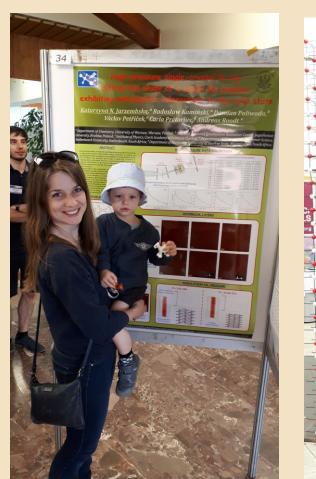
crystallographic time-resolved Laue data processing, was shown to worl well for the type of data collected at the Advanced Photon Source and in the case of standard single-crystal X-ray diffraction data. The reported algorithm enables reasonable separation of signal from the background in single

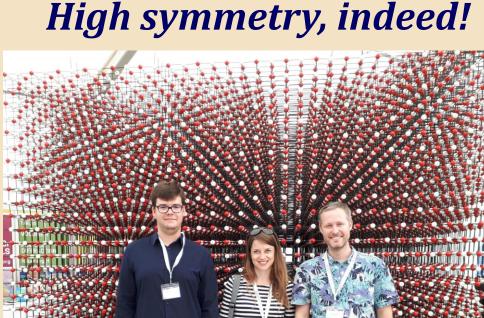
detection in time-resolved synchrotron Laue



Kasia, Maksio & Stasio

Conference workout by Ann Kate!





Kasia Patryk, Kasia, Radek

**Chillout** 

Piotrek, Patryk, Krysia (+ Maksio), Krysia, Radek, Kuba, Piotrek Kasia (+ Stasio), Radek, Darek

... and there it is! Coffee corner ready!

steady, go!

Krysia, Piotrek, Radek, Kasia and the Table



Ready,

Radek & Mark Warren

... 5 days of XFEL data collection ...

# Conferences more ...

House of cards

Patryk, Krysia, Piotrek





**Piotrek** 

Nice gloves!

Our first PhD promoted! Congratulations Sylwia!

Some applied physics...

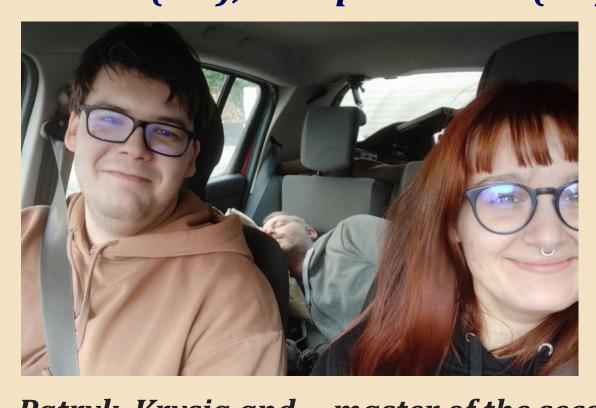




... last touches ...

Visits to Nancy (FR), Diamond (UK), European XFEL (DE)





Patryk, Krysia and ... master of the second plan (Radek)

### Research grants:

- K.N. Jarzembska, SONATA BIS, M:M-PROP: metallophilic interactions allies or enemies? 2021 (ongoing), National Science Centre (Poland), 2,889,000 PLN
- K.N. Jarzembska, PRELUDIUM BIS, MXO2-ISOMER: in search of colour-changing photoswitchable materials based on 4th-row transition-metal complexes with simple ambidentate ligands, 2020 (ongoing), National Science Centre (Poland), 532,800 PLN • R. Kamiński, OPUS, THIO-SWITCH: towards novel photo-active switchable materials – exploration of dithienylethene-based transition-metal complexes via advanced in situ
- photocrystallographic and spectroscopic approaches, 2020 (ongoing), National Science Centre (Poland), 1,999,880 PLN • R. Kamiński, SONATA, MMCT-XRAY: Communication between metallic centres in selected bridged mixed-valence coordination complexes - photocrystallographic studies
- combined with ultrafast spectroscopy, 2017 (ongoing), National Science Centre (Poland), 729,500 PLN
- K.N. Jarzembska, SONATA PHOTO-TRACE: Tracing of photo-excited species in crystals and solution samples of coinage-metal coordination complexes, 2015-2020, National Science Centre (Poland), 897,630 PLN
- S.E. Kutniewska, PRELUDIUM, NO2-SWITCH: Photocrystallographic studies of new photoswitchable 4th-row transition-metal nitro complexes, 2017-2021, National Science Centre (Poland), 180,000 PLN
- Other projects:

- Y. Jiang et al. (including K.N. Jarzembska & R. Kamiński), R&D proposal (accepted), XTRAS: ultrafast X-ray crysTallography with diveRse sAmple delivery methodS, 2022-2025, European XFEL (Germany)
- K. N. Jarzembska & P. Borowski, "Najlepsi z Najlepszych" programme, Co-SWITCH: badanie właściwości fotoprzełączalnych związków kompleksowych kobaltu(III), 2021, Ministry of Education and Science (Poland), 23,300 PLN
- K.N. Jarzembska, APS proposal (accepted), Tracing of photo-excited species in molecular crystals of polynuclear transitionmetal coordination complexes using the time-resolved X-ray Laue diffraction, 2021-2022, Advanced Photon Source (USA)

## Selected distinctions, lectures etc.

- K.N. Jarzembska, microsymposium chair at the IUCr Meeting in Prague, 2021
- S.E. Kutniewska, P. Łaski, oral presentations at the IUCr Meeting in Prague, 2021 • R. Kamiński, visiting professorship at the University of Lorraine & CNRS, Nancy (France), 2020
- R. Kamiński, UW Rector award enhancing the prestige of the university, 2020 • K.N. Jarzembska & R. Kamiński, UW Rector team award for scientific achievements, 2019
- K.N. Jarzembska, invited oral presentation at the ECM in Vienna, 2019

### Representative functions

• K.N. Jarzembska, Member of the Young Scientists Council of the Polish Ministry of Science and Higher Education (2018-2020)







Photocrystallographic and spectroscopic studies of

a model (N,N,O)-donor square-planar nickel(II) nitro complex: in search of high-conversion and

Sylwia E. Kutniewska, Adam Krówczyński, Radosław Kamiński, Katarzyna N rzembska, a\* Sébastien Pillet, b Emmanuel Wenger b and Dominik Schaniel b

A new, cheap, easy-to-synthesize and air-stable photoswitchable nickel(II) complex, QTNiNO2, is reported. The metal centre in QTNiNO2 is coordinated

ambient conditions. Irradiation of the solid-state form of QTNiNO2 with 530-

nitrito linkage isomer which is stable up to around 230 K, as indicated by IF

pectroscopy measurements. The structures of all species present in the

on the (photo)isomerization reaction taking place in a single crystal was additionally investigated. The experimental results are supported by computa

ties, either in solution or even more importantly in the solid

hould be chemically and thermodynamically stable at oper ating conditions), low cost, non-toxicity, and easy, high-yield

stable photoswitchable materials