Plan Overview

A Data Management Plan created using DMPonline

Title: Light-Induced Homolysis in C omplexes of Earth Abundant Transition Metals - Theoretical Investigations of Photochemical Pathways

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Funder: Swedish Research Council

Template: SU-VR template

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Project abstract:

Homogeneous photocatalysis involving transition metal complexes enables new sustainable routes in synthetic organic chemistry e.g. of active pharmaceutical substances. An emerging field of photoinduced ligand-to-metal charge transfer (LMC T) homolysis in complexes of earth-abundant transition metals offers means of regioselective synthesis without toxic compounds or precious metals with geopolitical issues. Progress in extending the synthetic protocols is hampered by lacking information of mechanistic details and even of the actual (photo)catalytic complexes. These details are difficult to obtain experimentally.

We propose theoretical modeling which can give valuable insight. However, it requires extensive simulations and experimental validation due to the challenges in simultaneously describing charge-transfer excitations and non- equilibrium dynamics in solution. First principle molecular dynamics simulations will be used to study "photocatalyzed decarboxylative azidation" - a specific process involving inner-sphere reactions. A LMCT excited state induces homolytic cleavage of a metal carboxylate bond leading to generation of an alkyl radical capable of C -N bond formation in a subsequent radical ligand transfer process. We will identify both the photoactive complex in the homolytic dissociation and the catalytic complex responsible for radical ligand transfer. Mechanistic details of excited state dynamics and ligand transfer will enable design of new photocatalytic routes.

ID: 195413

Start date: 01-01-2026

End date: 31-12-2029

Last modified: 20-01-2026

Grant number / URL: 2025-03596

Copyright information:

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Light-Induced Homolysis in C omplexes of Earth Abundant Transition Metals - Theoretical Investigations of Photochemical Pathways

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0: Note on personal data!

Q1: I have read and understood the above declaration and hereby certify that this DMP contains no personal data except for information about project members such as PI and contact person.

- Yes

I: Description of data – reuse of existing data and/or production of new data

Q1: Data Quality Assurance measures (FAIR data): please check multiple options that will apply to assure quality and integrity of data collected, created or reused.

- 3. Software specific file formats (e.g. Matlab - .mat; Stata - .dta)
- 6. Descriptive file names (e.g. '20200910SanFranciscoDaylight1pm.mp4')
- 1. Non-proprietary file formats (e.g. .csv, .txt, .json, netCDF)

Q2: Dataset ID: at this initial planning stage, please find one main identifier (e.g. a DOI, Handle, URL, ...) for the entire dataset(s) in the project where possible, even if it comprises several data files of different types.

2025-03596_VR

Q3: Dataset Identifier Type of your Dataset ID above in Q2, please select the corresponding option in the dropdown menu list below! (Default is 'other')

- other

Grant identifier

Q4: Dataset Description (Abstract) - please describe the dataset(s) in the project! The description can be at a rather simple conceptual level, which does not have to point to individual data files. However, it could preferably give an overview of what type of data files or other material the dataset(s) will include, e.g. images, spreadsheets etc.

Data from quantum chemical calculations and molecular dynamics simulations.

Q5: Title of dataset

Question not answered.

Q6: Are you re-using datasets that already have a definite *distribution* (that is, an *identifier*, access point or *location* URL)?

- no

Q10: Type of dataset(s) / resource type of the *main dataset(s)* of the project described by answers to Q2 / Q5 (thus, *not* of re-used datasets described in Q6-Q9).

- other

model structures, inputs, outputs, and derived results.

Q11: Issue date (YYYY-MM-DD) of *main dataset(s)* of the project described by answers to Q2 / Q5 (thus, not of re-used datasets described in Q6-Q9)

Question not answered.

II: Documentation and data quality

Q1: How will metadata be created for your dataset? If by *use of a repository* (*recommended*), please specify which, either from the given options, or - if Other - by giving a link(s) / URL(s) [if multiple separated by commas] as Additional Information below. Please*, do not write whole texts here* with line or paragraph breaks*, as this prevents automatic processing and evaluation of the DMP!*

- 1. Dataverse/StockholmUniversityLibrary
- 4. Zenodo/StockholmUniversityLibrary

For each publication, a Zenodo link will be created.

Q2: Which metadata standards and vocabularies will you employ for general and domain specific metadata?
(Multiple options possible. Some of them may overlap, then it is unnecessary to check all that hold a particular vocabulary specified in the text field.)

- 1. Metadata from II:Q1

Q3: Which of the following data quality documentation and safeguard measures, if any, would you consider applying to your dataset?
(Multiple options possible. For options 4. *Pre-registration,* 6. *Supplementary documentation* or 9. *Other*, please specify to the extent possible in the comment area, e.g. by giving the URLs of particular services you intend to use for certain data quality measures.)

- 2. File format and software description

III: Storage and backup

Q1: Where will you a) store and b) backup your accessible data during the project? (the data that you are using on a day-to-day basis). Please note that some options, in particular options 4-8, may not be suitable for storage and backup of *personal data* or other sensitive data!

- 9. NAISS (former SNIC-facility)
- X. Other option (please specify)
- 3. SUA workplace computer

Local data storage at Fysikum, SU. on workstation and cluster cap-fugu

Q2: What volume (X) of data will you need to store and backup?

- 1 TB < X < 10 TB

Q3: What security measures will you need to employ to protect your data during the research process? (Multiple options can be selected).

- 1. Password protection

IV: Legal and ethical aspects

Q1: Will the creation, collection or reuse of dataset(s) in your project entail processing of *personal data*, i.e. any information relating to an identified or identifiable natural person (a '*data subject*', that is a *living* person)?

- no

Q2: Will the creation, collection or reuse of dataset(s) in your project entail any of the following:

- **(a) processing of *special categories of personal data* according to the General Data Protection Regulation (EU 2016/679), i.e. personal data revealing racial or ethnic origin, political opinions, religious or philosophical beliefs, or trade union membership, and the processing of genetic data, biometric data for the purpose of uniquely identifying a natural person, data concerning health or data concerning a natural person's sex life or sexual orientation**
- **(b) processing of personal data regarding violations of law that include crimes, judgments in criminal cases, penal law sanctions, or administrative deprivation of liberty**
- **(c) physical interventions on research subjects or deceased persons**
- **(d) methods with the purpose of affecting a research person physically or mentally, or which includes an apparent risk of injuring the research subject either physically or mentally**
- **(e) studies of biological material that has been taken from a living or deceased person, and can be traced to that person**

Or, further, will the creation, collection or reuse of dataset(s) in your project include:

- **(F) Data from animal research**
- **(G) Data on genetic resources and/or traditional knowledge associated with genetic resources**
- **(H) Data that can be used for military purposes or concerning products that can be used for military purposes**
- **(I) Data that are sensitive in some other respect**

(Possible ethical review documentation applying to any of points (a-e) will be asked for separately.) If you answer yes to any of the points (F-I) and there is already relevant documentation or applications, please provide (a) reference(s) to any application(s)/ approval(s)/decision(s)/document(s), if possible by URL(s) / PID(s) such as DOI(s) giving direct access, or registration no. (Swe. *diarienr.*) in the text field below.

- no

Q5: Intellectual Property Rights - License(s) of data. Please select the usage license(s) for dataset(s) and/ or software *produced in your project*. (Multiple options possible. If *Other*, please specify by a URI or other file location for each of the additional license(s), separated by commas, in the comment area.)
[For *previously existing datasets* that you will be *re-using* , corresponding license(s) are entered in section *I:Q9 Description of data - re-use ...*]
If you choose no license at all from the options below, being aware that it *might* make your dataset less FAIR, please state the reason for this choice. [There are *fully legitimate reasons*, concerning e.g. personal data and sensitive data, that cannot be shared.]

- 05. CC-BY-NC-ND-4.0
- 04. CC-BY-NC-4.0
- 03. CC-BY-ND-4.0
- 02. CC-BY-SA-4.0
- 01. CC-BY-4.0

V: Accessibility and long-term storage

Q1: Where will datasets, documentation and/or metadata be made accessible? (Means or location of *distribution*).

- 3. SU Archive
- 4. On direct request from authorized users
- 1. Repository in answer to II:Q1
- 2. Supplement to journal article / publication

Q2: What will be made directly accessible (e.g. via repository in Q1, or as supplement to online journal)?

- Software scripts
- Metadata and some datafiles

Q3: When will data files and/ or metadata and documentation be made accessible?

- After embargo expires
- On completion of research project
- Only after publication of journal article / paper

Q4: How will you ensure that all data files, documentation and metadata are transferred to

SU digital archive for long-term preservation?

- Automatic harvest & transfer from repository

Q5: Will specific systems, software, source code or other types of services be necessary in order to understand, partake of or re-use / analyse data in the long term?

- yes

Q6: Will the software you will use to collect, create, handle, transform, refine or analyse data also be needed to replicate or rerun experiments, partake of your datasets or open datafiles?

- no

Q7: Will the software / code you will use to collect, create, handle, transform, refine or analyse data be ... (multiple options possible)

- 3. Other (please specify!)
- 1. Non-proprietary/Open Source (e.g. Python, R, XSLT)

Quantum chemical and Molecular Dynamics software will be required to run inputs

Q8: Will you be using Software in the "cloud" / Software-as-a-Service (SaaS) to create, handle, transform, refine or analyse data ?

- No

VI: Responsibility and resources

Q1: Who is responsible for data management and (possibly) supports the work with this while the research project is in progress?

- 1. PI

Q2: What resources will be required for data management to ensure that data fulfil the FAIR principles? (Multiple options possible.)

Q3: Please estimate total extra costs (C) for data management, that is not covered by grant funding (or regular SU services, such as RDM-team support).

- < 10000 SEK

VII: Funding requirement fulfilled for initial version

Q1: I hereby certify that the responsible PI (re)viewed this initial DMP as fulfilling the requirements for funding. I am aware that answering Yes will send this Initial version of the DMP to Archive for long-term preservation, and that future editing will then be in Phase 2, the final version.

- Yes

VIII: DMP administrative information

Q1: Please give an Identifier *of the Contact Person* (= yourself as creator/ owner) of this DMP, - *not* the *name* of the contact person, but only the identifier-string (that is within the " " in the examples below).

0000-0002-7023-2486

Q2: Please select Type of Identifier given as answer to Q1 above.

- orcid

Q3: Affiliation (Department / Institution) of Contact Person. Please select main Department / Institution affiliation *from drop-down menu* (ordered after faculties as in this list), or else choose "Other" and specify in comment area below!

- Physics

Q4: Language used for this DMP. Please select!

- eng: English

Q5: Funder(s). Multiple choice possible. If Other, please specify funder name(s) in the Additional Information text field, if more than one separated by commas.

- VR - Swedish Research Council

Q6: Grant ID. Please specify, if possible as a URL. (The Grant ID can often be the same as the PROJECT-ID in SweCris, e.g. https://www.vr.se/swecris#/project/2010-00383_VR)

https://www.vr.se/english/swecris.html?project=2025-03596_VR#/

Q7: Funding status. Please choose one from the dropdown menu.

- granted

IX: Full DMP - additional Datasets and identifiers, Reference list and Project end

Q1: Additional dataset(s)
Please fill in the *Default answer* table below in accordance with the given *Example answer* by replacing *None* in *Title, Identifier and Type* with *real values* for your dataset(s) after the *T1:, Id1: , Type1:* etc. You can add / delete rows if needed, but make sure the *new entries* are still in *italics* and leaving the last row without real values with *None* (as this will help us process your DMP data output for review.)
Identifier type: select from the same list as in section I-Q3: *ark, doi, handle, url, other.*
If *other*, please specify the type of dataset ID below the table as e.g. *"Local filename"* or *"Project-ID".*
The Description, Type of dataset (software, images, text, spreadsheets, sound, video, other) and Issue date for these additional datasets will as default be the same as for the main dataset described in section I: Q4, Q10 and Q11, so you might have to adjust these answers to fit for all datasets, or specify these new values for each additional dataset (below the table).

Question not answered.

Q2: List of References / Sources / Publications (other than reused datasets, in sec. I:Q6-9). To be updated during all research project.

Question not answered.

Q3: Research project ended?
Please indicate if the research project described by this DMP is completed, so the full and final version of this DMP can be sent to long-term archive.

- No