Solid catalysts for Functional group Shuttling

A Data Management Plan created using DMPonline.be

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Project abstract:

The project explores the benefit of solid porous (co-)catalysts in exchange reactions of functional groups between donors and acceptors. Target reactions are the transfer of -CN (nitrile) or –C(H)=O (formyl) groups to a C=C double bond. These reactions are particularly attractive since they allow to avoid hazardous chemicals (e.g. HCN; H2/CO) and/or high pressures during multistep organic syntheses. In the field of homogeneous catalysis, some metal coordination compounds or Lewis acids are emerging for these reactions, often in close synergy. However turnover frequencies for shuttling a functional group from a donor to an acceptor are so far low; catalyst recovery is poor, and due to the equilibrium nature of these isodesmic reactions, it is challenging to reach near-complete conversion. Here we introduce new concepts in these transfer hydrocyanations: (i) Lewis acids will be grafted on solid surfaces, enhancing their dispersion, making it easier to modulate and increase their activity and facilitating their recovery; (ii) olefin co-products will be withdrawn from the equilibrium by a consecutive reaction in a shape-selective material (zeolite, MOF) to which the other reactants have no access. Mechanistic insights will be gathered from a comprehensive spectroscopic-kinetic study. The project focuses on transfer hydrocyanation, but eventually the concept of e.g. equilibrium shifting is also tested in transfer hydroformylation.

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Research Data Summary

List and describe all datasets or research materials that you plan to generate/collect or reuse during your research project. For each dataset or data type (observational, experimental etc.), provide a short name & description (sufficient for yourself to know what data it is about), indicate whether the data are newly generated/collected or reused, digital or physical, also indicate the type of the data (the kind of content), its technical format (file extension), and an estimate of the upper limit of the volume of the data.

Dataset name / ID	Description	New or reuse	Digital or Physical data	Data Type	File format	Data volume	Physical volume
		Indicate: ***N****(ew data) or* ***E****(xisting data)*	Indicate: **D**(igital) or **P**(hysical)	Indicate: **A**udiovisual **I**mages **S**ound **N**umerical **T**extual **M**odel **SO**ftware Other (specify)		Indicate: <1GB <100GB <1TB <5TB >5TB NA	
GC	GC chromatograms	N	D	I,N	.gcd	<1GB	
NMR	NMR spectra	N	D	I,N	.fid	<100GB	
XRD	X-ray diffraction patterns	N	D	I,N	.xrdml	<1GB	
XAS	X-ray absorption spectra	N	D	I,N	.xdi	<100GB	
DFT	Density functional theory coordinates, energy calculations and structural models	N	D	T,N,M,I	.txt .log .chk .tiff	<100GB	
Lab notes	Notes of experiments and logbooks	N	P, D	T,I,N	.xlsx	<1GB	
Reports	Presentation and discussion of results	N	D	T,I,N	.doc;.ppt	<1GB	

If you reuse existing data, please specify the source, preferably by using a persistent identifier (e.g. DOI, Handle, URL etc.) per dataset or data type:

N/A

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? If so, refer to specific datasets or data types when appropriate and provide the relevant ethical approval number.

- No

Will you process personal data? If so, please refer to specific datasets or data types when appropriate and provide the KU Leuven or UZ Leuven privacy register number (G or S number).

- No

Does your work have potential for commercial valorization (e.g. tech transfer, for example spin-offs, commercial exploitation, …)? If so, please comment per dataset or data type where appropriate.

- Yes

The methods and applications developed in this project have potential for valorization, which will be subjected for discussion during the project. Patents will be submitted, transferred and valorized with the assistance of the intellectual property unit of KU Leuven Research & Development (LRD). Datasets relevant to commercial valorization include Reports.

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material or Data transfer agreements, Research collaboration agreements)? If so, please explain in the comment section to what data they relate and what restrictions are in place.

- No

Are there any other legal issues, such as intellectual property rights and ownership, to be managed related to the data you (re)use? If so, please explain in the comment section to what data they relate and which restrictions will be asserted.

- No

Documentation and Metadata

Clearly describe what approach will be followed to capture the accompanying information necessary to keep data understandable and usable, for yourself and others, now and in the future (e.g. in terms of documentation levels and types required, procedures used, Electronic Lab Notebooks, README.txt files, codebook.tsv etc. where this information is recorded).

Details to reproduce reaction procedures are described in a personal lab booklet. An overview of the analytical and experimental data will be maintained in excel sheets and word docs. Upon presentation or publication of data, procedures are described in sufficient detail to enable a reproduction of the generated results for an experienced user. ReadMe-files or recording methods for advanced characterization are stored in parallel with generated data.

Will a metadata standard be used to make it easier to find and reuse the data?
If so, please specify which metadata standard will be used.

If not, please specify which metadata will be created to make the data easier to find and reuse.

- No

Data Storage & Back-up during the Research Project

Where will the data be stored?

- OneDrive (KU Leuven)
- Personal network drive (I-drive)
- Shared network drive (J-drive)
- Sharepoint online

How will the data be backed up?

- Standard back-up provided by KU Leuven ICTS for my storage solution
- Personal back-ups I make (specify below)

External hard drives will be employed for personal data backups.

Is there currently sufficient storage & backup capacity during the project?

If no or insufficient storage or backup capacities are available, explain how this will be taken care of.

- Yes

How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?

The data will be stored in the university's secure environment for private data. The folders and data on the shared drives (in between persons working on the project) will be secured with passwords.

What are the expected costs for data storage and backup during the research project? How will these costs be covered?

Data storage costs on OneDrive are included in an internal service contract with the KU Leuven IT support service (SET-IT). No additional costs are expected for the storage of data. In case additional costs do arise, they will be covered by the project budget or reserve funds.

Data Preservation after the end of the Research Project

Which data will be retained for 10 years (or longer, in agreement with other retention policies that are applicable) after the end of the project?

In case some data cannot be preserved, clearly state the reasons for this (e.g. legal or contractual restrictions, storage/budget issues, institutional policies...).

- All data will be preserved for 10 years according to KU Leuven RDM policy

Where will these data be archived (stored and curated for the long-term)?

- Large Volume Storage (longterm for large volumes)
- Shared network drive (J-drive)

Upon termination of the contract, the data will be transferred and stored on an external hard drive (Samsung Portable SSD T5 1 TB), managed by Annelies Van Vlasselaer.

What are the expected costs for data preservation during the expected retention period? How will these costs be covered?

The high capacity of the available external hard drive (1 TB) enables the preservation of data from multiple terminated or finished projects. Currently, an average of 15 GB is used for the finished projects of each user, which allows to divide its cost over approximately 60 users. Given the cost of the available hard drive of 120 EUR, the expected costs are negligible. The involved IT-expenses are included in the project’s consumable expenses or covered by reserve funds.

Data Sharing and Reuse

Will the data (or part of the data) be made available for reuse after/during the project?
Please explain per dataset or data type which data will be made available.

- Yes, as restricted data (upon approval, or institutional access only)

Upon publication of the research results, the full datasets will be made available upon reasonable request.

If access is restricted, please specify who will be able to access the data and under what conditions.

Only uses for research purposes will be allowed and commercial reuse will be excluded.

Are there any factors that restrict or prevent the sharing of (some of) the data (e.g. as defined in an agreement with a 3rd party, legal restrictions)?

Please explain per dataset or data type where appropriate.

- No

Where will the data be made available?

If already known, please provide a repository per dataset or data type.

- KU Leuven RDR (Research Data Repository)
- Other data repository (specify below)

Besides KU Leuven RDR, via either journal-specific repositories (e.g. ACS) or public repositories (e.g. COD and CCDC).

When will the data be made available?

- Upon publication of research results

Which data usage licenses are you going to provide?

If none, please explain why.

- Other (specify below)

To be specified later.

Do you intend to add a persistent identifier (PID) to your dataset(s), e.g. a DOI or accession number? If already available, please provide it here.

- No

What are the expected costs for data sharing? How will these costs be covered?

No additional costs are expected as the data can be shared via online platforms (e.g. WeTransfer) or the already budgeted storage cloud from OneDrive. If additional costs would occur they will be covered from reserve funds.

Responsibilities

Who will manage data documentation and metadata during the research project?

PhD researchers: Jesse Dallenes, Jarne Leinders
PI: Prof. Dirk De Vos:

Who will manage data storage and backup during the research project?

PhD researchers: Jesse Dallenes, Jarne Leinders
PI: Prof. Dirk De Vos
Administrative contact: Annelies Van Vlasselaer

Who will manage data preservation and sharing?

PI: Prof. Dirk De Vos
Administrative contact: Annelies Van Vlasselaer

Who will update and implement this DMP?

PhD researchers: Jesse Dallenes, Jarne Leinders
PI: Prof. Dirk De Vos