
SYNTHETIC PLATFORM FOR THE CONTROLLED INCORPORATION OF MULTIPLE POLYOXOMETALATES INTO DISCRETE HYBRID STRUCTURES

A Data Management Plan created using DMPonline.be

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POLYOXOMETALATES INTO DISCRETE HYBRID STRUCTURES**

DPIA

DPIA

Have you performed a DPIA for the personal data processing activities for this project?

- Not applicable

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GDPR

GDPR

Have you registered personal data processing activities for this project?

- Not applicable

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Application DMP

Questionnaire

Describe the datatypes (surveys, sequences, manuscripts, objects ...) the research will collect and/or generate and /or (re)use. (use up to 700 characters)

The following data types will be created:

Physical:

Synthesized polyoxometalates samples

Digital:

1) Analytical raw data and chemical analysis of samples and equipment specific software-generated data such as NMR (.csv; .xls; Bruker NMR files...)

2) Textual and numerical experimental results such as interpreted data and processed data extracted from spectroscopic techniques as well as reports and presentations

A data storage capacity of 500GB - 1TB is expected to be sufficient for the whole project

Specify in which way the following provisions are in place in order to preserve the data during and at least 5 years after the end of the research? Motivate your answer. (use up to 700 characters)

1. Designation of responsible person: Head of the Lab of Bioinorganic Chemistry Prof. Tatjana N. Parac-Vogt
2. Storage capacity/repository
 - For better preservation of data, experimental methodology, planning and protocol will be logged in personal lab books and a word document. For each experiment, the experiment number, date, conditions, outcome, and characterization will be documented in a detailed fashion. Digital data will be saved on KU Leuven OneDrive
 - For long-term storage, an electronic copy of the data will be stored on one of KU Leuven online servers (K-drive)
Raw and processed data of every reaction will be stored in a separate folder. Folders of experiments that fall under a single subproject or correspond to data that will be used in a single publication will be merged in one folder to make sure that if any part of that work needs to be reused, all the data will be found in a single location.
An overview of the experiment number, the location in the lab book, the physical location of the sample, and the digital storage locations of the raw and processed data will be provided in a separate file.

What's the reason why you wish to deviate from the principle of preservation of data and of the minimum preservation term of 5 years? (max. 700 characters)

As KU Leuven's policy states that relevant research data must be stored for a minimum of 10 years, there will be no deviation from the principle of preservation of data.

Are there issues concerning research data indicated in the ethics questionnaire of this application form? Which specific security measures do those data require? (use up to 700 characters)

NA

Which other issues related to the data management are relevant to mention? (use up to 700 characters)

NA

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FWO DMP (Flemish Standard DMP)

1. 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.

				Only for digital data	Only for digital data	Only for digital data	Only for physical data
Dataset Name	Description	New or reused	Digital or Physical	Digital Data Type	Digital Data format	Digital data volume (MB/GB/TB)	Physical volume
		<i>Please choose from the following options:</i> <ul style="list-style-type: none"> • Generate new data • Reuse existing data 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> • Digital • Physical 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> • Observational • Experimental • Compiled/aggregated data • Simulation data • Software • Other • NA 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> • .por, .xml, .tab, .csv, .pdf, .txt, .rtf, .dwg, .gml, ... • NA 	<i>Please choose from the following options:</i> <ul style="list-style-type: none"> • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA 	
Analytical raw data	chemical analysis of samples and equipment specific software-generated data such as NMR and diffraction images	New	Digital	Experimental (textual/numerical)	.csv; .xls; .pdf; .txt; .cbf; .h5 Bruker NMR files;	< 500GB	
Experimental results	interpreted data and processed data extracted from spectroscopic techniques	New	Digital	Experimental (textual/numerical)	csv; .doc; .xls	<1GB	
Reports	presentations and results discussion	New	Digital	Experimental (textual/numerical)	doc; .pdf; .pptx	<1GB	
Polyoxometalate samples	synthesized during the project	New	Physical	Experimental (chemical compounds)			<50 vials

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:

NA

Are there any ethical issues concerning the creation and/or use of the data (e.g. experiments on humans or animals, dual use)? Describe these issues in the comment section. Please refer to specific datasets or data types when appropriate.

- No

Will you process personal data? If so, briefly describe the kind of personal data you will use in the comment section. Please refer to specific datasets or data types when appropriate.

- 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.

- No

Do existing 3rd party agreements restrict exploitation or dissemination of the data you (re)use (e.g. Material/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

2. 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).

For better preservation of data, experimental methodology, planning and protocol will be logged in personal lab books and a word document. For each experiment, the experiment number, date, conditions, outcome, and characterization will be documented in a detailed fashion. For long-term storage, an electronic copy of the data will be stored on OneDrive or one of KU Leuven online servers (J and K-Drive).

Raw and processed data of every reaction will be stored in a separate folder. Folders of experiments that fall under a single subproject or correspond to data that will be used in a single publication will be merged in one folder to make sure that if any part of that work needs to be reused, all the data will be found in a single location.

An overview of the experiment number, the location in the lab book, the physical location of the sample, and the digital storage locations of the raw and processed data will be provided in a separate file.

Will a metadata standard be used to make it easier to find and reuse the data? If so, please specify (where appropriate per dataset or data type) which metadata standard will be used. If not, please specify (where appropriate per dataset or data type) which metadata will be created to make the data easier to find and reuse.

- Yes

When conclusive data analyses is achieved, data will be deposited in the Research Data Repository (RDR) of KU Leuven (<https://rdr.kuleuven.be/>). The data will also be available in the open-access supplementary information of publications (with DOIs). All materials/resources newly generated in the project will be stored in-house and will be freely available to the community upon request. For scientific publications, peer-reviewed work will be deposited in the KU Leuven's repository system "Lirias" in case the work was published in non-open access journals.

3. Data storage & back-up during the research project

Where will the data be stored?

Shared network drive (J-Drive)
Archive (K-Drive)
OneDrive (KU Leuven)

How will the data be backed up?

Standard back-up provided by KU Leuven ICTS

**Is there currently sufficient storage & backup capacity during the project? If yes, specify concisely.
If no or insufficient storage or backup capacities are available, then 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?

KU Leuven servers managed by ICTS are protected from unauthorized persons. Files shared on OneDrive are only accessible to authorized people who are granted access by either the PI or the PhD/Postdoc researcher working on the project

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

OneDrive for business is free for staff and students of KU Leuven, and KU Leuven server costs are covered by the department.

4. Data preservation after the end of the research project

Which data will be retained for at least five 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)?

KU Leuven RDR
Shared network drive (J-drive)
KULEuven Archive storage (K-drive)

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

The costs are covered by project funding
Permanent storage is foreseen at the KULEuven Archive storage K-drive: €5,69 per 100GB per year

5. Data sharing and reuse

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

- Yes, in an Open Access repository
- Yes, in a restricted access repository (after approval, institutional access only, ...)

Most of the data will become available when published. Other data (not published yet as well as physical samples of synthesized POMs) can be obtained by researchers after request and approval by the PI (Tatjana N. Parac-Vogt).

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

All finalized work will be available publicly in open-access journal or on Lirias, the institutional repository of KU Leuven Association. Unpublished data can be obtained after request and approval of the PI (Tatjana N. Parac-Vogt).

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 in the comment section 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)
XRD data will be deposited on 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.

Data from the project that can be shared will be made available under a creative commons attribution license (cc-by 4.0), so that users have to give credit to the original data creators

Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, you have the option to provide it in the comment section.

- Yes

Yes, a PID will be added upon deposit in a data repository and a DOI will be provided through RDR

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

RDR is free for KU Leuven personnel, hence, no costs are expected for data sharing. Publication fees may be required to make articles open access in some peer-reviewed journals and these costs will be covered by the project when applicable.

6. Responsibilities

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

The PhD/Postdoc researcher will be responsible for data documentation & metadata, under the supervision of the PI (Tatjana N. Parac-Vogt)

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

The PhD/Postdoc researcher will be responsible for data storage and backup, as well as all researchers within the group that will collaborate on the project.

Who will manage data preservation and sharing?

The PI (Tatjana N. Parac-Vogt), as well as any delegated member of her group

Who will update and implement this DMP?

The PI (Tatjana N. Parac-Vogt), or a delegated researcher working on the project in her group.