The path to to chemically recyclable polymers: catalytic synthesis of 1,3-dioxacycloalkanes and their controlled polymerization to high MW polymers

A Data Management Plan created using DMPonline.be

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Project abstract:

The transition from a linear economy to a fully circular, closed loop economy goes along two tracks. First, for existing materials, improved recycling techniques are desired; but most current polymer types are hard to recycle to identical chemical building blocks. The alternative is to develop materials that are designed to be easily chemically recycled to their original monomers ('CRM'). In this PhD, the focus is on such a class of polymers, viz. polyacetals formed from the ring-opening polymerization of 1,3-dioxacycloalkanes, such as 1,3-dioxolane. First, we address the high yield preparation of the monomers from alpha,omega-diols and formaldehyde, using hydrophobic zeolites as the preferred catalysts. Next, solid catalysts are identified for the conversion of 1,3-dioxacycloalkanes to high molecular weight polyacetals, either via ring-opening polymerization (ROP) on Lewis acid sites, or via cationic ROP (CROP). The major asset of the solid catalysts is that they are easy to remove from the product, which impedes spontaneous depolymerization of the material. Double metal cyanides and Lewis acid zeolites are earmarked as platforms to design polymerization catalysts; to understand the catalysts' action, they are thoroughly characterized, also in catalytic operation, e.g. via X-ray absorption spectroscopy. The physicochemical properties of the high MW polymers are briefly explored, as well as their controlled depolymerization to monomers on Brønsted acid solids.

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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)

Question not answered.

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)

Question not answered.

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)

Question not answered.

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)

Question not answered.

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

Question not answered.

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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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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
		Please choose from the following options: • Generate new data • Reuse existing data	*Please choose from the following options:* • Digital • Physical	*Please choose from the following options:* • Observational • Experimental • Compiled/aggregated data • Simulation data • Software • Other • NA	*Please choose from the following options:* • .por, .xml, .tab, .cvs,.pdf, .txt, .rtf, .dwg, .gml, … • NA	*Please choose from the following options:* • <100MB • <1GB • <100GB • <1TB • <5TB • <10TB • <50TB • >50TB • NA	
Experimental data	Raw datafiles containing material characerization data (NMR, UV-Vis, XRD, physisorption and chemisorption data etc.) Chromatographic data (GPC, GC, GC-MS etc.	Generate new data	Digital	Experimental	NMR data .csv .gcd .xrdml .SPA	< 1 MB < 1 MB < 2 MB 20 kB 150 kB	
Physical samples	Catalysts, reaction products	Generate new data	Physical				1000 reaction vials
Data processing	excel files, summaries, manuscripts and/or patents, presentations	Generate new data	Digital	Summarized experimental data	.xlsx .docx .pdf .pptx .cdxml	< 1 MB < 500 kB < 500 kB 1 MB < 500 kB	

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:

/

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.

- Yes

The methods and reactor configurations 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).

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).

Details to reproduce reaction procedures are described in a personal lab booklet. 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 (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.

- No

Although no metadata standard is available for the advanced characterization in this project, most techniques store a non-standardized ReadMe-file containing recording parameters and file information in parallel with recorded datasets. Alternatively, some datasets contain metadata headers on recording parameters (e.g. XRD diffractograms). The data will be stored and named in a consistent manner with unambiguous identifiers. Descriptions of experiments and materials are kept in physical lab notes for each identifier. The data will be processed and summarized in a comprehensive excel worksheet with references to the identifiers. The resulting summaries will culminate in presentations, and finally in manuscripts and/or patents.

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

Where will the data be stored?

Physical hand-notes of procedures and initial observations are kept in lab books. Digital data, with unambiguous identifiers for reactions and materials, are kept in cloud storage from ‘Box’. KU Leuven offers an Enterprise Box account 3, which offers an easy and secure storage space of up to 100 GB for each user.

How will the data be backed up?

By using the cloud storage of ‘Box’, digital data will be stored in parallel on the cloud and on the personal computer of the applicant, guaranteeing back-up for this data. Most raw data is also stored and frequently backed up off-line on external hard drives.

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

The cloud storage provides a storage space up to 100 GB for each user, while the project is expected to generate less than 10 GB.

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. An Enterprise Box account 3 for cloud storage ensures a secure environment.

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

Data storage costs on Box 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.

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 retained for the expected 5 year period after the end of the project with exception of physical lab sampls.. Physical lab samples will be stored for 2 years or until a manuscript is peer-reviewed and published. This storage time is limited due to physical storage limitations regarding space and safety as well as the possibility of the chemical composition to change over time, yielding the samples unreliable.

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

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.

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.

- Other, please specify:

General data and summaries (explained under "Data processing" in part 1) will be made available through means of 'Supplementary Information' accompanying a publication. Extra data such as chromatograms or specific spectral data can be made available upon request by email.

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 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.

General data and summaries will be made available through means of 'Supplementary Information' accompanying a publication. Extra data such as chromatograms or specific spectral data can be made available upon request by email.

When will the data be made available?

Upon publication of the research results.

Which data usage licenses are you going to provide? If none, please explain why.

CC-BY-NC-SA-4.0

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.

- 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 Box. If additional costs would occur they will be covered from reserve funds.

6. Responsibilities

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

Margot Houbrechts (applicant)

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

The applicant (Margot Houbrechts), her supervisor (Dirk De Vos) and Annelies Van Vlasselaer.

Who will manage data preservation and sharing?

The supervisor (Dirk De Vos) and Annelies Van Vlasselaer.

Who will update and implement this DMP?

Margot Houbrechts (applicant)