

FWO DMP Template - Flemish Standard Data Management Plan

Project supervisors (from application round 2018 onwards) and fellows (from application round 2020 onwards) will, upon being awarded their project or fellowship, be invited to develop their answers to the data management related questions into a DMP. The FWO expects a **completed DMP no later than 6 months after the official start date** of the project or fellowship. The DMP should not be submitted to FWO but to the research co-ordination office of the host institute; FWO may request the DMP in a random check.

At the end of the project, the **final version of the DMP** has to be added to the final report of the project; this should be submitted to FWO by the supervisor-spokesperson through FWO's e-portal. This DMP may of course have been updated since its first version. The DMP is an element in the final evaluation of the project by the relevant expert panel. Both the DMP submitted within the first 6 months after the start date and the final DMP may use this template.

The DMP template used by the Research Foundation Flanders (FWO) corresponds with the Flemish Standard Data Management Plan. This Flemish Standard DMP was developed by the Flemish Research Data Network (FRDN) Task Force DMP which comprises representatives of all Flemish funders and research institutions. This is a standardized DMP template based on the previous FWO template that contains the core requirements for data management planning. To increase understanding and facilitate completion of the DMP, a standardized **glossary** of definitions and abbreviations is available via the following [link](#).

1. General Project Information

Name Grant Holder & ORCID	Ibrahim Khalil 0000-0003-0263-1079
Contributor name(s) (+ ORCID) & roles	
Project number ¹ & title	12A3M24N <i>“Novel IR spectroscopy methods for surface and diffusion characterization of small-pore zeolites using transient probe adsorption”</i>
Funder(s) GrantID ²	FWO 12A3M24N
Affiliation(s)	<input checked="" type="checkbox"/> KU Leuven <input type="checkbox"/> Universiteit Antwerpen <input type="checkbox"/> Universiteit Gent <input type="checkbox"/> Universiteit Hasselt <input type="checkbox"/> Vrije Universiteit Brussel <input type="checkbox"/> Other: Provide ROR ³ identifier when possible:
Please provide a short project description	<p>The interest in the production of platform chemicals such as light olefins by using atmospheric carbon dioxide (CO₂) is growing. Both commercial and academic interest is estimated to take off even more in coming years. This is directly related to the application of light olefins as starting materials for the synthesis of value-added chemicals such as polymers. The tandem one-pot CO₂ conversion to light olefins via the methanol route has been reported as a cost-effective and efficient way. It uses metal oxide catalysts for the CO₂-to-methanol and majorly small-pore zeolites (SPZ) for the methanol-to-olefins. However, challenges such as the development of stable SPZ catalysts still consist of a barrier to the tandem process. Understanding the reactivity of the acid sites in SPZ during the methanol adsorption and activation is essential yet not well established. The lack of analysis of these materials is mainly due to the lack of characterization methods adapted to probe the confined acidity in the small pores of these zeolites. This project tackles this issue by delivering in-depth analysis methods based on the adsorption of organic probes (alcohols and amines) followed by FT-IR spectroscopy. Monitoring the adsorption profiles, the interaction energies, and the diffusion kinetics of the probes with the surface of the zeolite will be keys to understanding the distribution of the acid sites inside the SPZ framework.</p>

¹ “Project number” refers to the institutional project number. This question is optional since not every institution has an internal project number different from the GrantID. Applicants can only provide one project number.

² Funder(s) GrantID refers to the number of the DMP at the funder(s), here one can specify multiple GrantIDs if multiple funding sources were used.

³ Research Organization Registry Community. <https://ror.org/>

2. Research Data Summary

The project aims to develop an FT-IR characterization method that allows analysis of the surface acidity of small-pore zeolites (SPZ) in order to correlate this parameter with catalytic activity. The selected application for the studied SPZ is the CO₂ to olefins. So far, an FT-IR cell to allow studying the catalysts has been successfully installed by optimizing some of the parameters of the existing IR tool (high sensitivity detector, addition of a line allowing the use of liquid probe molecules). A series of SPZ (CHA with Si/Al = 40 and AEI with Si/Al = 15-25) were prepared and tested in the FT-IR setup, where the adsorption of methanol (our first benchmark probe) was performed. The activity of these zeolites was tested in the CO₂-to-olefins in a parallel research project (colleagues from the Dusselier lab) and a comparison between the adsorption affinity of methanol and the reactivity of this latter were made. The steaming of the tested zeolites was also performed under several temperatures (650, 700, and 750°C → giving a total of 9 new materials) and the new obtained materials were also measured with methanol adsorption and progressive thermal desorption measurements. The evolution of the surface acidity was followed with the analysis of the OH zone (3800-3200 cm⁻¹) in the FT-IR spectra to reveal the effect of the steaming and depict the formation of new acidic sites on the surface.

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 data⁴.

Dataset Name	Description	New or Reused	Digital or Physical	ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR DIGITAL DATA	ONLY FOR PHYSICAL DATA
				Digital Data Type	Digital Data Format	Digital Data Volume (MB, GB, TB)	Physical Volume
Excel sheet	Qualitative data reporting the FT-IR spectra obtained for the different tested zeolites. The raw data is obtained from the analysis software (OMNIC). The raw data is saved as is and	<input type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data	<input checked="" type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input type="checkbox"/> .csv <input type="checkbox"/> .pdf <input type="checkbox"/> .txt	<input checked="" type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB	

⁴ Add rows for each dataset you want to describe.

	also converted to an excel file.			<input checked="" type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .rtf <input type="checkbox"/> .dwg <input type="checkbox"/> .tab <input type="checkbox"/> .gml <input checked="" type="checkbox"/> other: .xls <input type="checkbox"/> NA	<input type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
Descriptive notes for the measurements	Qualitative notes summarizing the properties of the studied zeolites (topology, Si/Al, activation conditions, steaming conditions, dimension of the analyzed samples).	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input checked="" type="checkbox"/> .pdf <input checked="" type="checkbox"/> other: .doc	<input checked="" type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
Source images	Images and Figures (print screen of plotted Figures) for the analyzed spectral zone from FT-IR spectroscopy data.	<input type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input type="checkbox"/> Digital <input type="checkbox"/> Physical	<input checked="" type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation data <input type="checkbox"/> Software <input type="checkbox"/> Other <input type="checkbox"/> NA	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input checked="" type="checkbox"/> .pdf <input type="checkbox"/> .tab <input checked="" type="checkbox"/> other: .jpg	<input type="checkbox"/> < 100 MB <input checked="" type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input type="checkbox"/> < 5 TB <input type="checkbox"/> < 10 TB <input type="checkbox"/> < 50 TB <input type="checkbox"/> > 50 TB <input type="checkbox"/> NA	
Calculation spreadsheet	Calculation reporting the results from the catalytic data (conversion, yield, selectivity, carbon balance, ...)	<input checked="" type="checkbox"/> Generate new data <input type="checkbox"/> Reuse existing data	<input checked="" type="checkbox"/> Digital <input type="checkbox"/> Physical	<input type="checkbox"/> Observational <input type="checkbox"/> Experimental <input checked="" type="checkbox"/> Compiled/aggregated data <input type="checkbox"/> Simulation	<input type="checkbox"/> .por <input type="checkbox"/> .xml <input type="checkbox"/> .tab <input type="checkbox"/> .csv <input type="checkbox"/> .pdf	<input checked="" type="checkbox"/> < 100 MB <input type="checkbox"/> < 1 GB <input type="checkbox"/> < 100 GB <input type="checkbox"/> < 1 TB <input type="checkbox"/> < 5 TB	

<p><i>GUIDANCE:</i></p> <p><i>DATA CAN BE DIGITAL OR PHYSICAL (FOR EXAMPLE BIOBANK, BIOLOGICAL SAMPLES, ...). DATA TYPE: DATA ARE OFTEN GROUPED BY TYPE (OBSERVATIONAL, EXPERIMENTAL ETC.), FORMAT AND/OR COLLECTION/GENERATION METHOD.</i></p> <p><i>EXAMPLES OF DATA TYPES: OBSERVATIONAL (E.G. SURVEY RESULTS, SENSOR READINGS, SENSORY OBSERVATIONS); EXPERIMENTAL (E.G. MICROSCOPY, SPECTROSCOPY, CHROMATOGRAMS, GENE SEQUENCES); COMPILED/AGGREGATED DATA⁵ (E.G. TEXT & DATA MINING, DERIVED VARIABLES, 3D MODELLING); SIMULATION DATA (E.G. CLIMATE MODELS); SOFTWARE, ETC.</i></p> <p><i>EXAMPLES OF DATA FORMATS: TABULAR DATA (.POR,. SPSS, STRUCTURED TEXT OR MARK-UP FILE XML, .TAB, .CSV), TEXTUAL DATA (.RTF, .XML, .TXT), GEOSPATIAL DATA (.DWG,. GML, ..), IMAGE DATA, AUDIO DATA, VIDEO DATA, DOCUMENTATION & COMPUTATIONAL SCRIPT.</i></p> <p><i>DIGITAL DATA VOLUME: PLEASE ESTIMATE THE UPPER LIMIT OF THE VOLUME OF THE DATA PER DATASET OR DATA TYPE.</i></p> <p><i>PHYSICAL VOLUME: PLEASE ESTIMATE THE PHYSICAL VOLUME OF THE RESEARCH MATERIALS (FOR EXAMPLE THE NUMBER OF RELEVANT BIOLOGICAL SAMPLES THAT NEED TO BE STORED AND PRESERVED DURING THE PROJECT AND/OR AFTER).</i></p>	
<p>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.</p>	<p>I am not reusing existing data.</p>
<p>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, please describe these issues further and refer to specific datasets or data types when appropriate.</p>	<p> <input type="checkbox"/> Yes, human subject data <input type="checkbox"/> Yes, animal data <input type="checkbox"/> Yes, dual use <input checked="" type="checkbox"/> No If yes, please describe: </p>

⁵ These data are generated by combining multiple existing datasets.

<p>Will you process personal data⁶? If so, briefly describe the kind of personal data you will use. Please refer to specific datasets or data types when appropriate. If available, add the reference to your file in your host institution's privacy register.</p>	<p><input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes:</p> <ul style="list-style-type: none"> - Short description of the kind of personal data that will be used: - Privacy Registry Reference:
<p>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.</p>	<p><input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes, please comment:</p>
<p>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 to what data they relate and what restrictions are in place.</p>	<p><input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes, please explain:</p>
<p>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 to what data they relate and which restrictions will be asserted.</p>	<p><input type="checkbox"/> Yes <input checked="" type="checkbox"/> No If yes, please explain:</p>

⁶ See Glossary Flemish Standard Data Management Plan

3. 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).

The collected data will be organized in a set of themed documents and folders. A README.txt file explaining the characteristics of the measurements will be available in each of the folders where these documents are stored. The titles of the files and documents will be labelled using a consistent code that can express the content of the file (codes are defined between me and my promotor); this will ensure the understandability and usability of the data by my colleagues.

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.

REPOSITORIES COULD ASK TO DELIVER METADATA IN A CERTAIN FORMAT, WITH SPECIFIED ONTOLOGIES AND VOCABULARIES, I.E. STANDARD LISTS WITH UNIQUE IDENTIFIERS.

☐ Yes

☒ No

If yes, please specify (where appropriate per dataset or data type) which metadata standard will be used:

4. Data Storage & Back-up during the Research Project

<p>Where will the data be stored?</p>	<p>The primary storage location for the data will be the researcher's personal laptop computer managed by SET-IT (local KU Leuven IT department). This pc is backed up via KU Leuven on a Personal Network Drive. A shared one-drive folder between me and my promotor will be used to store the data with automatic updates that will ensure their direct availability.</p> <p>The physical powder samples will be labelled and stored on a personal shelf in a laboratory cabinet meant for powder samples and will be accessible by the researcher and the promotor. An Excel sheet containing the description of the powder samples will be created and filled constantly and stored on the Shared one-drive folder.</p>
<p>How will the data be backed up?</p> <p><i>WHAT STORAGE AND BACKUP PROCEDURES WILL BE IN PLACE TO PREVENT DATA LOSS? DESCRIBE THE LOCATIONS, STORAGE MEDIA AND PROCEDURES THAT WILL BE USED FOR STORING AND BACKING UP DIGITAL AND NON-DIGITAL DATA DURING RESEARCH.⁷</i></p> <p><i>REFER TO INSTITUTION-SPECIFIC POLICIES REGARDING BACKUP PROCEDURES WHEN APPROPRIATE.</i></p>	<p>Project data will be backed up to the Personal KU Leuven Network Drive account. Data will also be backed up on the researcher's personal external hard-drive on a monthly basis.</p>
<p>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.</p>	<p><input checked="" type="checkbox"/> Yes <input type="checkbox"/> No</p> <p>If yes, please specify concisely: I estimated the data from this project to not exceed the 50 Gb.</p> <p>If no, please specify:</p>

⁷ Source: Ghent University Generic DMP Evaluation Rubric: <https://osf.io/2z5g3/>

<p>How will you ensure that the data are securely stored and not accessed or modified by unauthorized persons?</p> <p><i>CLEARLY DESCRIBE THE MEASURES (IN TERMS OF PHYSICAL SECURITY, NETWORK SECURITY, AND SECURITY OF COMPUTER SYSTEMS AND FILES) THAT WILL BE TAKEN TO ENSURE THAT STORED AND TRANSFERRED DATA ARE SAFE. ⁷</i></p>	<p>My personal laptop (where the data are first stored) is password and fingerprint-protected, which will help prevent the data from being misused. The external hard drive will be kept in a secure location in the office of my promotor.</p> <p>The KU Leuven OneDrive account is also password-protected and can be only accessed via KU Leuven Authenticator.</p>
<p>What are the expected costs for data storage and backup during the research project? How will these costs be covered?</p>	<p>No additional costs are required for data storage for this project.</p>

5. Data Preservation after the end of the Research Project

<p>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...).</p>	<p>All the stored data will be retained for at least 5 years after the research period. The data that are made available on the KU Leuven repository (RDR) will be preserved for at least 10 years.</p>
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Where will these data be archived (stored and curated for the long-term)?	Beyond the minimal storage period, the promotor can decide whether the retained data are worth keeping or not. Data referring to publications or ongoing projects are always maintained on the external drive and delivered to the newcomers.
What are the expected costs for data preservation during the expected retention period? How will these costs be covered?	The costs for buying an external drive has been already paid, no additional costs are needed.

6. Data Sharing and Reuse

<p>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.</p> <p><i>NOTE THAT 'AVAILABLE' DOES NOT NECESSARILY MEAN THAT THE DATA SET BECOMES OPENLY AVAILABLE, CONDITIONS FOR ACCESS AND USE MAY APPLY. AVAILABILITY IN THIS QUESTION THUS ENTAILS BOTH OPEN & RESTRICTED ACCESS. FOR MORE INFORMATION: HTTPS://WIKI.SURFNET.NL/DISPLAY/STANDARDS/INFO-EU-REPO/#INFOEU-REPO-ACCESSRIGHTS</i></p>	<p><input checked="" type="checkbox"/> Yes, in an Open Access repository</p> <p><input type="checkbox"/> Yes, in a restricted access repository (after approval, institutional access only, ...)</p> <p><input type="checkbox"/> No (closed access)</p> <p><input type="checkbox"/> Other, please specify:</p>
<p>If access is restricted, please specify who will be able to access the data and under what conditions.</p>	
<p>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.</p>	<p><input type="checkbox"/> Yes, privacy aspects</p> <p><input type="checkbox"/> Yes, intellectual property rights</p> <p><input type="checkbox"/> Yes, ethical aspects</p> <p><input type="checkbox"/> Yes, aspects of dual use</p> <p><input type="checkbox"/> Yes, other</p> <p><input checked="" type="checkbox"/> No</p> <p>If yes, please specify:</p>
<p>Where will the data be made available? If already known, please provide a repository per dataset or data type.</p>	<p>The KU Leuven institutional repository (RDR) can be used for data sharing.</p>

<p>When will the data be made available?</p> <p><i>THIS COULD BE A SPECIFIC DATE (DD/MM/YYYY) OR AN INDICATION SUCH AS 'UPON PUBLICATION OF RESEARCH RESULTS'.</i></p>	<p>Upon publication of research results, or by the end of the research period (whichever happens sooner).</p>
<p>Which data usage licenses are you going to provide? If none, please explain why.</p> <p><i>A DATA USAGE LICENSE INDICATES WHETHER THE DATA CAN BE REUSED OR NOT AND UNDER WHAT CONDITIONS. IF NO LICENCE IS GRANTED, THE DATA ARE IN A GREY ZONE AND CANNOT BE LEGALLY REUSED. DO NOTE THAT YOU MAY ONLY RELEASE DATA UNDER A LICENCE CHOSEN BY YOURSELF IF IT DOES NOT ALREADY FALL UNDER ANOTHER LICENCE THAT MIGHT PROHIBIT THAT.</i></p> <p><i>EXAMPLE ANSWER: E.G. "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." ⁸</i></p>	<p>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 (the researcher).</p>
<p>Do you intend to add a PID/DOI/accession number to your dataset(s)? If already available, please provide it here.</p> <p><i>INDICATE WHETHER YOU INTEND TO ADD A PERSISTENT AND UNIQUE IDENTIFIER IN ORDER TO IDENTIFY AND RETRIEVE THE DATA.</i></p>	<p><input checked="" type="checkbox"/> Yes <input type="checkbox"/> No If yes: Not yet available, but a published dataset in KU Leuven RDR gets its own DOI and is registered in Lirias.</p>
<p>What are the expected costs for data sharing? How will these costs be covered?</p>	<p>Costs for sharing the data during the retention period will be covered by the researcher's FWO bench fee.</p>

⁸ Source: Ghent University Generic DMP Evaluation Rubric: <https://osf.io/2z5g3/>

7. Responsibilities

Who will manage data documentation and metadata during the research project?	Ibrahim Khalil (the researcher)
Who will manage data storage and backup during the research project?	Ibrahim Khalil (the researcher)
Who will manage data preservation and sharing?	Ibrahim Khalil (the researcher)
Who will update and implement this DMP?	Ibrahim Khalil (the researcher)