
Rational Design and Synthesis of New ABC-6 Family Zeolites

A Data Management Plan created using DMPonline.be

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Project abstract:

Successful industrial uses of synthetic versions of chabazite (CHA), such as a catalyst for the methanol-to-olefins reaction (SAPO-34) and as a catalyst support for the selective catalytic reduction of NO_x with NH₃ (Cu-SSZ-13), reveal that the discovery of new zeolites and molecular sieves is valuable for advancing catalytic applications. The CHA topology is one of the framework types in the ABC-6 family, which is built by stacking of 6-ring layers in a different sequence along the c-axis. Despite high applicability and the chemical feasibility of 84292 ABC-6 structures, only 28 natural and synthetic ABC-6 molecular sieves have been reported so far. Here, we aim to design and execution of rational synthetic strategies for novel ABC-6 family zeolites. Our main synthetic strategies for new ABC-6 zeolites can be explained by the memory effect of 6-ring units for 6-ring layers and the synergistic effect of OSDAs for large cages. Based on these 2 concepts, understanding the mechanisms and driving forces is expected to provide insight into new tailored synthetic strategies for desired zeolites and fundamentally advance the generic understanding of zeolite (formation) chemistry. We will also evaluate the potential of best obtained zeolites as CO₂ adsorbents and catalysts.

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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 | |
| Catalyst | Solid powder | New | Physical | | | | >100g |
| Microscopy | Microscopy | New | Digital | Experimental | .jpeg, .tif | <100MB | |
| Spectroscopy | IR; TPD; TGA; NMR ... | New | Digital | Experimental | .spg, .csv | <100MB | |
| Diffraction patterns | XRD | New | Digital | Experimental | .raw | <100MB | |
| Manuscripts/presentations | Textual data | New | Digital | Observational | docx, .pptx, .pdf | <100MB | |
| Plotting worksheets | Worksheets | New | Digital | Observational | .xls, .pptx | <100MB | |

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:

Not applicable

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).

- Catalysts will be stored in accordance to safety standards. Labels will be added with inambiguous conection to an electronic list (i.e. an electronic lab notebook in .xls). The methodology and protocol during handling of the catalysts will be take from reported procedures as much as possible and/or described in details in a lab book.
- Microscopy images (.jpeg) will be noted as: sample code_conditions. A standard operation procedure (SOP) is used if possible. The methodology and protocol will be described in details in the lab book.
- X-ray diffraction patterns (.raw) will be noted as: sample code_conditions. A standard operation procedure (SOP) is used. The protocol of the sample preparation will be described in the lab book.
- IR spectra (.spg) will be noted as: sample code_conditions. A standard operation procedure (SOP) is used if possible. The analysis method and the sample preparation will be described in the lab book.
- NMR data (.zip folder) will be noted as: sample code_conditions. A standard operation procedure (SOP) is used if possible. The protocol of the sample preparation will be described in the lab book.
- Manuscripts/presentations - content related to dissemination (.docx, .pptx, .pdf), and will be noted as: title_year.
- Worksheets for basic calculations and making visualizations/plots (.xls)

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

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

Where will the data be stored?

All data during this project will be stored on the shared cloud (OneDrive).

How will the data be backed up?

The backup of the data during this project will be automatically done on the shared cloud (OneDrive). For extra security, the publishable data will be collected in a separate folder and also backed-up on an individual external device.

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

Maximum data storage should not exceed 500 GB.

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

The accesses to the OneDrive and sharepoint are only for researchers with permission. All users need to use an Authenticator (2FA app used at KUL). Furthermore, a log-out is always performed when leaving LAB PCs (where data is generated) to prevent modification of parameters by unauthorized persons.

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

With the project funding, an external offline hard drive will be purchased for offline storage.

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...).

Due to the estimated small size of the data, all the extracted data can be retained for the expected 5 year period after the end of the project.

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

After the project, key data (especially the 'publishable data' folder) will be stored on KU Leuven Drive with backup on an external hard drive (1TB) with the promotor.

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

The estimated cost of the external hard drive (1TB) is around 50-100euro.

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

All digital data will be made available.

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

With the approval of the PI (prof. Michiel Dusselier), all group members can access the data.

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.

Via RDR, the KU Leuven institutional repository.

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.

No data under licenses

Do you intend to add a PID/DOL/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?

RDR is free for KU Leuven personnel, hence, no costs are expected for data sharing

6. Responsibilities

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

Juna Bae

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

Juna Bae

Who will manage data preservation and sharing?

prof. Michiel Dusselier (PI)

Who will update and implement this DMP?

Juna Bae