



A Magneto-Electric Liquid - better sensing

Research and Innovation Action GA 899285

Deliverable D6.1 – Data Management Plan (update M12)

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Editor	F. Clemente (PRE)
Author(s)	A. Morandi (PRE), with contributions from all partners
Abstract	This document presents the Data Management Plan, developed in the framework of the Open Research Data Pilot in Horizon 2020.



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1 Summary

The MAGNELIQ project participates in the Open Research Data Pilot in Horizon 2020. The pilot aims to improve and maximise access to and re-use of research data generated by Horizon 2020 projects, taking into account:

- the need to balance openness and protection of scientific information;
- commercialisation and IPR;
- privacy concerns;
- security;
- data management and preservation questions.

The Open Research Data Pilot applies primarily to the data needed to validate the results presented in scientific publications.

A first draft of the Data Management Plan (DMP) is provided in this Deliverable. This defines which and how data generated during the project will be made publicly available. In particular, this details what data the project will generate, whether and how it will be exploited or made accessible for verification and re-use, and how it will be curated and preserved.

Specifically, at the current status of the project, partners were able to identify 10 datasets:

- Magnetic properties of hybrid materials
- Infrared spectroscopy of new hybrid materials
- Thermogravimetric analysis of new hybrid materials
- Organic ligands for hybridization of magnetic nanoplatelets
- Characterisation of organic ligands
- Studies of ligand's mesogenic properties
- Barium Hexaferrite surface properties
- Magnetic and electric dipole-dipole interactions for a-spherical particles
- Contactless magneto-optic rotation sensor characterisation
- All-optical external-field sensor characterisation

Given the heterogeneity of the data processed, it was considered preferable to treat each dataset separately, reporting, for each one, details about:

- Data set description
- Standards and metadata
- Data sharing
- Archiving and preservation (including storage and backup)

This DMP is not to be intended as a fixed document; it will evolve and gain more precision and substance during the lifespan of the project. This first version will be updated during mid-term and final reviews to fine-tune it to the data generated and the uses identified by the project consortium.

2 MAGNELIQ's Datasets

The following paragraphs summarize the contributions from all partners about the 10 datasets identified so far.

2.1 Magnetic properties of hybrid materials

2.1.1 Data set description

The data will consist of:

- magnetization vs. applied field curves measured at room temperature;
- saturation magnetization values.

The data could be useful to:

- scientists interested in modelling of such materials;
- scientists interested in the development of new magnetic materials.

2.1.2 Standards and metadata

The data will be collected following conventional procedure for the magnetic properties measurements using a vibrating sample magnetometer (VSM). This means:

- Test specimens of specific size and shape;
- Range of the applied magnetic field from -1T to $+1\text{T}$;
- Data stored in ASCII format with data and header including all necessary information about the data and measurement protocol.

2.1.3 Data sharing

The data set and the associated document will be made available to any researcher interested in the topic mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 20.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.1.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc. Examples of possible servers are:

- the storage system offered by Nature Scientific Data (this would be free of charge);
- servers of the Digital Repository of Research Organizations of Slovenia (DiRROS), accessible here: <http://dirros.openscience.si/info/index.php/slo/uvodnik>;
- Open Access platform like <https://zenodo.org/>.

2.2 Infrared spectroscopy of new hybrid materials

2.2.1 Data set description

The data will consist of:

- Fourier-transformed infrared (FTIR) spectra.

The data could be useful to:

- scientists interested in modelling of such materials;
- scientists interested in the development of new hybrid materials.

2.2.2 Standards and metadata

The data will be collected following conventional procedure with IR spectrometer. This means:

- Samples in powder form;
- Spectral range 500–3500 cm^{-1} ;
- Data stored in ASCII format and a header including all necessary information about the data and measurement protocol.

2.2.3 Data sharing

The data set and the associated document will be made available to any researcher interested in the topics mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 24.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.2.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc. Examples of possible servers are:

- the storage system offered by Nature Scientific Data (this would be free of charge);
- servers of the Digital Repository of Research Organizations of Slovenia (DIRROS), accessible here: <http://dirros.openscience.si/info/index.php/slo/uvodnik>;
- Open Access platform like <https://zenodo.org/>.

2.3 Thermogravimetric analysis of new hybrid materials

2.3.1 Data set description

The data will consist of:

- mass vs. temperature data.

The data could be useful to:

- scientists interested in modelling of such materials;
- scientists interested in the development of new hybrid materials.

2.3.2 Standards and metadata

The data will be collected following conventional procedure with a thermal analyser. This means:

- Samples in powder form;
- Temperature range up to 1000 °C;
- Data stored in ASCII format and a header including all necessary information about the data and measurement protocol

2.3.3 Data sharing

The data set and the associated document will be made available to any researcher interested in the topics mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 24.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.3.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc. Examples of possible servers are:

- the storage system offered by Nature Scientific Data (this would be free of charge);
- servers of the Digital Repository of Research Organizations of Slovenia (DiRROS), accessible here: <http://dirros.openscience.si/info/index.php/slo/uvodnik>;
- Open Access platform like <https://zenodo.org/>.

2.4 Characterisation of organic ligands

2.4.1 Data set description

The data will consist of:

- Identification, chemical and physical characterisation of polar organic ligands and their intermediates
- Synthetic protocols for polar organic ligands and their intermediates

The data could be useful to:

- general organic materials researchers
- materials' scientists designing and synthesising ligands for nanoparticles

2.4.2 Standards and metadata

- Data will include outputs from: UV-Vis spectrometry (185 – 900 nm), ¹H-NMR and ¹³C-NMR spectrometry, mass spectrometry.
- Data stored in ASCII, FID (NMR) and graphical formats including measurement parameters.
- Standard synthetic protocols files: schemes of chemical synthesis will be prepared in ChemOffice (possible to transform to graphical format, for example TIFF)

2.4.3 Data sharing

The data will be made available to any researcher interested in the topic mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 20. Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.4.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long-lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc.

2.5 Studies of ligand's mesogenic properties

2.5.1 Data set description

The data will consist of:

- differential scanning calorimetry (DSC) thermographs and a table collecting mesophase behaviour, the phase transition temperatures and corresponding enthalpy changes (graphical set in TIFF format and table in MS Word or MS Excel data set)
- mesophase characterization will be in the form of microscopic picture (JPEG format)
- X-ray intensity profile documenting mesophase identification (TIFF format)

The data could be useful to:

- scientists working in community of condensed matter, namely in specialization to liquid crystals
- scientists interested in the development of new hybrid materials.

2.5.2 Standards and metadata

The data will be collected following conventional procedure with a DSC calorimeter, polarizing optical microscope equipped with a heating/cooling stage. This means:

- DSC data stored in ASCII format for the heating and cooling runs
- Images from optical microscope will be in JPEG format

2.5.3 Data sharing

The data set and the associated document will be available to any researcher interested in the topics mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 24.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.5.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc. Examples of possible servers are:

- the storage system offered by Nature Scientific Data (this would be free of charge);
- servers of the Digital Repository of Research Organizations of Slovenia (DiRROS), accessible here: <http://dirros.openscience.si/info/index.php/slo/uvodnik>;
- Open Access platform like <https://zenodo.org/>.

2.6 Barium Hexaferrite surface properties

2.6.1 Data set description

The data will consist of:

- Textual Quantum-ESPRESSO inputs and outputs

The data could be useful to:

- scientists interested in modelling of such materials;
- scientists interested in the development of new magnetic materials.
- The data grant un-biased reproducibility of the results.

2.6.2 Standards and metadata

The data provided will be compliant with standard numerical convergence, and will only include final converged inputs and outputs. This means:

- Data stored in ASCII format (textual) including all necessary information to reproduce the calculations (software version).

2.6.3 Data sharing

The data set and the associated document will be made available to any researcher interested in the topic mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 20.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.6.4 Archiving and preservation (including storage and backup)

The data will be shared as part of the supplementary information of the expected publication. Alternatively, the data could be stored in servers such as NOMAD or Materials Cloud.

2.7 Magnetic and electric dipole-dipole interactions for a-spherical particles

2.7.1 Data set description

The data will consist of:

- Routines in C to be included in LAMMPS molecular dynamics simulator

The data could be useful to:

- scientists interested in modelling magneto-electric a-spherical particles and liquids;
- scientists interested in the rational design of new magneto-electric liquids.

2.7.2 Standards and metadata

The routines will be written following the standards of C programming language and will be compliant with LAMMPS programming philosophy. This means:

- Data stored in ASCII format (textual format) and a header including all necessary information about the implemented equations and copyrights.

2.7.3 Data sharing

The routines will be included in LAMMPS distribution after a first publication will be secured by the consortium (tentatively by month 39). LAMMPS is a freely available opensource software. The copyright included in the header of each routine will explicitly mention MAGNELIQ (H2020, GA #899285). In addition, the header will also strongly encourage users to explicitly acknowledge MAGNELIQ and to cite the reference publication.

2.7.4 Archiving and preservation (including storage and backup)

The routines will be shared as part as the LAMMPS distribution through LAMMPS git.

2.8 Contactless magneto-optic rotation sensor characterisation

2.8.1 Data set description

The data will consist of:

- sensors fabrication data
- measurements of magnetic fluid spectral and other optical characteristics

The data could be useful to:

- scientists interested in fibre optic sensor fabrication.
- scientists interested in fibre optic sensor interrogation.

2.8.2 Standards and metadata

The data will be collected following sensor design, principle of operation typical characteristics.

This means:

- Sensor fabrication procedures and initial sensor characteristics (splicing routines, micromachining routines, SEM imaging, etc)
- Range of the applied magnetic field from -1T to $+1\text{T}$.
- Data stored in ASCII format encapsulated with the necessary metadata (algorithms, sampling frequencies, magnetic field strength, etc.) information about the measurement protocol.

2.8.3 Data sharing

The data set and the associated document will be made available to any researcher interested in the topics mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 36.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.8.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long-lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc. Examples of possible servers are:

- the storage system offered by Nature Scientific Data (this would be free of charge);
- servers of the Digital library of University of Maribor (DKUM), available at the following link: <https://dk.um.si/info/index.php/slo/>.

2.9 All-optical external-field sensor characterisation

2.9.1 Data set description

The data will consist of:

- measurements of magnitude and direction of external electrical and/or magnetic fields

The data could be useful to:

- scientists interested in development fibre optic sensors for contactless measurements of electrical and/or magnetic magnitudes

2.9.2 Standards and metadata

The data will be collected following sensor design, principle of operation typical characteristics.

This means:

- Temperature effects on the sensor
- Applied magnetic field magnitudes.
- Unambiguous rotation angle from 0° to 360° for a vector sensor design.
- Data stored in ASCII format encapsulated with the necessary metadata (algorithms, sampling frequencies, magnetic field strength, etc.) information about the measurement protocol.

2.9.3 Data sharing

The data set and the associated document will be made available to any researcher interested in the topics mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 48.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.9.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long-lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc. Examples of possible servers are:

- the storage system offered by Nature Scientific Data (this would be free of charge);
- servers of the Digital library of University of Maribor (DKUM), available at the following link: <https://dk.um.si/info/index.php/slo/>.

2.10 Mechanical characterisation of compliant materials

2.10.1 Data set description

The data will consist of:

- Stress-strain curves of elastomers with different shore

The data could be useful to:

- scientists interested in modelling/simulating such materials
- scientists interested in designing new devices based on such materials

2.10.2 Standards and metadata

The data will be collected following state of the art engineering methods. This means:

- Test specimens of specific size and shape according to ISO 37-2017_EU for tensile test and to ASTM D575-91-2001 for compression test;
- Test duration, temperature and velocity of moving grip as specified in ISO 37-2017_EU for tensile test and in ASTM D575-91-2001 for compression test.

2.10.3 Data sharing

The data set and the associated document will be made available to any researcher interested in the topics mentioned above. The data set will be shared after a first publication will be secured by the Consortium. Tentatively this should happen within month 40.

Any researcher interested in pursuing this must consent to give acknowledgement to this effort by explicitly mentioning MAGNELIQ (H2020, GA #899285).

2.10.4 Archiving and preservation (including storage and backup)

The data will be shared through a reputable and long-lasting server and linked by the MAGNELIQ website. The choice of the server will be linked to the size of the dataset, the publications (eventually) linked to it, etc. An example of possible servers is the open access platforms, like Zenodo (<https://zenodo.org/>).

3 Allocation of resources

Prensilia is the lead beneficiary of WP6, and collaborates with all beneficiaries for the dissemination and exploitation of the MAGNELIQ project results. Prensilia is also responsible for the development and update of this Data Management Plan and, during the first part of the project, collaborated with the other beneficiaries for the identification and description of the relevant datasets.

With specific reference to costs for FAIR data management, beneficiaries already included personnel resources for this activity in their budget at the proposal stage. Moreover, other costs have been allocated when drafting the project budget (i.e. communication & dissemination costs, depreciation costs for server blade devoted to data management and data repository), and adequate coverage will be eventually guaranteed for any additional cost currently not foreseen. During the periodic meetings, the consortium will evaluate the resource consumption associated to data management and its appropriateness.

4 Data security

The MAGNELIQ project uses trusted third-party service and server providers in order to securely store and transfer non-sensitive research data in the course of the project. For data management and exchange within the consortium, two systems could be used:

- The private area of the magneliq.eu website;
- Microsoft-based services shared folders.

These platforms are only accessible to authenticated users from organisations involved in the project as beneficiaries. The access rights are managed depending on the nature of the data and the involvement in the specific project activities of accessing subjects.

The details on how data will be stored in certified repositories for long term preservation and curation will be defined along the project's lifecycle.

5 Ethical aspects

MAGNELIQ's data management does not concern any major ethical aspect. However, partners could deal with the collection and storage of personal data of subjects who directly participate to the project activities: for this reason, the partners agreed (art. 10.8 of the MAGNELIQ Consortium Agreement) that any Confidential Information and/or any and all data and/or information that is provided to other parties shall not include Personal Data, as defined by Article 4 of the (EU) 2016/679. Accordingly, each partner endeavours to ensure that all data and information contained in Shared Information is anonymized and functionally separated, whenever possible, such that it is no longer Personal Data, prior to providing the Shared Information to the other party.

Generally, the MAGNELIQ beneficiaries are committed to respect the EU legal requirements on privacy and data protection (i.e. GDPR (EU) 2016/679) and to adhere to the ethics standards applicable to Horizon 2020 research. In accordance with the data minimisation, data retention and purpose limitation principle, personal data will not be collected beyond the scope of the processing objectives and will not be stored for longer than necessary.