Plan Overview

A Data Management Plan created using DMPTuuli

Title: Halogen bond donor complexes with molecular tubes

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Copyright information:

Halogen bond donor complexes with molecular tubes

1. General description of data

1.1 What kinds of data is your research based on? What data will be collected, produced or reused? What file formats will the data be in? Also give a rough estimate of the size of the data produced or collected?

In the project both qualitative and quantitative structural data about the investigated chemical systems will be collected. The data will be obtained by synthetic, analytical and computational methods. It contains a lot of chemical coordinates and tables, spectral data and computational listings. Most of the data will be in standard ASCII type text file formats (.txt, .ins, .res, .hkl, .cif., .xyz, etc.) and in standard graphical file formats (.gif, .jpg, .eps, .tif, .bmp, etc.). Also word processing (.doc, .docx, .rtf) and portable document file formats (.pdf, .png) will be used. The analytical instruments used in the research may produce raw data formats of their own type. The project will produce rather large amount of electronic data, which in total means approximately one terabyte (1 TB) scale. Old-fashioned hard copy data is not produced in the project.

1.2 How will the consistency and quality of data be controlled?

Different analytical instruments in chemical laboratories produce deviating type of data. Anyway, the modern instruments produce data, which is error-free and adequate quality for high resolution analytical research. Fortunately, we have computer software capable to read the different types of data and we can reliably compare the data. The consistency of the data will also be maintained by immediate backup copies of the fresh data before further processing and refining of it.
University of Jyväskylä provides GitLab version control environment for research projects, hosted on university server. This can be used to secure documentation, consistency and recoverability of changes to data files, even where multiple persons are involved in handling them in different stages of research.

2. Ethical and legal compliance

2.1 What ethical issues are related to your data management, for example, in handling sensitive data, protecting the identity of participants, or gaining consent for data sharing?

Research subject has no direct ethical issues regarding the research, research utilization, or
research promotion. The research does not include processing of personal or sensitive data. The project will also be conducted completely in accordance with the "Responsible conduct of research" rules by the Finnish Advisory Board on Research Integrity. All the personnel involved in the project will be treated equally in respect of their gender, sexuality, race, nationality or religion.

2.2 How will data ownership, copyright and IPR issues be managed? Are there any copyrights, licences or other restrictions that prevent you from using or sharing the data?

The research data will be owned by the Universities, who have created it. When participating in
the project, researchers are given the rights to use the data for research and teaching for the time when they are employed by the university. The results will be published in peer-reviewed international scientific journals and open access manner will be preferred, when it will be
available at everyone's disposal. The original research data will also be available from authors or databases after the publication of results. Parallel open access publication in JyX database will be pursued when compatible with journals´ policies. Also, all authors contributing to this project will be credited in publications.

3. Documentation and metadata

3.1 How will you document your data to make them findable, accessible, interoperable and reusable for you and others? What kinds of metadata standards, README files or other documentation will you use to help others understand and use your data?

Data in ASCII type text file formats can be read by common word processing programs (e.g., Notepad or MS Word). The graphical data file formats can be opened with standard computer graphics programs (e.g., GIMP). The original raw data from the instruments are stored as such in the formats provided by the interface manufacturers of the instruments. Anyway, this raw data is usually converted to text or graphics files during the data processing and these files can be further delivered and saved. The data saved and obtained from databases can be accessed and used by the database interface, which shows the adequate documentation for it. If the data is obtained from PI or the researchers in the project, they will give the documentation as a textual form to the recipient. PI is responsible for all data produced in the project and also for monitoring and sufficient documentation of it.

4. Storage and backup during the research project

4.1 Where will your data be stored, and how will they be backed up?

Research data of the project will always be stored in a network drive provided and managed by IT-services of University of Jyväskylä. These network drives are also used to share files safely between participants using VPN. Systems will take automatic backups of the data to prevent catastrophic loss of data. In addition manual backups of master data files will be taken monthly and always before any major file-format or data conversions.

4.2 Who will be responsible for controlling access to your data, and how will secured access be controlled?

Right to access the data is controlled by PI and technical access control is provided by IT-services of University of Jyväskylä. The data deposited to database is handled by the database organization.
Data will be available to all researchers of the project via shared network drive (accessed via VPN in case of external partners).

5. Opening, publishing and archiving the data after the research project

5.1 What part of the data can be made openly available or published? Where and when will the data, or their metadata, be made available?

The resulting research material and data from the project will be stored by the authors and after the publication procedures are finished the material and data will be obtained free of charge from the publisher (open access) or from authors. The crystallographic data will also be included in Cambridge Structural Database (CSD), from where it is obtained free of charge by request. Data will be also archived in JYX.

5.2 Where will data with long-term value be archived, and for how long?

University of Jyväskylä will store all data archived in JYX for minimum of 10 years, in the format originally deposited in, but does no special packaging or continuous curation to guarantee long-term integrity and usability. The crystallographic data will be stored forever in CSD. The publication data will be stored by the publishers of the journals.

6. Data management responsibilities and resources

6.1. Who will be responsible for specific tasks of data management during the research project life cycle? Estimate also the resources (e.g. financial, time and effort) required for data management.

The University of Jyväskylä and FinELib provide the data storage capabilities and there are no further costs for the project (or they are covered by overheads by an amount which is not known at the moment). There is no need for any external data management in the project. The responsibilities and specific tasks of data management are already mentioned above.

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