Plan Overview

A Data Management Plan created using DMPonline

Title: Ultrafast Photochemistry in Organic Aerosols

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Project abstract:

Much of the current discussion of the causes of global warming and mitigation of its impacts focuses on greenhouse gas emissions and net-zero CO2 targets. However, atmospheric aerosols also contribute significantly, and in ways that remain more poorly quantified, to the radiative balance that determines Earth’s climate. The PHAERO project addresses a major gap in our knowledge of the sunlight-driven photochemistry of organic aerosol particles in the lower atmosphere. For the first time, PHAERO will apply cutting-edge time-resolved spectroscopy and mass spectrometry methods to explore directly the photochemistry of organic compounds dissolved in aqueous aerosol droplets with picolitre volumes, and with femtosecond to microsecond time resolution. The chosen organic compounds represent chemical species proposed to be responsible for organic aerosol growth, as well as those present in brown-carbon aerosol particles formed by the burning of plants and trees, for example in wildfires and agricultural land clearance. This project is timely because of the increasing incidences worldwide of such fires and their associated emissions of particulate matter, as exemplified by poor air quality in many cities and major fires in Europe, north America and the Arctic. PHAERO will explore how the photochemical pathways of atmospherically important organic molecules are changed by confinement in micron-dimension aqueous aerosol droplets, for example through solute accumulation at the water-air interface, supersaturated concentrations in evaporating aerosols, and inhibited diffusion in viscous aerosol particles. The outcomes will advance our understanding of climate science and air quality. Applying the same methods to the photochemistry of droplets containing molecules of biological importance, the project will also provide new insights into the UV-induced degradation of the molecular components of pathogens in exhaled respiratory droplets by sunlight or germicidal UVC radiation.

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Ultrafast Photochemistry in Organic Aerosols

Data Summary

Will you re-use any existing data and what will you re-use it for?

No existing data will be re-used.

What types and formats of data will the project generate or re-use?

Data will be produced in the form of time-resolved spectra from an ultrafast laser spectroscopy experiment. The data will be produced in .csv file format.

What is the purpose of the data generation or re-use and its relation to the objectives of the project?

The generated data will be used to understand how molecular photochemistry in micron-scale water droplets differs from bulk aqueous solution and the gas phase. The data are required to deliver all the objectives of the proposal.

What is the expected size of the data that you intend to generate or re-use?

Each data file will be approximately 1 MB in size. One data file is expected per day of experimental work. Data will be stored on the 5 TB storage provided by the University of Bristol.

What is the origin/provenance of the data, either generated or re-used?

All the data will be generated in my research laboratory located in the School of Chemistry at the University of Bristol.

To whom might your data be useful ('data utility'), outside your project?

Data will be useful to physical chemists, theoretical chemists, atmospheric chemists, aerosol scientists, environmental scientists.

FAIR data

2.1. Making data findable, including provisions for metadata: Will data be identified by a persistent identifier?

Yes. We will publish data sets with a DOI that is reported in associated publications.

2.1. Making data findable, including provisions for metadata: Will rich metadata be provided to allow discovery? What metadata will be created? What disciplinary or general standards will be followed? In case metadata standards do not exist in your discipline, please outline what type of metadata will be created and how.

Yes. Metadata will include a readme file explaining the structure of data folders and the contents they contain. File names will use standard formats that contain useful metadata about experimental conditions. The publications generated using the data files will also serve as metadata, for example by explaining how the data were obtained.

2.1. Making data findable, including provisions for metadata: Will search keywords be provided in the metadata to optimize the possibility for discovery and then potential re-use?

Yes.

2.1. Making data findable, including provisions for metadata: Will metadata be offered in such a way that it can be harvested and indexed?

Yes.

2.2. Making data accessible - Repository: Will the data be deposited in a trusted repository?

Yes. We will use the University of Bristol's Research Data Storage Facility (RDSF).

2.2. Making data accessible - Repository: Have you explored appropriate arrangements with the identified repository where your data will be deposited?

Yes. We will publish data sets open access and with an associated DOI.

2.2. Making data accessible - Repository: Does the repository ensure that the data is assigned an identifier? Will the repository resolve the identifier to a digital object?

Yes.

2.2. Making data accessible - Data:
Will all data be made openly available? If certain datasets cannot be shared (or need to be shared under restricted access conditions), explain why, clearly separating legal and contractual reasons from intentional restrictions. Note that in multi-beneficiary projects it is also possible for specific beneficiaries to keep their data closed if opening their data goes against their legitimate interests or other constraints as per the Grant Agreement.

Yes. All data will be made openly available.

2.2. Making data accessible - Data:
If an embargo is applied to give time to publish or seek protection of the intellectual property (e.g. patents), specify why and how long this will apply, bearing in mind that research data should be made available as soon as possible.

No embargoes are expected after the data have been used for our analysis and publication purposes.

2.2. Making data accessible - Data:
Will the data be accessible through a free and standardized access protocol?

Yes.

2.2. Making data accessible - Data:
If there are restrictions on use, how will access be provided to the data, both during and after the end of the project?

There will be no restrictions on use.

2.2. Making data accessible - Data:
How will the identity of the person accessing the data be ascertained?

The University of Bristol's Research Data team will use their protocols.

2.2. Making data accessible - Data:

Is there a need for a data access committee (e.g. to evaluate/approve access requests to personal/sensitive data)?

No.

2.2. Making data accessible - Metadata:

Will metadata be made openly available and licenced under a public domain dedication CC0, as per the Grant Agreement? If not, please clarify why. Will metadata contain information to enable the user to access the data?

Yes.

2.2. Making data accessible - Metadata:

How long will the data remain available and findable? Will metadata be guaranteed to remain available after data is no longer available?

The data will be published open access so will be indefinitely available.

2.2. Making data accessible - Metadata:

Will documentation or reference about any software be needed to access or read the data be included? Will it be possible to include the relevant software (e.g. in open source code)?

No specialist software will be needed. Information about readily available software will be provided in the metadata readme files.

2.3. Making data interoperable:

What data and metadata vocabularies, standards, formats or methodologies will you follow to make your data interoperable to allow data exchange and re-use within and across disciplines? Will you follow community-endorsed interoperability best practices? Which ones?

We will make the data available as arrays of numerical data values in .csv format files.

2.3. Making data interoperable:

In case it is unavoidable that you use uncommon or generate project specific ontologies or vocabularies, will you provide mappings to more commonly used ontologies? Will you openly publish the generated ontologies or vocabularies to allow reusing, refining or extending them?

Not applicable.

2.3. Making data interoperable:

Will your data include qualified references[1] to other data (e.g. other data from your project, or datasets from previous research)?

[1] ***A qualified reference is a cross-reference that explains its intent. For example, X is regulator of Y is a much more qualified reference than X is associated with Y, or X see also Y. The goal therefore is to create as many meaningful links as possible between (meta)data resources to enrich the contextual knowledge about the data. (Source: https://www.go-fair.org/fair-principles/i3-metadata-include-qualified-references-metadata/)***

No.

2.4. Increase data re-use:

How will you provide documentation needed to validate data analysis and facilitate data re-use (e.g. readme files with information on methodology, codebooks, data cleaning, analyses, variable definitions, units of measurement, etc.)?

Readme files will explain how the data were generated. Our own methods for data analysis will be explained in our published papers. We provide software on our group website that can be used to process the data.

2.4. Increase data re-use:

Will your data be made freely available in the public domain to permit the widest re-use possible? Will your data be licensed using standard reuse licenses, in line with the obligations set out in the Grant Agreement?

Yes.

2.4. Increase data re-use:

Will the data produced in the project be useable by third parties, in particular after the end of the project?

Yes.

2.4. Increase data re-use:

Will the provenance of the data be thoroughly documented using the appropriate standards?

Yes.

2.4. Increase data re-use:

Describe all relevant data quality assurance processes.

We will process the data ourselves using our own tried-and-tested software packages and will publish the results of this analysis.

2.4. Increase data re-use:

Further to the FAIR principles, DMPs should also address research outputs other than data, and should carefully consider aspects related to the allocation of resources, data security and ethical aspects.

Data security will be managed by the University of Bristol's Research Data team. There are no ethical considerations.

Other research outputs

In addition to the management of data, beneficiaries should also consider and plan for the management of other research outputs that may be generated or re-used throughout their projects. Such outputs can be either digital (e.g. software, workflows, protocols, models, etc.) or physical (e.g. new materials, antibodies, reagents, samples, etc.).

No other outputs are currently expected.

Beneficiaries should consider which of the questions pertaining to FAIR data above, can apply to the management of other research outputs, and should strive to provide sufficient detail on how their research outputs will be managed and shared, or made available for re-use, in line with the FAIR principles.

Not applicable.

Allocation of resources

What will the costs be for making data or other research outputs FAIR in your project (e.g. direct and indirect costs related to storage, archiving, re-use, security, etc.) ?

The costs are covered by the awarded grant and the University of Bristol.

How will these be covered? Note that costs related to research data/output management are eligible as part of the Horizon Europe grant (if compliant with the Grant Agreement conditions)

The costs are covered by the awarded grant and the University of Bristol.

Who will be responsible for data management in your project?

Professor Andrew Orr-Ewing

How will long term preservation be ensured? Discuss the necessary resources to accomplish this (costs and potential value, who decides and how, what data will be kept and for how long)?

The data will be stored on the University of Bristol's Research Data Storage Facility and repository.

Data security

What provisions are or will be in place for data security (including data recovery as well as secure storage/archiving and transfer of sensitive data)?

The data will be backed up according to the University of Bristol's RDSF practices.

Ethics

Are there, or could there be, any ethics or legal issues that can have an impact on data sharing? These can also be discussed in the context of the ethics review. If relevant, include references to ethics deliverables and ethics chapter in the Description of the Action (DoA).

No.

Will informed consent for data sharing and long term preservation be included in questionnaires dealing with personal data?

Not applicable.

Other issues

Do you, or will you, make use of other national/funder/sectorial/departmental procedures for data management? If yes, which ones (please list and briefly describe them)?

No.