

Project¹ Number: [H2020-MSCA-RISE-2019-872081]

Project Acronym: [ATMOS]

Project title: [Pollutants and greenhouse gases in the atmosphere - understanding gas-gas and gas-solid interactions towards a cleaner atmosphere]

DATA MANAGEMENT PLAN

¹ The term ‘project’ equates to an ‘action’ in certain other Horizon 2020 documentation

1. Data Summary

a) Purpose of the data collection/generation and its relation to the objectives of the project

The main objectives of ATMOS are the characterization of molecular systems and processes concerning atmosphere pollution and the description and evaluation of solid systems suitable for pollutant capture. Data generation (physical and chemical properties) is the main objective of the project.

The following sorts of data are expected:

-Spectroscopic and structural properties and parameters, as well as, observed lines (Work package 1); local potential energy surfaces.

-Kinetic rates and thermodynamic properties of chemical processes; potential energy surfaces; excitation energies to the excited states involved in photo-dissociation processes (Work package 2).

-Collisional rates and cross sections of non-reactive processes in the gas phase; structural parameters of porous solids, adsorption energies, and sorption isotherms (Work package 3)

b) Types and formats of data will the project generate/collect

Basically, the project will generate scientific articles in peer reviewed international journals and Open Research Europe, conference proceedings, topical special issues, and grey literature (informally published written material not controlled by scientific publishers, e.g. reports). In addition, it will generate data for specialized databases.

c) Origin of the data

Own laboratory measurements and own computational work using standardized and non-standardized codes.

d) Expected size of the data

With few exceptions, the size is limited and data can be published and collected in tables of the reviewed international journals. Exceptions are the spectral lines and the descriptors of the potential energy surfaces which are submitted to the journals as supplementary material or, if it is applicable, to the databases.

e) Data utility

Generated data can be relevant for scientists involved in the field of pollution and atmospheric sciences specially who interpret observations with the large scale instruments for atmosphere measurements. Some data can be relevant for astrophysicists and for diverse chemical applications. It has to be considered that many pollutants are not produced in situ in the atmosphere but they are emitted due to the human activity and industries. ATMOS species have many applications.

f) Previous existing data; origin

In general, our research concerning molecules does not require previous data as inputs because the sources are our instruments and computers. However, if previously other scientists have provided available information, they will always be considered. Our publications will provide a complete list of references. These previous data were derived from the same sources that we will employ to publish our results (articles, databases, repositories) which are the usually tools for experts in our fields.

Exception are the crystallographic data employed to start the solid state studies. Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals are provided by the Crystallography Open Database (<http://www.crystallography.net/cod/>) or by The Cambridge Crystallographic Data Centre (CCDC) (<https://www.ccdc.cam.ac.uk/>).

2. FAIR data

ATMOS Grant Agreement commitments: according to the Article 29 of the signed Grant Agreement:

- a) The beneficiaries must as soon as possible and at the latest on publication, deposit a machine-readable electronic copy of the published version or final peer-reviewed manuscript accepted for publication in a repository for scientific publications;
- b) The beneficiaries must aim to deposit at the same time the research data needed to validate the results presented in the deposited scientific publications.
- c) The beneficiaries must ensure open access (free-of-charge online access for any user) to all peer-reviewed scientific publications relating to their results. They must ensure open access — via the repository — to the bibliographic metadata that identify the deposited publication.

H2020 includes the "green" path (repositories) and the "golden" path (publication in open access) as valid tools to facilitate open access *to peer-reviewed articles published* in serial or periodical publications. Beneficiaries must ensure that any scientific peer-reviewed publications can be read online, downloaded and printed.

2. 1. Making data findable, including provisions for metadata

The metadata standard used to describe the dataset will be the Dublin Core Schema, as it is a flexible and common used standard and is also the one adopted by the European OpenAIRE repository (https://guidelines.openaire.eu/en/latest/literature/use_of_oai_pmh.html)

Metadata-Keywords

The data produced by ATMOS project is identifiable and locatable with the following **metadata**,

- 1) **dc.relation:** info:eu-repo/grantAgreement/EC/H2020/872081
- 2) **dc.contributor.funder:** European Union & Horizon 2020
- 3) **the name and reference of the action:** ATMOS & 872081, **publication** data, and length of the **embargo** period.

and by means of the **Digital Object Identifiers, DOIs**, and **ORCID** numbers,

Examples of **KEYWORDS** to optimize possibilities for re-use are given in section 2.3.

Repositories, journals and databases

To make data accessible (**green open access**), **repositories of the European Commission (ZENODO) and of the European institutions** involved in ATMOS, will be used. Access to all of them is possible through the global registry of research data repositories (**www.re3data.org**) and the global organization to provided identifiers (**datacite.org**).

When open access is facilitated through editorial publishing (**golden open access**), or once the embargo periods will be finished (**green open access**), ATMOS researchers will provide a copy to an open access repository and to the ATMOS consortium web page.

Given the interdisciplinary character of ATMOS, peer reviewed international journals specialized in different research fields as well as Open Research Europe will be selected. Some of these journals are open access journals or they offer open access as a possible option. Embargo periods of 12 months are common, although the open access mandate comprises providing open access to the articles. The embargo must be shorter than 6/12 months.

In case of too long embargos imposed by the journals, the preprints of the publications and their supplementary material will be uploaded in the free distribution service and an open access **arXiv.org e-Print archive** (<https://arxiv.org/>). **Creative Commons** offers licensing solutions. The **EUDAT B2SHARE tool** includes a built-in license wizard that facilitates the selection of adequate license for research data.

Frequently journals employed by the ATMOS researchers are the following:

Physical chemistry: **Physical Chemistry Chemical Physics** (ISSN: 1463-9076), **Chemical Science**, (ISSN: 2041-6520, 2041-6539, full Open Access journal), **The Journal of Chemical Physics**, (ISSN: 0021-9606), **Journal of Physical Chemistry A**, (ISSN: 1089-5639). **Journal of Physical Chemistry C**, edited by the American Chemical Society (ISSN: 1932-7447); **Journal of Physics B: Atomic and Molecular Physics** (ISSN: 0022-3700); **Molecules MDPI** (ISSN 1420-3049, full Open Access journal)

Terrestrial Atmosphere-gas-phase environments: **Atmospheric Chemistry and Physics** (ISSN: 1680-7316); **ACS Earth and Space Chemistry**, (ISSN: 2472-3452); **Environmental Science: Atmospheres** (ISSN:) **Monthly Notices of the Royal Astronomical Society** (ISSN: 0035-8711); The astrophysical journal (ISSN: **0004-637X**); **The Astrophysical Journal Supplement** (ISSN 0067-0049); **Astronomy & Astrophysics** (ISSN: 0004-6361).

Spectroscopic and atmosphere databases: spectroscopic data and kinetic results will be sent to international databases optimize the re-use of data. Examples are:

- 1) **JPL** (Jet Propulsion Laboratory (<http://www.jpl.nasa.gov>))
- 2) **HITRAN** molecular spectroscopy database (<https://www.cfa.harvard.edu/hitran/>)
- 3) **MPI-Mainz UV/VIS Spectral Atlas** (http://satellite.mpic.de/spectral_atlas)
- 4) **CDMS** (Cologne Database for Molecular Spectroscopy; <https://www.astro.uni-koeln.de/cdms>),
- 5) **KIDA** (<http://kida.obs.u-bordeaux1.fr/>), **PNN** (<https://secure2.pnl.gov/nsd/nsd.nsf/Welcome>)
- 6) **GEISA** (<http://ara.abct.lmd.polytechnique.fr/index.php?page=geisa-2>).

Acknowledgments

In all the papers, the H2020 program will be acknowledged using the terms: “This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement **No 872081**”. Then, the **contributor under the name and reference of the action:** will be categorized in the journal web page and in the **Scopus** (<https://www.scopus.com>) and **WOS** (<https://www.webofscience.com>) digital sites.

2.2. Making data openly accessible

The project will generate scientific articles in peer reviewed international journals, data for specialized databases, and, conference proceedings, topical special issues, and grey literature (informally published written material not controlled by scientific publishers, e.g. reports).

H2020 includes the "green" path (repositories) as the "golden" (publication in open access) as valid to facilitate open access *to peer-reviewed articles published* in serial or periodical publications. In addition, it is important to note that even in cases where open access is facilitated through editorial publishing, affected researchers should provide a copy to an open access repository.

To make data accessible, on line repositories of the institutions involved in ATMOS, the European repository **ZENODO**, and the ATMOS web site (<http://tct1.iem.csic.es/ATMOS.htm>), will be used. The documents contained in the repositories of the institutions will be disseminated and collected in other national and international repositories and directories.

ZENODO is the open-access repository developed under the European **OpenAIRE** program (<https://www.openaire.eu/>). **OpenAire** is an initiative of the European Commission that indexes and develops value-added services on scientific information resulting from research activity in European Union countries, neighbouring countries and other regions of the world. OpenAire's main functions is to index the research results of projects funded by the European Commission under the Horizon2020 programme with three objectives: 1) increase the international visibility of science resulting from European collaboration; 2) monitor the degree of compliance with the Commission's open access policies; 3) exercise transparency towards European taxpayers.

OpenAire identifies and indexes the research work that results from thousands of H2020 projects, and indicates which results from H2020 projects for which the open access pilot mandate has been extended to all areas of research. For the systematic recovery and identification of these works through OpenAire, the European Commission marks a number of technical requirements that must be present in the open access repositories and magazines that are consulted by the aggregator.

Software tools will not be needed to access the data.

Institutional on line repositories:

DIGITAL.CSIC (<https://digital.csic.es/>) produced by the CSIC (coordinator institution of ATMOS), began in 2008. DIGITAL.CSIC publishes research data, assigns DOIs, assume journal requirements and compliance with funding agency policies. The Storage and description of datasets obey to standards. One of **DIGITAL.CSIC**'s priorities is to support compliance with the European Commission's open access policy. The DIGITAL.CSIC Technical Office has developed a strategy to facilitate compliance with the European Commission's open access policies through the repository path. Training and support resources for scientific, library and institutional technical staff around open access in general and the European mandate in particular, internal tools available to the CSIC library network for the easy identification and monitoring of mandate-affected H2020 projects, collaboration with the **CSIC European Programme Service and OpenAire's** scientific and technical team are factors that have contributed to the consolidation of the strategy.

This priority is articulated by different advisory services to researchers according to the technical requirements set by the European Commission and OpenAire for their correct indexing. As a result, DIGITAL.CSIC appears as one of the main sources contributing to H2020 project results.

On line repositories of the beneficiary institutions:

ARIAS MONTANO (<http://rabida.uhu.es/dspace/?locale-attribute=en>), which is the institutional repository of the University of Huelva. It is a repository of digital documents, whose aim is to publicize the scientific and teaching production of the University community, and ensure the preservation of their productions in digital format, as well as those institutions with which the University of Huelva has established agreements for this purpose.

THE OPEN ARCHIVE HAL (<https://hal.archives-ouvertes.fr/>) is the repository employed by French institutions involved in ATMOS (CNRS and ULCO). HAL is run by the Centre pour la communication scientifique directe, which is part of the French National Centre for Scientific Research, CNRS.

HYDRA (hydra.hull.ac.uk) is the repository of Hull University (<https://libguides.hull.ac.uk/openaccess>)

2.3. Making data interoperable

The use of the Dublin Core standard will ensure the interoperability of the data.

Metadata-Keywords

The data produced by ATMOS project is identifiable and locatable with the following **metadata**,

- 4) **dc.relation:** info:eu-repo/grantAgreement/EC/H2020/872081
- 5) **dc.contributor.funder:** European Union & Horizon 2020
- 6) **the name and reference of the action:** ATMOS & 872081, **publication** data, and length of the **embargo** period.

and by means the **Digital Object Identifiers**, DOIs, and **ORCID** numbers,

Examples of Keywords to optimize possibilities for re-use

WP1: AIR-POLLUTION; VOC; ASTROCHEMISTRY; AB-INITIO DETERMINATION; POTENTIAL-ENERGY SURFACES; FORCE FIELD; ANHARMONICITY; BASIS-SET; ROTATIONAL SPECTRUM; MICROWAVE-SPECTRUM; TORSIONAL SPECTRUM; WAVE; NON-RIGIDITY; ASSIGNMENT; CONFIGURATION-INTERACTION; ELECTRONIC-SPECTRA; HYPERFINE-STRUCTURE; RAMAN-SPECTRA; INTERNAL-ROTATION; INFRARED-SPECTRA; molecule/radical identifiers (the chemical formulae, IUPAC) or customary names identifiers (ACS, IUPAC)

WP2: AIR-POLLUTION; VOC; REVERSE RATE CONSTANTS; TRANSITION-STATE; EXCITED-STATES; AB-INITIO; POTENTIAL-ENERGY SURFACES; DISSOCIATION; DYNAMICS; PHOTODISSOCIATION; PHOTOCHEMISTRY; OZONE CREATION POTENTIALS; HYDROXYL RADICALS; RATE COEFFICIENTS; FINE-PARTICLE; EMISSIONS; COMBUSTION; ABSORPTION; KINETICS

WP3: AIR-POLLUTION; DFT; ABINITIO; CARBON-DIOXIDE; FORCE-FIELD; SELECTIVE CAPTURE; STABILITY; DYNAMICS; GAS; SIMULATIONS; MIXTURES; PSEUDOPOTENTIALS; PREDICTIONS; ADAPTED PERTURBATION-THEORY; HYBRID DENSITY FUNCTIONALS; SET MODEL CHEMISTRY; MOLECULAR-STRUCTURE; HYDROGEN-BONDS;

2.4. Increase data re-use (through clarifying licences)

When open access is facilitated through editorial publishing (**golden open access**), or once the embargo periods will be finished (**green open access**), ATMOS researchers will provide a copy to an open access repository and to the ATMOS consortium web page. In addition, scientific journals usually accept the distributions of pre-prints to institutional repositories before the end of the embargo period. Authors must read the open access information and policy of the different journals and repositories.

Given the interdisciplinary character of ATMOS, peer reviewed international journals specialized in different research fields as well as Open Research Europe will be selected. Some of these journals are open access journals or they offer open access as a possible option. Embargo periods of 12 months are common. However, the open access mandate comprises providing open access to the articles. The embargo must be shorter than 6/12 months. In addition, the preprints of the publications and their supplementary material will be uploaded in the free distribution service and an open access [arXiv.org](https://arxiv.org) e-Print archive.

arXiv (pronounced "archive") is an open-access repository of electronic preprints and postprints (known as **e-prints**) approved for posting after moderation, but not peer review. It consists of scientific papers in, which can be accessed online. In many fields of mathematics and physics, almost all scientific papers are self-archived on the arXiv repository before publication in a peer-reviewed journal. Some publishers also grant permission for authors to archive the peer-reviewed postprint. **arXiv** begun on 1991.

[Creative Commons](https://creativecommons.org/) offers licensing solutions. The [EUDAT B2SHARE tool](https://eudat.eu/) includes a built-in license wizard that facilitates the selection of adequate license for research data.

3. Allocation of resources

Open access to scientific publications is a general principle of H2020: on the one hand, eligibility of publication costs in open access and, on the other hand, embargoes permitted for the fulfilment of the mandate by the green way of the repositories.

The data publication by the ATMOS Partners is also supported by their own institutions.

4. Data security

We can expect that the data will be safely stored in certified repositories for long term preservation and curation because institutional repositories and Open Air will be used for this aim.

Zenodo (<https://zenodo.org/features>) have properly addressed this issue.

5. Ethical aspects

The project has no Ethics issues identified by the experts in the Ethics Summary Report.

6. Other issues

Open access mandates of the institutions involved in ATMOS can be found in the following links:

CSIC: [CSIC institutional open access mandate.pdf](#)

Huelva University: <http://rabida.uhu.es/dspace/handle/10272/10023>

CNRS: https://www.science-ouverte.cnrs.fr/wp-content/uploads/2021/04/Cnrs_Research-Data-Plan_mars21.pdf

Hull University: <https://hydra.hull.ac.uk/resources/hull:18307>;

ULCO University:

Wuppertal University: <https://www.bib.uni-wuppertal.de/de/open-access.html>

7. Further support in developing your DMP

The institutional repositories provide their own tools.

The Research Data Alliance provides a [Metadata Standards Directory](#) that can be searched for discipline-specific standards and associated tools.

Useful listings of repositories include: [Registry of Research Data Repositories](#)

[DMP online](#) and platforms for making individual scientific observations available such as [ScienceMatters](#).

SUMMARY TABLE 1

FAIR Data Management at a glance: issues to cover in your Horizon 2020 DMP

DMP component	Issues
1. Data summary	<p>State the purpose of the data collection/generation; relation to the objectives of the project: The main objectives of ATMOS are the characterization of molecular systems and processes concerning atmosphere pollution and the description and evaluation of solid systems suitable for pollutant capture. Data generation (physical and chemical properties) is the main objective of the project. The following sorts of data are expected: a) spectroscopic and structural properties and parameters, as well as, observed lines (Work package 1); local potential energy surfaces; b) kinetic rates and thermodynamic properties of chemical processes; potential energy surfaces; excitation energies to the excited states involved in photo-dissociation processes (Work package 2); c) collisional rates and cross sections of non-reactive processes in the gas phase; structural parameters of porous solids, adsorption energies, and sorption isotherms (Work package 3)</p> <p>Specify the types and formats of data generated/collected: Basically, the project will generate scientific articles in peer reviewed international journals and Open Research Europe, conference proceedings, topical special issues, and grey literature (informally published written material not controlled by scientific publishers, e.g. reports). In addition, it will generate data for specialized databases.</p> <p>Origin of the data: Own laboratory measurements and own computational work using standardized and non-standardized codes.</p> <p>Expected size of the data: With few exceptions, the size is limited and data can be published collected in tables of the reviewed international journals. Exceptions are the spectral lines and the descriptors of the potential energy surfaces which are submitted to the journals as supplementary material or, if it is applicable, to the databases.</p> <p>Outline the data utility; to whom will it be useful: Generated data can be relevant for scientists involved in the field of pollution and atmospheric sciences specially who interpret observations with the large scale instruments for atmosphere measurements. Some data can be relevant for astrophysicists and for diverse chemical applications. It has to be considered that many pollutants are not produced in situ in the atmosphere but they are emitted due to the human activity and industries. ATMOS species have many applications.</p> <p>Specify if existing data is being re-used: In general, our research concerning molecules does not require previous data as inputs because the sources are our instruments and computers. However, if previously other scientists have provided available information, they will always be considered. Our publications will provide a complete list of references. These previous data derive from the same sources that we will employ to publish our results (articles, databases, repositories) which are the usually tools for experts in our fields. Exception are the crystallographic data employed to start the solid state studies. Open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals are provided by the Crystallography Open Database (http://www.crystallography.net/cod/) or by The Cambridge Crystallographic Data Centre (CCDC) (https://www.ccdc.cam.ac.uk/).</p>
2. FAIR Data 2.1. Making data findable, including provisions for metadata	<p>Discoverability of data (metadata provision): To make data accessible (green open access), repositories of the European Commission (ZENODO) and of the European institutions involved in ATMOS, will be used. Access to all of them is possible through the global registry of research data repositories (www.re3data.org) and the global organization to provided identifiers (datacite.org). When open access is facilitated through editorial publishing (golden open access), or once the embargo periods will be finished (green open access), ATMOS researchers will provide a copy to an open access repository and to the ATMOS consortium web page. Given the interdisciplinary character of ATMOS, peer reviewed international journals specialized in different research fields as well as Open Research Europe will be selected. Some of these journals are open access journals or they offer open access as a possible option. Embargo periods of 12 months are common, although the open access mandate comprises providing open access to the articles. The embargo must be shorter than 6/12 months. In case of too long embargos imposed by the journals, the preprints of the publications and their supplementary material will be uploaded in the free distribution service and an open access arXiv.org e-Print archive (https://arxiv.org). Creative Commons offers licensing solutions. The EUDAT B2SHARE tool includes a built-in license wizard that facilitates the selection of adequate license for research data.</p> <p>Identifiability of data and refer to standard identification mechanism: the metadata standard used to describe the dataset will be the Dublin Core Schema, as it is a flexible and common used standard and is also the one adopted by the European OpenAIRE repository (https://guidelines.openaire.eu/en/latest/literature/use_of_oai_pmh.html)</p> <p>The data produced by ATMOS project is identifiable and locatable with the following metadata: a) dc.relation: info:eu-repo/grantAgreement/EC/H2020/872081 ;</p>

	<p>b) dc.contributor.funder: European Union & Horizon 2020; c) the name and reference of the action: ATMOS & 872081, publication data, and length of the embargo period.</p> <p>In addition, the data will be identifiable means of the Digital Object Identifiers, DOIs, and ORCID numbers, and Keywords.</p> <p>Naming conventions used and outline the approach towards search keyword: Examples of KEYWORDS to optimize possibilities for re-use are given in section 2.3.</p> <p>Type of metadata will be created and how: metadata will be created following the policy of the used repositories</p>
2.2 Making data openly accessible	<p>The project will generate scientific articles in peer reviewed international journals, data for specialized databases, and, conference proceedings, topical special issues, and grey literature (informally published written material not controlled by scientific publishers, e.g. reports).</p> <p>H2020 includes the "green" path (repositories) as the "golden" (publication in open access) as valid to facilitate open access <i>to peer-reviewed articles published</i> in serial or periodical publications. In addition, it is important to note that even in cases where open access is facilitated through editorial publishing, affected researchers should provide a copy to an open access repository.</p> <p>To make data accessible, on line repositories of the institutions involved in ATMOS, the European repository ZENODO, and the ATMOS web site (http://tct1.iem.csic.es/ATMOS.htm), will be used. The documents contained in the repositories of the institutions will be disseminated and collected in other national and international repositories and directories.</p> <p>ZENODO is the open-access repository developed under the European OpenAIRE program (https://www.openaire.eu/). OpenAire is an initiative of the European Commission that indexes and develops value-added services on scientific information resulting from research activity in European Union countries, neighbouring countries and other regions of the world. OpenAire's main functions is to index the research results of projects funded by the European Commission under the Horizon2020 programme with three objectives: 1) increase the international visibility of science resulting from European collaboration; 2) monitor the degree of compliance with the Commission's open access policies;3) exercise transparency towards European taxpayers.</p> <p>OpenAire identifies and indexes the research work that results from thousands of H2020 projects, and indicates which results from H2020 projects for which the open access pilot mandate has been extended to all areas of research. For the systematic recovery and identification of these works through OpenAire, the European Commission marks a number of technical requirements that must be present in the open access repositories and magazines that are consulted by the aggregator.</p> <p><u>Software tools will not be needed to access the data.</u></p> <p>Institutional on line repositories: DIGITAL.CSIC (https://digital.csic.es/) produced by the CSIC (coordinator institution of ATMOS), began in 2008. DIGITAL.CSIC publishes research data, assigns DOIs, assume journal requirements and compliance with funding agency policies. The Storage and description of datasets obey to standards. One of DIGITAL.CSIC's priorities is to support compliance with the European Commission's open access policy. The DIGITAL.CSIC Technical Office has developed a strategy to facilitate compliance with the European Commission's open access policies through the repository path. Training and support resources for scientific, library and institutional technical staff around open access in general and the European mandate in particular, internal tools available to the CSIC library network for the easy identification and monitoring of mandate-affected H2020 projects, collaboration with the CSIC European Programme Service and OpenAire's scientific and technical team are factors that have contributed to the consolidation of the strategy. This priority is articulated by different advisory services to researchers according to the technical requirements set by the European Commission and OpenAire for their correct indexing. As a result, DIGITAL.CSIC appears as one of the main sources contributing to H2020 project results.</p> <p><u>On line repositories of the beneficiary institutions:</u> ARIAS MONTANO (http://rabida.uhu.es/dspace/?locale-attribute=en), which is the institutional repository of the University of Huelva. It is a repository of digital documents, whose aim is to publicize the scientific and teaching production of the University community, and ensure the preservation of their productions in digital format, as well as those institutions with which the University of Huelva has established agreements for this purpose. THE OPEN ARCHIVE HAL (https://hal.archives-ouvertes.fr/) is the repository employed by French institutions involved in ATMOS (CNRS and ULCO). HAL is run by the Centre pour la communication scientifique directe, which is part of the French National Centre for Scientific Research, CNRS.</p> <p>HYDRA (hydra.hull.ac.uk) is the repository of Hull University (https://libguides.hull.ac.uk/openaccess)</p>
2.3. Making data interoperable	<p>Metadata-Keywords: The data produced by ATMOS project is identifiable and locatable with the following metadata, 1) dc.relation: info:eu-repo/grantAgreement/EC/H2020/872081 ; 2) dc.contributor.funder: European Union & Horizon 2020; 3) the name and reference of the action: ATMOS &</p>

	<p>872081, publication data, and length of the embargo period. and by means the Digital Object Identifiers, DOIs, and ORCID numbers,</p> <p>Examples of Keywords to optimize possibilities for re-use: WP1: AIR-POLLUTION; VOC; ASTROCHEMISTRY; AB-INITIO DETERMINATION; POTENTIAL-ENERGY SURFACES; FORCE FIELD; ANHARMONICITY; BASIS-SET; ROTATIONAL SPECTRUM; MICROWAVE-SPECTRUM; TORSIONAL SPECTRUM; WAVE; NON-RIGIDITY; ASSIGNMENT; CONFIGURATION-INTERACTION; ELECTRONIC-SPECTRA; HYPERFINE-STRUCTURE; RAMAN-SPECTRA; INTERNAL-ROTATION; INFRARED-SPECTRA; molecule/radical identifiers (the chemical formulae, IUPAC) or customary names identifiers (ACS, IUPAC) WP2: AIR-POLLUTION; VOC; REVERSE RATE CONSTANTS; TRANSITION-STATE; EXCITED-STATES; AB-INITIO; POTENTIAL-ENERGY SURFACES; DISSOCIATION; DYNAMICS; PHOTODISSOCIATION; PHOTOCHEMISTRY; OZONE CREATION POTENTIALS; HYDROXYL RADICALS; RATE COEFFICIENTS; FINE-PARTICLE; EMISSIONS; COMBUSTION; ABSORPTION; KINETICS WP3: AIR-POLLUTION; DFT; ABINITIO; CARBON-DIOXIDE; FORCE-FIELD; SELECTIVE CAPTURE; STABILITY; DYNAMICS; GAS; SIMULATIONS; MIXTURES; PSEUDOPOTENTIALS; PREDICTIONS; ADAPTED PERTURBATION-THEORY; HYBRID DENSITY FUNCTIONALS; SET MODEL CHEMISTRY; MOLECULAR-STRUCTURE; HYDROGEN-BONDS;</p>
2.4. Increase data re-use (through clarifying licences)	<p>When open access is facilitated through editorial publishing (golden open access), or once the embargo periods will be finished (green open access), ATMOS researchers will provide a copy to an open access repository and to the ATMOS consortium web page. In addition, scientific journals usually accept the distributions of pre-prints to institutional repositories before the end of the embargo period. <u>Authors must read the open access information and policy of the different journals and repositories.</u></p> <p>Given the interdisciplinary character of ATMOS, peer reviewed international journals specialized in different research fields as well as Open Research Europe will be selected. Some of these journals are open access journals or they offer open access as a possible option. Embargo periods of 12 months are common. However, the open access mandate comprises providing open access to the articles. The embargo must be shorter than 6/12 months. In addition, the preprints of the publications and their supplementary material will be uploaded in the free distribution service and an open access arXiv.org e-Print archive. arXiv (pronounced "archive") is an open-access repository of electronic preprints and postprints (known as e-prints) approved for posting after moderation, but not peer review. It consists of scientific papers in, which can be accessed online. In many fields of mathematics and physics, almost all scientific papers are self-archived on the arXiv repository before publication in a peer-reviewed journal. Some publishers also grant permission for authors to archive the peer-reviewed postprint. arXiv begun on 1991. Creative Commons offers licensing solutions. The EUDAT B2SHARE tool includes a built-in license wizard that facilitates the selection of adequate license for research data.</p>
3. Allocation of resources	Open access to scientific publications is a general principle of H2020: on the one hand, eligibility of publication costs in open access and, on the other hand, embargoes permitted for the fulfilment of the mandate by the green way of the repositories. The data publication by the ATMOS Partners is also supported by their own institutions.
4. Data security	<p>We can expect that the data will be safely stored in certified repositories for long term preservation and curation because institutional repositories and Open Air will be used for this aim.</p> <p>Zenodo (https://zenodo.org/features) have properly addressed this issue.</p>
5. Ethical aspects	The project <u>has no Ethics issues identified</u> by the experts in the Ethics Summary Report.
6. Other	<p>Open access mandates of the institutions involved in ATMOS can be found in the following links:</p> <p>CSIC institutional open access mandate.pdf http://rabida.uhu.es/dspace/handle/10272/10023 https://www.science-ouverte.cnrs.fr/wp-content/uploads/2021/04/Cnrs_Research-Data-Plan_mars21.pdf https://hydra.hull.ac.uk/resources/hull:18307; https://www.bib.uni-wuppertal.de/de/open-access.html</p>

HISTORY OF CHANGES		
Version	Publication date	Change
1.0	13.10.2016	▪ Initial version