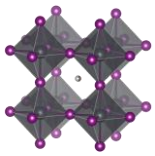


The perovskite database

Descriptions of what is found in the database

Document version 5.4

General instructions

This document describes all fields in the Perovskite Database, how it is formatted, and a few things that that could be good to know when analysing the data

One cell per column

The database uses the individual solar cell as the basic organisational unit. Every entry should represent data for one specific cell. For example, if EQE was measured on one cell, stability under illumination on another cell, and stability in the dark on a third cell, this data should have been split into three different entries as the data comes from three individual cells. Historically that has not always been the case, and it happens that some data are a means for a number of devices.

A left to right, and a substrate first paradigm

When defining the stack sequence for a cell, the substrate is to the left. For any subsequent layer (e.g. substrate, electron transport layer, perovskite, hole transport layer, back contact, etc.) the material closes to the substrate is written to the left, and the material furthest from the substrate is written to the right.

Grammar of the database, i.e. the specific meaning of specific delimiters

The vertical bar, i.e. (' | ')

If a filed contains data for more than one layer, the data belonging to the different layers is separated by a vertical bar with a space on both sides, i.e. (' | ')
Layers are sorted left to right with the substrate first, i.e. to the left.

The semicolon. i.e. ('; ')

If several materials, solvents, gases, etc. are occurring in one layer or during one reaction step, e.g. A and B, are listed in alphabetic order and separated with semicolons, as in (A; B)

The double forward angel bracket, i.e. (' >> ')

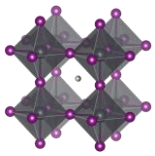
When a layer in a stack is deposited, there may be more than one reaction step involved. If that is the case, the information concerning the different reaction steps, e.g. A, and B, are separated by a double forward angel bracket with one blank space on both sides, as in ('A >> B')

The decimal point, i.e. (' . ')

Numbers have been entered with decimal points and not decimal commas.

Alphabetic ordering of lists

When several elements of information are connected to one layer or to one reaction step, the elements are ordered in alphabetic order to simplify downstream data processing. The exceptions to that principle is when a list is describing another list that is sorted in alphabetic order, e.g. a solution contains the three components A, B, and C whereas another field specifies the concentrations for A, B, and C. In that field, the order of the concentrations must line up with components. Otherwise, it would be hard to interpret which concentration that are linked to which component.



Correctness of data

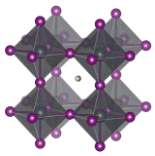
The original data based on how well we understood what was written
For newer data, we rely on that authors have reported data honestly, and that they have used correct formatting. There are checks and balances in place but be aware that we have no possibility to guarantee the correctness of every data point.

Descriptions of the columns in the database

There are 410 columns in the database.
Those are grouped in a number of topics. The number of columns has been expanded gradually which means that for older data there will be more gaps than for newer data. Below is a description of all the columns, with explanation to the formation, when they were implemented, estimates of reliability, and warnings concerning ambiguities.

The columns are grouped into 15 topics

- Reference information
- Cell definition
- Module definition (for modules only)
- Substrate
- Electron transport layer
- The perovskite layer
- The perovskite deposition
- The hole transport layer
- The back contact
- Additional layers, e.g. encapsulation, antireflective coatings, etc.
- JV data
- Stabilised efficiencies
- Quantum efficiency
- Stability
- Outdoor testing



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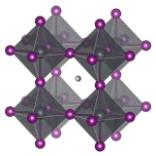

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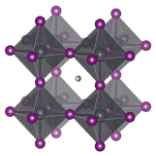

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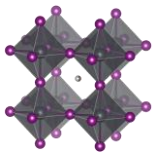

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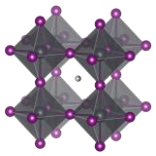

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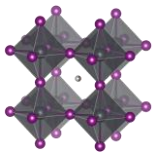

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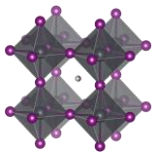

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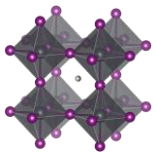


Reference information

Ref_ID_temp

Format: Integer
Implemented: In the original data hunt
Description: A temporary reference number to keep track of the devices before they are submitted to the database. Does not bear any particular meaning but is there for traceability reasons

Ref_ID

Format: Integer
Implemented: In the original data hunt
Description: The primary database key

Ref_name_of_person_entering_the_data

Format: String
Default: Empty string
Implemented: In the original data hunt
Description: name of person entering the database

Ref_data_entered_by_author

Format: Boolean. i.e. TRUE or FALSE
Default: False
Implemented: In the original data hunt
Description: If the data is entered by an author to the publication where it is found

Ref_DOI_number

Format: Text string
Default: Empty string
Implemented: In the original data hunt
Description: The DOI number referring to the published paper or dataset where the data can be found

Ref_lead_author

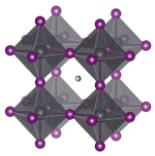
Format: Text string
Default: Empty string
Implemented: In the original data hunt
Description: The surname of the first author. Programmatically obtained from www.corsref.org by the DOI number

Ref_publication_date

Format: Date
Default: Empty string
Format: Year:mm:dd
Implemented: In the original data hunt
Description: Publication date. If the DOI number was given correctly, this was extracted automatically from www.crossref.org

Ref_journal

Format: String
Default: Empty string
Implemented: In the original data hunt
Description: The journal name. If the DOI number was given correctly, this was extracted automatically from www.crossref.org

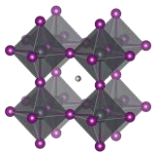


Ref_part_of_initial_dataset
Format: Boolean. i.e. TRUE or FALSE
Default: False
Implemented: In the original data hunt
Description: True if the data was part of the initial dataset of the project

Ref_original_filename_data_upload
Format: String
Default: Empty string
Implemented: In the original data hunt
Description: The name of the file with data uploaded to the database. Only for traceability reasons in case the database must be restored from original submitted files.

Ref_free_text_comment
Format: Text string
Default: Empty string
Implemented: In the original data hunt
Description: This could be anything given additional description to the cell that is not captured by any other field.

Ref_internal_sample_id
Format: Text string
Default: Empty string
Implemented: In the original data hunt
Description: This is supposed to be a unique cell identifier. With this text string alone, you should in principle be able to identify the cell in original data source.
Concerns: Seldom used properly in the original dataset



Cell definition

Cell_stack_sequence

Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The stack sequence describing the cell. The following guidelines apply

- Start with the substrate to the left and list the materials in each layer of the device
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- The perovskite layer is stated as "Perovskite", regardless of composition, mixtures, dimensionality etc. There are plenty of other fields specifically targeting the perovskite.
- If a material is doped, or have an additive, state the pure material here and specify the doping in the columns specifically targeting the doping of those layers.
- There is no sharp well-defined boundary between a when a material is best considered as doped to when it is best considered as a mixture of two materials. When in doubt if your material is doped or a mixture, use the notation that best capture the metaphysical essence of the situation
- Use common abbreviations when possible but spell it out when there is risk for confusion. For consistency, please pay attention to the abbreviation specified under the headline Abbreviations found earlier in this document.
- There are several thousand stack sequences described in the literature. Try to find your one in the list of alternatives in the data template. If it is not there (i.e. you may have done something new) define a new stack sequence according to the instructions.

Concerns: Is considered a primary descriptor of a cell. It could happen that more than one label can refer to the same thing.

Cell_area_total

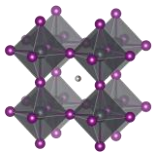
Format: Float. [cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total cell area in cm^2. The total area is defined as the area that would provide photovoltaic performance when illuminated without any shading, i.e. in practice the geometric overlap between the top and bottom contact.

Cell_area_measured

Format: Float. [cm^2]
Default: nan
Implemented: In the original data hunt
Description: The effective area of the cell during IV and stability measurements under illumination. If measured with a mask, this corresponds to the area of the hole in the mask. Otherwise this area is the same as the total cell area.
Concerns: Arias is sometimes not stated properly. There could be confusion about which type of area that is referred to. Initially a default area of 0.1 cm^2 was used when no data was stated.

Cell_number_of_cells_per_substrate

Format: Integer
Default: 0
Implemented: In the original data hunt
Description: The number of individual solar cells, or pixels, on the substrate on which the reported cell is made



Cell_architecture
Format: Text string
Default: "Unknown"
Implemented: In the original data hunt
Description: The cell architecture with respect to the direction of current flow and the order in which layers are deposited. The two most common are nip (also referred to as normal) and pin (also referred to as inverted) but there are also a few others, e.g. Back contacted

- nip architecture means that the electrons are collected at the substrate side. The typical example is when a TiO_2 electron selective contact is deposited between the perovskite and the substrate (e.g. SLG | FTO | TiO2-c |Perovskite | …)
- pin architecture means that it instead is the holes that are collected at the substrate side. The typical example is when a PEDOT:PSS hole selective contact is deposited between the perovskite and the substrate (e.g. SLG | FTO | PEDOT:PSS |Perovskite | …)

Cell_flexible
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell flexible and bendable.
Concerns: This does not discriminate between different levels of flexibility

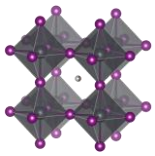
Cell_flexible_min_bending_radius
Format: Float
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The minimum bending radius possible without degrading the cells performance

Cell_semitransparent
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell is semi-transparent, which usually is the case when there are no thick completely covering metal electrodes.
Concerns: Does not discriminate between different levels of transparency. In practice this is True for any cell that does not have metal contacts.

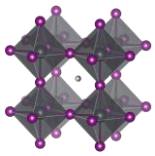
Cell_semitransparent_AVT
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The average visible transmittance in the wavelength range stated in the next field. In %
Concerns. Not tested at the time of project implementation

Cell_semitransparent_wavelength_range
Format: text string. [lambda_min; lambda_max]
Default: none
Implemented: After the initial data hunt but before initial release
Description: the wavelength range under which the average visible transmittance is determined
Example:

Cell_semitransparent_raw_data
Format: text string
Default:
Implemented: After the initial data hunt but before initial release



Description: Link to experimental data trace.
Concern. Central storage and dealing with data traces is not yet implemented within the project.



Module definition

Module

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell is a module composed of connected individual sub cells
Concerns. Historically module papers have seldom contained data for more than one module

Module_number_of_cells_in_module

Format: Integer
Default: 0
Implemented: In the original data hunt
Description: The number of cells in the module

Module_area_total

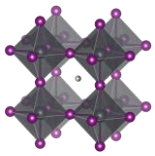
Format: Float. [cm^2]
Default: nan
Implemented: In the original data hunt
Description: The total area of the module in cm^2. This includes scribes, contacts, boundaries, etc. and represent the module's geometrical footprint.
Concerns. Sometimes mixed up with effective area

Module_area_effective

Format: Float [cm^2]
Default: nan
Implemented: In the original data hunt
Description: The active area of the module in cm^2.

Module_JV_data_recalculated_per_cell

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: The preferred way to report IV data for modules is to recalculate the IV data to average data per sub-cells in the module. That simplifies downstream comparisons, and it ensures that there is no erroneous transformation that otherwise may occur when error checking the IV data. Mark this as TRUE if the conversation is done. In the historical dataset, this transformation has been done for all cells. Potentials should be reported in V but it happens that people report it in mV, and to deal with that problem, all potential values over a threshold indicating that it probably is stated in mV is divided by 1000. For series interconnected modules, the total module potential can be over that threshold, so if data not is calculated per cell, this could be wrong with a factor 1000.



Substrate

Substrate_stack_sequence

Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The stack sequence describing the substrate.

- With the substrate, we refer to any layer below the electron transport layer in a nip-device, and any layer below the hole transport layer in a pin-device.
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- Use common abbreviations when appropriate but spell it out if risk for confusion.
- There are a lot of stack sequences described in the literature. Try to find your one in the list. If it is not there (i.e. you may have done something new) define a new stack sequence according to the instructions.

Substrate_thickness

Format: Text string. [Th.1 | Th.2 | … | Th.n] [mm]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: A list of thicknesses of the individual layers in the stack. Use the following guidelines

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- The layers must line up with the previous filed.
- State thicknesses in nm
- Every layer in the stack has a thickness. If it is unknown, state this as 'nan'
- If there are uncertainties, state the best estimate, e.g. write 100 and not 90-110
- If you only know the total thickness, e.g. you have a 2 mm thick commercial FTO substrate and you do not know how thick the FTO layer is, state that as '2 | nan'

Substrate_area

Format: Float. [cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total area in cm^2 of the substrate over which the perovskite is deposited. This may be significantly larger than the cell area

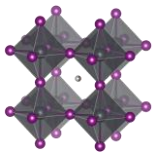
Substrate_supplier

Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description. The supplier of the substrate.

- Most substrates in the perovskite field are bought commercially, but if it is made in the lab, state this as "lab made"
- If the supplier is unknown, stat that as: 'Unknown'
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Substrate_brand_name

Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description. The specific brand name of the substrate. e.g. NGO11, TEC15, etc.



Substrate_deposition_procedure

Format: Text string
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description. A list of the deposition procedures for the substrate

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- Make sure that you describe as many layers as there are layers in the stack. Otherwise it will be difficult to interpret which layer the deposition procedure is referring to. It should thus be as many vertical bars in this field as when describing the substrate stack.
- When more than one reaction step, separate them by a double forward angel bracket with one blank space on both sides (' >> ')
- If the deposition procedure for a layer unknown, state that as: 'Unknown'
- If a substrate is bought commercially and you do not know, indicate this by the label "Commercial"

Substrate_surface_roughness_rms

Format: Float, [nm]
Default: nan
Implemented: After the initial data hunt but before initial release
Implemented: After the initial data hunt but before initial release
Description: The root mean square value (RMS) of the surface roughness expressed in nm

Substrate_etching_procedure

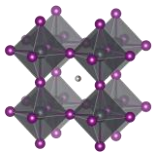
Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description. For the most common substrates, i.e. FTO and ITO it is common that part of the conductive layer is removed before perovskite deposition. State the method by which it was removed

- If there is more than one cleaning step involved, separate the steps by a double forward angel bracket (' >> ')

Substrate_cleaning_procedure

Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description. The schematic cleaning sequence of the substrate. The Extraction protocol does not capture the fine details in the cleaning procedures, e.g. times, temperatures, etc. but state the general sequence. Refers to the cleaning of the entire substrate before the deposition of the rest of the cell stack starts.

- If there is more than one cleaning step involved, separate the steps by a double forward angel bracket (' >> ')
- If more than one procedure is occurring simultaneously, e.g. Soap washing an ultrasonic bath, separate simultaneously occurring steps with a semicolon.



Electron transport layer

ETL_stack_sequence

Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The stack sequence describing the electron transport layer. Use the following formatting guidelines

- With the ETL, we refer to any layer between the substrate and the perovskite in a nip-device, and any layer between the perovskite and the back contact in a pin-device.
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- If no electron transport layer, state that as 'non'
- Use common abbreviations when appropriate but spell it out if risk for confusion.
- If a material is doped, or have an additive, state the pure material here and specify the doping in the columns specifically targeting the doping of those layers.
- There is no sharp well-defined boundary between when a material is best considered as doped or as a mixture of two materials. When in doubt if your material is best described as doped or as a mixture, use the notation that best capture the metaphysical essence of the situation.

ETL_thickness

Format: Text string. [Th.1 | Th.2 | … | Th.n] [nm]
Default: nan
Implemented: In the original data hunt
Description: A list of thicknesses of the individual layers in the stack. Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')

- The layers must line up with the previous filed.
- State thicknesses in nm
- Every layer in the stack has a thickness. If it is unknown, state this as 'nan'
- If there are uncertainties, state the best estimate, e.g. write 100 and not 90-110

ETL_additives_compounds

Format: Text string. [Addt.1; Addt.2; ... | Addt.3; … | Addt.4 | ...]
Default: Empty text string
Implemented: In the original data hunt
Description: List of the dopants and additives that are in each layer of the ETL-stack

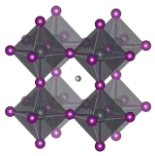
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- The layers must line up with the previous fields.
- If several dopants/additives, e.g. A and B, are present in one layer, list the dopants/additives in alphabetic order and separate them with semicolons, as in (A; B)
- If no dopants/additives, state that as "Undoped"
- If the doping situation is unknown, stat that as: 'Unknown'

Concerns: This is a category with a lot of uncertainty. Historically a lot of dopants have not been added properly. A blank field may thus not guarantee that the layer was undoped. Sometimes it has been a confusion if something should be treated as a dopant, or an extra layer, or a part of the previous layer and just involve an extra deposition step for that layer. An example is $TiCl_4$ treatment of TiO_2

ETL_additives_concentrations

Format: Text string. [c1 M; c2 wt%; … | c3 vol%; ... | c4 mg/ml | ...]
Default: nan
Implemented: In the original data hunt
Description: The concentration of the dopants/additives.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')



- If more than one dopant/additive in the layer, e.g. A and B, separate the concentration for each dopant/additive with semicolons, as in (A; B)
- For each dopant/additive in the layer, state the concentration.
- The order of the dopants/additives must be the same as in the previous filed.
- For layers with no dopants/additives, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used.
- The preferred way to state the concentration of a dopant/additive is to refer to the amount in the final product, i.e. the material in the layer. When possible, use on the preferred units:
    - wt%, mol%, vol%, ppt, ppm, ppb
- When the concentration of the dopant/additive in the final product is unknown, but where the concentration of the dopant/additive in the solution is known, state that concentration instead. When possible, use on the preferred units:
    - M, mM, molal; g/ml, mg/ml, μg/ml
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Concerns. In the initial instructions, concentrations should be stated as fraction of total amount, but that was ambiguous and was interpreted differently.

ETL_deposition_procedure

Format: Text string. [Proc. 1 >> Proc. 2 >> ... | Proc. 3 >> … | Proc. 4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The deposition procedures for the ETL stack.

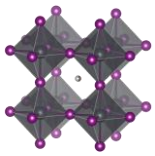
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate them by a double forward angel bracket with one blank space on both sides (' >> ')
- Thermal annealing is generally not considered as an individual reaction step. The philosophy behind this is that every deposition step has a thermal history, which is specified in a separate filed. In exceptional cases with thermal annealing procedures clearly disconnected from other procedures, state 'Thermal annealing' as a separate reaction step.
- Please read the instructions under "*Perovskite. Deposition. Procedure*" for descriptions and distinctions between common deposition procedures and how they should be labelled for consistency in the database.

Concerns. Much effort was put to make this correct in the original dataset, but it happens that we have misunderstood the descriptions in the original publications.

ETL_deposition_aggregation_state_of_reactants

Format: Text string.) [Agr. 1 >> Agr. 2 >> ... | Agr. 3 >> … | Agr. 4 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The physical state of the reactants

- The three basic categories are Solid/Liquid/Gas
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the aggregation state associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- Most cases are clear cut, e.g. spin-coating involves species in solution and evaporation involves species in gas phase. For less clear-cut cases, consider where the reaction really is happening as in:
    - For a spray-coating procedure, it is droplets of liquid that enters the substrate (thus a liquid phase reaction)
    - For sputtering and thermal evaporation, it is species in gas phase that reaches the substrate (thus a gas phase reaction)



ETL_deposition_synthesis_atmosphere
Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The synthesis atmosphere

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

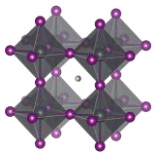
ETL_deposition_synthesis_atmosphere_pressure_total
Format: Text string. [P.1 >> P.2 >> ... | P.3 >> … | P.4 | ...] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total pressure during each synthesis step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- Pressures can be stated in different units suited for different situations. Therefore, specify the unit. The preferred units are:
    - atm, bar, mbar, mmHg, Pa, torr, psi
- If a pressure is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 100 pa and not 80-120 pa.

ETL_deposition_synthesis_atmosphere_pressure_partial
Format: Text string. [P.1; P.2 >> P.3 >> ... | P.4 >> … | P.5 | ...] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The partial pressures for the gases present during each reaction step.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the partial pressures and separate them with semicolons, as in (A; B). The list of partial pressures must line up with the gases they describe.
- In cases where no gas mixtures are used, this field will be the same as the previous filed.

ETL_deposition_synthesis_atmosphere_relative_humidity
Format: Text string. [RH1 >> RH2 >> ... | RH3 >> … | RH4 | ...] [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relative humidity during each deposition step



- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the relative humidity associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The number and order of layers and deposition steps must line up with the previous columns
- If the relative humidity for a step is not known, stat that as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 35 and not 30-40.

ETL_deposition_solvents

Format: Text string. [Sol.1; Sol.2 >> Sol.3; ... >> ... | Sol.4 >> … | Sol.5 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The solvents used in each deposition procedure for each layer in the stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the solvents associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solvent is a mixture of different solvents, e.g. A and B, list the solvents in alphabetic order and separate them with semicolons, as in (A; B)
- The number and order of layers and deposition steps must line up with the previous columns.
- For non-liquid processes with no solvents, state the solvent as ‘none’
- If the solvent is not known, state this as ‘Unknown’
- Use common abbreviations when appropriate but spell it out when risk for confusion
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

ETL_deposition_solvents_mixing_ratios

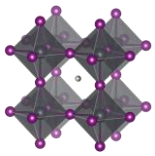
Format: Text string. [V1; V2 >> V3; V4 >> ... | V5; V6 >> … | 1 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The mixing ratios for mixed solvents

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the solvent mixing ratios associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The number and order of layers and deposition steps must line up with the previous columns.
- For pure solvents, state the mixing ratio as 1
- For non-solvent processes, state the mixing ratio as 1
- For unknown mixing ratios, state the mixing ratio as ‘nan’
- For solvent mixtures, i.e. A and B, state the mixing ratios by using semicolons, as in (V_A; V_B)
- The preferred metrics is the volume ratios. If that is not available, mass or mol ratios can be used instead, but it the analysis the mixing ratios will be assumed to be based on volumes.

ETL_deposition_solvents_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: ‘Unknown’
Implemented: After the initial data hunt but before initial release
Description: The suppliers of all the solvents.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the solvent suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.



- For non-liquid processes with no solvents, mark the supplier as 'none'
- If the supplier for a solvent is unknown, state this as 'Unknown'

ETL_deposition_solvents_purity
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the solvents used.

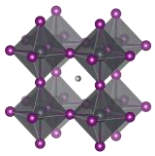
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For non-liquid processes with no solvents, state the purity as 'none'
- If the purity for a solvent is not known, state this as 'Unknown'

ETL_deposition_reaction_solutions_compounds
Format: Text string. [C1; C2 >> C3; … >> … | C4; C5 | C6 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The non-solvent precursor chemicals used in each reaction step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemicals associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several compounds, e.g. A and B, list the associated compounds in alphabetic order and separate them with semicolons, as in (A; B)
- Note that also dopants/additives should be included
- When several precursor solutions are made and mixed before the reaction step, it is the properties of the final mixture used in the reaction we here describe.
- The number and order of layers and reaction steps must line up with the previous columns.
- For gas phase reactions, state the reaction gases as if they were in solution.
- For solid-state reactions, state the compounds as if they were in solution.
- For reaction steps involving only pure solvents, state this as 'none'
- If the compounds for a deposition step is not known, state this as 'Unknown'

ETL_deposition_reaction_solutions_compounds_supplier
Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemical suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For gas phase reactions, state the suppliers for the gases or the targets/evaporation sources that are evaporated/sputtered/etc.



- For solid state reactions, state the suppliers for the compounds in the same way.
- For reaction steps involving only pure solvents, state the supplier as 'none' (as that that is entered in a separate filed)
- For chemicals that are lab made, state that as "Lab made" or "Lab made (name of lab)"
- If the supplier for a compound is unknown, state this as 'Unknown'

ETL_deposition_reaction_solutions_compounds_purity
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the non-solvent chemicals.

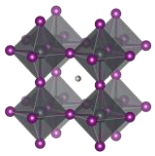
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the compound purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, i.e. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For reaction steps involving only pure solvents, state this as 'none' (as that is stated in another field)
- If the purity for a compound is not known, state this as 'Unknown'

ETL_deposition_reaction_solutions_concentrations
Format: Text string. [c1 M; c2 mol/dm3 >> c3 mg/ml; … >> ... | c4 wt%; c5 vol% | c6 ppm |...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the non-solvent precursor chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the concentrations associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated concentrations and separate them with semicolons, as in (A; B)
- The order of the compounds must be the same as in the previous filed.
- For reaction steps involving only pure solvents, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used. When possible, use one of the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml, wt%, mol%, vol%, ppt, ppm, ppb
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

ETL_deposition_reaction_solutions_volumes
Format: Text string. [V1 >> V2 >> ... | V3 >> … | V4 | ...] [ml]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The volume of the reaction solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the volumes associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The volumes refer the volumes used, not the volume of the stock solutions. Thus if 0.15 ml of a solution is spin-coated, the volume is 0.15 ml
- For reaction steps without solvents, state the volume as 'nan'
- When volumes are unknown, state that as 'nan'



ETL_deposition_reaction_solutions_age
Format: Text string. [A1 >> A2 >> ... | A3 >> … | A4 | ...] [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the age of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- As a general guideline, the age refers to the time from the preparation of the final precursor mixture to the reaction procedure.
- When the age of a solution is not known, state that as ‘nan’
- For reaction steps where no solvents are involved, state this as ‘nan’
- For solutions that are stored a long time, an order of magnitude estimate is adequate.

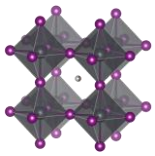
ETL_deposition_reaction_solutions_temperature
Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the reaction solutions.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the temperatures of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a reaction solution undergoes a temperature program, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons, e.g. 25; 100
- When the temperature of a solution is unknown, state that as ‘nan’
- For reaction steps where no solvents are involved, state the temperature of the gas or the solid if that make sense. Otherwise state this as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume an undetermined room temperature to be 25

ETL_deposition_substrate_temperature
Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the substrate.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the temperatures of the substrates (i.e. the last deposited layer) associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The temperature of the substrate refers to the temperature when the deposition of the layer is occurring.
- If a substrate undergoes a temperature program before the deposition, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- When the temperature of a substrate is not known, state that as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume that an undetermined room temperature is 25

ETL_deposition_thermal_annealing_temperature
Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperatures of the thermal annealing program associated with depositing the layers



- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the annealing temperatures associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If the thermal annealing involves a temperature program with multiple temperature stages, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- If no thermal annealing is occurring after the deposition of a layer, state that by stating the room temperature (assumed to 25°C if not further specified)
- If the thermal annealing program is not known, state that by ‘nan’

ETL_deposition_thermal_annealing_time

Format: Text string. [t1; t2 >> t3; ... >> ... | t4 >> … | t5 | ...] [min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time program associated to the thermal annealing program.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the annealing times associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If the thermal annealing involves a temperature program with multiple temperature stages, list the associated times at those temperatures and separate them with semicolons.
- The annealing times must align in terms of layers, reaction steps and annealing temperatures in the previous filed.
- If a time is not known, state that by ‘nan’
- If no thermal annealing is occurring after the deposition of a layer, state that by ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 20 and not 10-30.

ETL_deposition_thermal_annealing_atmosphere

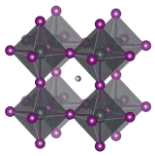
Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: “Unknown”
Implemented: After the initial data hunt but before initial release
Description: The atmosphere during thermal annealing

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the atmospheres associated to each annealing step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The number and order of layers and deposition steps must line up with the previous columns.
- If the atmosphere is a mixture of different gases, i.e. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- “Dry air” represents air with low relative humidity but where the relative humidity is not known
- “Ambient” represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as “Air”
- “Vacuum” (of unspecified pressure) is for this purpose considered as an atmospheric gas.
- This is often the same as the atmosphere under which the deposition is occurring, but not always.

ETL_storage_time_until_next_deposition_step

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time between the HTL stack is finalised and the next layer is deposited

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.



ETL_storage_atmosphere

Format: Text string. [Gas1; Gas2; ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the sample with the finalised HTL stack is stored until the next deposition step.

ETL_storage_relative_humidity

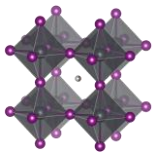
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relive humidity under which the sample with the finalised HTL stack is stored until next deposition step

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

ETL_surface_treatment_before_next_deposition_step

Format: Text string
Default: nan
Implemented: After the initial data hunt but before initial release
Description: Description of any type of surface treatment or other treatment the sample with the finalised ETL-stack undergoes before the next deposition step.

- If more than one treatment, list the treatments and separate them by a double forward angel bracket (' >> ')
- If no special treatment, state that as 'none'



The perovskite

Perovskite_single_crystal

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell is based on a perovskite single crystal
Concerns. This distinction was not made in the initial instructions, which means that some single crystal cells may be marked as False

Perovskite_dimension_0D

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell is based on a perovskite quantum dots. Perovskite nanoparticle architectures can also be counted here unless they more have the characteristics of a standard polycrystalline cell
Concerns. This distinction was not made in the initial instructions, which means that some QD cells probably is marked as False

Perovskite_dimension_2D

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell is based on 2D perovskites, i.e. a layered perovskite with a large A-cation
Concerns. This distinction was not made in the initial instructions, which means that some 2D cells may be marked as False, but as dimensionality often can be deduced from the composition this should not be a big problem

Perovskite_dimension_2D3D_mixture

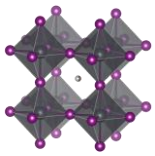
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell is based on a mixture of 2D and 3D perovskites. This is sometimes referred to as reduced dimensional perovskites (but not as reduced as to be a pure 2D perovskite)
Concerns. This distinction was not made in the initial instructions, which means that some cells that should be here may be marked as False. It is also not always obvious from the papers if this is the case, in part because it is non-trivial to measure.

Perovskite_dimension_3D

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE for standard three-dimensional perovskites with ABC_3 structures. TRUE also for the case where the bulk of the perovskite is 3D but where there exist a thin 2D-capping layer
Concern. Mya also include some 2D, and 1D perovskites

Perovskite_dimension_3D_with_2D_capping_layer

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the bulk of the perovskite layer is 3D but there is a top layer with lower dimensionality.



Concerns. This distinction was not made in the initial instructions which means that some cells that should be here may be marked as False. It is also not always obvious from the papers if this is the case, in part because it is non-trivial to measure.

Perovskite. Dimension. List of layers

Format: Text string. [Dim.1 | Dim.2 | …]
Default: nan
Implemented: In the original data hunt
Description: A list of the perovskite dimensionalities

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- In most cases, there will be only one layer
- For a perovskite that is a mixture of a 2D and a 3D phase, mark this is as: 2.5

Concerns. Most entries are single numbers stored as strings, but when converting them to numbers one must remember that there could be more than one layer

Perovskite_composition_perovskite_ABC3_structure

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the photo-absorber has a perovskite structure

- The typical perovskite has an ABC_3 structure and that is clearly a TRUE
- This category is inclusive in the sense that also 2D perovskite analogues should be labelled as TRUE

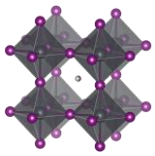
Perovskite_composition_perovskite_inspired_structure

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the photo absorber does not have a perovskite structure. In the literature we sometimes see cells based on non-perovskite photo absorbers, but which claims to be "perovskite inspired" regardless if the crystal structure has any resemblance to the perovskite ABC_3 structure or not. This category is for enabling those cells to easily be identified and filtered.

Perovskite_composition_a_ions

Format: Text string. [Ion.1; Ion.2; … | Ion.3; … | ...]
Default: nan
Implemented: In the original data hunt
Description: List of the A-site ions in the perovskite structure

- We have experimented with letting users write the perovskite structure and from that extract ions and coefficients. Due to the multitude of formatting variations, that has not worked out very well, wherefor we now define the perovskite ion by ion.
- List all the A-site ions in alphabetic order and separate them by semicolons
- For ions which labels are three characters or longer, enclose them in parenthesis. That improves readability and simplifies downstream data treatment.
- In case of a layered perovskite structure, separate layers by a space, a vertical bar, and a space, i.e. (' | ')
- Only include ions that go into the perovskite structure. Ions that only are found in secondary phases, or amorphous grain boundaries, or that disappears during synthesis, should instead be added as dopants/additives in the field dedicated to dopants and additives.
    - On example is Rb in MAFAPbBrI-perovskites. As far as we know, Rb does not go into the perovskite structure, even if that was believed to be the case in the beginning, but rather form secondary phases. For MAFAPbBrI-perovskites, Rb should thus not be considered as a A-site cation, but as a dopant/additive.



Perovskite_composition_a_ions_coefficients

Format: Text string. [Cof.1; Cof.2; … | Cof.3; … | ...]
Default: nan
Implemented: In the original data hunt
Description: A list of the perovskite coefficients for the A-site ions

- The list of coefficients must line up with the list of the A-site ions
- If a coefficient is unknown, state that with an 'x'
- If there are uncertainties in the coefficient, only state the best estimate, e.g. write 0.4 and not 0.3-0.5.
- A common notation is '1-x'. Write that as x
- If the coefficients are not known precisely, a good guess is worth more than to state that we have absolutely no idea.

Perovskite_composition_b_ions

Format: Text string. [Ion.1; Ion.2; … | Ion.3; … | ...]
Default: nan
Implemented: In the original data hunt
Description: List of the B-site ions in the perovskite structure

- We have experimented with letting users write the perovskite structure and from that extract ions and coefficients. Due to the multitude of formatting variations, that has not worked out very well, wherefor we now define the perovskite ion by ion.
- List all the B-site ions in alphabetic order and separate them by semicolons
- In case of a layered perovskite structure, separate layers by a space, a vertical bar, and a space, i.e. (' | ')
- Only include ions that go into the perovskite structure. Ions that only are found in secondary phases, or amorphous grain boundaries, or that disappears during synthesis, should instead be added as dopants/additives in the field dedicated to dopants and additives.

Perovskite_composition_b_ions_coefficients

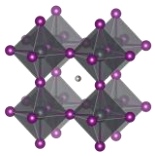
Format: Text string. [Cof.1; Cof.2; … | Cof.3; … | ...]
Default: nan
Implemented: In the original data hunt
Description: A list of the perovskite coefficients for the B-site ions

- The list of coefficients must line up with the list of the B-site ions
- If a coefficient is unknown, mark that with an 'x'
- If there are uncertainties in the coefficient, only state the best estimate, e.g. write 0.4 and not 0.3-0.5.
- A common notation is '1-x'. Write that as x
- If the coefficients are not known precisely, a good guess is worth more than to state that we have absolutely no idea.

Perovskite_composition_c_ions

Format: Text string. [Ion.1; Ion.2; … | Ion.3; … | ...]
Default: nan
Implemented: In the original data hunt
Description: List of the C-site ions in the perovskite structure

- We have experimented with letting users write the perovskite structure and from that extract ions and coefficients. Due to the multitude of formatting variations, that has not worked out very well, wherefor we now define the perovskite ion by ion.
- List all the A-site ions in alphabetic order and separate them by semicolons
- For ions which labels are three characters or longer, enclose them in parenthesis. That improves readability and simplifies downstream data treatment.



- In case of a layered perovskite structure, separate layers by a space, a vertical bar, and a space, i.e. (' | ')
- Only include ions that go into the perovskite structure. Ions that only are found in secondary phases, or amorphous grain boundaries, or that disappears during synthesis, should instead be added as dopants/additives in the field dedicated to dopants and additives.

One example is chloride in $MAPbI_3$. As far as we know, Cl does not go into the perovskite structure even if that was believed to be the case in the beginning. For $MAPbI_3$ Cl should thus not be considered as a C-site cation, but as a dopant/additive

Perovskite_composition_c_ions_coefficients

Format: Text string. [Cof.1; Cof.2; … | Cof.3; … | ...]
Default: nan
Implemented: In the original data hunt
Description: A list of the perovskite coefficients for the C-site ions

- The list of coefficients must line up with the list of the C-site ions
- If a coefficient is unknown, mark that with an 'x'
- If there are uncertainties in the coefficient, only state the best estimate, e.g. write 0.4 and not 0.3-0.5.
- A common notation is '1-x'. Write that as x
- If the coefficients are not known precisely, a good guess is worth more than to state that we have absolutely no idea.

Perovskite_composition_none_stoichiometry_components_in_excess

Format: Text string. [Com.1; Com.2; … | Com.3; … | ...]
Default: nan
Implemented: In during the original data hunt
Description: Components that are in excess in the perovskite synthesis. E.g. to form stoichiometric $MAPbI_3$, PbI_2 and MAI are mixed in the proportions 1:1. If one of them are in excess compared to the other, then that component is considered to be in excess. This information can be inferred from data entered on the concentration for all reaction solutions, but this gives a convenient shorthand filtering option.

- If more than one component is in excess, order them in alphabetic order and separate them by semicolons.
- It there are no components that are in excess, write Stoichiometric

Perovskite_composition_short_form

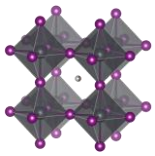
Format: Text string
Default: 'Unknown'
Implemented: In the original data hunt
Description: The perovskite composition written in shorthand notation, i.e. without coefficients. Not given by users but inferred from the previous columns. This is because it turned out to be impossible to get people to follow instructions and state the perovskite structures in a consistent and machine-readable form.

Perovskite_composition_long_form

Format: Text string
Default: 'Unknown'
Implemented: In the original data hunt
Description: The perovskite composition Not given by users but inferred from the previous columns. This is because it turned out to be impossible to get people to follow instructions and state the perovskite structures in a consistent and machine-readable form.

Perovskite_composition_assumption

Format: Text string. [Solution composition/Experimental verification/Literature/ …]



Default: nan
Implemented: After the initial data hunt but before initial release
Description: The knowledge base from which the perovskite composition is inferred. Is the assumed perovskite composition based on the composition of the precursor solutions and the assumption that the final perovskite will have the same composition (i.e. Solution composition), or is it based on literature claims (i.e. Literature) or has it been experimentally verified with some technique, e.g. XRD, EDX, XRF, etc.?

Perovskite_composition_inorganic

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the perovskite does not contain any organic ions.

Perovskite_composition_leadfree

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the perovskite is completely lead free.

Perovskite_additives_compounds

Format: Text string. [Addt.1; Addt.2; ... | Addt.3; … | Addt.4 | ...]
Default: Empty text string
Implemented: In the original data hunt
Description: List of the dopants and additives that are in the perovskite

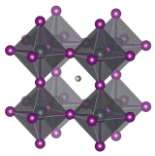
- If the perovskite is layered (e.g. 3D perovskite with a 2D capping layer), separate the layers by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- If several dopants/additives, e.g. A and B, are present in one layer, list the dopants/additives in alphabetic order and separate them with semicolons: as in (A; B)
- If no dopants/additives, state that as “Undoped”
- If the doping situation is unknown, stat that as: ‘Unknown’
- Include any non-solvent that does not go into the perovskite structure. This includes compounds that are found in secondary phases, or amorphous grain boundaries, or that disappears during synthesis.
    - One example is Rb in MAFAPbBrI-perovskites. As far as we know, Rb does not go into the perovskite structure, even if that was believed to be the case in the beginning, but rather form secondary phases. For MAFAPbBrI-perovskites, Rb should thus not be considered as a A-site cation, but as a dopant/additive.
    - One other example is chloride in $MAPbI_3$. As far as we know, Cl does not go into the perovskite structure even if that was believed to be the case in the beginning. For $MAPbI_3$ Cl should thus not be considered as a C-site cation, but as a dopant/additive.

Concerns: This is a category with a lot of uncertainty. Historically a lot of dopants have not been added properly. A blank field may thus not guarantee that the layer was undoped.

Perovskite_additives_concentrations

Format: Text string. [c1 M; c2 wt%; … | c3 vol%; ... | c4 mg/ml | ...]
Default: nan
Implemented: In the original data hunt
Description: The concentration of the dopants/additives.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- If more than one dopant/additive in the layer, e.g. A and B, separate the concentration for each dopant/additive with semicolons, as in (A; B)
- For each dopant/additive in the layer, state the concentration.
- The order of the dopants/additives must be the same as in the previous filed.



- For layers with no dopants/additives, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used.
- The preferred way to state the concentration of a dopant/additive is to refer to the amount in the final product, i.e. the material in the layer. When possible, use on the preferred units:
    - wt%, mol%, vol%, ppt, ppm, ppb
- When the concentration of the dopant/additive in the final product is unknown, but where the concentration of the dopant/additive in the solution is known, state that concentration instead. When possible, use on the preferred units:
    - M, mM, molal; g/ml, mg/ml, μg/ml
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Perovskite_thickness

Format: Text string. [Th.1 | Th.2 | … | Th.n] [nm]
Default: nan
Implemented: In the original data hunt
Description: The thickness of the perovskite layer

- If the perovskite contains more than one layer, separate those by a space, a vertical bar, and a space, i.e. (' | ')
- State thicknesses in nm
- Every layer in the stack has a thickness. If it is unknown, state this as 'nan'
- If there are uncertainties, state the best estimate, e.g. write 100 and not 90-110
- For cells where the perovskite infiltrates a mesoporous scaffold, state the thickness as starting from the bottom of the infiltrated mesoporous layer to the top of the perovskite layer (i.e. include the thickness of the infiltrated mesoporous layer)

Concern. A category with a lot of uncertainty. The practice of deposition on mesoporous substrates make direct comparisons harder

Perovskite_band_gap

Format: Text string
Default: nan
Implemented: In the original data hunt
Description: The band gap of the perovskite

- If the perovskite contains more than one layer, separate the band gaps for the respective layer by a space, a vertical bar, and a space, i.e. (' | ')
- If there are uncertainties, state the best estimate, e.g. write 1.62 and not 1.6-1.64

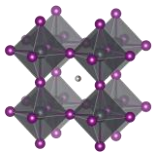
Concern. When values have not been stated, default values have been used for $MAPbI_3$ and $FAPbI_3$

Perovskite_band_gap_graded

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: After the initial data hunt but before initial release
Description: TRUE if the band gap varies as a function of the vertical position in the perovskite layer.

Perovskite_band_gap_estimation_basis

Format: Text string. [Absorption/Composition/Literature/EQE/…]
Default: nan
Implemented: In the original data hunt
Description: The method by which the band gap was estimated. The band gap can be estimated from absorption data, EQE-data, UPS-data, or it can be estimated based on literature values for the recipe, or it could be inferred from the composition and what we know of similar but not identical compositions.



Perovskite_pl_max

Format: Text string. [PL.1; PL.2; … | PL.3; … | ...] [nm]
Default: nan
Implemented: In the original data hunt
Description: The maximum from steady-state PL measurements

- If more than one PL-max, separate those by a semicolon

Perovskite deposition

Perovskite_deposition_number_of_deposition_steps

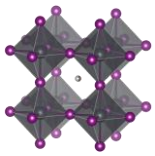
Format: Integer
Default: 0
Implemented: In the original data hunt
Description: The number of production steps involved in making the perovskite-stack

- A spin coating program that are composed of several segments with different spin speed are still counted as one step (1)
- A spin coating program involving an antisolvent step counts as a 1-step method (1).
- Depositing PbI_2 first and subsequently converting it to a perovskite count as a 2-step procedure (2)
- Thermal annealing is considered separately. The motivation for this is that every step is considered to have its own thermal history.

Perovskite_deposition_procedure

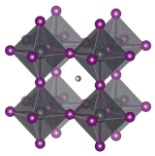
Format: Text string. [Proc. 1 >> Proc. 2 >> ... | Proc. 3 >> … | Proc. 4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The deposition procedures for the perovskite block.

- The perovskite stack is considered as one block/layer when we consider the synthesis. Thus, even if the perovskite is layered, consider it as one block, i.e. no vertical bars in this field
- When more than one reaction step, separate them by a double forward angel bracket with one blank space on both sides (' >> ')
- There should be as many reaction steps described here as indicated in the field "Perovskite. Deposition. Number of deposition steps"
- Thermal annealing is generally not considered as an individual reaction step. The philosophy behind this is that every deposition step has a thermal history, which is specified in a separate filed. In exceptional cases with thermal annealing procedures clearly disconnected from other procedures, state 'Thermal annealing' as a separate reaction step.
- Antisolvent treatment is considered in a separate filed. The motivation for that is that it usually is conducted simultaneously as a spin-coating procedure, and thus acts as an additional aspect of reaction step already accounted for. Exception to this is if there is an antisolvent step that is distinctly separated in time, e.g. a film with a spin-coated perovskite solution is immersed in an antisolvent. In that case, this could be added as a dipp-coating event, while also being reported in the antisolvent field.
- Even if the most common deposition procedures have been used for 95 % of all reported devise, do not be surprised if you do not find your deposition procedure in the list of reported deposition procedure, as the original dataset tended to use a simplified notation.
- A few clarifications
- Air brush spray
    - Deposition with something looking like an old perfume bottle. Classified as a solution technique.
- Brush painting
    - A precursor ink is applied with a brush
- CBD:



- Chemical bath deposition. Refers to procedures where a film has been immersed in a solution where a reaction occurs. The typical example is when a PbI_2 film is immerse in an IPA solution with MAI in which the PbI_2 is converted to the perovskite.

- Co-evaporation
  - Simultaneous evaporation from multiple sources with line of sight deposition.
- CVD
  - Chemical vapour deposition. A gas phase process where a chemical reaction is occurring in the gas phase. If a MA-containing compound is evaporated and reacted with PbI_2 where another species is released to the gas phase, it is labelled as CVD. A process where MAI in gas phase react with PbI_2 in gas phase is labelled as CVD. A process where MAI or MA gas is reacting with solid PbI_2 is instead labelled as a gas reaction as no chemical reaction is occurring the gas phase. Note that all reactions labelled as CVD in the literature may not be CVD even if it is conducted in a CVD reactor, and should instead be labelled as a gas reaction.
- Diffusion
  - Solid state reaction where two solid components are mixed. E.g. solid MAI is bought in direct contact with solid PbI_2
- Diffusion-gas reaction
  - A special case. Where one compound, e.g. MAI is placed on top of another e.g. PbI_2 where it is evaporated. It is thus a combination of a gas phase reaction and solid-solid diffusion.
- Dipp-coating
  - The thing that separates dipp-coating from CBD is the occurrence of a reaction. If you have component A in solution, dip your substrate in the solution, take it up and you have component A on your substrate, then you have done a dipp-coating. If you have substance A in solution, dip your substrate in the solution, take it up and have something else than A on your substrate, you have done a CBD (e.g. PbI_2 dipped in MAI/IPA which gives $MAPbI_3$ and not MAI on the substrate)
- Dropcasting
  - A drop is applied to a substrate where it is left to dry without any additional procedures.
- Drop-infiltration
  - A mesoporous scaffold in which a drop of the precursor solution is infiltrated without the aid of spin-coating.
- Doctor blading:
  - There is a family of related techniques, but if it could be described as doctor blading, that is the label to use.
- Evaporation
  - Refers to thermal evaporation with line-of-sigh deposition. i.e. PVD
- Flash evaporation
  - Fast evaporation (in a flash) of a perovskite that sublimes on another substrate. Line of sight deposition.
- Closed space sublimation
  - Evaporation of a well controlled amount of substance (usually in the form of a thin film) in a small container containing the final substrate.
- Gas reaction
  - A gas phase reaction. **Not** a line of sight deposition. In the typical case, MAI is evaporated and the MAI gas builds up a pressure in the reaction chamber in which it reacts with a PbI_2 film forming the perovskite.
- Ion exchange
  - One perovskite is dipped into a solution (or exposed to a gas) which leads to an ion exchange, e.g. I is replaced by Br.
- Lamination
  - A readymade film is transferred directly to the device stack. A rather broad concept. An everyday kitchen related example of lamination would eb to place a thin plastic film over a slice of pie.



- Recrystallization
  - A perovskite that already have been formed is deformed and then recrystallised. E.g. $MAPbI_3$ is exposed to Methylamine gas for a short while which dissolved the perovskite which then can crystallize again
- Rinsing
  - Cleaning step with a solvent
- Sandwiching
  - When a readymade top stack simply is placed on top of the device stack. Could be held together with clams.
- Ultrasonic spray
  - A bit like air brush spray but with better control of droplet size. Classified as a solution technique.

Perovskite_deposition_aggregation_state_of_reactants

Format: Text string.) [Agr. 1 >> Agr. 2 >> … | Agr. 3 >> … | Agr. 4 | …]
Default: "Unknown"
Implemented: In the original data hunt
Description: The physical state of the reactants

- The three basic categories are Solid/Liquid/Gas
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the aggregation state associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- Most cases are clear cut, e.g. spin-coating involves species in solution and evaporation involves species in gas phase. For less clear-cut cases, consider where the reaction really is happening as in:
  - For a spray-coating procedure, it is droplets of liquid that enters the substrate (thus a liquid phase reaction)
  - For sputtering and thermal evaporation, it is species in gas phase that reaches the substrate (thus a gas phase reaction)

Perovskite_deposition_synthesis_atmosphere

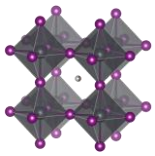
Format: Text string. [Gas1; Gas2 >> Gas3; … >> … | Gas4 >> … | Gas5 | …]
Default: "Unknown"
Implemented: In the original data hunt
Description: The synthesis atmosphere

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas

Perovskite_deposition_synthesis_atmosphere_pressure_total

Format: Text string. [P.1 >> P.2 >> … | P.3 >> … | P.4 | …] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total pressure during each synthesis step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')



- The number and order of layers and deposition steps must line up with the previous columns.
- Pressures can be stated in different units suited for different situations. Therefore, specify the unit. The preferred units are:
    - atm, bar, mbar, mmHg, Pa, torr, psi
- If a pressure is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 100 pa and not 80-120 pa.

Perovskite_deposition_synthesis_atmosphere_pressure_partial

Format: Text string. [P.1; P.2 >> P.3 >> ... | P.4 >> … | P.5 | ...] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The partial pressures for the gases present during each reaction step.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the partial pressures and separate them with semicolons, as in (A; B). The list of partial pressures must line up with the gases they describe.
- In cases where no gas mixtures are used, this field will be the same as the previous filed.

Perovskite_deposition_synthesis_atmosphere_relative_humidity

Format: Text string. [RH1 >> RH2 >> ... | RH3 >> … | RH4 | ...] [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relative humidity during each deposition step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the relative humidity associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns
- If the relative humidity for a step is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 35 and not 30-40.

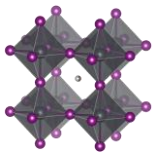
Perovskite_deposition_solvents

Format: Text string. [Sol.1; Sol.2 >> Sol.3; ... >> ... | Sol.4 >> … | Sol.5 | ...]
Default: nan
Implemented: In the original data hunt
Description: The solvents used in each deposition procedure for each layer in the stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvents associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the solvents in alphabetic order and separate them with semicolons, as in (A; B)
- The number and order of layers and deposition steps must line up with the previous columns.
- For non-liquid processes with no solvents, state the solvent as 'none'
- If the solvent is not known, state this as 'Unknown'
- Use common abbreviations when appropriate but spell it out when risk for confusion

Perovskite_deposition_solvents_mixing_ratios

Format: Text string. [V1; V2 >> V3; V4 >> ... | V5; V6 >> … | 1 | ...]
Default: nan
Implemented: In the original data hunt



Description: The mixing ratios for mixed solvents

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent mixing ratios associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- For pure solvents, state the mixing ratio as 1
- For non-solvent processes, state the mixing ratio as 1
- For unknown mixing ratios, state the mixing ratio as 'nan'
- For solvent mixtures, i.e. A and B, state the mixing ratios by using semicolons, as in (V_A; V_B)
- The preferred metrics is the volume ratios. If that is not available, mass or mol ratios can be used instead, but it the analysis the mixing ratios will be assumed to be based on volumes.

Perovskite_deposition_solvents_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of all the solvents.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For non-liquid processes with no solvents, mark the supplier as 'none'
- If the supplier for a solvent is unknown, state this as 'Unknown'

Perovskite_deposition_solvents_purity

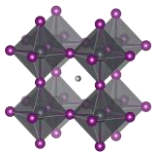
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the solvents used.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For non-liquid processes with no solvents, state the purity as 'none'
- If the purity for a solvent is not known, state this as 'Unknown'

Perovskite_deposition_reaction_solutions_compounds

Format: Text string. [C1; C2 >> C3; … >> … | C4; C5 | C6 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The non-solvent precursor chemicals used in each reaction step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemicals associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')



- If a solution contains several compounds, e.g. A and B, list the associated compounds in alphabetic order and separate them with semicolons, as in (A; B)
- Note that also dopants/additives should be included
- When several precursor solutions are made and mixed before the reaction step, it is the properties of the final mixture used in the reaction we here describe.
- The number and order of layers and reaction steps must line up with the previous columns.
- For gas phase reactions, state the reaction gases as if they were in solution.
- For solid-state reactions, state the compounds as if they were in solution.
- For reaction steps involving only pure solvents, state this as 'none'
- If the compounds for a deposition step is not known, state this as 'Unknown'

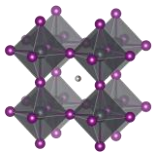
Perovskite_deposition_reaction_solutions_compounds_supplier
Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemical suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For gas phase reactions, state the suppliers for the gases or the targets/evaporation sources that are evaporated/sputtered/etc.
- For solid state reactions, state the suppliers for the compounds in the same way.
- For reaction steps involving only pure solvents, state the supplier as 'none' (as that that is entered in a separate filed)
- For chemicals that are lab made, state that as "Lab made" or "Lab made (name of lab)"
- If the supplier for a compound is unknown, state this as 'Unknown'

Perovskite_deposition_reaction_solutions_compounds_purity
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the compound purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, i.e. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For reaction steps involving only pure solvents, state this as 'none' (as that is stated in another field)
- If the purity for a compound is not known, state this as 'Unknown'

Perovskite_deposition_reaction_solutions_concentrations
Format: Text string. [c1 M; c2 mol/dm3 >> c3 mg/ml; … >> ... | c4 wt%; c5 vol% | c6 ppm |...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the non-solvent precursor chemicals.



- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the concentrations associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solution contains several dissolved compounds, e.g. A and B, list the associated concentrations and separate them with semicolons, as in (A; B)
- The order of the compounds must be the same as in the previous filed.
- For reaction steps involving only pure solvents, state this as ‘none’
- When concentrations are unknown, state that as ‘nan’
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used. When possible, use one of the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml, wt%, mol%, vol%, ppt, ppm, ppb
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Perovskite_deposition_reaction_solutions_volumes

Format: Text string. [V1 >> V2 >> … | V3 >> … | V4 | …] [ml]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The volume of the reaction solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the volumes associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The volumes refer the volumes used, not the volume of the stock solutions. Thus if 0.15 ml of a solution is spin-coated, the volume is 0.15 ml
- For reaction steps without solvents, state the volume as ‘nan’
- When volumes are unknown, state that as ‘nan’

Perovskite_deposition_reaction_solutions_age

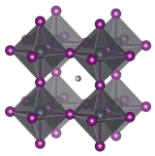
Format: Text string. [A1 >> A2 >> … | A3 >> … | A4 | …] [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the age of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- As a general guideline, the age refers to the time from the preparation of the final precursor mixture to the reaction procedure.
- When the age of a solution is not known, state that as ‘nan’
- For reaction steps where no solvents are involved, state this as ‘nan’
- For solutions that are stored a long time, an order of magnitude estimate is adequate.

Perovskite_deposition_reaction_solutions_temperature

Format: Text string. [A1 >> A2 >> … | A3 >> … | A4 | …] [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the age of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- As a general guideline, the age refers to the time from the preparation of the final precursor mixture to the reaction procedure.
- When the age of a solution is not known, state that as ‘nan’
- For reaction steps where no solvents are involved, state this as ‘nan’



- For solutions that are stored a long time, an order of magnitude estimate is adequate.

Perovskite_deposition_substrate_temperature

Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the substrate.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the temperatures of the substrates (i.e. the last deposited layer) associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The temperature of the substrate refers to the temperature when the deposition of the layer is occurring.
- If a substrate undergoes a temperature program before the deposition, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- When the temperature of a substrate is not known, state that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume that an undetermined room temperature is 25

Perovskite_deposition_quenching_induced_crystallisation

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE is measures were taken to discontinuously accelerate the crystallisation process without significantly changing the temperature. i.e. an antisolvent treatment or an analogue process was used.

- The most common case is the antisolvent treatment where a volume of a solvent in which the perovskite is not soluble is poured on the substrate during spin coating.
- The same effect can also be achieved by blowing a gas on the sample
- If the sample quickly after spin coating is subjected to a vacuum, this also counts as quenched induced crystallisation

Perovskite_deposition_quenching_media

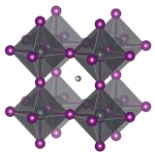
Format: Text string. [Sol.1; Sol.2; …]
Default: 'Unknown'
Implemented: In the original data hunt
Description: The solvents used in the antisolvent treatment

- If the antisolvent is a mixture of different solvents, e.g. A and B, list the solvents in alphabetic order and separate them with semicolons: as in (A; B)
- If gas quenching was used, state the gas used
- If the sample quickly after spin coating was subjected to a vacuum, state this as 'Vacuum'
- If an antisolvent was used but it is unknown which one, stat this as "Antisolvent"
- If no antisolvent was used, leave this field blank

Perovskite_deposition_quenching_media_mixing_ratios

Format: Text string. [V1; V2: ...]
Default: nan
Implemented: In the original data hunt
Description: The mixing ratios of the antisolvent

- The order of the solvent must line up with the previous column
- For solvent mixtures, i.e. A and B, state the mixing ratios by using semicolons, as in (V_A; V_B)
- The preferred metrics is the volume ratios. If that is not available, mass or mol ratios can be used instead, but it the analysis the mixing ratios will be assumed to be based on volumes.



- For pure solvents, give the mixing ratio as 1
- For non-solvent processes, give the mixing ratio as 1

Perovskite_deposition_quenching_media_volume

Format: Text string. [µl]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The volume of the antisolvent

- For gas and vacuum assisted quenching, stat the volume as 'nan'
- If the sample is dipped or soaked in the antisolvent, state the volume of the entire solution

Perovskite_deposition_quenching_media_additives_compounds

Format: Text string. [Addt.1; Addt.2; ...]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: List of the dopants and additives in the antisolvent

- If several dopants/additives, e.g. A and B, are present, list the dopants/additives in alphabetic order and separate them with semicolons: as in (A; B)
- If no dopants/additives, leave the field blank

Perovskite_deposition_quenching_media_additives_concentrations

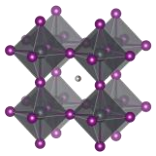
Format: Text string. [c1 M; c2 wt%; c3 mg/ml; ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the dopants/additives in the antisolvent

- If more than one dopant/additive in the layer, e.g. A and B, separate the concentration for each dopant/additive with semicolons, as in (A; B)
- For each dopant/additive, state the concentration.
- The order of the dopants/additives must be the same as in the previous filed.
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used.
- The preferred way to state the concentration of a dopant/additive is to refer to the amount in the final product, i.e. the material in the layer. When possible, use on the preferred units:
    - wt%, mol%, vol%, ppt, ppm, ppb
- When the concentration of the dopant/additive in the final product is unknown, but where the concentration of the dopant/additive in the solution is known, state that concentration instead. When possible, use on the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Perovskite_deposition_thermal_annealing_temperature

Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: In the original data hunt
Implemented: After the initial data hunt but before initial release
Description: The temperatures of the thermal annealing program associated with depositing the layers

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the annealing temperatures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.



- If no thermal annealing is occurring after the deposition of a layer, state that by stating the room temperature (assumed to 25°C if not further specified)
- If the thermal annealing program is not known, state that by 'nan'

Perovskite_deposition_thermal_annealing_time

Format: Text string. [t1; t2 >> t3; ... >> ... | t4 >> … | t5 | ...] [min]
Default: nan
Implemented: In the original data hunt
Implemented: After the initial data hunt but before initial release
Description: The time program associated to the thermal annealing program.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the annealing times associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the associated times at those temperatures and separate them with semicolons.
- The annealing times must align in terms of layers, reaction steps and annealing temperatures in the previous filed.
- If a time is not known, state that by 'nan'
- If no thermal annealing is occurring after the deposition of a layer, state that by 'nan'
- For values with uncertainties, state the best estimate, e.g. write 20 and not 10-30.

Perovskite_deposition_thermal_annealing_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere during thermal annealing

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each annealing step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the atmosphere is a mixture of different gases, i.e. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas.
- This is often the same as the atmosphere under which the deposition is occurring, but not always.

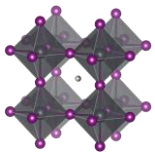
Perovskite_deposition_thermal_annealing_relative_humidity

Format: Text string. [RH1 >> RH2 >> ... | RH3 >> … | RH4 | ...] [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relative humidity during the thermal annealing

- If there is more than one annealing step involved, list the associate relative humidity in the surrounding atmosphere and separate them by a double forward angel bracket (' >> ')
- The number and order of annealing steps must line up with the previous column
- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.
- If a humidity is not known, stat that as 'nan'

Perovskite_deposition_thermal_annealing_pressure

Format: Text string. [P.1 >> P.2 >> ... | P.3 >> … | P.4 | ...] [atm/Torr/Pa/bar/mmHg
Default: nan



Implemented: After the initial data hunt but before initial release
Description: The atmospheric pressure during the thermal annealing

- If there is more than one annealing step involved, list the associate atmospheric pressures and separate them by a double forward angel bracket (' >> ')
- The number and order of annealing steps must line up with the previous column
- Pressures can be stated in different units suited for different situations. Therefore, specify the unit. The preferred units are:
    - atm, bar, mbar, mmHg, Pa, torr, psi
- If a pressure is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 100 pa and not 80-120 pa.

Perovskite_deposition_solvent_annealing

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: During the initial data hunt
Description: TRUE if there has been a separate solvent annealing step, i.e. a step where the perovskite has been annealing in an atmosphere with a significant amount of solvents. This step should also be included deposition procedure sequence but is also stated separately here to simplify downstream filtering.

Perovskite_deposition_solvent_annealing_time_vs_thermal_annealing

Format: Text string. [Before/Under/After/...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The timing of the solvent annealing with respect to the thermal annealing step under which the perovskite is formed. There are three options.

- The solvent annealing is conducted before the perovskite is formed.
- The solvent annealing is conducted under the same annealing step in which the perovskite is formed
- The solvent annealing is conducted after the perovskite has formed.

Perovskite_deposition_solvent_annealing_solvent_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The solvents used in the solvent annealing step

- If the solvent atmosphere is a mixture of different solvents and gases, e.g. A and B, list them in alphabetic order and separate them with semicolons: as in (A; B)

Perovskite_deposition_solvent_annealing_time

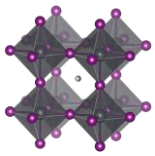
Format: Text string. [t1; t2 >> t3; ... >> ... | t4 >> … | t5 | ...] [min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The extend of the solvent annealing step in minutes

- If the time is not known, state that by 'nan'
- If the solvent annealing involves a temperature program with multiple temperature stages, list the associated times at each temperature and separate them with a semicolon (e.g. 5; 10)

Perovskite_deposition_solvent_annealing_temperature

Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature during the solvent annealing step

- The temperature refers to the temperature of the sample



- If the solvent annealing involves a temperature program with multiple temperature stages, list the associated temperatures and separate them with a semicolon (e.g. 5; 10) and make sure they align with the times in the previous field.
- If the temperature is not known, state that by 'nan'

Perovskite_deposition_after_treatment_of_formed_perovskite
Format: Text string
Default: nan
Implemented: In the original data hunt
Description: Any after treatment of the formed perovskite. Most possible reaction steps should have been entered before this point. This is an extra category for procedures that just does not fit into any of the other categories.

Perovskite_deposition_after_treatment_of_formed_perovskite_metrics
Format: Text string
Default: nan
Implemented: After the initial data hunt but before initial release
Description: Connected to the previous field (After treatment of formed perovskite). The label describing the method should be in the previous filed, and the associated metrics in this one. For example: The sample is intense gamma radiation at a flux of X under 45 minutes. The "gamma radiation" is the label, and the time and the flux is the metrics. Give the units when you state the metrics

Perovskite_storage_time_until_next_deposition_step
Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time between the HTL stack is finalised and the next layer is deposited

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

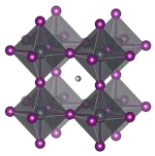
Perovskite_storage_atmosphere
Format: Text string. [Gas1; Gas2; ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the sample with the finalised HTL stack is stored until the next deposition step.

Perovskite_storage_relative_humidity
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relive humidity under which the sample with the finalised HTL stack is stored until next deposition step

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

Perovskite_surface_treatment_before_next_deposition_step
Format: Text string
Default: nan
Implemented: After the initial data hunt but before initial release
Description: Description of any type of surface treatment or other treatment the sample with the finalised ETL-stack undergoes before the next deposition step.

- If more than one treatment, list the treatments and separate them by a double forward angel bracket (' >> ')
- If no special treatment, state that as 'none'



Hole transport layer

HTL_stack_sequence

Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The stack sequence describing the hole transport layer. Use the following formatting guidelines

- With the HTL, we refer to any layer between the substrate and the perovskite in a pin-device, and any layer between the perovskite and the back contact in a nip-device.
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- If no hole transport layer, state that as 'non'
- Use common abbreviations when appropriate but spell it out if risk for confusion.
- If a material is doped, or have an additive, state the pure material here and specify the doping in the columns specifically targeting the doping of those layers.
- There is no sharp well-defined boundary between when a material is best considered as doped or as a mixture of two materials. When in doubt if your material is best described as doped or as a mixture, use the notation that best capture the metaphysical essence of the situation.

HTL_thickness_list

Format: Text string. [Th.1 | Th.2 | … | Th.n] [nm]
Default: nan
Implemented: In the original data hunt
Description: A list of thicknesses of the individual layers in the stack. Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')

- The layers must line up with the previous filed.
- State thicknesses in nm
- Every layer in the stack has a thickness. If it is unknown, state this as 'nan'
- If there are uncertainties, state the best estimate, e.g. write 100 and not 90-110

HTL_additives_compounds

Format: Text string. [Addt.1; Addt.2; ... | Addt.3; … | Addt.4 | ...]
Default: Empty text string
Implemented: In the original data hunt
Description: List of the dopants and additives that are in each layer of the HTL-stack

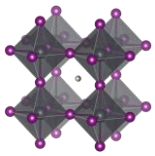
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- The layers must line up with the previous fields.
- If several dopants/additives, e.g. A and B, are present in one layer, list the dopants/additives in alphabetic order and separate them with semicolons, as in (A; B)
- If no dopants/additives, state that as "Undoped"
- If the doping situation is unknown, stat that as: 'Unknown'

Concerns: This is a category with a lot of uncertainty. Historically a lot of dopants have not been added properly. A blank field may thus not guarantee that the layer was undoped.

HTL_additives_concentrations

Format: Text string. [c1 M; c2 wt%; … | c3 vol%; ... | c4 mg/ml | ...]
Default: nan
Implemented: In the original data hunt
Description: The concentration of the dopants/additives.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If more than one dopant/additive in the layer, e.g. A and B, separate the concentration for each dopant/additive with semicolons, as in (A; B)



- For each dopant/additive in the layer, state the concentration.
- The order of the dopants/additives must be the same as in the previous filed.
- For layers with no dopants/additives, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used.
- The preferred way to state the concentration of a dopant/additive is to refer to the amount in the final product, i.e. the material in the layer. When possible, use on the preferred units:
    - wt%, mol%, vol%, ppt, ppm, ppb
- When the concentration of the dopant/additive in the final product is unknown, but where the concentration of the dopant/additive in the solution is known, state that concentration instead. When possible, use on the preferred units:
    - M, mM, molal; g/ml, mg/ml, μg/ml
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Concerns. In the initial instructions, concentrations should be stated as fraction of total amount, but that was ambiguous and was interpreted differently.

HTL_deposition_procedure

Format: Text string. [Proc. 1 >> Proc. 2 >> ... | Proc. 3 >> … | Proc. 4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The deposition procedures for the HTL stack.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate them by a double forward angel bracket with one blank space on both sides (' >> ')
- Thermal annealing is generally not considered as an individual reaction step. The philosophy behind this is that every deposition step has a thermal history, which is specified in a separate filed. In exceptional cases with thermal annealing procedures clearly disconnected from other procedures, state 'Thermal annealing' as a separate reaction step.
- Please read the instructions under "*Perovskite. Deposition. Procedure*" for descriptions and distinctions between common deposition procedures and how they should be labelled for consistency in the database.

Concerns. Much effort was put to make this correct in the original dataset, but it happens that we have misunderstood the descriptions in the original publications.

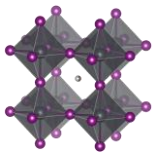
HTL_deposition_aggregation_state_of_reactants

Format: Text string.) [Agr. 1 >> Agr. 2 >> ... | Agr. 3 >> … | Agr. 4 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The physical state of the reactants

- The three basic categories are Solid/Liquid/Gas
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the aggregation state associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- Most cases are clear cut, e.g. spin-coating involves species in solution and evaporation involves species in gas phase. For less clear-cut cases, consider where the reaction really is happening as in:
    - For a spray-coating procedure, it is droplets of liquid that enters the substrate (thus a liquid phase reaction)
    - For sputtering and thermal evaporation, it is species in gas phase that reaches the substrate (thus a gas phase reaction)

HTL_deposition_synthesis_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]



Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The synthesis atmosphere

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

HTL_deposition_synthesis_atmosphere_pressure_total

Format: Text string. [P.1 >> P.2 >> ... | P.3 >> … | P.4 | ...] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total pressure during each synthesis step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- Pressures can be stated in different units suited for different situations. Therefore, specify the unit. The preferred units are:
    - atm, bar, mbar, mmHg, Pa, torr, psi
- If a pressure is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 100 pa and not 80-120 pa.

HTL_deposition_synthesis_atmosphere_pressure_partial

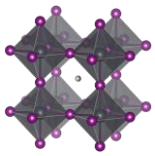
Format: Text string. [P.1; P.2 >> P.3 >> ... | P.4 >> … | P.5 | ...] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The partial pressures for the gases present during each reaction step.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the partial pressures and separate them with semicolons, as in (A; B). The list of partial pressures must line up with the gases they describe.
- In cases where no gas mixtures are used, this field will be the same as the previous filed.

HTL_deposition_synthesis_atmosphere_relative_humidity

Format: Text string. [RH1 >> RH2 >> ... | RH3 >> … | RH4 | ...] [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relative humidity during each deposition step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')



- When more than one reaction step, separate the relative humidity associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns
- If the relative humidity for a step is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 35 and not 30-40.

HTL_deposition_solvents

Format: Text string. [Sol.1; Sol.2 >> Sol.3; ... >> ... | Sol.4 >> … | Sol.5 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The solvents used in each deposition procedure for each layer in the stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvents associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the solvents in alphabetic order and separate them with semicolons, as in (A; B)
- The number and order of layers and deposition steps must line up with the previous columns.
- For non-liquid processes with no solvents, state the solvent as 'none'
- If the solvent is not known, state this as 'Unknown'
- Use common abbreviations when appropriate but spell it out when risk for confusion
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

HTL_deposition_solvents_mixing_ratios

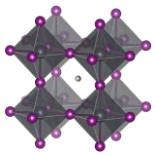
Format: Text string. [V1; V2 >> V3; V4 >> ... | V5; V6 >> … | 1 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The mixing ratios for mixed solvents

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent mixing ratios associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- For pure solvents, state the mixing ratio as 1
- For non-solvent processes, state the mixing ratio as 1
- For unknown mixing ratios, state the mixing ratio as 'nan'
- For solvent mixtures, i.e. A and B, state the mixing ratios by using semicolons, as in (V_A; V_B)
- The preferred metrics is the volume ratios. If that is not available, mass or mol ratios can be used instead, but it the analysis the mixing ratios will be assumed to be based on volumes.

HTL_deposition_solvents_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of all the solvents.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For non-liquid processes with no solvents, mark the supplier as 'none'



- If the supplier for a solvent is unknown, state this as 'Unknown'

HTL_deposition_solvents_purity

Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the solvents used.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For non-liquid processes with no solvents, state the purity as 'none'
- If the purity for a solvent is not known, state this as 'Unknown'

HTL_deposition_reaction_solutions_compounds

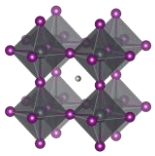
Format: Text string. [C1; C2 >> C3; … >> … | C4; C5 | C6 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The non-solvent precursor chemicals used in each reaction step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemicals associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several compounds, e.g. A and B, list the associated compounds in alphabetic order and separate them with semicolons, as in (A; B)
- Note that also dopants/additives should be included
- When several precursor solutions are made and mixed before the reaction step, it is the properties of the final mixture used in the reaction we here describe.
- The number and order of layers and reaction steps must line up with the previous columns.
- For gas phase reactions, state the reaction gases as if they were in solution.
- For solid-state reactions, state the compounds as if they were in solution.
- For reaction steps involving only pure solvents, state this as 'none'
- If the compounds for a deposition step is not known, state this as 'Unknown'

HTL_deposition_reaction_solutions_compounds_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemical suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For gas phase reactions, state the suppliers for the gases or the targets/evaporation sources that are evaporated/sputtered/etc.
- For solid state reactions, state the suppliers for the compounds in the same way.



- For reaction steps involving only pure solvents, state the supplier as 'none' (as that that is entered in a separate filed)
- For chemicals that are lab made, state that as "Lab made" or "Lab made (name of lab)"
- If the supplier for a compound is unknown, state this as 'Unknown'

HTL_deposition_reaction_solutions_compounds_purity

Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the compound purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, i.e. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For reaction steps involving only pure solvents, state this as 'none' (as that is stated in another field)
- If the purity for a compound is not known, state this as 'Unknown'

HTL_deposition_reaction_solutions_concentrations

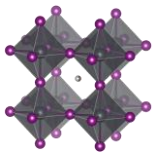
Format: Text string. [c1 M; c2 mol/dm3 >> c3 mg/ml; … >> ... | c4 wt%; c5 vol% | c6 ppm |...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the non-solvent precursor chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the concentrations associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated concentrations and separate them with semicolons, as in (A; B)
- The order of the compounds must be the same as in the previous filed.
- For reaction steps involving only pure solvents, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used. When possible, use one of the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml, wt%, mol%, vol%, ppt, ppm, ppb
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

HTL_deposition_reaction_solutions_volumes

Format: Text string. [V1 >> V2 >> ... | V3 >> … | V4 | ...] [ml]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The volume of the reaction solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the volumes associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The volumes refer the volumes used, not the volume of the stock solutions. Thus if 0.15 ml of a solution is spin-coated, the volume is 0.15 ml
- For reaction steps without solvents, state the volume as 'nan'
- When volumes are unknown, state that as 'nan'



HTL_deposition_reaction_solutions_age

Format: Text string. [A1 >> A2 >> … | A3 >> … | A4 | …] [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the age of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- As a general guideline, the age refers to the time from the preparation of the final precursor mixture to the reaction procedure.
- When the age of a solution is not known, state that as ‘nan’
- For reaction steps where no solvents are involved, state this as ‘nan’
- For solutions that are stored a long time, an order of magnitude estimate is adequate.

HTL_deposition_reaction_solutions_temperature

Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the reaction solutions.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the temperatures of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a reaction solution undergoes a temperature program, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons, e.g. 25; 100
- When the temperature of a solution is unknown, state that as ‘nan’
- For reaction steps where no solvents are involved, state the temperature of the gas or the solid if that make sense. Otherwise state this as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume an undetermined room temperature to be 25

HTL_deposition_substrate_temperature

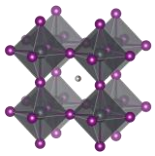
Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the substrate.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the temperatures of the substrates (i.e. the last deposited layer) associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The temperature of the substrate refers to the temperature when the deposition of the layer is occurring.
- If a substrate undergoes a temperature program before the deposition, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- When the temperature of a substrate is not known, state that as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume that an undetermined room temperature is 25

HTL_deposition_thermal_annealing_temperature

Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperatures of the thermal annealing program associated with depositing the layers

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)



- When more than one reaction step, separate the annealing temperatures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- If no thermal annealing is occurring after the deposition of a layer, state that by stating the room temperature (assumed to 25°C if not further specified)
- If the thermal annealing program is not known, state that by 'nan'

HTL_deposition_thermal_annealing_time

Format: Text string. [t1; t2 >> t3; ... >> ... | t4 >> … | t5 | ...] [min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time program associated to the thermal annealing program.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the annealing times associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the associated times at those temperatures and separate them with semicolons.
- The annealing times must align in terms of layers, reaction steps and annealing temperatures in the previous filed.
- If a time is not known, state that by 'nan'
- If no thermal annealing is occurring after the deposition of a layer, state that by 'nan'
- For values with uncertainties, state the best estimate, e.g. write 20 and not 10-30.

HTL_deposition_thermal_annealing_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere during thermal annealing

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each annealing step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the atmosphere is a mixture of different gases, i.e. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas.
- This is often the same as the atmosphere under which the deposition is occurring, but not always.

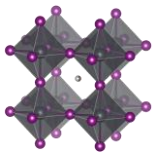
HTL_storage_time_until_next_deposition_step

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time between the HTL stack is finalised and the next layer is deposited

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

HTL_storage_atmosphere

Format: Text string. [Gas1; Gas2; ...]



Default: “Unknown”
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the sample with the finalised HTL stack is stored until the next deposition step.

HTL_storage_relative_humidity

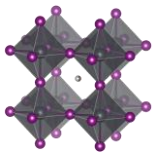
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relive humidity under which the sample with the finalised HTL stack is stored until next deposition step

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

HTL_surface_treatment_before_next_deposition_step

Format: Text string
Default: nan
Implemented: After the initial data hunt but before initial release
Description: Description of any type of surface treatment or other treatment the sample with the finalised HTL-stack undergoes before the next deposition step.

- If more than one treatment, list the treatments and separate them by a double forward angel bracket (‘ >> ‘)
- If no special treatment, state that as ‘none’



Back contact

Backcontact_stack_sequence

Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The stack sequence describing the electron transport layer. Use the following formatting guidelines

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- If no electron transport layer, state that as 'non'
- Use common abbreviations when appropriate but spell it out if risk for confusion.
- If a material is doped, or have an additive, state the pure material here and specify the doping in the columns specifically targeting the doping of those layers.
- There is no sharp well-defined boundary between when a material is best considered as doped or as a mixture of two materials. When in doubt if your material is best described as doped or as a mixture, use the notation that best capture the metaphysical essence of the situation.

Concerns. Where to draw the line between which layers tat are a part of the HTL-stack and part of the Backcontact layer stack is somewhat arbitrary

Backcontact_thickness

Format: Text string. [Th.1 | Th.2 | … | Th.n] [nm]
Default: nan
Implemented: In the original data hunt
Description: A list of thicknesses of the individual layers in the stack. Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')

- The layers must line up with the previous filed.
- State thicknesses in nm
- Every layer in the stack has a thickness. If it is unknown, state this as 'nan'
- If there are uncertainties, state the best estimate, e.g. write 100 and not 90-110

Backcontact_additives_compounds

Format: Text string. [Addt.1; Addt.2; ... | Addt.3; … | Addt.4 | ...]
Default: Empty text string
Implemented: In the original data hunt
Description: List of the dopants and additives that are in each layer of the Backcontact-stack

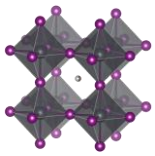
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- The layers must line up with the previous fields.
- If several dopants/additives, e.g. A and B, are present in one layer, list the dopants/additives in alphabetic order and separate them with semicolons, as in (A; B)
- If no dopants/additives, state that as "Undoped"
- If the doping situation is unknown, stat that as: 'Unknown'

Concerns: Back contacts are seldom doped

Backcontact_additives_concentrations

Format: Text string. [c1 M; c2 wt%; … | c3 vol%; ... | c4 mg/ml | ...]
Default: nan
Implemented: In the original data hunt
Description: The concentration of the dopants/additives.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If more than one dopant/additive in the layer, e.g. A and B, separate the concentration for each dopant/additive with semicolons, as in (A; B)
- For each dopant/additive in the layer, state the concentration.



- The order of the dopants/additives must be the same as in the previous filed.
- For layers with no dopants/additives, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used.
- The preferred way to state the concentration of a dopant/additive is to refer to the amount in the final product, i.e. the material in the layer. When possible, use on the preferred units:
    - wt%, mol%, vol%, ppt, ppm, ppb
- When the concentration of the dopant/additive in the final product is unknown, but where the concentration of the dopant/additive in the solution is known, state that concentration instead. When possible, use on the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Concerns. In the initial instructions, concentrations should be stated as fraction of total amount, but that was ambiguous and was interpreted differently. Most back contacts are however evaporated metal contacts.

Backcontact_deposition_procedure

Format: Text string. [Proc. 1 >> Proc. 2 >> ... | Proc. 3 >> … | Proc. 4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The deposition procedures for the Backcontact stack.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate them by a double forward angel bracket with one blank space on both sides (' >> ')
- Thermal annealing is generally not considered as an individual reaction step. The philosophy behind this is that every deposition step has a thermal history, which is specified in a separate filed. In exceptional cases with thermal annealing procedures clearly disconnected from other procedures, state 'Thermal annealing' as a separate reaction step.
- Please read the instructions under "*Perovskite. Deposition. Procedure*" for descriptions and distinctions between common deposition procedures and how they should be labelled for consistency in the database.

Concerns. Much effort was put to make this correct in the original dataset, but it happens that we have misunderstood the descriptions in the original publications.

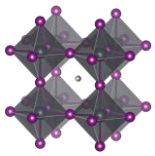
Backcontact_deposition_aggregation_state_of_reactants

Format: Text string.) [Agr. 1 >> Agr. 2 >> ... | Agr. 3 >> … | Agr. 4 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The physical state of the reactants

- The three basic categories are Solid/Liquid/Gas
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the aggregation state associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- Most cases are clear cut, e.g. spin-coating involves species in solution and evaporation involves species in gas phase. For less clear-cut cases, consider where the reaction really is happening as in:
    - For a spray-coating procedure, it is droplets of liquid that enters the substrate (thus a liquid phase reaction)
    - For sputtering and thermal evaporation, it is species in gas phase that reaches the substrate (thus a gas phase reaction)

Backcontact_deposition_synthesis_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]



Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The synthesis atmosphere

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas

Backcontact_deposition_synthesis_atmosphere_pressure_total

Format: Text string. [P.1 >> P.2 >> ... | P.3 >> … | P.4 | ...] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total pressure during each synthesis step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- Pressures can be stated in different units suited for different situations. Therefore, specify the unit. The preferred units are:
    - atm, bar, mbar, mmHg, Pa, torr, psi
- If a pressure is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 100 pa and not 80-120 pa.

Backcontact_deposition_synthesis_atmosphere_pressure_partial

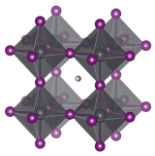
Format: Text string. [P.1; P.2 >> P.3 >> ... | P.4 >> … | P.5 | ...] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The partial pressures for the gases present during each reaction step.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the partial pressures and separate them with semicolons, as in (A; B). The list of partial pressures must line up with the gases they describe.
- In cases where no gas mixtures are used, this field will be the same as the previous filed.

Backcontact_deposition_synthesis_atmosphere_relative_humidity

Format: Text string. [RH1 >> RH2 >> ... | RH3 >> … | RH4 | ...] [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relative humidity during each deposition step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the relative humidity associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns
- If the relative humidity for a step is not known, stat that as 'nan'



- For values with uncertainties, state the best estimate, e.g. write 35 and not 30-40.

Backcontact_deposition_solvents

Format: Text string. [Sol.1; Sol.2 >> Sol.3; ... >> ... | Sol.4 >> … | Sol.5 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The solvents used in each deposition procedure for each layer in the stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvents associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the solvents in alphabetic order and separate them with semicolons, as in (A; B)
- The number and order of layers and deposition steps must line up with the previous columns.
- For non-liquid processes with no solvents, state the solvent as 'none'
- If the solvent is not known, state this as 'Unknown'
- Use common abbreviations when appropriate but spell it out when risk for confusion

Backcontact_deposition_solvents_mixing_ratios

Format: Text string. [V1; V2 >> V3; V4 >> ... | V5; V6 >> … | 1 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The mixing ratios for mixed solvents

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent mixing ratios associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- For pure solvents, state the mixing ratio as 1
- For non-solvent processes, state the mixing ratio as 1
- For unknown mixing ratios, state the mixing ratio as 'nan'
- For solvent mixtures, i.e. A and B, state the mixing ratios by using semicolons, as in (V_A; V_B)
- The preferred metrics is the volume ratios. If that is not available, mass or mol ratios can be used instead, but it the analysis the mixing ratios will be assumed to be based on volumes.

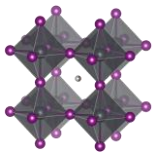
Backcontact_deposition_solvents_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of all the solvents.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For non-liquid processes with no solvents, mark the supplier as 'none'
- If the supplier for a solvent is unknown, state this as 'Unknown'

Backcontact_deposition_solvents_purity

Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release



Description: The purity of the solvents used.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the solvent purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For non-liquid processes with no solvents, state the purity as ‘none’
- If the purity for a solvent is not known, state this as ‘Unknown’

Backcontact_deposition_reaction_solutions_compounds

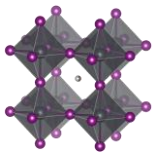
Format: Text string. [C1; C2 >> C3; … >> … | C4; C5 | C6 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The non-solvent precursor chemicals used in each reaction step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the non-solvent chemicals associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solution contains several compounds, e.g. A and B, list the associated compounds in alphabetic order and separate them with semicolons, as in (A; B)
- Note that also dopants/additives should be included
- When several precursor solutions are made and mixed before the reaction step, it is the properties of the final mixture used in the reaction we here describe.
- The number and order of layers and reaction steps must line up with the previous columns.
- For gas phase reactions, state the reaction gases as if they were in solution.
- For solid-state reactions, state the compounds as if they were in solution.
- For reaction steps involving only pure solvents, state this as ‘none’
- If the compounds for a deposition step is not known, state this as ‘Unknown’

Backcontact_deposition_reaction_solutions_compounds_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: ‘Unknown’
Implemented: After the initial data hunt but before initial release
Description: The suppliers of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the non-solvent chemical suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solution contains several dissolved compounds, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For gas phase reactions, state the suppliers for the gases or the targets/evaporation sources that are evaporated/sputtered/etc.
- For solid state reactions, state the suppliers for the compounds in the same way.
- For reaction steps involving only pure solvents, state the supplier as ‘none’ (as that that is entered in a separate filed)
- For chemicals that are lab made, state that as “Lab made” or “Lab made (name of lab)”
- If the supplier for a compound is unknown, state this as ‘Unknown’



Backcontact_deposition_reaction_solutions_compounds_purity

Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the compound purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, i.e. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For reaction steps involving only pure solvents, state this as 'none' (as that is stated in another field)
- If the purity for a compound is not known, state this as 'Unknown'

Backcontact_deposition_reaction_solutions_concentrations

Format: Text string. [c1 M; c2 mol/dm3 >> c3 mg/ml; … >> ... | c4 wt%; c5 vol% | c6 ppm |...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the non-solvent precursor chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the concentrations associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated concentrations and separate them with semicolons, as in (A; B)
- The order of the compounds must be the same as in the previous filed.
- For reaction steps involving only pure solvents, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used. When possible, use one of the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml, wt%, mol%, vol%, ppt, ppm, ppb
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Backcontact_deposition_reaction_solutions_volumes

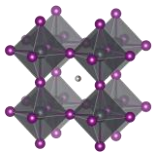
Format: Text string. [V1 >> V2 >> ... | V3 >> … | V4 | ...] [ml]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The volume of the reaction solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the volumes associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The volumes refer the volumes used, not the volume of the stock solutions. Thus if 0.15 ml of a solution is spin-coated, the volume is 0.15 ml
- For reaction steps without solvents, state the volume as 'nan'
- When volumes are unknown, state that as 'nan'

Backcontact_deposition_reaction_solutions_age

Format: Text string. [A1 >> A2 >> ... | A3 >> … | A4 | ...] [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')



- When more than one reaction step, separate the age of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- As a general guideline, the age refers to the time from the preparation of the final precursor mixture to the reaction procedure.
- When the age of a solution is not known, state that as 'nan'
- For reaction steps where no solvents are involved, state this as 'nan'
- For solutions that are stored a long time, an order of magnitude estimate is adequate.

Backcontact_deposition_reaction_solutions_temperature

Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the reaction solutions.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the temperatures of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a reaction solution undergoes a temperature program, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons, e.g. 25; 100
- When the temperature of a solution is unknown, state that as 'nan'
- For reaction steps where no solvents are involved, state the temperature of the gas or the solid if that make sense. Otherwise state this as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume an undetermined room temperature to be 25

Backcontact_deposition_substrate_temperature

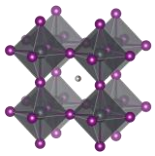
Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the substrate.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the temperatures of the substrates (i.e. the last deposited layer) associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The temperature of the substrate refers to the temperature when the deposition of the layer is occurring.
- If a substrate undergoes a temperature program before the deposition, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- When the temperature of a substrate is not known, state that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume that an undetermined room temperature is 25

Backcontact_deposition_thermal_annealing_temperature

Format: Text string. [T1; T2 >> T3; ... >> ... | T4 >> … | T5 | ...] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperatures of the thermal annealing program associated with depositing the layers

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the annealing temperatures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)



- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- If no thermal annealing is occurring after the deposition of a layer, state that by stating the room temperature (assumed to 25°C if not further specified)
- If the thermal annealing program is not known, state that by 'nan'

Backcontact_deposition_thermal_annealing_time

Format: Text string. [t1; t2 >> t3; ... >> ... | t4 >> … | t5 | ...] [min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time program associated to the thermal annealing program.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the annealing times associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the associated times at those temperatures and separate them with semicolons.
- The annealing times must align in terms of layers, reaction steps and annealing temperatures in the previous filed.
- If a time is not known, state that by 'nan'
- If no thermal annealing is occurring after the deposition of a layer, state that by 'nan'
- For values with uncertainties, state the best estimate, e.g. write 20 and not 10-30.

Backcontact_deposition_thermal_annealing_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere during thermal annealing

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each annealing step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the atmosphere is a mixture of different gases, i.e. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas.
- This is often the same as the atmosphere under which the deposition is occurring, but not always.

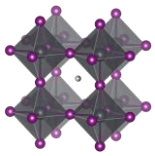
Backcontact_storage_time_until_next_deposition_step

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time between the HTL stack is finalised and the next layer is deposited

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

Backcontact_storage_atmosphere

Format: Text string. [Gas1; Gas2; ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the sample with the finalised HTL stack is stored until the next deposition step.



Backcontact_storage_relative_humidity

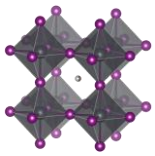
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relive humidity under which the sample with the finalised HTL stack is stored until next deposition step

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

Backcontact_surface_treatment_before_next_deposition_step

Format: Text string
Default: nan
Implemented: After the initial data hunt but before initial release
Description: Description of any type of surface treatment or other treatment the sample with the finalised Backcontact-stack undergoes before the next deposition step.

- If more than one treatment, list the treatments and separate them by a double forward angel bracket (' >> ')
- If no special treatment, state that as 'none'



Additional layers

Add_lay_front

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: During the original data hunt
Description: TRUE if there is a functional layer below the substrate, i.e. on the opposite side of the substrate from with respect to the perovskite.

Add_lay_front_function

Format: Text string. [A.R.C./Upconversion/Down conversion/Back reflection/ ...]
Default: Empty text string
Implemented: During the original data hunt
Description: The function of the additional layers on the substrate side

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- If a layer has more than one function, e.g. A and B, list the functions in order and separate them with semicolons, as in (A; B)

Add_lay_front_stack_sequence

Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: “Unknown”
Implemented: During the original data hunt
Description: The stack sequence describing the additional layers on the substrate side

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- Use common abbreviations when appropriate but spell it out if risk for confusion.
- There are now separate filed for doping. Indicate doping with colons. E.g. wither aluminium doped NiO-np as Al:NiO-np

Add_lay_front_thickness_list

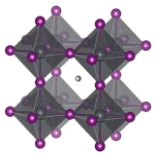
Format: Text string. [Th.1 | Th.2 | … | Th.n] [nm]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: A list of thicknesses of the individual layers in the stack. Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)

- The layers must line up with the previous filed.
- State thicknesses in nm
- Every layer in the stack has a thickness. If it is unknown, state this as ‘nan’
- If there are uncertainties, state the best estimate, e.g. write 100 and not 90-110

Add_lay_front_additives_compounds

Format: Text string. [Addt.1; Addt.2; ... | Addt.3; … | Addt.4 | ...]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: List of the dopants and additives that are in each layer of the ETL-stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- The layers must line up with the previous fields.
- If several dopants/additives, e.g. A and B, are present in one layer, list the dopants/additives in alphabetic order and separate them with semicolons, as in (A; B)
- If no dopants/additives, state that as “Undoped”
- If the doping situation is unknown, stat that as: ‘Unknown’



Add_lay_front_additives_concentrations

Format: Text string. [c1 M; c2 wt%; … | c3 vol%; … | c4 mg/ml | …]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the dopants/additives.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- If more than one dopant/additive in the layer, e.g. A and B, separate the concentration for each dopant/additive with semicolons, as in (A; B)
- For each dopant/additive in the layer, state the concentration.
- The order of the dopants/additives must be the same as in the previous filed.
- For layers with no dopants/additives, state this as ‘none’
- When concentrations are unknown, state that as ‘nan’
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used.
- The preferred way to state the concentration of a dopant/additive is to refer to the amount in the final product, i.e. the material in the layer. When possible, use on the preferred units:
    - wt%, mol%, vol%, ppt, ppm, ppb
- When the concentration of the dopant/additive in the final product is unknown, but where the concentration of the dopant/additive in the solution is known, state that concentration instead. When possible, use on the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Add_lay_front_deposition_procedure

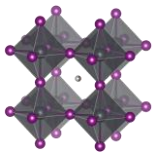
Format: Text string. [Proc. 1 >> Proc. 2 >> … | Proc. 3 >> … | Proc. 4 | …]
Default: “Unknown”
Implemented: In the original data hunt
Description: The deposition procedures for the ETL stack.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- When more than one reaction step, separate them by a double forward angel bracket with one blank space on both sides (‘ >> ’)
- Thermal annealing is generally not considered as an individual reaction step. The philosophy behind this is that every deposition step has a thermal history, which is specified in a separate filed. In exceptional cases with thermal annealing procedures clearly disconnected from other procedures, state ‘Thermal annealing’ as a separate reaction step.
- Please read the instructions under “*Perovskite. Deposition. Procedure*” for descriptions and distinctions between common deposition procedures and how they should be labelled for consistency in the database.

Add_lay_front_deposition_aggregation_state_of_reactants

Format: Text string.) [Agr. 1 >> Agr. 2 >> … | Agr. 3 >> … | Agr. 4 | …]
Default: “Unknown”
Implemented: After the initial data hunt but before initial release
Description: The physical state of the reactants

- The three basic categories are Solid/Liquid/Gas
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- When more than one reaction step, separate the aggregation state associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ’)
- Most cases are clear cut, e.g. spin-coating involves species in solution and evaporation involves species in gas phase. For less clear-cut cases, consider where the reaction really is happening as in:
    - For a spray-coating procedure, it is droplets of liquid that enters the substrate (thus a liquid phase reaction)



- For sputtering and thermal evaporation, it is species in gas phase that reaches the substrate (thus a gas phase reaction)

Add_lay_front_deposition_synthesis_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; … >> … | Gas4 >> … | Gas5 | …]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The synthesis atmosphere

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Add_lay_front_deposition_synthesis_atmosphere_pressure_total

Format: Text string. [P.1 >> P.2 >> … | P.3 >> … | P.4 | …] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total pressure during each synthesis step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- Pressures can be stated in different units suited for different situations. Therefore, specify the unit. The preferred units are:
  - atm, bar, mbar, mmHg, Pa, torr, psi
- If a pressure is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 100 pa and not 80-120 pa.

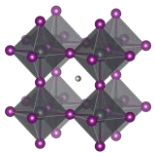
Add_lay_front_deposition_synthesis_atmosphere_pressure_partial

Format: Text string. [P.1; P.2 >> P.3 >> … | P.4 >> … | P.5 | …] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The partial pressures for the gases present during each reaction step.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the partial pressures and separate them with semicolons, as in (A; B). The list of partial pressures must line up with the gases they describe.
- In cases where no gas mixtures are used, this field will be the same as the previous filed.

Add_lay_front_deposition_synthesis_atmosphere_relative_humidity

Format: Text string. [RH1 >> RH2 >> … | RH3 >> … | RH4 | …] [%]
Default: nan



Implemented: After the initial data hunt but before initial release
Description: The relative humidity during each deposition step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the relative humidity associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The number and order of layers and deposition steps must line up with the previous columns
- If the relative humidity for a step is not known, stat that as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 35 and not 30-40.

Add_lay_front_deposition_solvents

Format: Text string. [Sol.1; Sol.2 >> Sol.3; … >> … | Sol.4 >> … | Sol.5 | …]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The solvents used in each deposition procedure for each layer in the stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the solvents associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solvent is a mixture of different solvents, e.g. A and B, list the solvents in alphabetic order and separate them with semicolons, as in (A; B)
- The number and order of layers and deposition steps must line up with the previous columns.
- For non-liquid processes with no solvents, state the solvent as ‘none’
- If the solvent is not known, state this as ‘Unknown’
- Use common abbreviations when appropriate but spell it out when risk for confusion
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Add_lay_front_deposition_solvents_mixing_ratios

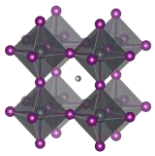
Format: Text string. [V1; V2 >> V3; V4 >> … | V5; V6 >> … | 1 | …]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The mixing ratios for mixed solvents

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the solvent mixing ratios associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The number and order of layers and deposition steps must line up with the previous columns.
- For pure solvents, state the mixing ratio as 1
- For non-solvent processes, state the mixing ratio as 1
- For unknown mixing ratios, state the mixing ratio as ‘nan’
- For solvent mixtures, i.e. A and B, state the mixing ratios by using semicolons, as in (V_A; V_B)
- The preferred metrics is the volume ratios. If that is not available, mass or mol ratios can be used instead, but it the analysis the mixing ratios will be assumed to be based on volumes.

Add_lay_front_deposition_solvents_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; … >> … | Sup.4 >> … | Sup.5 | …]
Default: ‘Unknown’
Implemented: After the initial data hunt but before initial release
Description: The suppliers of all the solvents.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the solvent suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)



- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For non-liquid processes with no solvents, mark the supplier as 'none'
- If the supplier for a solvent is unknown, state this as 'Unknown'

Add_lay_front_deposition_solvents_purity
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the solvents used.

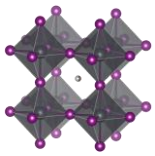
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For non-liquid processes with no solvents, state the purity as 'none'
- If the purity for a solvent is not known, state this as 'Unknown'

Add_lay_front_deposition_reaction_solutions_compounds
Format: Text string. [C1; C2 >> C3; … >> … | C4; C5 | C6 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The non-solvent precursor chemicals used in each reaction step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemicals associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several compounds, e.g. A and B, list the associated compounds in alphabetic order and separate them with semicolons, as in (A; B)
- Note that also dopants/additives should be included
- When several precursor solutions are made and mixed before the reaction step, it is the properties of the final mixture used in the reaction we here describe.
- The number and order of layers and reaction steps must line up with the previous columns.
- For gas phase reactions, state the reaction gases as if they were in solution.
- For solid-state reactions, state the compounds as if they were in solution.
- For reaction steps involving only pure solvents, state this as 'none'
- If the compounds for a deposition step is not known, state this as 'Unknown'

Add_lay_front_deposition_reaction_solutions_compounds_supplier
Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemical suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.



- For gas phase reactions, state the suppliers for the gases or the targets/evaporation sources that are evaporated/sputtered/etc.
- For solid state reactions, state the suppliers for the compounds in the same way.
- For reaction steps involving only pure solvents, state the supplier as 'none' (as that that is entered in a separate filed)
- For chemicals that are lab made, state that as "Lab made" or "Lab made (name of lab)"
- If the supplier for a compound is unknown, state this as 'Unknown'

Add_lay_front_deposition_reaction_solutions_compounds_purity
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the non-solvent chemicals.

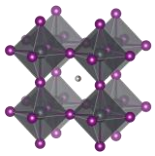
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the compound purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, i.e. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For reaction steps involving only pure solvents, state this as 'none' (as that is stated in another field)
- If the purity for a compound is not known, state this as 'Unknown'

Add_lay_front_deposition_reaction_solutions_concentrations
Format: Text string. [c1 M; c2 mol/dm3 >> c3 mg/ml; … >> ... | c4 wt%; c5 vol% | c6 ppm |...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the non-solvent precursor chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the concentrations associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated concentrations and separate them with semicolons, as in (A; B)
- The order of the compounds must be the same as in the previous filed.
- For reaction steps involving only pure solvents, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used. When possible, use one of the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml, wt%, mol%, vol%, ppt, ppm, ppb
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Add_lay_front_deposition_reaction_solutions_volumes
Format: Text string. [V1 >> V2 >> ... | V3 >> … | V4 | ...] [ml]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The volume of the reaction solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the volumes associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The volumes refer the volumes used, not the volume of the stock solutions. Thus if 0.15 ml of a solution is spin-coated, the volume is 0.15 ml



- For reaction steps without solvents, state the volume as 'nan'
- When volumes are unknown, state that as 'nan'

Add_lay_front_deposition_reaction_solutions_age
Format: Text string. [A1 >> A2 >> … | A3 >> … | A4 | …] [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the age of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- As a general guideline, the age refers to the time from the preparation of the final precursor mixture to the reaction procedure.
- When the age of a solution is not known, state that as 'nan'
- For reaction steps where no solvents are involved, state this as 'nan'
- For solutions that are stored a long time, an order of magnitude estimate is adequate.

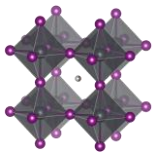
Add_lay_front_deposition_reaction_solutions_temperature
Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the reaction solutions.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the temperatures of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a reaction solution undergoes a temperature program, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons, e.g. 25; 100
- When the temperature of a solution is unknown, state that as 'nan'
- For reaction steps where no solvents are involved, state the temperature of the gas or the solid if that make sense. Otherwise state this as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume an undetermined room temperature to be 25

Add_lay_front_deposition_substrate_temperature
Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the substrate.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the temperatures of the substrates (i.e. the last deposited layer) associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The temperature of the substrate refers to the temperature when the deposition of the layer is occurring.
- If a substrate undergoes a temperature program before the deposition, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- When the temperature of a substrate is not known, state that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume that an undetermined room temperature is 25

Add_lay_front_deposition_thermal_annealing_temperature
Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]



Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperatures of the thermal annealing program associated with depositing the layers

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the annealing temperatures associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If the thermal annealing involves a temperature program with multiple temperature stages, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- If no thermal annealing is occurring after the deposition of a layer, state that by stating the room temperature (assumed to 25°C if not further specified)
- If the thermal annealing program is not known, state that by ‘nan’

Add_lay_front_deposition_thermal_annealing_time

Format: Text string. [t1; t2 >> t3; ... >> ... | t4 >> … | t5 | ...] [min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time program associated to the thermal annealing program.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the annealing times associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If the thermal annealing involves a temperature program with multiple temperature stages, list the associated times at those temperatures and separate them with semicolons.
- The annealing times must align in terms of layers, reaction steps and annealing temperatures in the previous filed.
- If a time is not known, state that by ‘nan’
- If no thermal annealing is occurring after the deposition of a layer, state that by ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 20 and not 10-30.

Add_lay_front_deposition_thermal_annealing_atmosphere

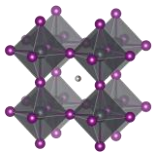
Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: “Unknown”
Implemented: After the initial data hunt but before initial release
Description: The atmosphere during thermal annealing

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the atmospheres associated to each annealing step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The number and order of layers and deposition steps must line up with the previous columns.
- If the atmosphere is a mixture of different gases, i.e. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- “Dry air” represents air with low relative humidity but where the relative humidity is not known
- “Ambient” represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as “Air”
- “Vacuum” (of unspecified pressure) is for this purpose considered as an atmospheric gas.
- This is often the same as the atmosphere under which the deposition is occurring, but not always.

Add_lay_front_storage_time_until_next_deposition_step

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time between the HTL stack is finalised and the next layer is deposited

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.



Add_lay_front_storage_atmosphere

Format: Text string. [Gas1; Gas2; ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the sample with the finalised HTL stack is stored until the next deposition step.

Add_lay_front_storage_relative_humidity

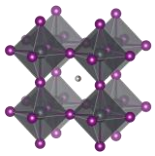
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relive humidity under which the sample with the finalised HTL stack is stored until next deposition step

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

Add_lay_front_surface_treatment_before_next_deposition_step

Format: Text string
Default: nan
Implemented: After the initial data hunt but before initial release
Description: Description of any type of surface treatment or other treatment the sample with the finalised ETL-stack undergoes before the next deposition step.

- If more than one treatment, list the treatments and separate them by a double forward angel bracket (' >> ')
- If no special treatment, state that as 'none'



Add_lay_back
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: During the original data hunt
Description: TRUE if there is a functional layer below the substrate, i.e. on the opposite side of the substrate from with respect to the perovskite.

Add_lay_back_function
Format: Text string. [A.R.C./Upconversion/Down conversion/Back reflection/ ...]
Default: Empty text string
Implemented: During the original data hunt
Description: The function of the additional layers on the back side

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If a layer has more than one function, e.g. A and B, list the functions in order and separate them with semicolons, as in (A; B)

Add_lay_back_stack_sequence
Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: "Unknown"
Implemented: During the original data hunt
Description: The stack sequence describing the additional layers on the substrate side

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- Use common abbreviations when appropriate but spell it out if risk for confusion.
- There are now separate filed for doping. Indicate doping with colons. E.g. wither aluminium doped NiO-np as Al:NiO-np

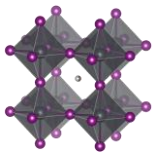
Add_lay_back_thickness_list
Format: Text string. [Th.1 | Th.2 | … | Th.n] [nm]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: A list of thicknesses of the individual layers in the stack. Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')

- The layers must line up with the previous filed.
- State thicknesses in nm
- Every layer in the stack has a thickness. If it is unknown, state this as 'nan'
- If there are uncertainties, state the best estimate, e.g. write 100 and not 90-110

Add_lay_back_additives_compounds
Format: Text string. [Addt.1; Addt.2; ... | Addt.3; … | Addt.4 | ...]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: List of the dopants and additives that are in each layer of the ETL-stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- The layers must line up with the previous fields.
- If several dopants/additives, e.g. A and B, are present in one layer, list the dopants/additives in alphabetic order and separate them with semicolons, as in (A; B)
- If no dopants/additives, state that as "Undoped"
- If the doping situation is unknown, stat that as: 'Unknown'

Add_lay_back_additives_concentrations
Format: Text string. [c1 M; c2 wt%; … | c3 vol%; ... | c4 mg/ml | ...]



Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the dopants/additives.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- If more than one dopant/additive in the layer, e.g. A and B, separate the concentration for each dopant/additive with semicolons, as in (A; B)
- For each dopant/additive in the layer, state the concentration.
- The order of the dopants/additives must be the same as in the previous filed.
- For layers with no dopants/additives, state this as ‘none’
- When concentrations are unknown, state that as ‘nan’
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used.
- The preferred way to state the concentration of a dopant/additive is to refer to the amount in the final product, i.e. the material in the layer. When possible, use on the preferred units:
    - wt%, mol%, vol%, ppt, ppm, ppb
- When the concentration of the dopant/additive in the final product is unknown, but where the concentration of the dopant/additive in the solution is known, state that concentration instead. When possible, use on the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Add_lay_back_deposition_procedure

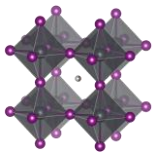
Format: Text string. [Proc. 1 >> Proc. 2 >> … | Proc. 3 >> … | Proc. 4 | …]
Default: “Unknown”
Implemented: In the original data hunt
Description: The deposition procedures for the ETL stack.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- When more than one reaction step, separate them by a double forward angel bracket with one blank space on both sides (‘ >> ’)
- Thermal annealing is generally not considered as an individual reaction step. The philosophy behind this is that every deposition step has a thermal history, which is specified in a separate filed. In exceptional cases with thermal annealing procedures clearly disconnected from other procedures, state ‘Thermal annealing’ as a separate reaction step.
- Please read the instructions under “*Perovskite. Deposition. Procedure*” for descriptions and distinctions between common deposition procedures and how they should be labelled for consistency in the database.

Add_lay_back_deposition_aggregation_state_of_reactants

Format: Text string.) [Agr. 1 >> Agr. 2 >> … | Agr. 3 >> … | Agr. 4 | …]
Default: “Unknown”
Implemented: After the initial data hunt but before initial release
Description: The physical state of the reactants

- The three basic categories are Solid/Liquid/Gas
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ’)
- When more than one reaction step, separate the aggregation state associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ’)
- Most cases are clear cut, e.g. spin-coating involves species in solution and evaporation involves species in gas phase. For less clear-cut cases, consider where the reaction really is happening as in:
    - For a spray-coating procedure, it is droplets of liquid that enters the substrate (thus a liquid phase reaction)
    - For sputtering and thermal evaporation, it is species in gas phase that reaches the substrate (thus a gas phase reaction)



Add_lay_back_deposition_synthesis_atmosphere
Format: Text string. [Gas1; Gas2 >> Gas3; … >> … | Gas4 >> … | Gas5 | …]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The synthesis atmosphere

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Add_lay_back_deposition_synthesis_atmosphere_pressure_total
Format: Text string. [P.1 >> P.2 >> … | P.3 >> … | P.4 | …] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The total pressure during each synthesis step

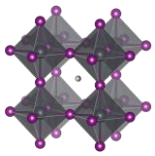
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- Pressures can be stated in different units suited for different situations. Therefore, specify the unit. The preferred units are:
    - atm, bar, mbar, mmHg, Pa, torr, psi
- If a pressure is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 100 pa and not 80-120 pa.

Add_lay_back_deposition_synthesis_atmosphere_pressure_partial
Format: Text string. [P.1; P.2 >> P.3 >> … | P.4 >> … | P.5 | …] [atm/Torr/Pa/bar/mmHg]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The partial pressures for the gases present during each reaction step.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the pressures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the synthesis atmosphere is a mixture of different gases, e.g. A and B, list the partial pressures and separate them with semicolons, as in (A; B). The list of partial pressures must line up with the gases they describe.
- In cases where no gas mixtures are used, this field will be the same as the previous filed.

Add_lay_back_deposition_synthesis_atmosphere_relative_humidity
Format: Text string. [RH1 >> RH2 >> … | RH3 >> … | RH4 | …] [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relative humidity during each deposition step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')



- When more than one reaction step, separate the relative humidity associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns
- If the relative humidity for a step is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 35 and not 30-40.

Add_lay_back_deposition_solvents

Format: Text string. [Sol.1; Sol.2 >> Sol.3; ... >> ... | Sol.4 >> … | Sol.5 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The solvents used in each deposition procedure for each layer in the stack

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvents associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the solvents in alphabetic order and separate them with semicolons, as in (A; B)
- The number and order of layers and deposition steps must line up with the previous columns.
- For non-liquid processes with no solvents, state the solvent as 'none'
- If the solvent is not known, state this as 'Unknown'
- Use common abbreviations when appropriate but spell it out when risk for confusion
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Add_lay_back_deposition_solvents_mixing_ratios

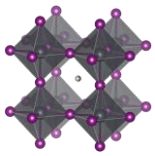
Format: Text string. [V1; V2 >> V3; V4 >> ... | V5; V6 >> … | 1 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The mixing ratios for mixed solvents

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent mixing ratios associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- For pure solvents, state the mixing ratio as 1
- For non-solvent processes, state the mixing ratio as 1
- For unknown mixing ratios, state the mixing ratio as 'nan'
- For solvent mixtures, i.e. A and B, state the mixing ratios by using semicolons, as in (V_A; V_B)
- The preferred metrics is the volume ratios. If that is not available, mass or mol ratios can be used instead, but it the analysis the mixing ratios will be assumed to be based on volumes.

Add_lay_back_deposition_solvents_supplier

Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of all the solvents.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For non-liquid processes with no solvents, mark the supplier as 'none'



- If the supplier for a solvent is unknown, state this as 'Unknown'

Add_lay_back_deposition_solvents_purity
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the solvents used.

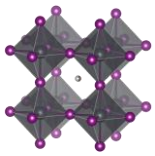
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the solvent purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solvent is a mixture of different solvents, e.g. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For non-liquid processes with no solvents, state the purity as 'none'
- If the purity for a solvent is not known, state this as 'Unknown'

Add_lay_back_deposition_reaction_solutions_compounds
Format: Text string. [C1; C2 >> C3; … >> … | C4; C5 | C6 | ...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The non-solvent precursor chemicals used in each reaction step

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemicals associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several compounds, e.g. A and B, list the associated compounds in alphabetic order and separate them with semicolons, as in (A; B)
- Note that also dopants/additives should be included
- When several precursor solutions are made and mixed before the reaction step, it is the properties of the final mixture used in the reaction we here describe.
- The number and order of layers and reaction steps must line up with the previous columns.
- For gas phase reactions, state the reaction gases as if they were in solution.
- For solid-state reactions, state the compounds as if they were in solution.
- For reaction steps involving only pure solvents, state this as 'none'
- If the compounds for a deposition step is not known, state this as 'Unknown'

Add_lay_back_deposition_reaction_solutions_compounds_supplier
Format: Text string. [Sup.1; Sup.2 >> Sup.3; ... >> ... | Sup.4 >> … | Sup.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The suppliers of the non-solvent chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the non-solvent chemical suppliers associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated suppliers and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- For gas phase reactions, state the suppliers for the gases or the targets/evaporation sources that are evaporated/sputtered/etc.
- For solid state reactions, state the suppliers for the compounds in the same way.



- For reaction steps involving only pure solvents, state the supplier as 'none' (as that that is entered in a separate filed)
- For chemicals that are lab made, state that as "Lab made" or "Lab made (name of lab)"
- If the supplier for a compound is unknown, state this as 'Unknown'

Add_lay_back_deposition_reaction_solutions_compounds_purity
Format: Text string. [Pur.1; Pur.2 >> Pur.3; ... >> ... | Pur.4 >> … | Pur.5 | ...]
Default: 'Unknown'
Implemented: After the initial data hunt but before initial release
Description: The purity of the non-solvent chemicals.

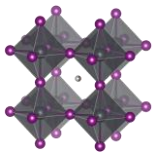
- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the compound purities associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, i.e. A and B, list the associated purities and separate them with semicolons, as in (A; B)
- The number and order of layers, reaction steps, and solvents must line up with the previous columns.
- Use standard nomenclature for purities, e.g. pro analysis, puris, extra dry, etc.
- For reaction steps involving only pure solvents, state this as 'none' (as that is stated in another field)
- If the purity for a compound is not known, state this as 'Unknown'

Add_lay_back_deposition_reaction_solutions_concentrations
Format: Text string. [c1 M; c2 mol/dm3 >> c3 mg/ml; … >> ... | c4 wt%; c5 vol% | c6 ppm |...]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The concentration of the non-solvent precursor chemicals.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the concentrations associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If a solution contains several dissolved compounds, e.g. A and B, list the associated concentrations and separate them with semicolons, as in (A; B)
- The order of the compounds must be the same as in the previous filed.
- For reaction steps involving only pure solvents, state this as 'none'
- When concentrations are unknown, state that as 'nan'
- Concentrations can be stated in different units suited for different situations. Therefore, specify the unit used. When possible, use one of the preferred units:
    - M, mM, molal; g/ml, mg/ml, µg/ml, wt%, mol%, vol%, ppt, ppm, ppb
- For values with uncertainties, state the best estimate, e.g. write 4 wt% and not 3-5 wt%.

Add_lay_back_deposition_reaction_solutions_volumes
Format: Text string. [V1 >> V2 >> ... | V3 >> … | V4 | ...] [ml]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The volume of the reaction solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the volumes associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- The volumes refer the volumes used, not the volume of the stock solutions. Thus if 0.15 ml of a solution is spin-coated, the volume is 0.15 ml
- For reaction steps without solvents, state the volume as 'nan'
- When volumes are unknown, state that as 'nan'



Add_lay_back_deposition_reaction_solutions_age

Format: Text string. [A1 >> A2 >> … | A3 >> … | A4 | …] [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the solutions

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the age of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- As a general guideline, the age refers to the time from the preparation of the final precursor mixture to the reaction procedure.
- When the age of a solution is not known, state that as ‘nan’
- For reaction steps where no solvents are involved, state this as ‘nan’
- For solutions that are stored a long time, an order of magnitude estimate is adequate.

Add_lay_back_deposition_reaction_solutions_temperature

Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the reaction solutions.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the temperatures of the solutions associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- If a reaction solution undergoes a temperature program, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons, e.g. 25; 100
- When the temperature of a solution is unknown, state that as ‘nan’
- For reaction steps where no solvents are involved, state the temperature of the gas or the solid if that make sense. Otherwise state this as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume an undetermined room temperature to be 25

Add_lay_back_deposition_substrate_temperature

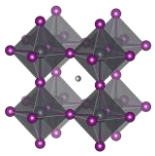
Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the substrate.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)
- When more than one reaction step, separate the temperatures of the substrates (i.e. the last deposited layer) associated to each reaction step by a double forward angel bracket with one blank space on both sides (‘ >> ‘)
- The temperature of the substrate refers to the temperature when the deposition of the layer is occurring.
- If a substrate undergoes a temperature program before the deposition, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- When the temperature of a substrate is not known, state that as ‘nan’
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- Assume that an undetermined room temperature is 25

Add_lay_back_deposition_thermal_annealing_temperature

Format: Text string. [T1; T2 >> T3; … >> … | T4 >> … | T5 | …] [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperatures of the thermal annealing program associated with depositing the layers

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (‘ | ‘)



- When more than one reaction step, separate the annealing temperatures associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the temperatures (e.g. start, end, and other important points) and separate them with semicolons (e.g. 25; 100)
- For values with uncertainties, state the best estimate, e.g. write 120 and not 110-130.
- If no thermal annealing is occurring after the deposition of a layer, state that by stating the room temperature (assumed to 25°C if not further specified)
- If the thermal annealing program is not known, state that by 'nan'

Add_lay_back_deposition_thermal_annealing_time

Format: Text string. [t1; t2 >> t3; ... >> ... | t4 >> … | t5 | ...] [min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time program associated to the thermal annealing program.

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the annealing times associated to each reaction step by a double forward angel bracket with one blank space on both sides (' >> ')
- If the thermal annealing involves a temperature program with multiple temperature stages, list the associated times at those temperatures and separate them with semicolons.
- The annealing times must align in terms of layers, reaction steps and annealing temperatures in the previous filed.
- If a time is not known, state that by 'nan'
- If no thermal annealing is occurring after the deposition of a layer, state that by 'nan'
- For values with uncertainties, state the best estimate, e.g. write 20 and not 10-30.

Add_lay_back_deposition_thermal_annealing_atmosphere

Format: Text string. [Gas1; Gas2 >> Gas3; ... >> ... | Gas4 >> … | Gas5 | ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere during thermal annealing

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- When more than one reaction step, separate the atmospheres associated to each annealing step by a double forward angel bracket with one blank space on both sides (' >> ')
- The number and order of layers and deposition steps must line up with the previous columns.
- If the atmosphere is a mixture of different gases, i.e. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas.
- This is often the same as the atmosphere under which the deposition is occurring, but not always.

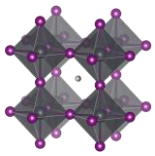
Add_lay_back_storage_time_until_next_deposition_step

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time between the HTL stack is finalised and the next layer is deposited

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

Add_lay_back_storage_atmosphere

Format: Text string. [Gas1; Gas2; ...]



Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the sample with the finalised HTL stack is stored until the next deposition step.

Add_lay_back_storage_relative_humidity

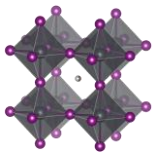
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relive humidity under which the sample with the finalised HTL stack is stored until next deposition step

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

Add_lay_back_surface_treatment_before_next_deposition_step

Format: Text string
Default: nan
Implemented: After the initial data hunt but before initial release
Description: Description of any type of surface treatment or other treatment the sample with the finalised ETL-stack undergoes before the next deposition step.

- If more than one treatment, list the treatments and separate them by a double forward angel bracket (' >> ')
- If no special treatment, state that as 'none'



Encapsulation

Encapsulation

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the cell is encapsulated

Encapsulation_stack_sequence

Format: Text string. [Mat.1; Mat.2; ... | Mat.3; ... | Mat.4 | ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The stack sequence of the encapsulation

- Every layer should be separated by a space, a vertical bar, and a space, i.e. (' | ')
- If two materials, e.g. A and B, are mixed in one layer, list the materials in alphabetic order and separate them with semicolons, as in (A; B)
- Use common abbreviations when appropriate but spell it out if risk for confusion.
- There are now separate filed for doping. Indicate doping with colons. E.g. wither aluminium doped NiO-np as Al:NiO-np

Encapsulation_edge_sealing_materials

Format: Text string. [Mat.1; Mat.2; ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: Edge sealing materials

- If two materials, e.g. A and Bare used, list the materials in alphabetic order and separate them with semicolons, as in (A; B)

Encapsulation_atmosphere_for_encapsulation

Format: Text string
Default: "Unknown"
Implemented: In the original data hunt
Description: The surrounding atmosphere during encapsulation.

- If the surrounding atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas

Encapsulation_water_vapour_transmission_rate

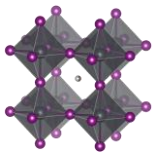
Format: Float. [g/m^2/d]
Default: nan
Implemented: In the original data hunt
Description: The water vapour transmission rate trough the encapsulation.

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

Encapsulation_oxygen_transmission_rate

Format: Float. [cm^3/m^2/d]
Default: nan
Implemented: In the original data hunt
Description: The oxygen transmission rate trough the encapsulation.

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.



JV data

JV_measured

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if IV-data has been measured and is reported.

JV_average_over_n_number_of_cells

Format: Integer
Default: 0
Implemented: In the original data hunt
Description: The number of cells the reported IV data is based on.

- The preferred way to enter data is to give every individual cell its own entry in the data template/data base. If that is done, the data is an average over 1 cell.
- If the reported IV data is not the data from one individual cell, but an average over N cells. Give the number of cells.
- If the reported value is an average, but it is unknown over how many cells the value has been averaged (and no good estimate is available), state the number of cells as 2, which is the smallest number of cells that qualifies for an averaging procedure.

Concerns. Generally, not very reliable

JV_certified_values

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the IV data is measured by an independent and certification institute. If your solar simulator is calibrated by a calibrated reference diode, that does **not** count as a certified result.

JV_certification_institute

Format: Text string
Default: Empty text string
Implemented: In the original data hunt
Description: The name of the certification institute that has measured the certified device.
Example:

JV_storage_age_of_cell

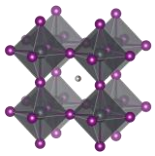
Format: Float. [days]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The age of the cell with respect to when the last deposition step was finalised.

- If there are uncertainties, only state the best estimate, e.g. write 3 and not 1-5.

JV_storage_atmosphere

Format: Text string. [Gas1; Gas2; ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the sample was stored between the device finalisation and the IV measurement.

- If the atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"



- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas
- If the atmosphere has changed during the storing time, separate the different atmospheres by a double forward angel bracket with one blank space on both sides (' >> ')

JV_storage_relative_humidity

Format: Text string. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relative humidity in the atmosphere in which the sample was stored between the device finalisation and the IV measurement.

- If the relative humidity has changed during the storing time, separate the different relative humidity by a double forward angel bracket with one blank space on both sides (' >> ')
- If the relative humidity is not known, stat that as 'nan'
- For values with uncertainties, state the best estimate, e.g. write 35 and not 30-40.

JV_test_atmosphere

Format: Text string. [Gas1; Gas2; ...]
Default: "Unknown"
Implemented: After the initial data hunt but before initial release
Description: The atmosphere in which the IV measurement is conducted

- If the atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas

JV_test_relative_humidity

Format: Text string. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The relive humidity in which the IV measurement is conducted

- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.
- If the relative humidity is not known, stat that as 'nan'

JV_test_temperature

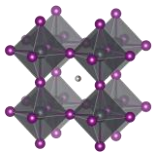
Format: Float. [deg. C]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature of the device during the IV-measurement

- If the temperature is not controlled and not is known, assume a standard room temperature of 25°C.
- If there are uncertainties, only state the best estimate, e.g. write 35 and not 20-50.

JV_light_source_type

Format: Text string. [Dark/White LED/Metal halide/ ...]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The type of light source used during the IV-measurement

- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.
- The category Solar simulator should only be used when you do not really know which type of light source you have in your solar simulator.



JV_light_source_brand_name
Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The brand name and model number of the light source/solar simulator used

- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

JV_light_source_simulator_class
Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The class of the solar simulator

- A three-letter code of As, Bs, and Cs. The order of the letters represents the quality of: spectral match, spatial non-uniformity, and temporal instability

JV_light_intensity
Format: Float. [mW/cm^2]
Default: nan
Implemented: In the original data hunt
Description: The light intensity during the IV measurement

- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- Standard AM 1.5 illumination correspond to 100 mW/cm^2
- If you need to convert from illumination given in lux; at 550 nm, 1 mW/cm^2 corresponds to 6830 lux. Be aware that the conversion change with the spectrum used. As a rule of thumb for general fluorescent/LED light sources, around 0.31mW corresponded to 1000 lux. If your light intensity is measured in lux, it probably means that your light spectra deviates quite a lot from AM 1.5, wherefore it is *very* important that you also specify the light spectra in the next column.

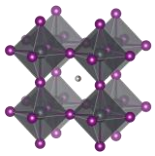
JV_light_spectra
Format: Text string. [AM 1.5/UVA/UVB/Monochromatic/ …]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The light spectrum used (or simulated as best as possible) during the IV measurement

JV_light_wavelength_range
Format: Text string. [lambda min; lambda max] or [lambda constant] [nm]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The wavelength range of the light source

- Separate the lower and upper bound by a semicolon.
- For monochromatic light sources, only give the constant value.
- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- State unknown values as 'nan'

JV_light_illumination_direction
Format: Text string. [Substrate/superstrate]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The direction of the illumination with respect to the device stack

- If the cell is illuminated trough the substrate, state this as 'Substrate'
- If the cell is illuminated trough the top contact, state this as 'Superstrate'



- For back contacted cells illuminated from the non-contacted side, state this as 'Superstrate'

JV_light_masked_cell
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: After the initial data hunt but before initial release
Description: TRUE if the cell is illuminated trough a mask with an opening that is smaller than the total cell area.

JV_light_mask_area
Format: Float. [cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The area of the opening in the mask trough with the cell is illuminated (if there is a mask)

- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- If there is no light mask, leave this field empty.

JV_scan_speed
Format: Float. [mV/s]
Default: nan
Implemented: In the original data hunt
Description: The speed of the potential sweep during the IV measurement

JV_scan_delay_time
Format: Float. [ms]
Default: nan
Implemented: In the original data hunt
Description: The time at each potential value before integration in the potential sweep.

- For some potentiostats you need to specify this value, whereas for others it is set automatically and is not directly accessible.
- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- If unknown, leave this field empty.

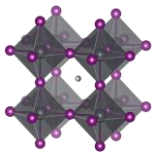
JV_scan_integration_time
Format: Float. [ms]
Default: nan
Implemented: In the original data hunt
Description: The integration time at each potential value in the potential sweep.

- For some potentiostats you need to specify this value, whereas for others it is set automatically and is not directly accessible.
- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- If unknown, leave this field empty.

JV._scan_voltage_step
Format: Float. [mV]
Default: nan
Implemented: In the original data hunt
Description: The distance between the measurement point in the potential sweep

- If unknown, leave this field empty.

JV_preconditioning_protocol
Format: Text string. [none/Light soaking/Potential biasing/ …]
Default: Empty text string



Implemented: In the original data hunt
Description: Any preconditioning protocol done immediately before the IV measurement

- If no preconditioning was done, state this as 'none'
- If more than one preconditioning protocol was conducted in parallel, separate them with semicolons
- If more than one preconditioning protocol was conducted in sequence, separate them by a double forward angel bracket (' >> ')

Concerns. It is reasonable to assume that a lot of cells with no data about preconditioning protocols actually have been subjected to some sort of preconditioning

JV_preconditioning_time

Format: Float. [s]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The duration of the preconditioning protocol

- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- If unknown or not applicable, leave this field empty.

JV_preconditioning_potential

Format: Float. [V]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The potential at any potential biasing step

- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- If unknown or not applicable, leave this field empty.

JV_preconditioning_light_intensity

Format: Float. [mW/cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The light intensity at any light soaking step

- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- If unknown or not applicable, leave this field empty.

JV_reverse_scan_Voc

Format: Float. [V]
Default: nan
Implemented: In the original data hunt
Description: The open circuit potential, Voc, at the reverse voltage sweep (when U scanned from Voc to 0)

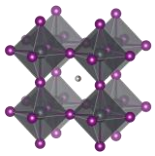
- Give Voc in volts [V]
- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)

JV_reverse_scan_Jsc

Format: Float. [mA/cm^2]
Default: nan
Implemented: In the original data hunt
Description: The short circuit current, Jsc, at the reverse voltage sweep (when U scanned from Voc to 0)

- Give Jsc in mA/cm^2
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20



- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)

JV_reverse_scan_FF
Format: Float. [number between 0 and 1]
Default: nan
Implemented: In the original data hunt
Description: The fill factor, FF, at the reverse voltage sweep (when U scanned from Voc to 0)

- Give FF as the ratio between Vmp*Jmp/(Voc*Jsc) which gives it a value between 0 and 1
- If there are uncertainties, only state the best estimate, e.g. write 0.73 and not 0.7-0.76
- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)

JV_reverse_scan_PCE
Format: Float. [%]
Default: nan
Implemented: In the original data hunt
Description: The fill factor, FF, at the reverse voltage sweep (when U scanned from Voc to 0)

- Give FF as the ratio between Vmp*Jmp/(Voc*Jsc) which gives it a value between 0 and 1
- If there are uncertainties, only state the best estimate, e.g. write 0.73 and not 0.7-0.76
- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)

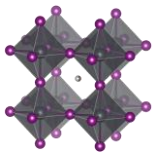
JV_reverse_scan_Vmp
Format: Float. [V]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The potential at the maximum power point, Vmp, at the reverse voltage sweep (when U scanned from Voc to 0)

- Give Vmp in volts [V]
- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

JV_reverse_scan_Jmp
Format: Float. [mA/cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The current density at the maximum power point, Jmp, at the reverse voltage sweep (when U scanned from Voc to 0)

- Give Jmp in mA/cm^2
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

JV_reverse_scan_series_resistance
Format: Float. [ohmcm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The series resistance as extracted from the reverse voltage sweep (when U scanned from Voc to 0)



JV_reverse_scan_shunt_resistance
Format: Float. [ohmcm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The shunt resistance as extracted from the reverse voltage sweep (when U scanned from Voc to 0)

JV_forward_scan_Voc
Format: Float. [V]
Default: nan
Implemented: In the original data hunt
Description: The open circuit potential, Voc, at the forward voltage sweep (when U scanned from 0 to Voc)

- Give Voc in volts [V]
- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)

JV_forward_scan_Jsc
Format: Float. [mA/cm^2]
Default: nan
Implemented: In the original data hunt
Description: The short circuit current, Jsc, at the forward voltage sweep (when U scanned from 0 to Voc)

- Give Jsc in mA/cm²
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)

JV_forward_scan_FF
Format: Float. [number between 0 and 1]
Default: nan
Implemented: In the original data hunt
Description: The fill factor, FF, at the forward voltage sweep (when U scanned from 0 to Voc)

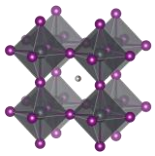
- Give FF as the ratio between Vmp*Jmp/(Voc*Jsc) which gives it a value between 0 and 1
- If there are uncertainties, only state the best estimate, e.g. write 0.73 and not 0.7-0.76
- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)

JV_forward_scan_PCE
Format: Float. [%]
Default: nan
Implemented: In the original data hunt
Description: The efficiency, PCE, at the forward voltage sweep (when U scanned from 0 to Voc)

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Concerns. When the scan direction not is stated, it has generally been assumed to be in the reverse direction (i.e. when U scanned from Voc to 0)



JV_forward_scan_Vmp
Format: Float. [V]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The potential at the maximum power point, Vmp, at the forward voltage sweep (when U scanned from 0 to Voc)

- Give Vmp in volts [V]
- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

JV_forward_scan_Jmp
Format: Float. [mA/cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The current density at the maximum power point, Jmp, at the forward voltage sweep (when U scanned from 0 to Voc)

- Give Jmp in mA/cm^2
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

JV_forward_scan_series_resistance
Format: Float. [ohmcm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The series resistance as extracted from the forward voltage sweep (when U scanned from 0 to Voc)

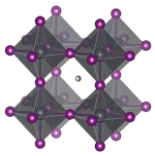
JV_forward_scan_shunt_resistance
Format: Float. [ohmcm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The shunt resistance as extracted from the forward voltage sweep (when U scanned from 0 to Voc)

JV_link_raw_data
Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: A link to where the data file for the IV-data is stored

- This is a beta feature. The plan is to create a file repository where the raw files for IV data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw IV-data.

JV_default_Voc
Format: Float. [V]
Default: nan
Implemented: In the original data hunt
Description: The open circuit potential, Voc. Data for the reverse sweep if available, otherwise data for the forward sweep.

JV_default_Jsc
Format: Float. [mA/cm^2]
Default: nan
Implemented: In the original data hunt



Description: The short circuit current, Jsc. Data for the reverse sweep if available, otherwise data for the forward sweep.

JV_default_FF
Format: Float. [number between 0 and 1]
Default: nan
Implemented: In the original data hunt
Description: The fill factor, FF. Data for the reverse sweep if available, otherwise data for the forward sweep.

JV_default_PCE
Format: Float. [%]
Default: nan
Implemented: In the original data hunt
Description: The cell efficiency. Data for stabilised efficiency if available, otherwise data for the reverse scan if available, otherwise data for the forward sweep.

JV_default_Voc_scan_direction
Format. String
Default: empty string
Implemented: In the original data hunt
Description. The scan direction for " JV_default_Voc"

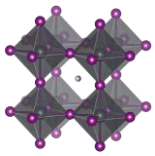
JV_default_Jsc_scan_direction
Format. String
Default: empty string
Implemented: In the original data hunt
Description. The scan direction for " JV_default_Jsc"

JV_default_FF_scan_direction
Format. String
Default: empty string
Implemented: In the original data hunt
Description. The scan direction for " JV_default_FF"

JV_default_PCE_scan_direction
Format. String
Default: empty string
Implemented: In the original data hunt
Description. The scan direction for " JV_default_PCE"

JV_hysteresis_index
Format: Float.
Default: nan
Implemented: In the original data hunt
Description: Hysteresis index calculated from given data. H = f1 * f2 * f3 * f4 – 1
f1 = Jsc_f/Jsc_r
f2 = Voc_f/Voc_r
f3 = FF_f/FF_r
f4 = PCE_f/PCE_r

fx = 1/fx for each fx < 1



Stabilised efficiency

Stabilised_performance_measured

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if a stabilised cell efficiency has been measured

- A stabilised efficiency requires a continuous measurement. Measuring an IV-curve, storing the cell in the dark for a while, and then measure a new IV-curve does thus not count as a stabilised efficiency measurement.

Stabilised_performance_procedure

Format: Text string. [MPPT/Constant potential/Constant current/ …]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The Potentiostatic load condition during the stabilised performance measurement

Stabilised_performance_procedure_metrics

Format: Text string. [Potential in V, Current in mA/cm^2, ...]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The metrics associated to the load condition in the previous filed

- For measurement under constant current, state the current in mA/cm^2
- For measurement under constant potential. State the potential in V
- For a measurement under constant resistive load, state the resistance in ohm

Stabilised_performance_measurement_time

Format: Float. [min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The duration of the stabilised performance measurement.

Stabilised_performance_PCE

Format: Float. [%]
Default: nan
Implemented: In the original data hunt
Description: The stabilised efficiency, PCE

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

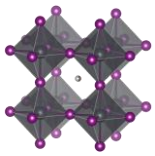
Stabilised_performance_Vmp

Format: Float. [V]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The stabilised Vmp

- Give Vmp in volts [V]
- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

Stabilised_performance_Jmp

Format: Float. [mA/cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release

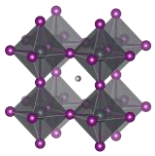


Description: The stabilised Jmp

- Give Jmp in mA/cm^2
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Stabilised_performance_link_raw_data
Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: A link to where the data file for the stability measurement is stored

- This is a beta feature. The plan is to create a file repository where the raw files for IV data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw IV-data.



Quantum efficiency

EQE_measured

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the external quantum efficiency has been measured

EQE_light_bias

Format: Float. [mW/cm^2]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The light intensity of any bias light during the EQE measurement

- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- If unknown or not applicable, leave this field empty.

EQE_integrated_Jsc

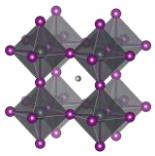
Format: Float. [mA/cm^2]
Default: nan
Implemented: In the original data hunt
Description: The integrated current from the EQE measurement

- Give Jmp in mA/cm^2
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

EQE_link_raw_data

Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: A link to where the data file for the EQE measurement is stored

- This is a beta feature. The plan is to create a file repository where the raw files for IV data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw IV-data.



Stability

Stability_measured

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if some kind of stability measurement has been done.

- There is no sharp boundary between a stability measurement and a measurement of stabilised efficiency. Generally, a measurement under a few minutes is considered as a measurement of stabilised efficiency, whereas a stability measurement is sufficiently long for degradation to be seen (unless the device is really good)

Stability_protocol

Format: Text string
Default: Empty text string. [ISOS x/IEC x/ …]
Implemented: In the original data hunt
Description: The stability protocol used for the stability measurement.

- For a more detailed discussion on protocols and standard nomenclature for stability measurements, please see the following paper:
    - Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures by: M. V. Khenkin et al. Nat. Energ. 2020. DOI: 10.1038/s41560-019-0529-5

Stability_average_over_n_number_of_cells

Format: Integer
Default: 1
Implemented: In the original data hunt
Description: The number of cells the reported stability data is based on.

- The preferred way to enter data is to give every individual cell its own entry in the data template/data base. If that is done, the data is an average over 1 cell.
- If the reported stability data is not the data from one individual cell, but an average over N cells. Give the number of cells.
- If the reported value is an average, but it is unknown over how many cells the value has been averaged (and no good estimate is available), state the number of cells as 2, which is the smallest number of cells that qualifies for an averaging procedure.

Stability_light_source_type

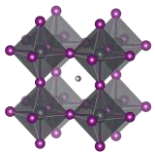
Format: Text string. [Dark/White LED/Metal halide/ ...]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The type of light source used during the IV-measurement

- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.
- The category Solar simulator should only be used when you do not really know which type of light source you have in your solar simulator.

Stability_light_source_brand_name

Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The brand name and model number of the light source/solar simulator used

- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.



Stability_light_source_simulator_class
Format: Text string
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The class of the solar simulator

- A three-letter code of As, Bs, and Cs. The order of the letters represents the quality of: spectral match, spatial non-uniformity, and temporal instability

Stability_light_intensity
Format: Float. [mW/cm^2]
Default: nan
Implemented: In the original data hunt
Description: The light intensity during the stabiliy measurement

- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- Standard AM 1.5 illumination correspond to 100 mW/cm^2
- If you need to convert from illumination given in lux; at 550 nm, 1 mW/cm^2 corresponds to 6830 lux. Be aware that the conversion change with the spectrum used. As a rule of thumb for general fluorescent/LED light sources, around 0.31mW corresponded to 1000 lux. If your light intensity is measured in lux, it probably means that your light spectra deviates quite a lot from AM 1.5, wherefore it is *very* important that you also specify the light spectra in the next column.

Stability_light_spectra
Format: Text string. [AM 1.5/UVA/UVB/Monochromatic/ …]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The light spectrum used (or simulated as best as possible) during the stability measurement

Stability_light_wavelength_range
Format: Text string. [lambda min; lambda max] or [lambda constant] [nm]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The wavelength range of the light source

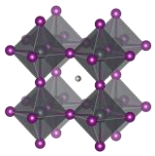
- Separate the lower and upper bound by a semicolon.
- For monochromatic light sources, only give the constant value.
- If there are uncertainties, only state the best estimate, e.g. write 100 and not 90-100.
- State unknown values as 'nan'

Stability_light_illumination_direction
Format: Text string. [Substrate/superstrate]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The direction of the illumination with respect to the device stack

- If the cell is illuminated trough the substrate, state this as 'Substrate'
- If the cell is illuminated trough the top contact, state this as 'Superstrate'
- For back contacted cells illuminated from the non-contacted side, state this as 'Superstrate'

Stability_light_load_condition
Format: Text string. [Continious/Cycled/Day-nigh/ …]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The load situation of the illumination during the stability measurement.

- If the illumination is constant during the entire stability measurement, or if the cell is stored in the dark, state this as 'Constant'.



- If the situation periodically is interrupted by IV-measurements, continue to consider the load condition as constant
- If there is a cycling between dark and light, state this as 'Cycled'
- If the illumination varies in an uncontrolled way, state this as 'Uncontrolled'
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Stability_light_cycling_times

Format: Text string. [time in low light; time in high light] [h]
Default: 'nan; nan'
Implemented: After the initial data hunt but before initial release
Description: If the illumination load is cycled during the stability measurement, state the time in low light followed by the time in high light for the cycling period.

- If not applicable, leave blank

Stability_light_UV_filter

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if a UV-filter of any kind was placed between the illumination source and the device during the stability measurement.

Stability_potential_bias_load_condition

Format: Text string. [Open circuit/MPPT/Constant potential/ …]
Default: Empty text string
Implemented: In the original data hunt
Description: The Potentiostatic load condition during the stability measurement

- When the cell is not connected to anything, state this as 'Open circuit'

Stability_potential_bias_range

Format: Text string. [U.min; U.max] or [U.constant] [V]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The potential range during the stability measurement

- Separate the lower and upper bound by a semicolon.
- For constant values, state only that value.
- For open circuit conditions, state this as 'nan'
- If there are uncertainties, only state the best estimate, e.g. write 1 and not 0.90-1.1
- State unknown values as 'nan'

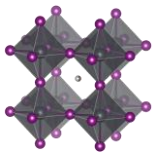
Stability_potential_bias_passive_resistance

Format: Float. [ohm]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The passive resistance in the measurement circuit if a resistor was used

- Give the value in ohm
- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

Stability_temperature_load_condition

Format: Text string. [Constant/Uncontrolled/Cycled/ ...]
Default: Empty text string
Implemented: After the initial data hunt but before initial release



Description: The load situation of the temperature during the stability measurement.

- If the temperature is constant during the entire stability measurement, state this as 'Constant'.
- If there is a cycling between colder and hotter conditions, state this as 'Cycled'
- If the temperature varies in an uncontrolled way, state this as 'Uncontrolled'
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Stability_temperature_range

Format: Text string. [T.min; T.max] or [T.constant] [deg. C]
Default: Empty text string
Implemented: In the original data hunt
Description: The temperature range during the stability measurement

- Separate the lower and upper bound by a semicolon.
- For constant values, state only that value.
- If there are uncertainties, only state the best estimate, e.g. write 1 and not 0.90-1.1
- State unknown values as 'nan'

Stability_temperature_cycling_times

Format: Text string. [t at T.min; t at T.max] [h]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: If the temperature is cycled during the stability measurement, state the time in low temperature followed by the time in high temperature for the cycling period.

- If not applicable, leave blank
- Separate the lower and upper bound by a semicolon.
- If there are uncertainties, only state the best estimate, e.g. write 1 and not 0.90-1.1
- State unknown values as 'nan'

Stability_temperature_ramp_speed

Format: Float. [deg. C/min]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The temperature ramp speed

- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

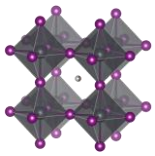
Stability_atmosphere

Format: Text string. [Gas1; Gas2; ...]
Default: "Unknown"
Implemented: In the original data hunt
Description: The atmosphere in which the stability measurement is conducted

- If the atmosphere is a mixture of different gases, e.g. A and B, list the gases in alphabetic order and separate them with semicolons, as in (A; B)
- "Dry air" represents air with low relative humidity but where the relative humidity is not known
- "Ambient" represents air where the relative humidity is not known. For ambient conditions where the relative humidity is known, state this as "Air"
- "Vacuum" (of unspecified pressure) is for this purpose considered as an atmospheric gas

Stability_atmosphere_oxygen_concentration

Format: Float [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The oxygen concentration in the atmosphere



- If unknown, leave this field empty.

Stability_relative_humidity_load_conditions

Format: Text string. [Ambient/Controlled/Cycled/ …]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The load situation of the relative humidity during the stability measurement.

- If the relative humidity is constant during the entire stability measurement, state this as 'Constant'.
- If there is a cycling between dryer and damper conditions, state this as 'Cycled'
- If the relative humidity varies in an uncontrolled way, i.e. the cell is operated under ambient conditions, state this as 'Ambient'
- This category was included after the projects initial phase wherefor the list of reported categories is short. Thus, be prepared to expand the given list of alternatives in the data template.

Stability_relative_humidity_range

Format: Text string. [RH.min; RH.max] [%]
Default: Empty text string
Implemented: After the initial data hunt but before initial release
Description: The relative humidity range during the stability measurement

- Separate the lower and upper bound by a semicolon.
- For constant values, state only that value.
- If there are uncertainties, only state the best estimate, e.g. write 1 and not 0.90-1.1
- State unknown values as 'nan'

Stability_relative_humidity_average_value

Format: Float [%]
Default: nan
Implemented: In the original data hunt
Description: The average relative humidity during the stability measurement.

- If there are uncertainties, only state the best estimate, e.g. write 1 and not 0.90-1.1
- If unknown, leave this field empty.

Stability_time_total_exposure

Format: Float [h]
Default: nan
Implemented: In the original data hunt
Description: The total duration of the stability measurement.

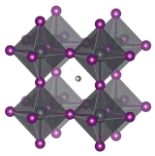
- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050

Stability_periodic_JV_measurements

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: After the initial data hunt but before initial release
Description: TRUE if the stability measurement periodically is interrupted for JV-measurements. A typical example is a cell that is stored in the dark and once in a wile is take out from storage for an IV-measurement.

Stability_periodic_JV_measurements_time_between_measurements

Format: Float [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The average time between JV-measurement during the stability measurement.



Stability_PCE_initial_value

Format: Float. [%]
Default: nan
Implemented: In the original data hunt
Description: The efficiency, PCE, of the cell before the stability measurement routine starts

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Concerns. Often not stated. For some cells there is separate JV data. In the historical dataset, that JV data is, however, most likely for other cells, but have in the original data hunt been merged into one entry (i.e. assumed to be the same cell)

Stability_PCE_burn_in_observed

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the performance has a relatively fast initial decay after which the decay rate stabilises at a lower level.

- There is no sharp boundary between an initial burn in phase and a catastrophic failure, but if the performance of the cell quickly degrade by more than half, it is stretching it a bit to label this as an initial burn in phase.

Stability_PCE_end_of_experiment

Format: Float. [% of initial PCE]
Default: nan
Implemented: In the original data hunt
Description: The efficiency, PCE, of the cell at the end of the stability routine

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Stability_PCE_T95

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time after which the cell performance has degraded by 5 % with respect to the initial performance.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

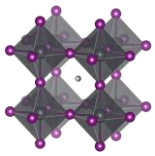
Concerns. Values often extracted by hand from figures, which affects the precision.

Stability_PCE_Ts95

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time after which the cell performance has degraded by 5 % with respect to the performance after any initial burn in phase.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.



Stability_PCE_T80
Format: Float. [h]
Default: nan
Implemented: In the original data hunt
Description: The time after which the cell performance has degraded by 20 % with respect to the initial performance.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Stability_PCE_Ts80
Format: Float. [h]
Default: nan
Implemented: In the original data hunt
Description: The time after which the cell performance has degraded by 20 % with respect to the performance after any initial burn in phase.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Stability_PCE_Te80
Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: An estimated T80 for cells that were not measured sufficiently long for them to degrade by 20 %. with respect to the initial performance.

- This value will by definition have a significant uncertainty to it, as it is not measured but extrapolated under the assumption linearity but without a detailed and stabilised extrapolation protocol. This estimate is, however, not without value as it enables a rough comparison between all cells for with the stability has been measured.

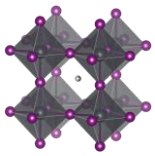
Stability_PCE_Tse80
Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: An estimated T80s for cells that was not measured sufficiently long for them to degrade by 20 %. with respect to the performance after any initial burn in phase.

- This value will by definition have a significant uncertainty to it, as it is not measured but extrapolated under the assumption linearity but without a detailed and stabilised extrapolation protocol. This estimate is, however, not without value as it enables a ruff comparison between all cells for with the stability has been measured.
- If there is an experimental T80s, leave this field empty.

Stability_PCE_after_1000_h
Format: Float. [% of initial PCE]
Default: nan
Implemented: In the original data hunt
Description: The efficiency, PCE, of the cell after 1000 hours

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.



Stability_lifetime_energy_yield
Format: Float. [kWh/m^2]
Default: nan
Implemented: In the original data hunt
Description: The lifetime energy yield

- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Stability_flexible_cell_number_of_bending_cycles
Format: Integer
Default: 0
Implemented: After the initial data hunt but before initial release
Description: Number of bending cycles for a flexible cell in a mechanical stability test

Stability_flexible_cell_bending_radius
Format: Float. [degrees]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The bending radius of the flexible cell during the mechanical stability test

Stability_flexible_cell_PCE_initial_value
Format: Float. [%]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The efficiency, PCE, of the cell before the mechanical stability measurement routine starts

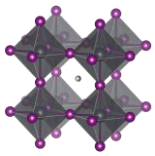
- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Stability_flexible_cell_PCE_end_of_experiment
Format: Float. [% of initial PCE]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The efficiency, PCE, of the cell after the mechanical stability measurement routine

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Stability_link_raw_data_for_stability_trace
Format: Text string
Default: Empty text string
Implemented: In the original data hunt
Description: A link to where the data file for the stability data is stored

- This is a beta feature. The plan is to create a file repository where the raw files for stability data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw stability data.



Outdoor testing

Outdoor_tested

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the performance of the cell has been tested outdoors.

Outdoor_protocol

Format: Text string. [ISOS x/IEC x/ …]
Default: Empty text string
Implemented: In the original data hunt
Description: The protocol used for the outdoor testing.

- For a more detailed discussion on protocols and standard nomenclature for stability measurements, please see the following paper:
    - Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures by: M. V. Khenkin et al. Nat. Energ. 2020. DOI: 10.1038/s41560-019-0529-5

Outdoor_average_over_n_number_of_cells

Format: Integer
Default: 1
Implemented: In the original data hunt
Description: The number of cells the reported outdoor data is based on.
Example:

- The preferred way to enter data is to give every individual cell its own entry in the data template/data base. If that is done, the data is an average over 1 cell.
- If the reported data is not the data from one individual cell, but an average over N cells. Give the number of cells.
- If the reported value is an average, but it is unknown over how many cells the value has been averaged (and no good estimate is available), state the number of cells as 2, which is the smallest number of cells that qualifies for an averaging procedure.

Outdoor_location_country

Format: Text string. [Country]
Default: Empty text string
Implemented: In the original data hunt
Description: The country where the outdoor testing was occurring

- For measurements conducted in space, state this as 'Space International'

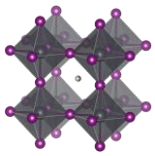
Outdoor_location_city

Format: Text string. [City]
Default: Empty text string
Implemented: In the original data hunt
Description: The city where the outdoor testing was occurring

Outdoor_location_coordinates

Format: Text string
Default: 'nan; nan'
Implemented: In the original data hunt
Description: The coordinates fort the places where the outdoor testing was occurring.

- Use decimal degrees (DD) as the format.



Outdoor_location_climate_zone
Format: Text string. [Tropical/Subtropical/Temperate/Cold]
Default: Empty text string
Implemented: In the original data hunt
Description: The climate zone for the places where the outdoor testing was occurring.

Outdoor_installation_tilt
Format: Float. [degrees]
Default: 'nan'
Implemented: In the original data hunt
Description: The tilt of the installed solar cell.

- A module lying flat on the ground have a tilt of 0
- A module standing straight up has a tilt of 90

Outdoor_installation_cardinal_direction
Format: Float. [degrees]
Default: 'nan'
Implemented: In the original data hunt
Description: The cardinal direction of the installed solar cell.

- North is 0
- East is 90
- South is 180
- West is 270

Outdoor_installation_number_of_solar_tracking_axis
Format: Integer. [0/1/2]
Default: 0
Implemented: In the original data hunt
Description: The number of tracking axis in the installation.

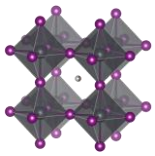
Outdoor_time_season
Format: Text string. [Winter/Summer/ …]
Default: Empty text string
Implemented: In the original data hunt
Description: The time of year the outdoor testing was occurring.

- Order the seasons in alphabetic order and separate them with semicolons.
- For time periods longer than a year, state all four seasons once.

Outdoor_time_start
Format: Date. [year:mm:dd:hh:mm]
Default: Empty string
Implemented: In the original data hunt
Description: The starting time for the outdoor measurement.

Outdoor_time_end
Format: Date. [year:mm:dd:hh:mm]
Default: Empty string
Implemented: In the original data hunt
Description: The ending time for the outdoor measurement.

Outdoor_time_total_exposure
Format: Float. [days]
Default: nan



Implemented: In the original data hunt
Description: The total duration of the outdoor measurement.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050

Outdoor_potential_bias_load_condition

Format: Text string. [Open circuit/MPPT/Constant potential/ …]
Default: Empty text string
Implemented: In the original data hunt
Description: The Potentiostatic load condition during the outdoor measurement

- When the cell is not connected to anything, state this as 'Open circuit'

Outdoor_potential_bias_range

Format: Text string. [U.min; U.max] or [U.constant] [V]
Default: Empty text string
Implemented: In the original data hunt
Description: The potential range during the outdoor measurement

- Separate the lower and upper bound by a semicolon.
- For constant values, state only that value.
- For open circuit conditions, state this as 'nan'
- If there are uncertainties, only state the best estimate, e.g. write 1 and not 0.90-1.1
- State unknown values as 'nan'

Outdoor_potential_bias_passive_resistance

Format: Float. [ohm]
Default: nan
Implemented: In the original data hunt
Description: The passive resistance in the measurement circuit if a resistor was used

- Give the value in ohm
- If there are uncertainties, only state the best estimate, e.g. write 1.03 and not 1.01-1.05
- If unknown or not applicable, leave this field empty.

Outdoor_temperature_load_condition

Format: Text string. [Constant/Uncontrolled/Cycled/ ...]
Default: Empty text string
Implemented: In the original data hunt
Description: The load situation of the temperature during the outdoor measurement.

- If the temperature is constant during the entire stability measurement, state this as 'Constant'.
- If there is a cycling between colder and hotter conditions, state this as 'Cycled'
- If the temperature varies in an uncontrolled way, state this as 'Uncontrolled'

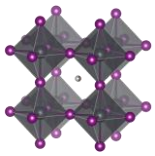
Outdoor_temperature_range

Format: Text string. [T.min; T.max] or [T.constant] [deg. C]
Default: Empty text string
Implemented: In the original data hunt
Description: The temperature range during the outdoor measurement

- Separate the lower and upper bound by a semicolon.
- For constant values, state only that value.
- If there are uncertainties, only state the best estimate, e.g. write 1 and not 0.90-1.1
- State unknown values as 'nan'

Outdoor_temperature_tmodule

Format: Float. [degrees C]



Default: nan
Implemented: In the original data hunt
Description: The effective temperature of the module during peak hours.

Outdoor_periodic_JV_measurements
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the outdoor measurement periodically is interrupted for JV-measurements.

Outdoor_periodic_JV_measurements_time_between_measurements
Format: Float. [h]
Default: nan
Implemented: In the original data hunt
Description: The average time between JV-measurement during the outdoor measurement.

Outdoor_PCE_initial_value
Format: Float. [%]
Default: nan
Implemented: In the original data hunt
Description: The efficiency, PCE, of the cell before the measurement routine starts

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Outdoor_PCE_burn_in_observed
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if the performance has a relatively fast initial decay after which the decay rate stabilises at a lower level.

Outdoor_PCE_end_of_experiment
Format: Float. [% of initial PCE]
Default: nan
Implemented: In the original data hunt
Description: The efficiency, PCE, of the cell at the end of the experiment

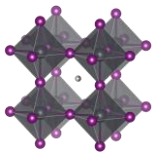
- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Outdoor_PCE_T95
Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time after which the cell performance has degraded by 5 % with respect to the initial performance.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Outdoor_PCE_Ts95
Format: Float. [h]



Default: nan
Implemented: After the initial data hunt but before initial release
Description: The time after which the cell performance has degraded by 5 % with respect to the performance after any initial burn in phase.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Outdoor_PCE_T80

Format: Float. [h]
Default: nan
Implemented: In the original data hunt
Description: The time after which the cell performance has degraded by 20 % with respect to the initial performance.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Outdoor_PCE_Ts80

Format: Float. [h]
Default: nan
Implemented: In the original data hunt
Description: The time after which the cell performance has degraded by 20 % with respect to the performance after any initial burn in phase.

- If there are uncertainties, only state the best estimate, e.g. write 1000 and not 950-1050
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Outdoor_PCE_Te80

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: An estimated T80 for cells that were not measured sufficiently long for them to degrade by 20 %. with respect to the initial performance.

- This value will by definition have a significant uncertainty to it, as it is not measured but extrapolated under the assumption linearity but without a detailed and stabilised extrapolation protocol. This estimate is, however, not without value as it enables a rough comparison between all cells for with the stability has been measured.

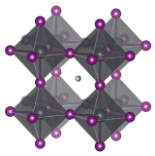
Outdoor_PCE_Tse80

Format: Float. [h]
Default: nan
Implemented: After the initial data hunt but before initial release
Description: An estimated T80s for cells that was not measured sufficiently long for them to degrade by 20 %. with respect to the performance after any initial burn in phase.

- This value will by definition have a significant uncertainty to it, as it is not measured but extrapolated under the assumption linearity but without a detailed and stabilised extrapolation protocol. This estimate is, however, not without value as it enables a ruff comparison between all cells for with the stability has been measured.
- If there is an experimental T80s, leave this field empty.

Outdoor_PCE_after_1000_h

Format: Float. [% of initial PCE]
Default: nan



Implemented: In the original data hunt
Description: The efficiency, PCE, of the cell after 1000 hours

- Give the efficiency in %
- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Concerns. Values often extracted by hand from figures, which affects the precision.

Outdoor_power_generated

Format: Float. [kWh/year/m^2]
Default: nan
Implemented: In the original data hunt
Description: The yearly power generated during the measurement period

- If there are uncertainties, only state the best estimate, e.g. write 20.5 and not 19-20
- If unknown or not applicable, leave this field empty.

Outdoor_link_raw_data_for_outdoor_trace

Format: Text string
Default: Empty text string
Implemented: In the original data hunt
Description: A link to where the data file for the measurement is stored

- This is a beta feature. The plan is to create a file repository where the raw files for stability data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw data.

Outdoor_detaild_weather_data_available

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE if detailed weather data is available for the measurement period

Outdoor_link_detailed_weather_data

Format: Text string
Default: Empty text string
Implemented: In the original data hunt
Description: A link to where the data file for the measurement is stored

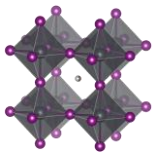
- This is a beta feature. The plan is to create a file repository where the raw files for stability data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw data.

Outdoor_spectral_data_available

Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE measured spectral data are available for the measurement period

Outdoor_link_spectral_data

Format: Text string
Default: Empty text string
Implemented: In the original data hunt
Description: A link to where the data file for the measurement is stored



- This is a beta feature. The plan is to create a file repository where the raw files for stability data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw data.

Outdoor_irradiance_measured
Format: Boolean. i.e. TRUE or FALSE
Default: FALSE
Implemented: In the original data hunt
Description: TRUE measured irradiance data are available for the measurement period

Outdoor_link_irradiance_data
Format: Text string
Default: Empty text string
Implemented: In the original data hunt
Description: A link to where the data file for the measurement is stored

- This is a beta feature. The plan is to create a file repository where the raw files for stability data can be stored and disseminated. With the link and associated protocols, it should be possible to programmatically access and analyse the raw data.