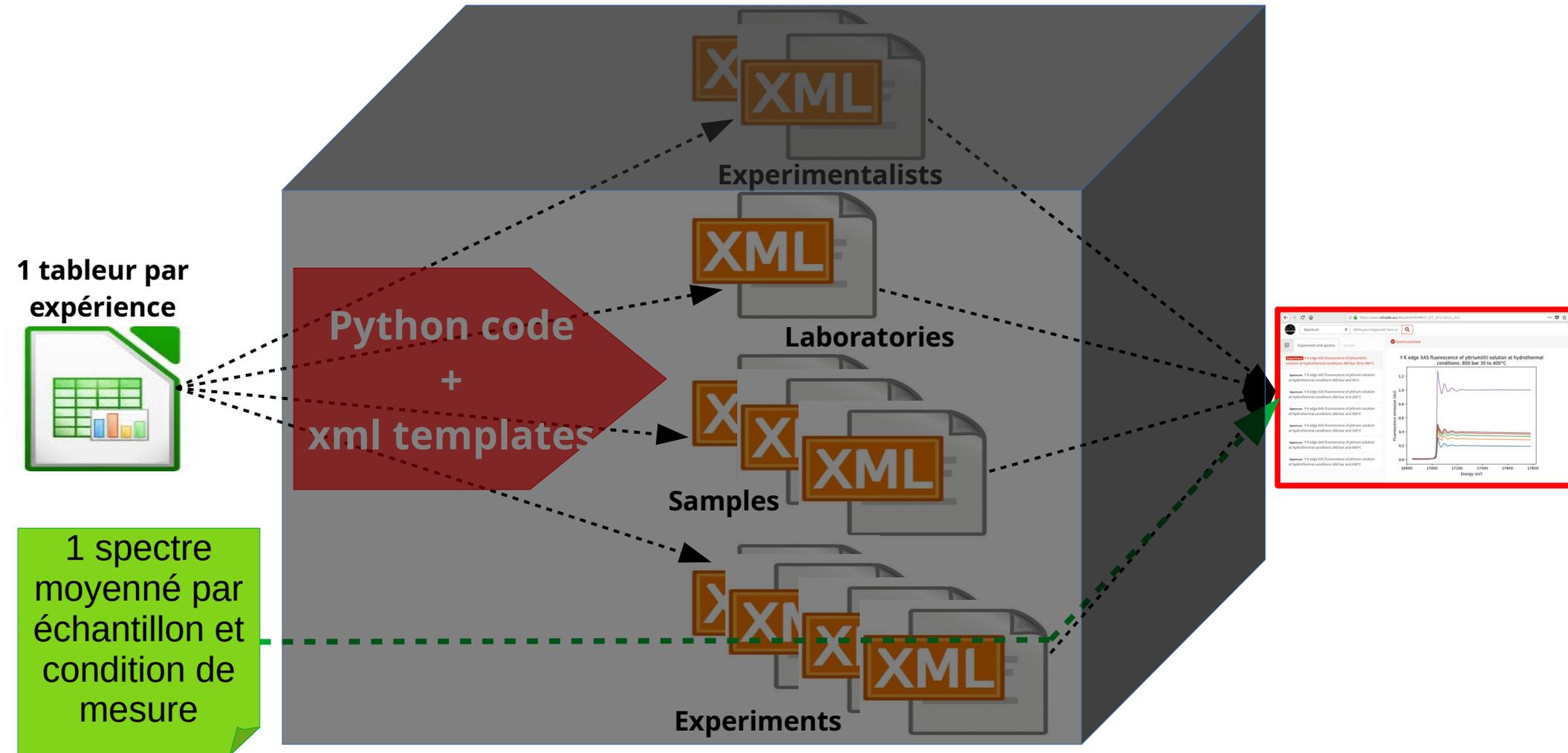


Quelques outils pour l'import dans SSHADE/FAME

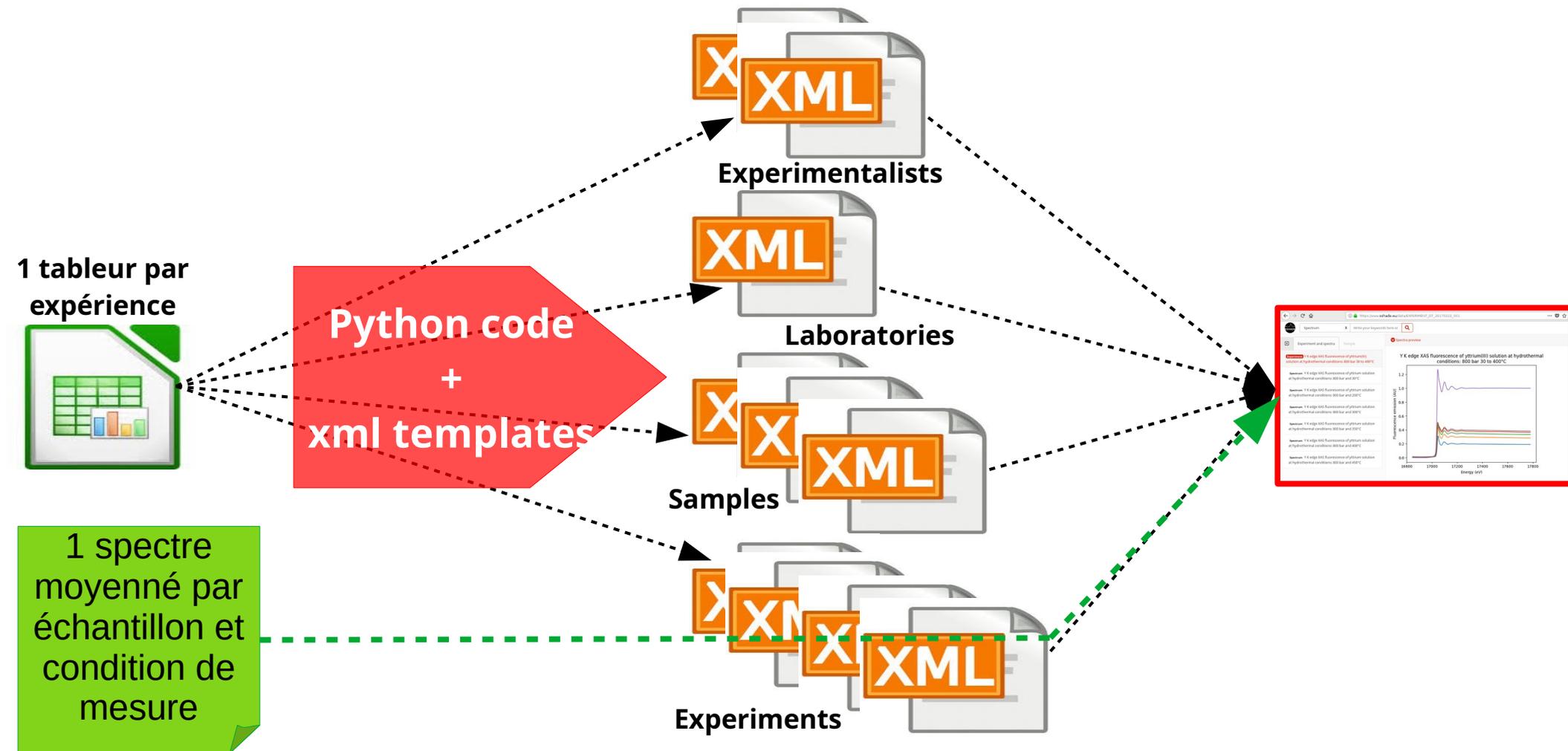
- **Motivation**
- **Présentation des fichiers**
- **Limitations**
- **Démonstration**



Motivation



Motivation



Présentation globale

- 1 fichier **ods** par experiment
 - ↳ 1 onglet par fichier xml final
 - **Laboratory**
 - **Experimentalist**
 - Types de **sample** supportés :
 - ✓ Pellet
 - ✓ Frozem solution
 - ✓ HP/HT solution
 - **Experiment** :
 - ✓ Simple
 - ✓ Multiple
- 1 fichier pour les phases :
 - **Solid**
 - **Molecule**
 - **Molecule ion**



- Autant de templates **xml** que de types d'onglets
 - ↳ Adaptation
 - ↳ Simplification
 - ↳ Remplissage par défaut des valeurs fixes



- Un code **Python**
 - ↳ Conversion des ods en csv
 - ↳ Remplissage des xml à partir des csv
- Un **jupyter notebook**
 - ↳ Interface utilisateur

Required Data: the files to be filled by the user to prepare the data ingestion into the database

-  **Expemiment spreadsheet**
-  **Phases spreadsheet**

<https://wiki.sshade.eu/ssshade/databases/fame>



<https://gitlab.esrf.fr/letard/ssshade>

Exemple de fichier ods

	A	B	C	D	E
1	PARAMETRE	VALUE	EXAMPLE	COMMENTS	
2	sample_uid	DT_20211206_002	DT_20181214_001		
3	sample_import_mode	first import	MENU	New data → first import	
4	sample_date	2021-12-06	2018-01-01		
5	material_name	Cu(SO4) with glycerol	MgO	Name of the main contituent	
6	material_origin	commercial	MENU		
7	comments		Prepared in a glove box	Preparation precautions...	
8	sample_provider	Sigma	Sigma-Aldrich, Pierre Dupond...		
9	specie_quantity_unit	mol/l	MENU		
10					
11	publication_uid	NULL	PUBLI ... (filled by fame staff)	Users, please put the DOI.	The block can be duplicated
12					
13	experimentalist_uid	EXPER_Olivier_Proux	MENU	Will be created from the experimentalist tab. Ex: EXPER_MarieJosephine_DeNo	The block can be duplicated
14					
15	specie_uid	MOLEC_H2O	MOLEC ... or ATOM ... or ATION ...	FAME staff: To be found in the database (or via Bernard...)	The block can be duplicated
16	specie_state	solvent	MENU		
17	specie_relevance	main	MENU		
18	specie_quantity				
19	specie_comments	Pure water (milliQ)	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
20					
21	specie_uid	MOLEC_glycerol	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	The block can be duplicated
22	specie_state	solute	MENU		
23	specie_relevance	main	MENU		
24	specie_quantity				
25	specie_comments	Quantity :50 % in volume	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
26					
27	specie_uid	ATION_Cu2+	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	The block can be duplicated
28	specie_state	solute	MENU		
29	specie_relevance	impurity	MENU		
30	specie_quantity	0.002			
31	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
32					
33	specie_uid	MOLION_SO4_2-	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	The block can be duplicated
34	specie_state	solute	MENU		
35	specie_relevance	impurity	MENU		
36	specie_quantity	0.002			
37	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
38					

Exemple de fichier ods

	A	B	C	D	E
1	PARAMETRE	VALUE	EXAMPLE	COMMENTS	
2	sample_uid	DT_20211206_002	DT_20181214_001		
3	sample_import_mode	first import	MENU	New data → first import	
4	sample_date	2021-12-06	2018-01-01		
5	material_name	Cu(SO4) with glycerol	MgO	Name of the main contituent	
6	material_origin	commercial	MENU		
7	comments		Prepared in a glove box	Preparation precautions...	
8	sample_provider	Sigma	Sigma-Aldrich, Pierre Dupond...		
9	specie_quantity_unit	mol/l	MENU		
10					
11	publication_uid	NULL	PUBLI ... (filled by fame staff)	Users, please put the DOI.	The block can be duplicated
12					
13	experimentalist_uid	EXPER_Olivier_Proux	MENU	Will be created from the experimentalist tab. Ex: EXPER_MarieJosephine_DeNo	The block can be duplicated
14					
15	specie_uid	MOLEC_H2O		ME staff: To be found in the database (or via Bernard...)	
16	specie_state	solvent			
17	specie_relevance	main			The block can be duplicated
18	specie_quantity				
19	specie_comments	Pure water (m...		...d reacted with GSH in a glove box	
20					
21	specie_uid	MOLEC_glyce...		To be found in the database (or via Bernard...)	
22	specie_state	solute			
23	specie_relevance	main			The block can be duplicated
24	specie_quantity				
25	specie_comments	Quantity :50 % in volume	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
26					
27	specie_uid	ATION_Cu2+	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	
28	specie_state	solute	MENU		
29	specie_relevance	impurity	MENU		The block can be duplicated
30	specie_quantity	0.002			
31	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
32					
33	specie_uid	MOLION_SO4_2-	MOI ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	
34	specie_state	solute	MENU		
35	specie_relevance	impurity	MENU		The block can be duplicated
36	specie_quantity	0.002			
37	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
38					

Onglets à dupliquer
autant de fois que
nécessaire

Exemple de fichier ods (frozen_solution)

	A	B	C	D	E
1	PARAMETRE	VALUE	EXAMPLE	COMMENTS	
2	sample_uid	DT_20211206_002	DT_20181214_001		
3	sample_import_mode	first import	MENU	New data → first import	
4	sample_date	2021-12-06	2018-01-01		
5	material_name	Cu(SO4) with glycerol	MgO	Name of the main constituent	
6	material_origin	commercial	MENU		
7	comments		Prepared in a glove box	Preparation precautions...	
8	sample_provider	Sigma	Sigma-Aldrich, Pierre Dupond...		
9	specie_quantity_unit	mol/l	MENU		
10					
11	publication_uid	NULL	PUBLI ... (filled by fame staff)	Users, please put the DOI.	The block can be duplicated
12					
13	experimentalist_uid	EXPER_Olivier_Proux	MENU	... to be created from the experimentalist tab. Ex: EXPER_MarieJosephine_DeNo	The block can be duplicated
14					
15	specie_uid	MOLEC_H2O		... to be found in the database (or via Bernard...)	
16	specie_state	main			
17	specie_relevance	main			The block can be duplicated
18	specie_quantity				
19	specie_comments	Pure water (m...		... with GSH in a glove box	
20					
21	specie_uid	MOLEC_glycerol		... to be found in the database (or via Bernard...)	
22	specie_state	solute			
23	specie_relevance	main			The block can be duplicated
24	specie_quantity				
25	specie_comments	Quantity :50 % in volume	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
26					
27	specie_uid	ATION_Cu2+	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	
28	specie_state	solute	MENU		
29	specie_relevance	impurity	MENU		The block can be duplicated
30	specie_quantity	0.002			
31	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
32					
33	specie_uid	MOLION_SO4_2-	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	
34	specie_state	solute	MENU		
35	specie_relevance	impurity	MENU		The block can be duplicated
36	specie_quantity	0.002			
37	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
38					

Sélection de mots-clés de sshade utiles pour nous (en rose si mandatory)

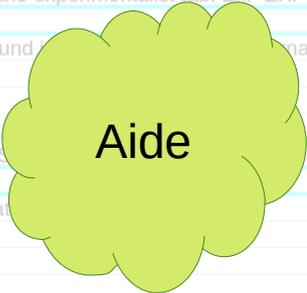
Exemple de fichier ods (frozen_solution)

	A	B	C	D	E
1	PARAMETRE	VALUE	EXAMPLE	COMMENTS	
2	sample_uid	DT_20211206_002	DT_20181214_001		
3	sample_import_mode	first import	MENU	New data → first import	
4	sample_date	2021-12-06	2018-01-01		
5	material_name	Cu(SO4) with glycerol	MgO	Name of the main contituent	
6	material_origin	commercial	MENU		
7	comments		Prepared in a glove box	Preparation precautions...	
8	sample_provider	Sigma	Sigma-Aldrich, Pierre Dupond...		
9	specie_quantity_unit	mol/l	MENU		
10					
11	publication_uid	NULL	PUBLI ... (filled by fame staff)	Users, please put the DOI.	The block can be duplicated
12					
13	experimentalist_uid	EXPER_Olivier_Proux	MENU	Will be created from the experimentalist tab. Ex: EXPER_MarieJosephine_DeNo	The block can be duplicated
14					
15	specie_uid	MOLEC_H2O	MOLEC ... or ATOM ...	To be found in the database (or via Bernard...)	
16	specie_state	solvent	MENU		
17	specie_relevance	main	MENU		The block can be duplicated
18	specie_quantity				
19	specie_comments	Pure water (milliQ)	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
20					
21	specie_uid	MOLEC_glycerol	MOLEC ... or ATOM ...	To be found in the database (or via Bernard...)	
22	specie_state	solute	MENU		
23	specie_relevance	main	MENU		The block can be duplicated
24	specie_quantity				
25	specie_comments	Quantity :50 % in volume	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
26					
27	specie_uid	ATION_Cu2+	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	
28	specie_state	solute	MENU		
29	specie_relevance	impurity	MENU		The block can be duplicated
30	specie_quantity	0.002			
31	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
32					
33	specie_uid	MOLION_SO4_2-	MOLEC ... or ATOM ... or ATION ...	To be found in the database (or via Bernard...)	
34	specie_state	solute	MENU		
35	specie_relevance	impurity	MENU		The block can be duplicated
36	specie_quantity	0.002			
37	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
38					

Champs vides à remplir

Exemple de fichier ods (frozen_solution)

	A	B	C	D	E
1	PARAMETRE	VALUE	EXAMPLE	COMMENTS	
2	sample_uid	DT_20211206_002	DT_20181214_001		
3	sample_import_mode	first import	MENU	New data → first import	
4	sample_date	2021-12-06	2018-01-01		
5	material_name	Cu(SO4) with glycerol	MgO	Name of the main contituent	
6	material_origin	commercial	MENU		
7	comments		Prepared in a glove box	Preparation precautions...	
8	sample_provider	Sigma	Sigma-Aldrich, Pierre Dupond...		
9	specie_quantity_unit	mol/l	MENU		
10					
11	publication_uid	NULL	PUBLI ... (filled by fame staff)	Users, please put the DOI.	The block can be duplicated
12					
13	experimentalist_uid	EXPER_Olivier_Proux	MENU	Will be created from the experimentalist tab. Ex: EXPER_MarieJosephine_DeNo	The block can be duplicated
14					
15	specie_uid	MOLEC_H2O	MOLEC_... or ATOM_... or ATION_...	FAME staff: To be found in the database (or via Bernard...)	
16	specie_state	solvent	MENU		
17	specie_relevance	main	MENU		The block can be duplicated
18	specie_quantity				
19	specie_comments	Pure water (milliQ)	Quantity: 3mM, AgNO3 dissolved in water	and reacted with GSH in a glove box	
20					
21	specie_uid	MOLEC_glycerol	MOLEC_... or ATOM_... or ATION_...	To be found in the database (or via Bernard...)	
22	specie_state	solute	MENU		
23	specie_relevance	main	MENU		The block can be duplicated
24	specie_quantity				
25	specie_comments	Quantity :50 % in volume	Quantity: 3mM, AgNO3 dissolved in water	and reacted with GSH in a glove box	
26					
27	specie_uid	ATION_Cu2+	MOLEC_... or ATOM_... or ATION_...	To be found in the database (or via Bernard...)	
28	specie_state	solute	MENU		
29	specie_relevance	impurity	MENU		The block can be duplicated
30	specie_quantity	0.002			
31	specie_comments		Quantity: 3mM, AgNO3 dissolved in water	and reacted with GSH in a glove box	
32					
33	specie_uid	MOLION_SO4_2-	MOLEC_... or ATOM_... or ATION_...	To be found in the database (or via Bernard...)	
34	specie_state	solute	MENU		
35	specie_relevance	impurity	MENU		The block can be duplicated
36	specie_quantity	0.002			
37	specie_comments		Quantity: 3mM, AgNO3 dissolved in water	and reacted with GSH in a glove box	
38					

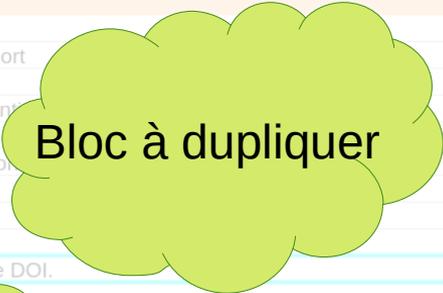


Exemple de fichier ods (Content of the menus)

	A	B	C	D	E	F	G	H
1	import_mode	laboratory_uid	experimentalist_uid	state	status	diluent_uid	material_origin	specie_state
2	first import	LAB_ADELAIDE_UNIVERSITY	EXPER_Abdallah_Nassereddine	current	engineer	BN	commercial	pure
3	no change	LAB_BIAM	EXPER_Agnes_Gorczyca	previous	master student	cellulose	extraterrestrial	mixed
4	correction	LAB_CEDLEFT	EXPER_Amazigh_Ouaksel		PhD student	PVP	laboratory	matrix
5		LAB_Cerege	EXPER_Ana_Pradas		post-doc	NULL	natural terrestrial	solute
6		LAB_CSIRO	EXPER_AnaTeresa_FialhoBatista		researcher		simulated	solvent
7		LAB_DCM	EXPER_Angelika_Rosa		undergraduate student			liquid solution
8		LAB_EGC	EXPER_Anthony_Lannes					solid solution
9		LAB_EMPA	EXPER_Antonio_AguilarTapia					clathrate network
10		LAB_ERDW	EXPER_Ashis_Biswas					clathrate guest
11		LAB_ESRF	EXPER_Barbara_Etschmann					hydration
12		LAB_FAME	EXPER_Bhoopesh_Mishra					hydrated
13		LAB_Geollinois	EXPER_Blanche_Collin					in complex
14		LAB_GeoResources	EXPER_Blake_Tooth					monomers
15		LAB_GET	EXPER_Carmen_Sanchez					dimers
16		LAB_GFZ	EXPER_Carole_Duboc					multimers
17		LAB_GIN	EXPER_Caroline_Bissardon					physically adsorbed
18		LAB_ICCF	EXPER_Cecile_DaSilva					chemically adsorbed
19		LAB_ICMG	EXPER_Charles_Paleo					interlayer physically adsorbed
20		LAB_ICSM	EXPER_Charlotte_Vichery					other
21		LAB_IFMWWU	EXPER_Chinh_NguyenTrung					unknown
22		LAB_IFPEN	EXPER_Christele_Legens					
23		LAB_ILM	EXPER_Christian_Schmidt					
24		LAB_IMBE	EXPER_Christophe_Geantet					
25		LAB_IMRB	EXPER_Claire_Lallemand					
26		LAB_IPREM	EXPER_Clement_Laskar					
27		LAB_IRCELYON	EXPER_Clement_Levard					
28		LAB_ISTerre	EXPER_Damien_LeRoy					
29		LAB_KCC	EXPER_David_Pignol					
30		LAB_LCBM	EXPER_Denis_Testemale					
31		LAB_LEG	EXPER_Dominique_Luneau					
32		LAB_LMI	EXPER_Elena_Bazarkina					
33		LAB_MEG	EXPER_Francesco_Stellato					
34		LAB_MONASH_UNIVERSITY	EXPER_Geraldine_Sarret					
35		LAB_Neel	EXPER_Giulia_Veronesi					
36		LAB_PMC	EXPER_Gleb_Pokrovski					
37		LAB_PSI	EXPER_Ina_Vollmer					
38		LAB_PotsdamGeosciences	EXPER_Isabelle_Hazemann					
39		LAB_SCIB	EXPER_Isabelle_Kieffer					
40		LAB_SCPE	EXPER_Isabelle_Maurin					
41		LAB_SES	EXPER_Isabelle_MichaudSoret					
42		LAB_SNBL	EXPER_Jacques_Pecaut					
43		LAB_SYMMES	EXPER_JeanFrancois_Gaillard					
44		LAB_UMS_OSUG	EXPER_JeanLouis_Hazemann					
45		LAB_UniToV	EXPER_Jeanne_Perrin					
46			EXPER_Jeremy_Domergue					
47			EXPER_Jerome_Rose					
48			EXPER_Joel_Brugger					
49			EXPER_Julien_Couturier					
50			EXPER_Laetitia_Laversenne					
51			EXPER_Laurent_Truche					
52			EXPER_Manuela_Borchert					
53			EXPER_Maria_Kokh					
54			EXPER_Marie_Carriere					
55			EXPER_Maria_Diana_Jacobs					

Exemple de fichier ods (frozen_solution)

	A	B	C	D	E
1	PARAMETRE	VALUE	EXAMPLE	COMMENTS	
2	sample_uid	DT_20211206_002	DT_20181214_001		
3	sample_import_mode	first import	MENU	New data → first import	
4	sample_date	2021-12-06	2018-01-01		
5	material_name	Cu(SO4) with glycerol	MgO	Name of the main component	
6	material_origin	commercial	MENU		
7	comments		Prepared in a glove box	Preparation precautions	
8	sample_provider	Sigma	Sigma-Aldrich, Pierre Dupond...		
9	specie_quantity_unit	mol/l	MENU		
10					
11	publication_uid	NULL	PUBLI ... (filled by fame staff)	Users, please put the DOI.	The block can be duplicated
12					
13	experimentalist_uid	EXPER_Olivier_Proux	MENU	Will be created from the experimentalist tab. Ex: EXPER_MarieJosephine_DeNo	The block can be duplicated
14					
15	specie_uid	MOLEC_H2O	MOLEC_... or ATOM_... or ATION_...	FAME To be found in the database (or via Bernard...)	The block can be duplicated
16	specie_state	solvent	MENU		
17	specie_relevance	main	MENU		
18	specie_quantity				
19	specie_comments	Pure water (milliQ)	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
20					
21	specie_uid	MOLEC_glycerol	MOLEC_... or ATOM_... or ATION_...	To be found in the database (or via Bernard...)	The block can be duplicated
22	specie_state	solute	MENU		
23	specie_relevance	main	MENU		
24	specie_quantity				
25	specie_comments	Quantity :50 % in volume	Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
26					
27	specie_uid	ATION_Cu2+	MOLEC_... or ATOM_... or ATION_...	To be found in the database (or via Bernard...)	The block can be duplicated
28	specie_state	solute	MENU		
29	specie_relevance	impurity	MENU		
30	specie_quantity	0.002			
31	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
32					
33	specie_uid	MOLION_SO4_2-	MOLEC_... or ATOM_... or ATION_...	To be found in the database (or via Bernard...)	The block can be duplicated
34	specie_state	solute	MENU		
35	specie_relevance	impurity	MENU		
36	specie_quantity	0.002			
37	specie_comments		Quantity: 3mM, AgNO3 dissolved in water and reacted with GSH in a glove box		
38					



Exemple de template xml (frozen_solution)

```
sample_frozen_solution.xml x
1 <import type="sample" ssdm_version="0.9.0">
2
3 <sample><!-- multiple -->
4 <import_mode>first import</import_mode> <!-- sample import mode -->
5 <uid>SAMPLE_$$$</uid> <!-- sample uid - Ex: SAMPLE_OP_20180717_001 -->
6
7 <owner_databases>
8 <database_uid>DB_FAME</database_uid>
9 </owner_databases>
10
11 <provider><![CDATA[]]></provider> <!-- sample provider -->
12 <experimentalists> <!-- Ex: EXPER_Olivier_Proux -->
13 <experimentalist_uid>$$$</experimentalist_uid>
14 </experimentalists>
15
16 <!-- SAMPLE NAME and REFERENCES -->
17 <name>Frozen solution of @@@</name> <!-- sample name -->
18 <date>$$$</date> <!-- Ex: 2006-09-02 -->
19
20 <is_generic>no</is_generic>
21 <surface_roughness>NULL</surface_roughness>
22 <size_unit>mm</size_unit>
23 <substrate_material>NULL</substrate_material>
24
25 <parameters_environment>
26 <time_unit>min</time_unit>
27 <temperature>
28 <unit>K</unit>
29 <value>77</value>
30 <error>NULL</error>
31 <max>NULL</max>
32 </temperature>
33 <fluid>
34 <type>molecular liquid</type>
35 <temperature>77</temperature>
36 <pressure_unit>bar</pressure_unit>
37 <pressure>1</pressure>
38 <composition_species>
39 <composition_specie>
40 <uid>MOLEC_N2</uid>
41 <mole fraction>1</mole fraction>
42 </composition_specie>
43 </composition_species>
44 </fluid>
45 </parameters_environment>
46 </sample>
47 </import>
```

Champ rempli par défaut

Champ rempli et/ou dupliqué par le code

124 lignes au lieu de 1300 pour un sample

Limitations

- Fait peur aux utilisateurs (complexe à prendre en main)
 - ↳ Interface graphique ?
 - ↳ Intégrée à sshade (vérification des erreurs en live)
- Pas de gestion des **erreurs de syntaxe**
 - ↳ Erreurs humaines
 - ↳ Passage excel / libre office
- Nombre limité de **templates** :
 - ↳ types d'échantillons :
 - Solutions
 - Solides bulk
 - ↳ conditions expérimentales :
 - Atmosphères variées
 - ...