batchcalculator Documentation

Release 0.3.0

Lukasz Mentel

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Contents:

CHAPTER 1

Installation

1.1 Dependencies

- Python 2.7.x
- wxPython
- ObjectListView,
- reportlab
- numpy
- jinja2
- SQLAlchemy

If you want to export your calculations to a TeX report and be able to automatically typeset the pdf you should have a TeX distribution installed. If you don't know what TeX is TUG (TeX Users Group) is a good place to start.

1.2 Installing from source

Currently the preferred way is to install the package from source and manually setup the link and/or shortcuts if you want an launcher on you desktop.

You can either download the code from the repository and run:

```
[sudo] pip install batchcalc-x.x.x.tgz
```

or:

```
[sudo] easy_install batchcalc-x.x.x.tgz
```

or clone the repository:

```
git clone https://github.com/lmmentel/batchcalculator.git
```

pull the latest version and update:

```
git pull
```

then *cd* to the package directory and run:

```
[sudo] python setup.py install
```

If the installation finishes without errors you should be able to start the GUI from the command line by typing:

```
$ zbc
```

CHAPTER 2

Tutorial

To illustrate the usage of the **Batch Calculator** we will calculate the the amounts of reactants required to perform the synthesis of ZSM-22 described by Ernst et al. [1].

The batch composition is given as (p. 139 of [1]):

- 13 K_2O
- Al_2O_3
- 91 SiO_2
- 3670 H_20
- 27 $NH_2(CH_2)_6NH_2$

The reactants used are:

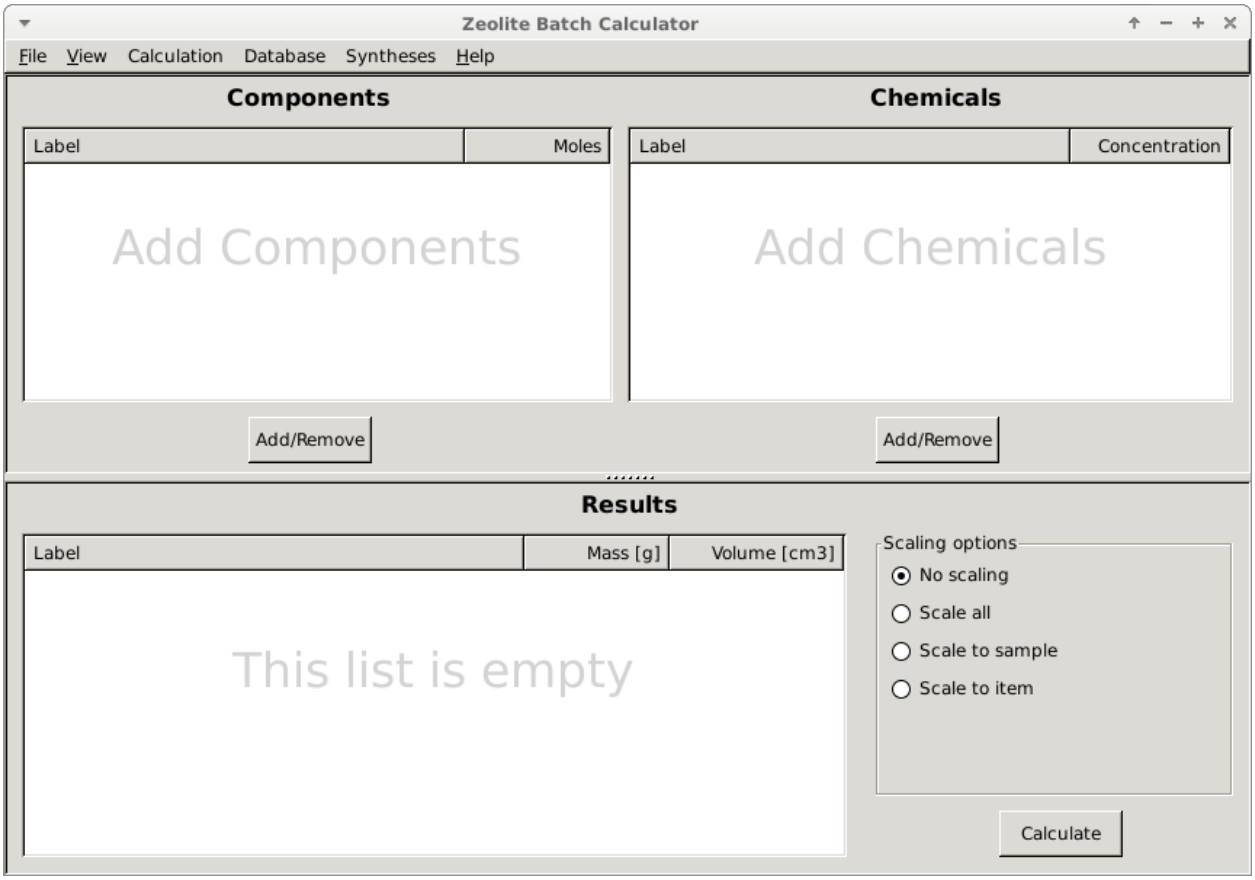
- silica sol (40% silica; Ludox AS40, DuPont) was
- $Al_2(SO_4)_3$* 18H_2 O
- KOH
- 1,6-diaminohexane (HMDA)
- water

The amounts of reactants used in the synthesis are presented in the table below for reference

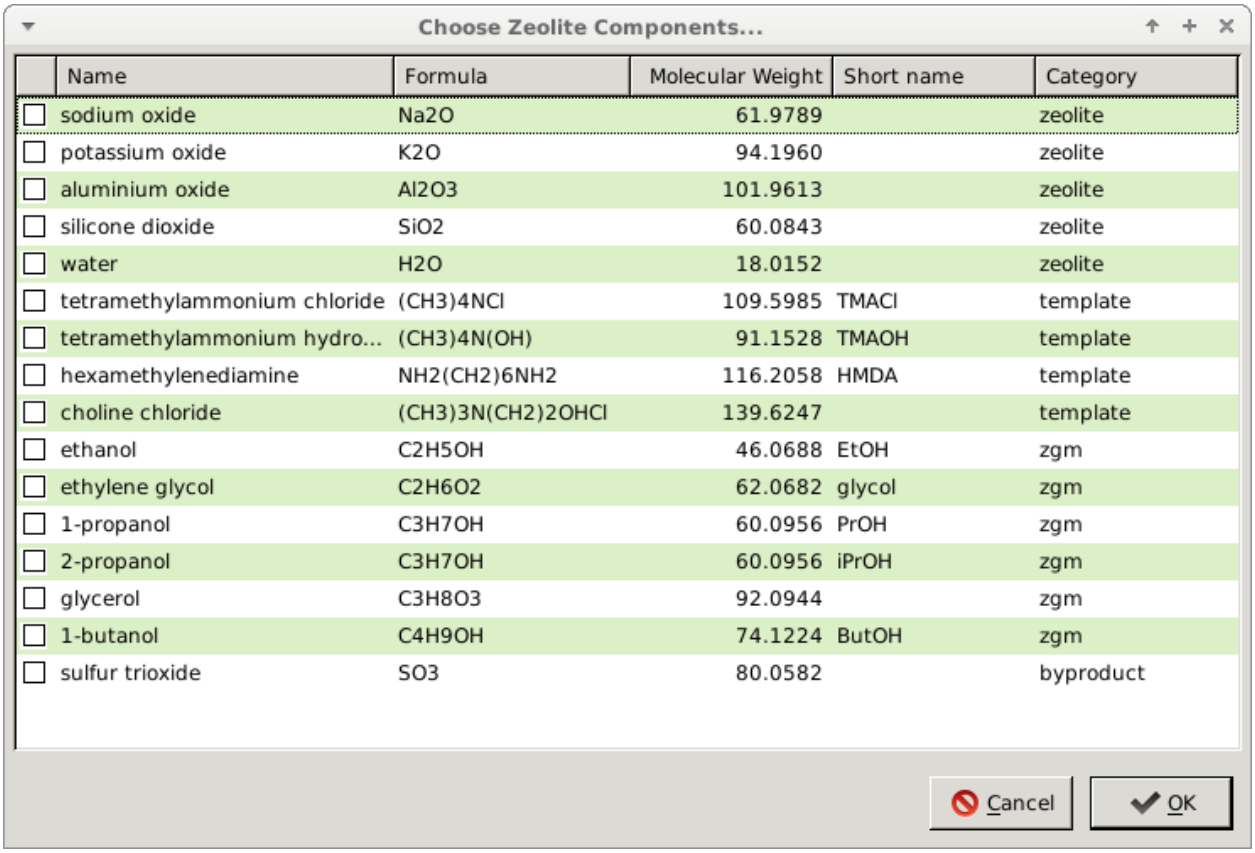
Name	Amoung [g]
KOH	7.8
Al2(SO4)3	3.5
silica sol	72
water	301
HDMA	16.7

After starting the **Batch Calculator** the main window appears. As a first step we need to add the components by clicking on the **Add/Remove** button in the **Components** panel.

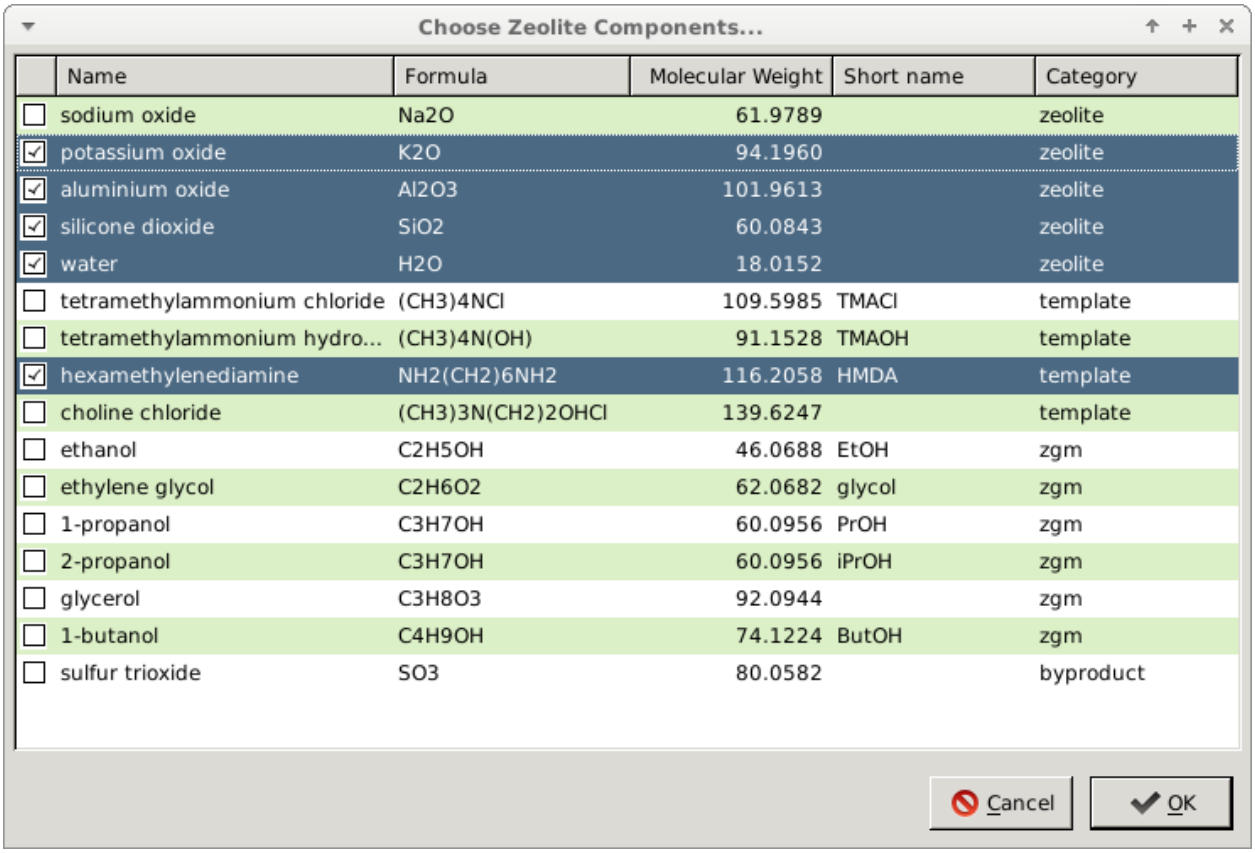
[1] Ernst, S., Weitkamp, J., Martens, J. A., & Jacobs, P. A. (1989). Synthesis and shape-selective properties of ZSM-22. Applied Catalysis, 48(1), 137–148. doi:/10.1016/S0166-9834(00)80271-7



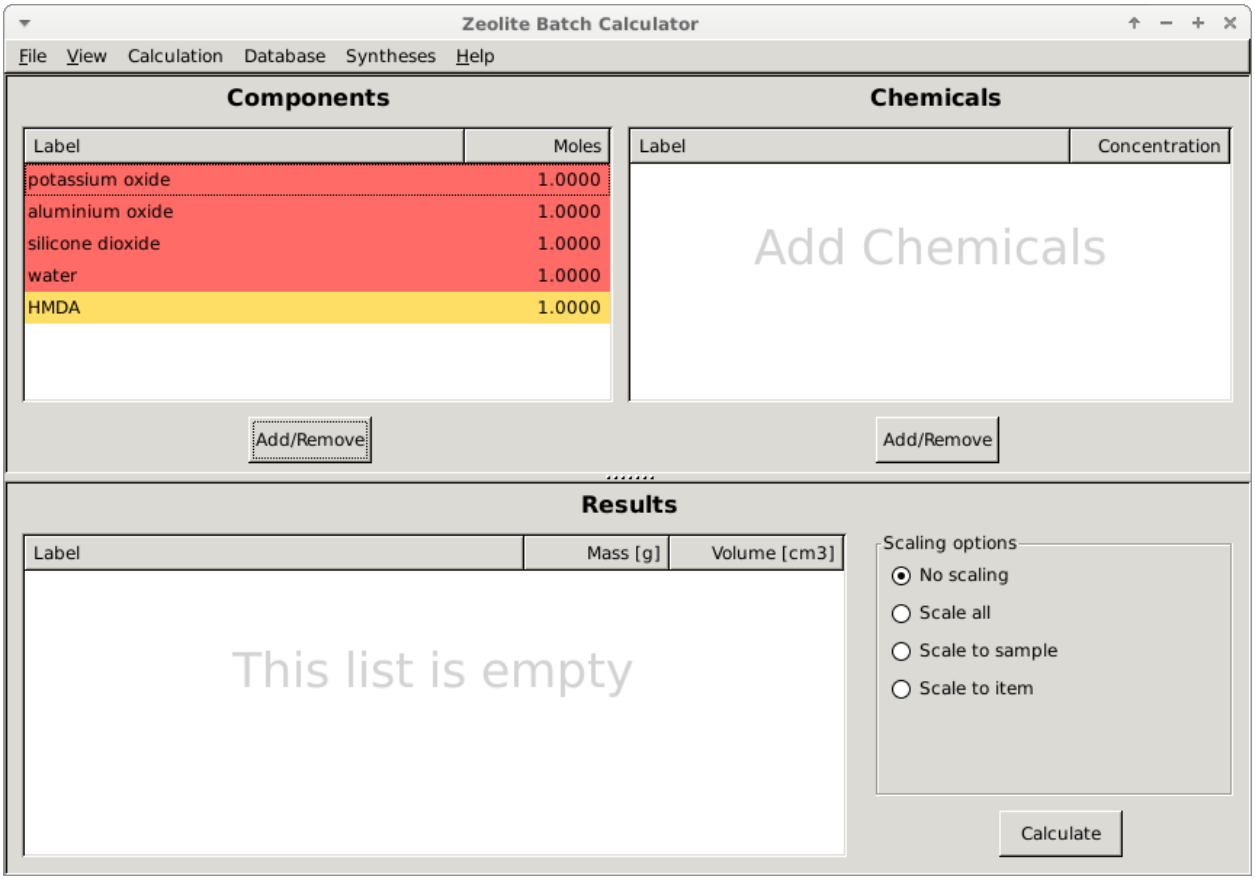
A dialog window should appear with all the components that are currently available in the database.



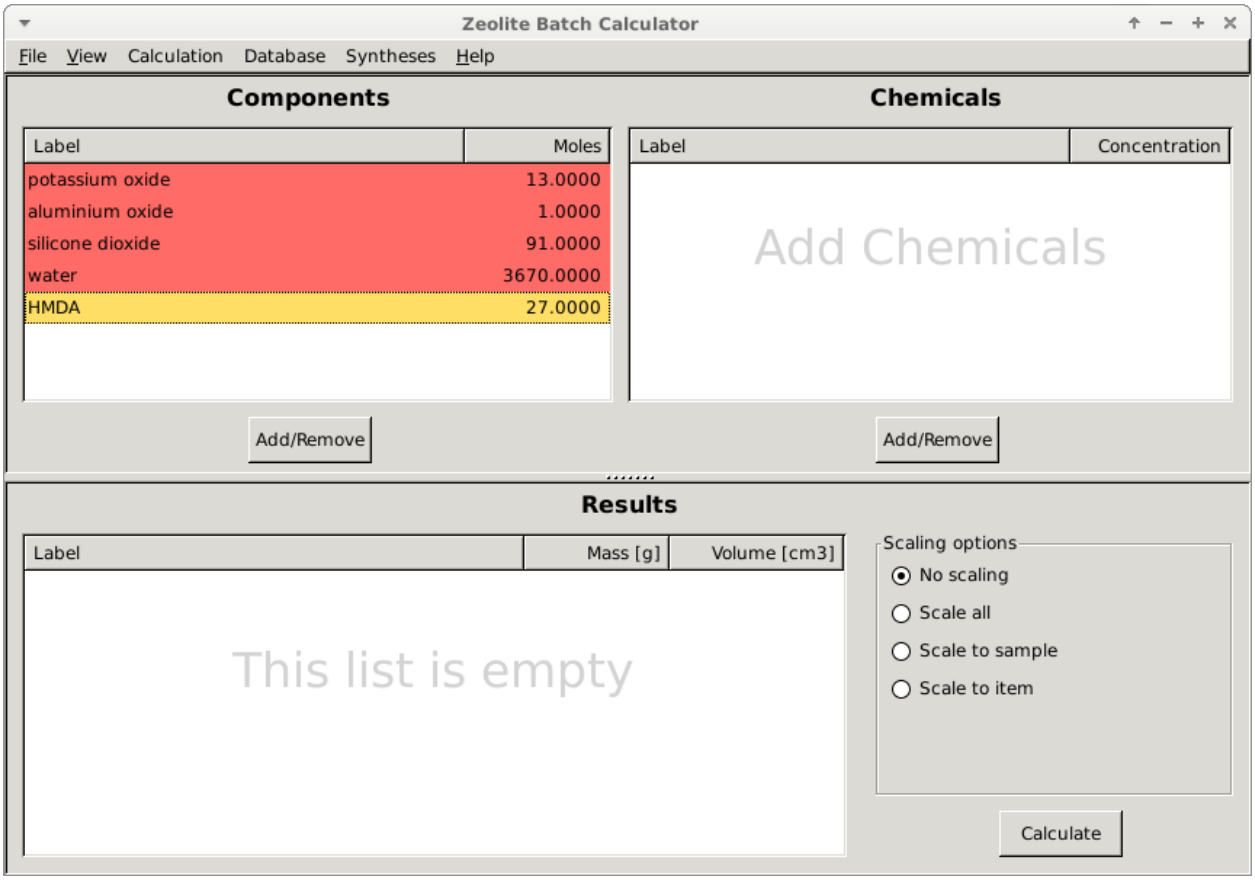
We need to choose the appropriate components by ticking the correct boxes as shown below and click the **OK** button.



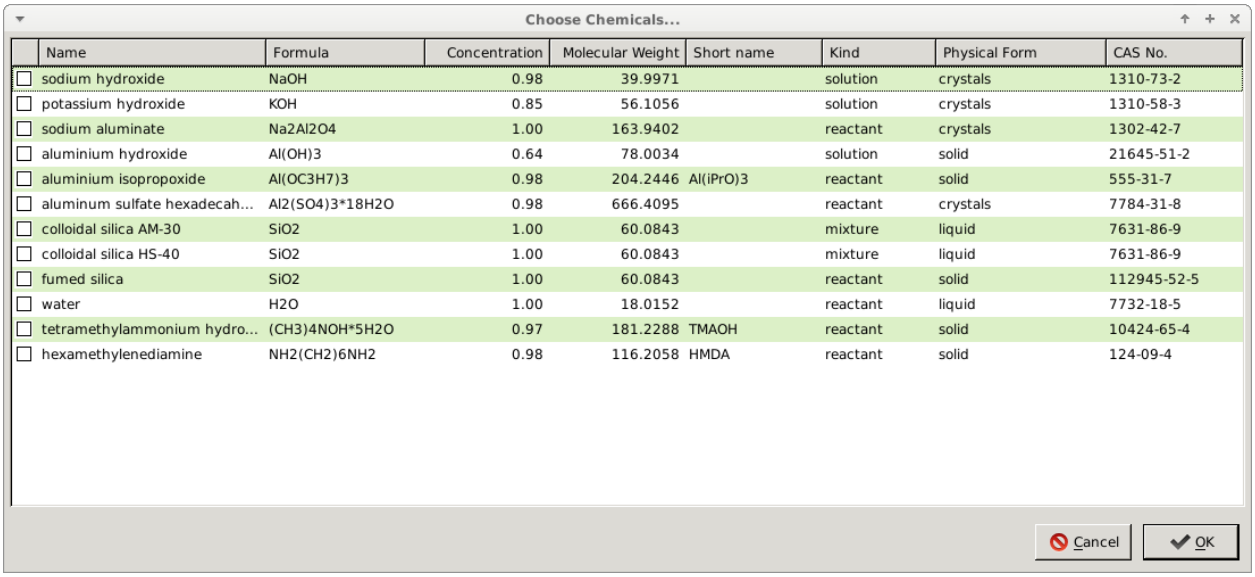
By doing that the selected components are now shown in the main window with the default amounts equal to 1.



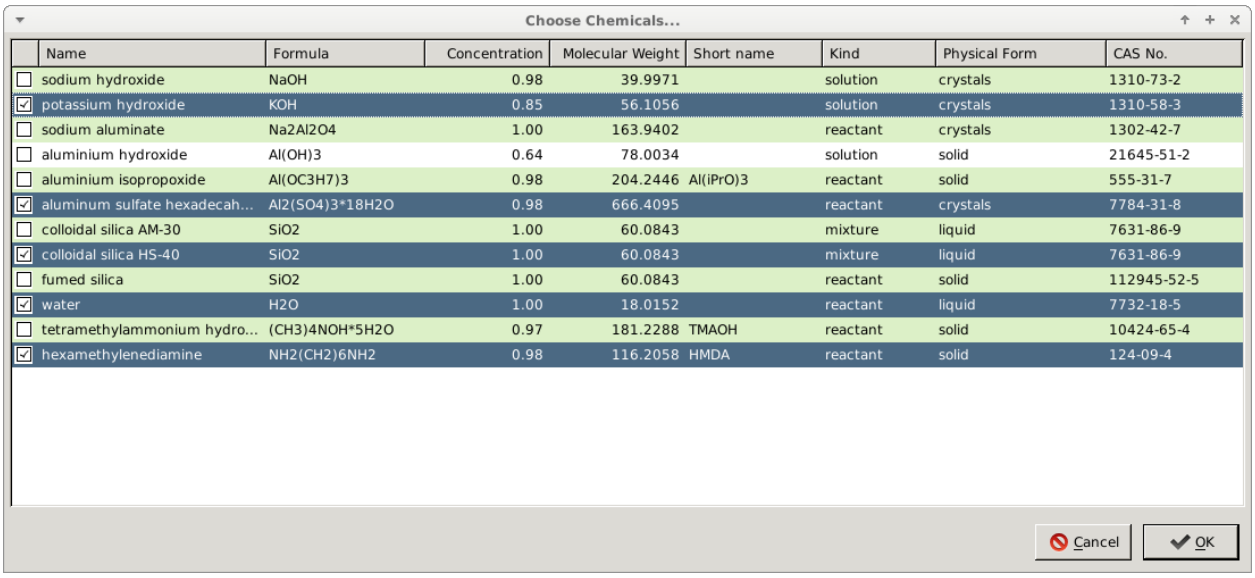
To adjust the amount double click on the appropriate number and enter the correct amount, in our case the amounts are:



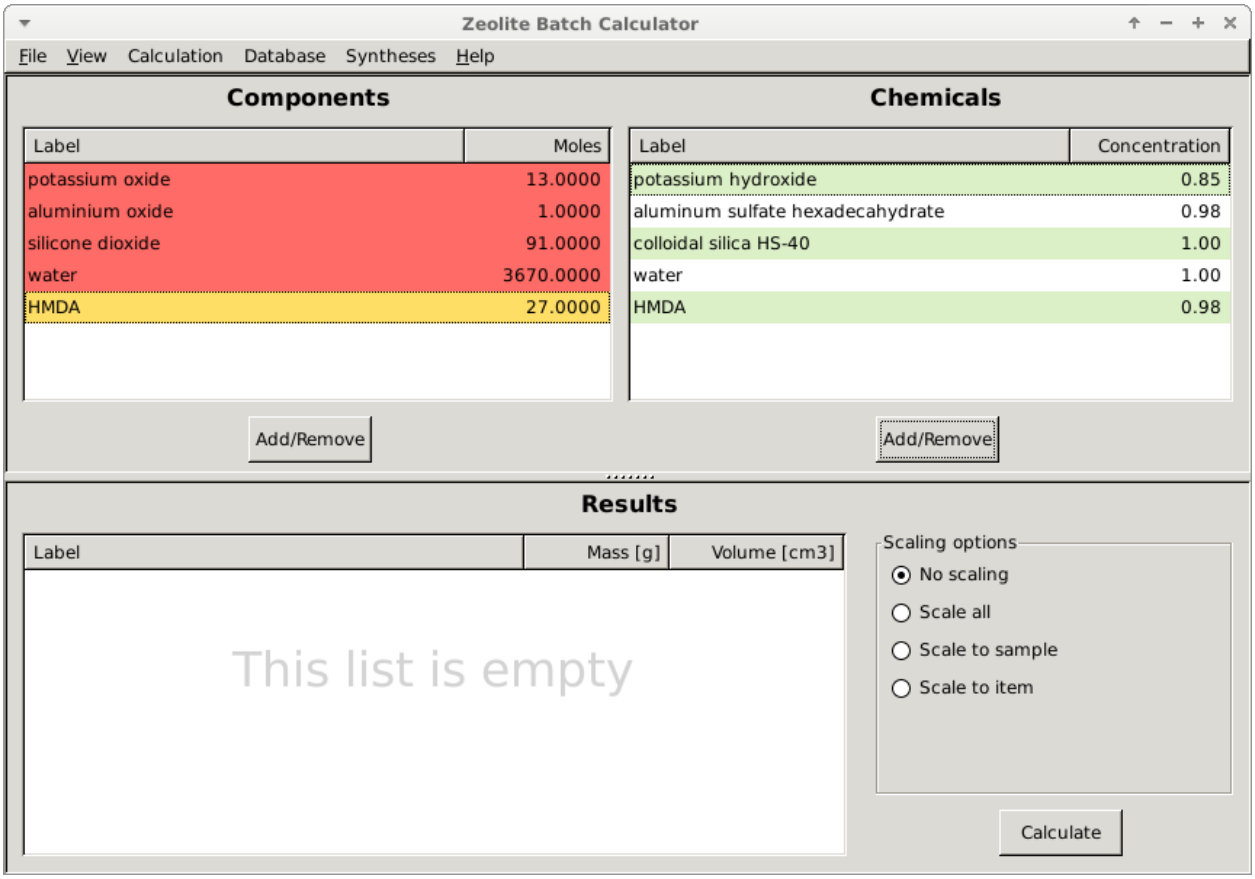
Now we need to add the chemicals by clicking the **Add/Remove** button in the **Chemicals** panel to open the dialog with all the chemicals in the database that are potential sources for the selected components



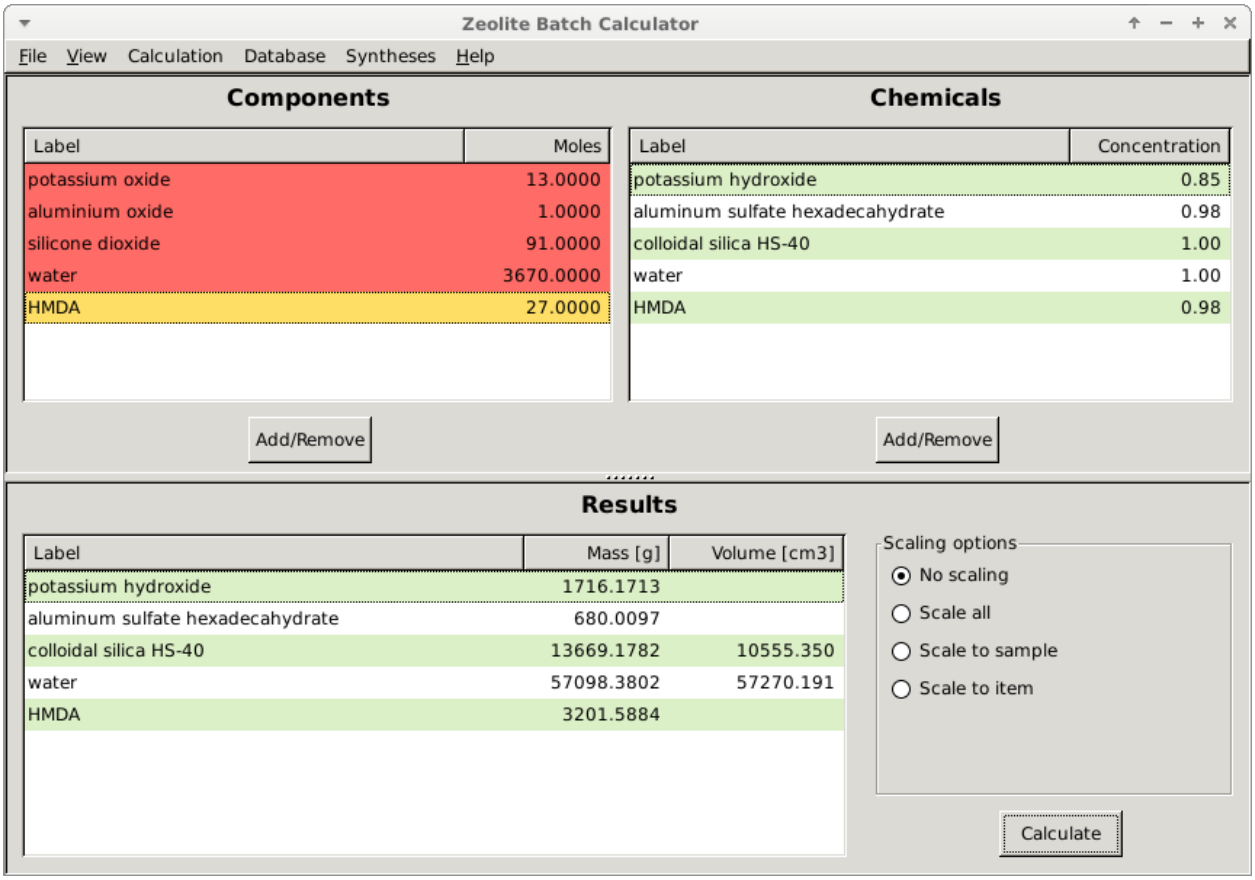
We can now select the appropriate chemicals by ticking the boxes in the first column and click **OK**.



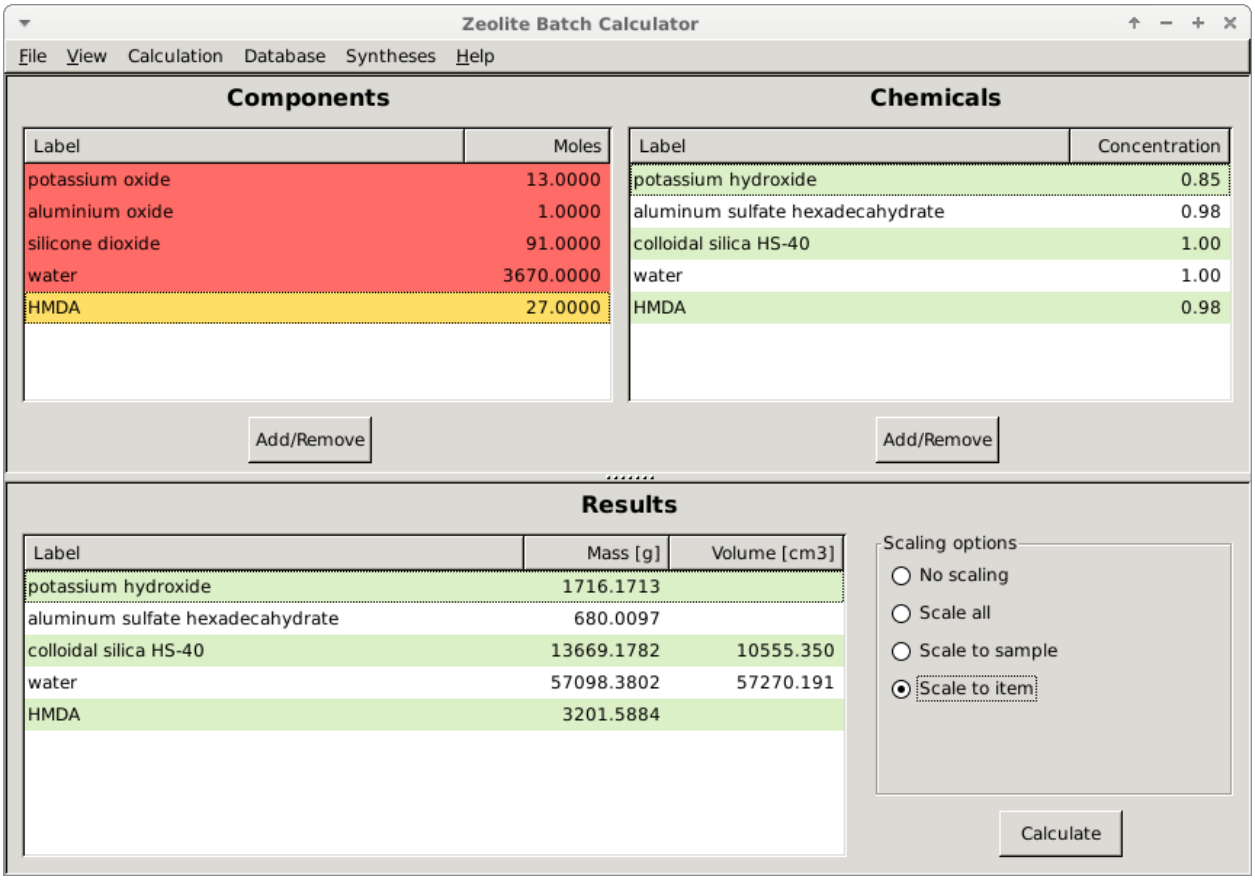
We can see that the chemical we successfully added to the main window with their default concentration/purities depending on the kind of chemical. The concentrations/purities can be adjusted in the same way as the amounts of components by double clicking the fields and entering the desired values.



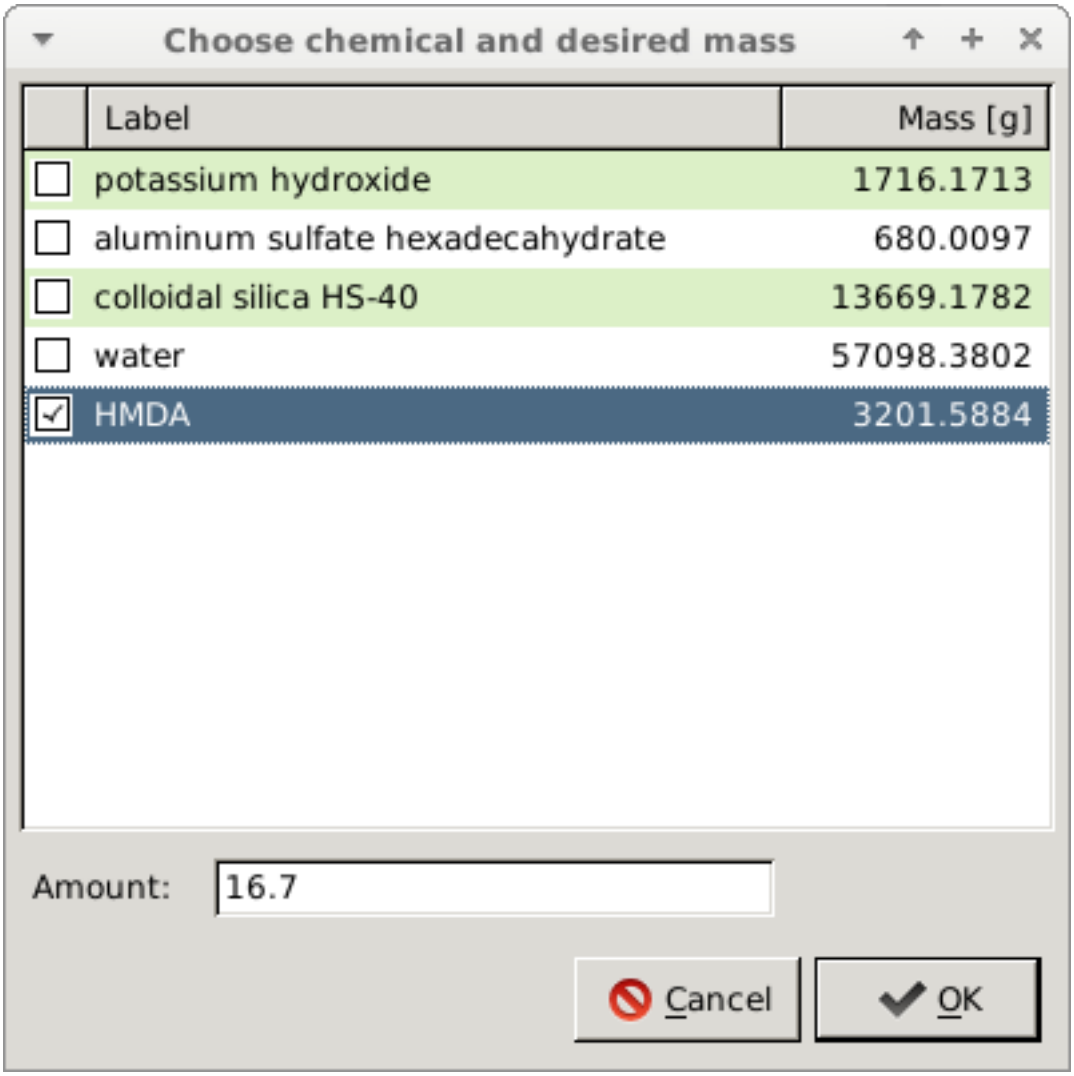
By clicking the **Calculate** button, the calculation will be performed and the result will appear in the **Results** panel.



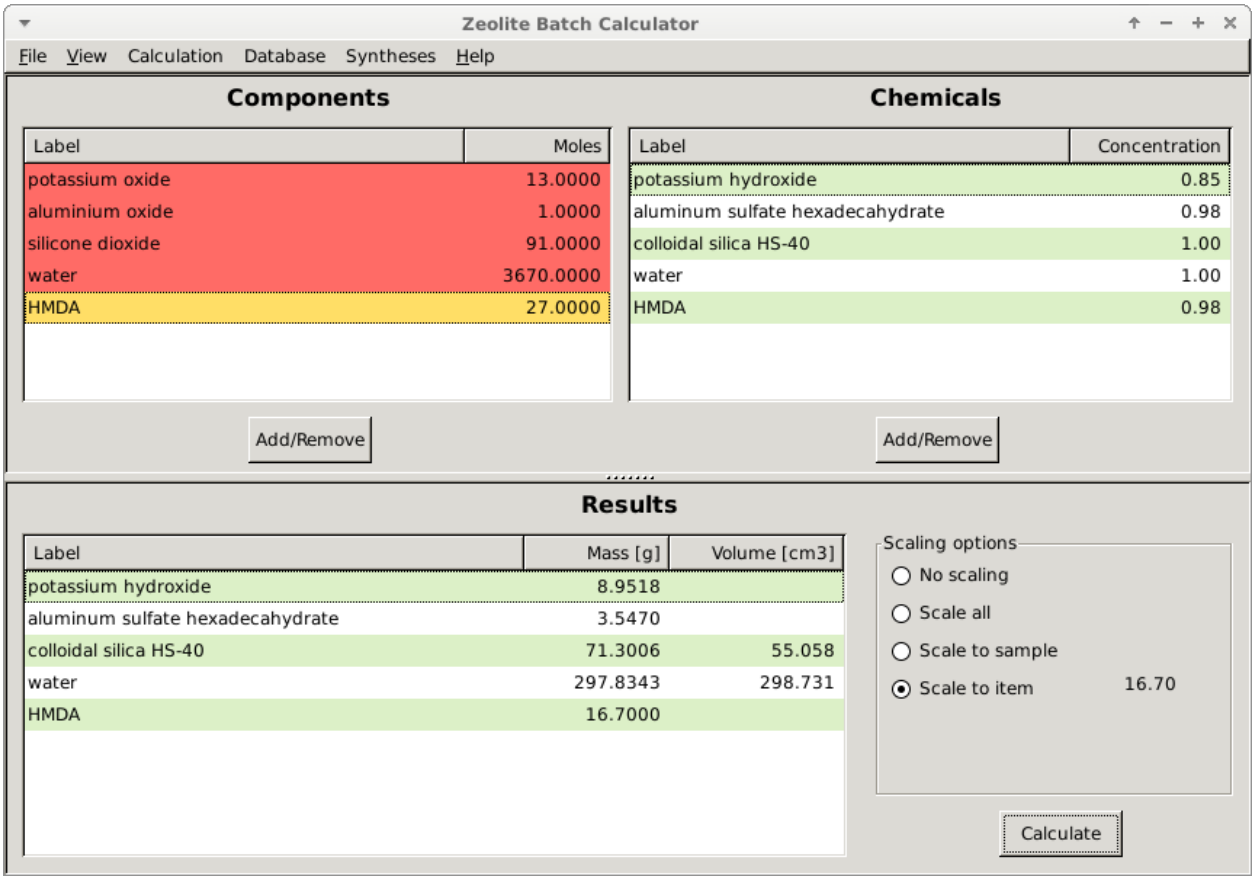
On the right hand side of the **Results** panel are the scaling options to adjust the batch size. In order to compare our results to the ones used in the paper we will rescale all the masses to the 16.7 g of HDMA using the **Scale to item** option.



After selecting that option and clicking **Calculate** again a dialog will appear where we will select **HMDA** and enter a value of **16.7** to scale all the masses (and volumes) to 16.7 g of **HMDA** and click **OK**.

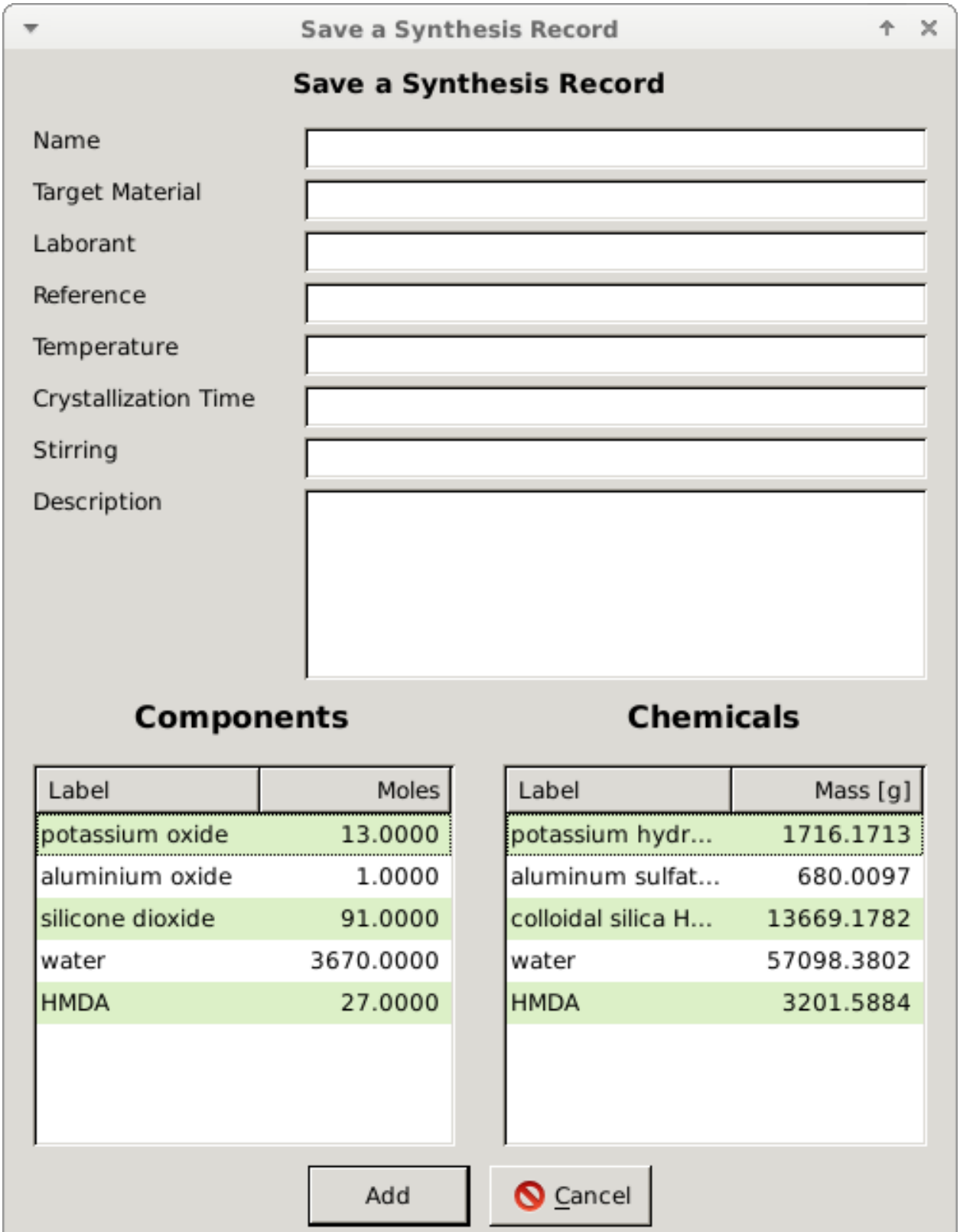


The updated masses are now shown in the **Results** panel instead of the initial results.

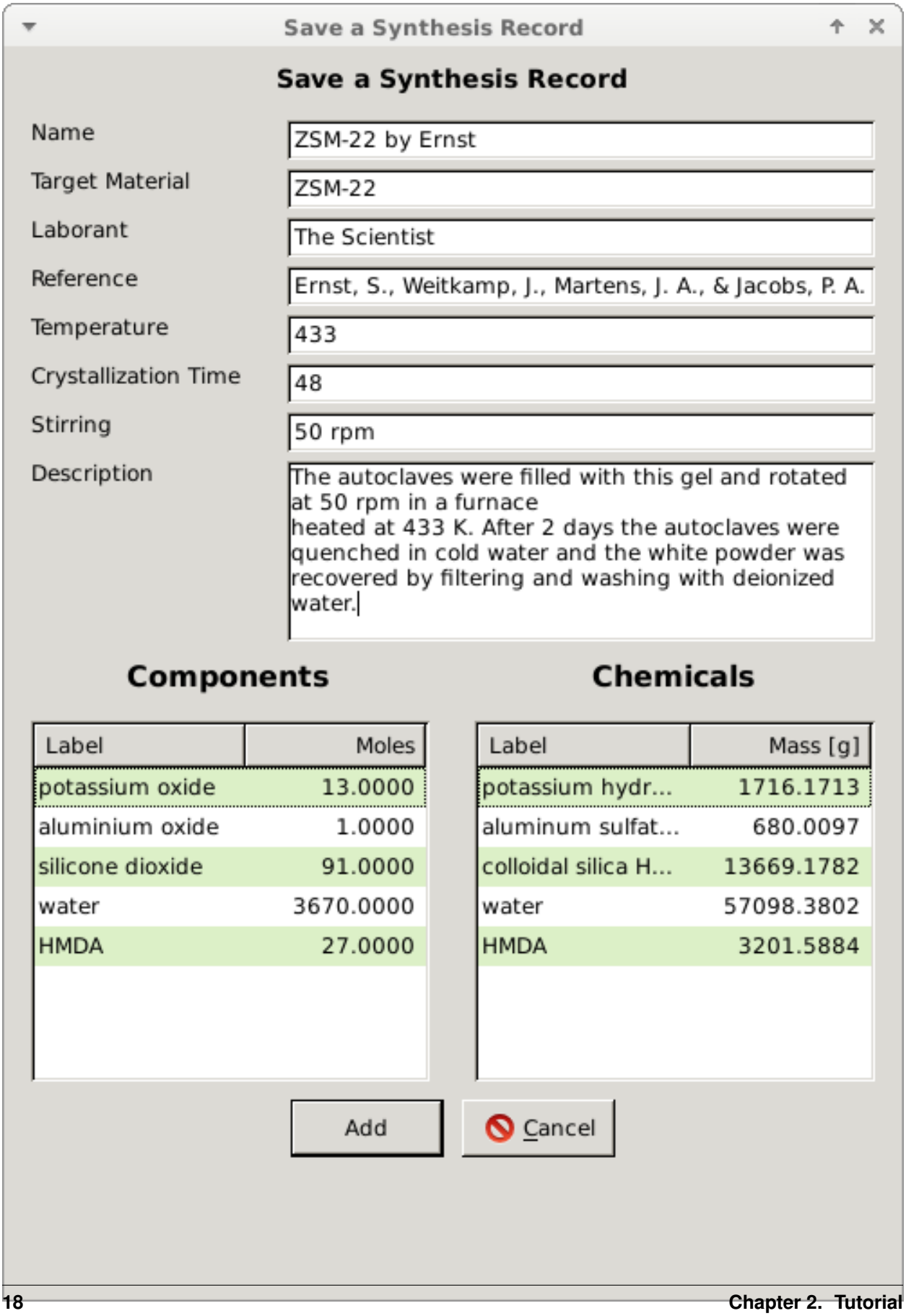


The result can be stored internally for further reference or modification by clicking the **Add current** option from the **Syntheses** drop down menu

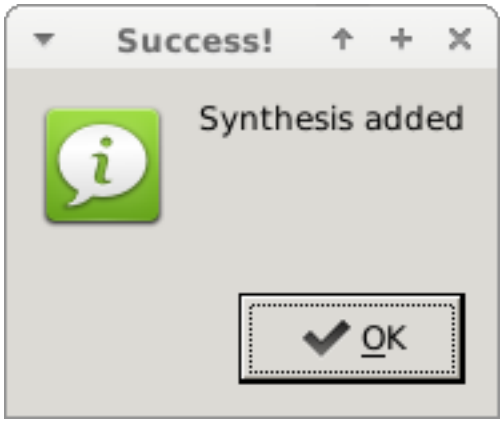
A dialog will be opened with an option to provide additional information about the synthesis of the material


Save a Synthesis Record
Save a Synthesis Record
Name
Target Material
Laborant
Reference
Temperature
Crystallization Time
Stirring
Description
Components
Label
Moles
potassium oxide
13.0000
aluminium oxide
1.0000
silicone dioxide
91.0000
water
3670.0000
HMDA
27.0000
Chemicals
Label
Mass [g]
potassium hydr...
1716.1713
aluminum sulfat...
680.0097
colloidal silica H...
13669.1782
water
57098.3802
HMDA
3201.5884
Add
Cancel

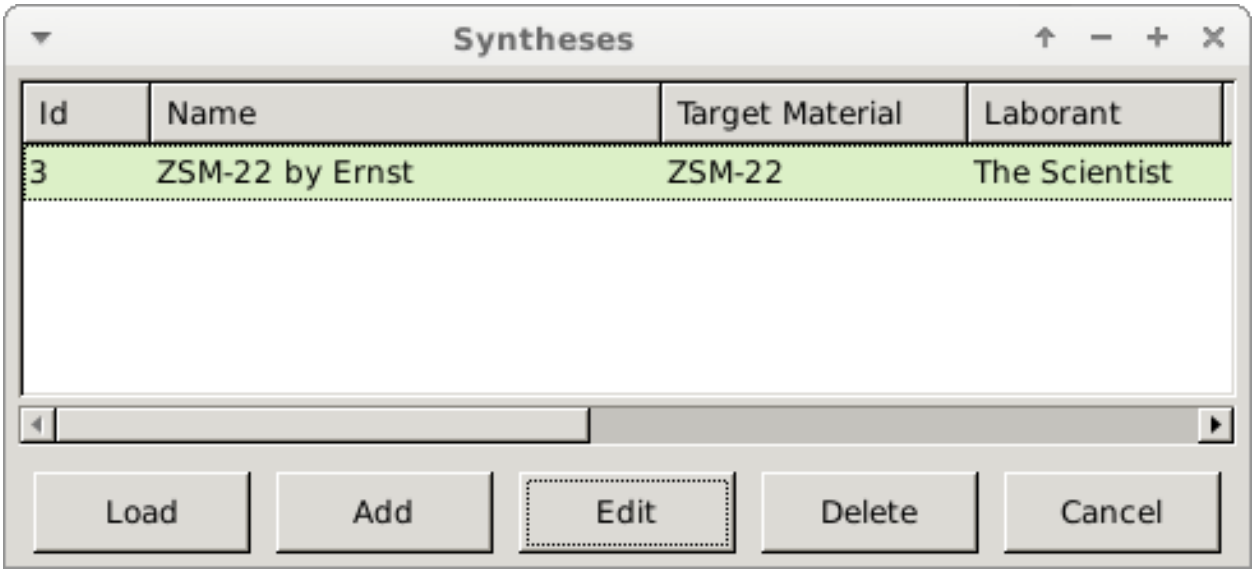
After filling in the form we can click the **Add** button that will store the information in the internal database.


Save a Synthesis Record
Save a Synthesis Record
Name
ZSM-22 by Ernst
Target Material
ZSM-22
Laborant
The Scientist
Reference
Ernst, S., Weitkamp, J., Martens, J. A., & Jacobs, P. A.
Temperature
433
Crystallization Time
48
Stirring
50 rpm
Description
The autoclaves were filled with this gel and rotated at 50 rpm in a furnace
heated at 433 K. After 2 days the autoclaves were quenched in cold water and the white powder was recovered by filtering and washing with deionized water.
Components
Label
Moles
potassium oxide
13.0000
aluminium oxide
1.0000
silicone dioxide
91.0000
water
3670.0000
HMDA
27.0000
Chemicals
Label
Mass [g]
potassium hydr...
1716.1713
aluminum sulfat...
680.0097
colloidal silica H...
13669.1782
water
57098.3802
HMDA
3201.5884
Add
Cancel

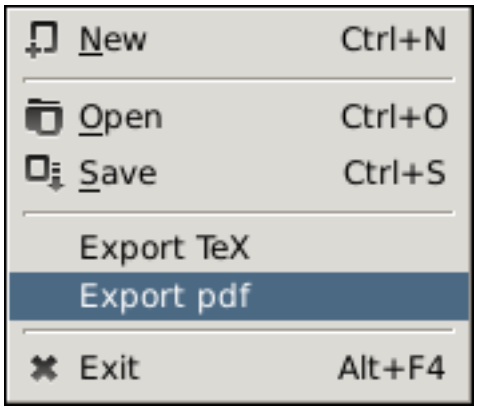
The dialog confirming the success of the modification should be displayed.



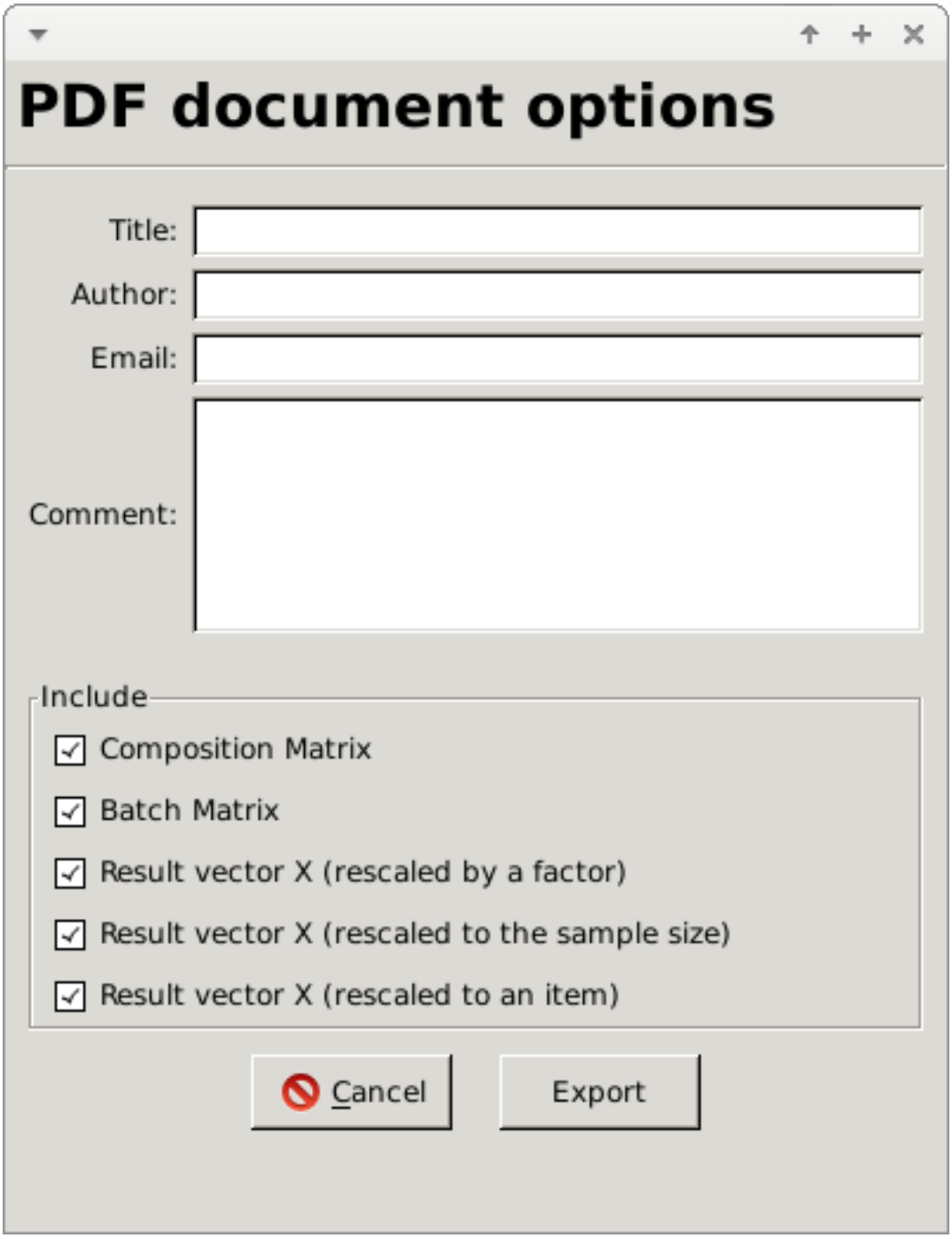
To verify or access the stored syntheses go to the **Syntheses** menu and select **Show All** which will open up a dialog with the stored records. From here the syntheses can be loaded back into the *Batch Calculator* deleted or modified.



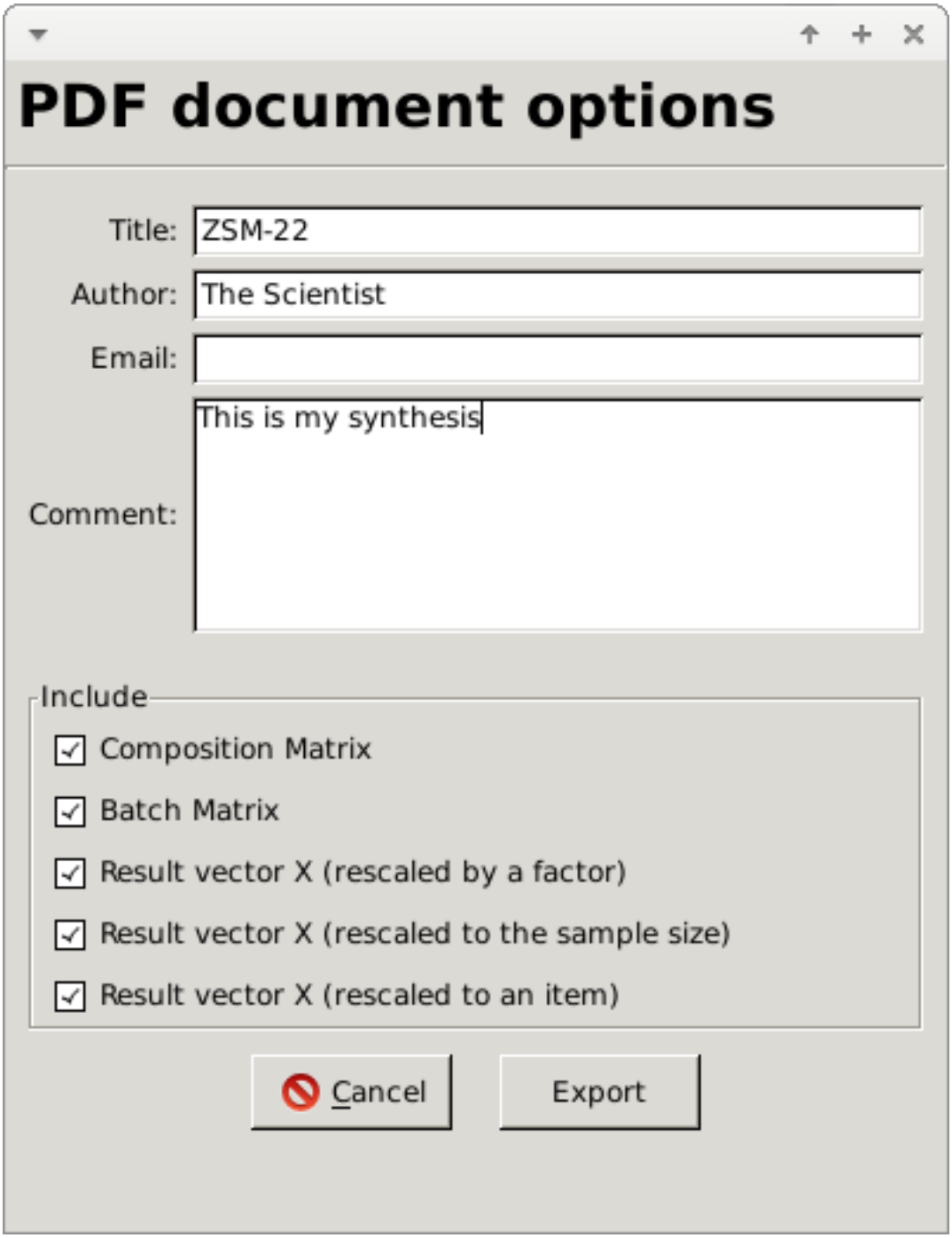
To finalize we can export a lab report for this synthesis by selecting the **Export to pdf** option from the **File** menu



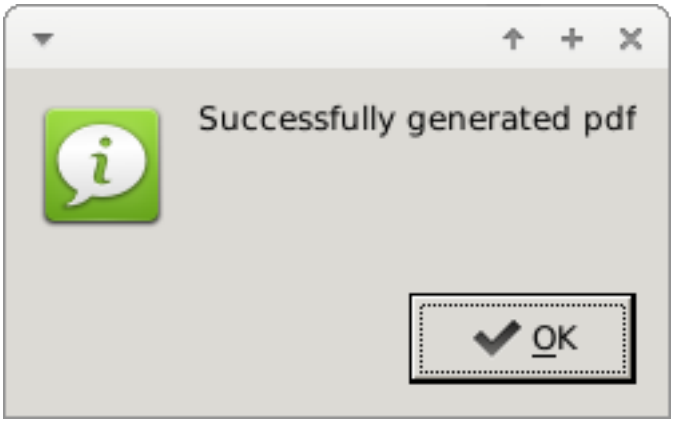
Another dialog appears with additional options for the report, where also the sections of the report can be chosen



After filling out the details and clicking **Export**



a dialog will appear to choose the file name and finally a message should appear that the pdf was successfully generated.



The report should like similar to the one below

19:56:25 04.09.2016

ZSM-22

$13.0K_2O:1.0Al_2O_3:91.0SiO_2:3670.0H_2O:27.0HMDA$

The Scientist

Composition Matrix [C]

Compound	K2O	Al2O3	SiO2	H2O	NH2(CH2)6NH2
Mole ratio	13.000	1.000	91.000	3670.000	27.000
Weight [g]	1224.548	101.961	5467.671	66115.784	3137.557
Mol. wt. [g/mol]	94.196	101.961	60.084	18.015	116.206

Batch Matrix [B]

Compound	K2O	Al2O3	SiO2	H2O	NH2(CH2)6NH2
KOH (85.00%)	0.7135	0.0000	0.0000	0.2865	0.0000
Al2(SO4)3*18H2O (98.00%)	0.0000	0.1530	0.0000	0.4866	0.0000
SiO2 (100.00%)	0.0000	0.0000	0.4000	0.6000	0.0000
H2O (100.00%)	0.0000	0.0000	0.0000	1.0000	0.0000
NH2(CH2)6NH2 (98.00%)	0.0000	0.0000	0.0000	0.0000	1.0000

Results [X] (SF=100.0000)

Substance	Formula	Mass [g]	Volume [cm3]	Weighted Mass [g]
potassium hydroxide	KOH	17.1617		
aluminum sulfate hexadecahydrate	Al2(SO4)3*18H2O	6.8001		
colloidal silica HS-40	SiO2	136.6918	105.5535	
water	H2O	570.9838	572.7019	
HMDA	NH2(CH2)6NH2	32.0159		
Sum		763.6533	678.2554	

Results [X] (SF= 1.0000)

Substance	Formula	Mass [g]	Volume [cm3]	Weighted Mass [g]
potassium hydroxide	KOH	1716.1713		
aluminum sulfate hexadecahydrate	Al2(SO4)3*18H2O	680.0097		
colloidal silica HS-40	SiO2	13669.1782	10555.3500	
water	H2O	57098.3802	57270.1907	
HMDA	NH2(CH2)6NH2	3201.5884		
Sum		76365.3277	67825.5407	

Results [X] (SF=191.7119)

Substance	Formula	Mass [g]	Volume [cm3]	Weighted Mass [g]
potassium hydroxide	KOH	8.9518		
aluminum sulfate hexadecahydrate	Al2(SO4)3*18H2O	3.5470		
colloidal silica HS-40	SiO2	71.3006	55.0584	
water	H2O	297.8343	298.7305	
HMDA	NH2(CH2)6NH2	16.7000		
Sum		398.3338	353.7889	

Comments

This is my synthesis

CHAPTER 3

Indices and tables

- genindex
- modindex
- search