

PROCEDURE

to plot Mass Spectroscopy
and Thermogravimetry data
from Netzsch Dispsav and Proteus
in Origin software

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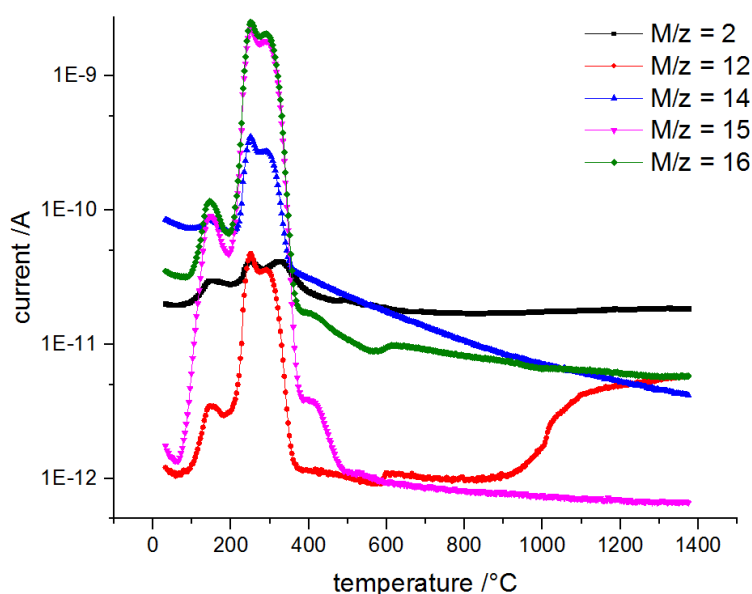
This is a guide to process and plot the mass spectroscopy (MS) and thermogravimetry (TG) data recorded from the Netzsch pieces of equipment in Origin 2016 software.¹ This also includes some scripts to automate the process.

The script source files and setup can be found at :

<https://github.com/sylvain-kern/tgmsplot-script>

along with this very procedure in .pdf or .md formats for user convenience.

¹ Origin 2016 -
<https://www.originlab.com/index.aspx?go=PRODUCTS/Origin>

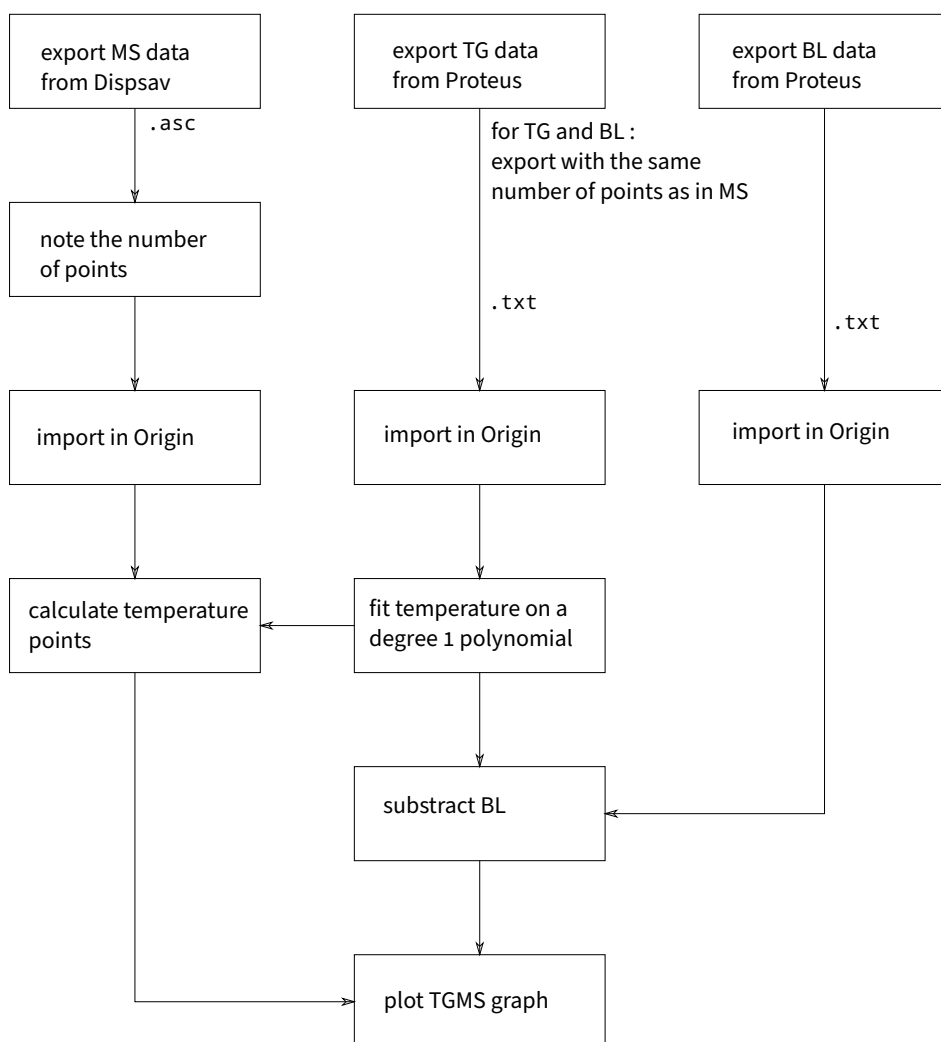


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1 Manual procedure

Here is a way to get TGMS plots from data collected in the different Netzsch pieces of software, using Origin.



This is a visual overview of the procedure explained below.

However, this procedure can be quite repetitive, so a script that executes it automatically is presented in section 2.

1.1 Exports

1.1.1 Export MS data from Dispsav

1. Open Aëolos Dispsav.
2. Go to the **Process** tab, go to **Cycles...** and open the desired **.mdc**.
3. Then go to **File > Convert to ASCII...**.
4. Save the **.asc** file into a chosen folder.

5. Open this `.asc` file with a notepad and note the number of points and the maximum time, which appear in the header lines or in the last line of the two firsts columns.

1.1.2 Export TG data form Netzsch Proteus

1. Open Proteus Analysis.
2. Go to `File > Open...` and open the `.ngb-ss1` file of your choice.
3. Then go to `Extras > Export Data...`. Choose the range and number of points². The number of points must be exactly the same as in the `.asc` file exported from Dispsav. Check that the maximum time matches too.

² Since the TG and MS experiments have been made at the same time with the same temperature increase, the temperature measurements and the step should match for the MS and TG.

1.1.3 Export baseline data

The baseline data is in the same form than the TG data, so the steps are exactly similar than those on the paragraph above. Again, export it with exactly the same number of points and maximum time as in the MS.

1.2 Imports in Origin

The data treatments will be executed on Origin software. To continue, open Origin.

1.2.1 Import MS data in ASCII format

Here are the steps to import the first MS data worksheet, *i.e* the relative intensity extrema for each M/z .

1. On Origin, go to `File > Import > Import Wizard` or press `Ctrl+3`.
2. On the `Import Wizard - Source` window, select the MS data file you saved. Make sur the data type ASCII is selected, and click `Next`.

This procedure has been made using Origin 2016 version 93E. The software may differ a bit if you use more recent versions of the software. For more help, see Origin's user guide: www.originlab.com/doc/User-Guide

If the `Import` line does not appear on the `File` menu, make sure an Origin project is open by clicking `File > New > Project`.

Data Type

☒ ASCII ☐ Binary ☐ User Defined

Data Source

☒ File C:\Users\Admin\Desktop\sylvain_stage\procedures origin\donnees-test\MS\He\ae36 phms40c ... ☐ Clipboard

Import Filter

☒ List filters applicable to both Data Type and file name

Import Filters for current Data Type User Files Folder: ASCII

Description

Target Window

☒ Worksheet ☐ Matrix ☐ None (User Defined filter needs to create window)

Template <default>

Template could be used only when import mode is start new books or start new sheets

Import Mode Replace Existing Data

Cancel << Back Next >> Finish

- On the Import Wizard - Header Lines window, specify the number of header lines –i.e. the number of lines which will be ignored by Origin. Leave the Number of subheader lines at 0, and Long Names at 0 too.

Number of main header lines(exclude subheader lines) 9

Number of subheader lines 0

☐ Auto determine header lines

Column Label Assignment from Subheader Lines

Short Names <None>

Long Names <None>

Units <None>

☐ Extract Long Names and Units from Same Line

Comments <None> to 0

System Parameters <None> to 0

User Parameters <None> to 0

Characters to skip on each line 0

Preview Font System Preview Lines 50

Prefix: S=Short Name, L=Long Name, U=Units, P=Parameters, C=Comment, MH=Main Header, SH=Subheader

```

001 001MH ASCII SAMPLE CYCLES : e36 phms40dub 412mg monolith
002 002MH DATE : 19/11/2013 TIME : 09:50:23
003 003MH CONVERTED CYCLES : 186
004 004MH
005 005MH Number of stored cycles 186
006 006MH Printed start cycle 1
007 007MH Printed end cycle 186
008 008MH Number of stored datablocks 4
009 009MH
010 Datablock 0 Analog Input [V]
011 '0/0' [V] TC min: 0.234409 max: 8.54384
012 Datablock 1 Ion Current [A]
013 '1/0' 2.00 min: -2.3045E-014 max: 7.54705E-013
014 '1/1' 12.00 min: -3.38069E-014 max: 1.20491E-014
015 '1/2' 14.00 min: 1.68903E-013 max: 3.98264E-013
016 '1/3' 15.00 min: -3.20437E-014 max: 1.54455E-012
017 '1/4' 16.00 min: 6.96464E-014 max: 2.06829E-012
018 '1/5' 18.00 min: 7.4644E-014 max: 0.04650E-014
  
```

Cancel << Back Next >> Finish

The data preview should look like this: header lines in black and data lines

in gray.

Then, click **Next**.

- On **Variable Extraction** window, verify that the **Save file into a workbook** box is ticked. Leave the other boxes blank and click **Next**.

Extract variables from file names and file headers

- ☐ Specify location of variable names and values using delimiters
- ☐ Specify location of variable names and values using character positions
- ☐ Specify delimiter and Wizard scans for variable names and values
- ☐ Call a user defined Origin C function

Source File

Function Name

- ☐ Add variables to page info
- ☐ Create User Parameter rows for each variable

File Info

- ☒ Save file info. in workbook

- On **File name options**, tick the **Worksheet with filename** box and leave the others alone. Then go **Next**.

Rename

- ☐ Auto
- ☒ worksheet with filename
- ☐ worksheet with variable
- ☐ workbook with file name
- ☐ workbook with variable
- ☐ Rename Long Name for Book only
- ☐ Include path when rename workbook

Append

- ☐ file name to workbook comments
- ☐ file name to column comments
- ☒ Include path when appending file name

- On **Data Columns**, select the number of columns there are in the imported file, – here 6, click **Apply** and make sure that the data is properly formatted in the preview window. Select the **1,000.00** numeric separator and go to the **Next** page.

Column Separator

☒ Delimiter ☐ Tab/Space ☐ Tab ☐ Comma ☐ Semicolon ☐ Space ☐ Other ☐

☐ Treat consecutive delimiters as one

☐ Fixed Width

Column Designations

<Unchanged>

Right click column heading to set format and designation for individual column.

Number of columns

Text Qualifier ☐ Remove

☐ Keep target column format

☒ Remove leading zeroes from numbers

☐ Force Rows to same size by filling missing value

☐ Column Width Preview (Click and drag edge of column header to resize columns)

Custom Date Format

Custom Time Format

Numeric Separator

Add Sparklines

A(V)(T&N)	B(V)(T&N)	C(V)(T&N)	D(V)(T&N)	E(V)(T&N)
Datablock 0	Analog Input	[U]		--
'0/0'	[U] TC	min:	0,23441	max:
Datablock 1	Ion Current	[A]		--
'1/0'	2	min:	-2,3045E-14	max:
'1/1'	12	min:	-3,38069E-14	max:
'1/2'	14	min:	1,68903E-13	max:
'1/3'	15	min:	-3,20437E-14	max:
'1/4'	16	min:	6,96464E-14	max:
'1/5'	18	min:	-7,16411E-15	max:
'1/6'	28	min:	8,48202E-13	max:
'1/7'	30	min:	1,51461E-13	max:
'1/8'	31	min:	-3,55389E-14	max:
'1/9'	42	min:	-3,7694E-14	max:
'1/10'	43	min:	-3,74612E-14	max:
'1/11'	44	min:	-3,22126E-14	max:
'1/12'	45	min:	-3,75118E-14	max:
'1/13'	46	min:	-3,59657E-14	max:

7. On Data Selection, just leave Partial import to None click Next – the data should be correctly displayed in the window below, just like in the last step. Then go Next .

Partial Import

From Column To Skip Columns Read Columns

From Row To Skip Rows Read Rows

Non-numeric data in a numeric field

A(V)(T&N)	B(V)(T&N)	C(V)(T&N)	D(V)(T&N)	E(V)(T&N)
Datablock 0	Analog Input	[U]		--
'0/0'	[U] TC	min:	0,23441	max:
Datablock 1	Ion Current	[A]		--
'1/0'	2	min:	-2,3045E-14	max:
'1/1'	12	min:	-3,38069E-14	max:
'1/2'	14	min:	1,68903E-13	max:
'1/3'	15	min:	-3,20437E-14	max:
'1/4'	16	min:	6,96464E-14	max:
'1/5'	18	min:	-7,16411E-15	max:
'1/6'	28	min:	8,48202E-13	max:
'1/7'	30	min:	1,51461E-13	max:
'1/8'	31	min:	-3,55389E-14	max:
'1/9'	42	min:	-3,7694E-14	max:
'1/10'	43	min:	-3,74612E-14	max:
'1/11'	44	min:	-3,22126E-14	max:
'1/12'	45	min:	-3,75118E-14	max:
'1/13'	46	min:	-3,59657E-14	max:

8. On Save Filters, leave everything as it is, unless you want to save this

Number of main header lines(exclude subheader lines) 35 ☐ Line number start from bottom

Number of subheader lines 1 ☐ Auto determine header lines

Column Label Assignment from Subheader Lines

Short Names <None> Comments <None> to 0

Long Names 1 System Parameters <None> to 0

Units <None> User Parameters <None> to 0

☐ Extract Long Names and Units from Same Line Characters to skip on each line 0

Preview Font System Preview Lines 50

Prefix: S=Short Name, L=Long Name, U=Units, P=Parameters, C=Comment, MH=Main Header, SH=Subheader

028 028MH '1/15' 59.00 min: -3.7519E-014 max: 1.19628E-014

029 029MH '1/16' 73.00 min: -3.71024E-014 max: -1.42418E-014

030 030MH '1/17' 91.00 min: -3.75622E-014 max: -1.78932E-014

031 031MH Datablock 2 Analog Input [mbar]

032 032MH '2/0' AI 1 min: 3.63425E-006 max: 4.22764E-006

033 033MH Datablock 3 Float Var. []

034 034MH '3/0' Temp [°C] min: 39 max: 1452

035 035MH

036 001SH L Cucle Date Time RelTime[s] '0/0' '1/0' '1/1' '1/2' '1'

037 1 19/11/2013 09:50:23:01 0.015 0.234409 -4.01502E-015

038 2 19/11/2013 09:50:23:01 0.015 0.234409 -4.01502E-015

039 3 19/11/2013 09:51:18:66 55.661 0.234721 -1.60586E-01

040 4 19/11/2013 09:52:14:30 111.308 0.249389 -1.72305E-0

041 5 19/11/2013 09:53:09:92 166.923 0.285593 -1.59787E-0

042 6 19/11/2013 09:54:05:55 222.553 0.334594 -1.76531E-0

043 7 19/11/2013 09:55:01:18 278.185 0.414492 -1.70443E-0

044 8 19/11/2013 09:55:56:81 333.816 0.499072 -1.6465E-01

045 0 19/11/2013 09:56:52:45 388.445 0.58075 -1.77605E-01

Cancel << Back Next >> Finish

The data preview should look like this, with the subheader lines highlighted in blue.

Then, click Next .

- On Variable Extraction window, verify that the Save file into a workbook box is ticked. Leave the other boxes blank and click Next .
- On File name options , tick the Worksheet with filename box and leave the others alone. Then go Next .
- On Data Columns , select the number of columns there are in the imported file, – here 25, click Apply and make sure that the data is properly formatted in the preview window. Select the 1,000.00 numeric separator and go to the Next page.

Column Separator

☒ Delimiter ☐ Tab/Space ☐ Tab ☐ Comma
☐ Semicolon ☐ Space ☐ Other ☐

☐ Treat consecutive delimiters as one

☐ Fixed Width 4

Column Designations

<Unchanged>

Right click column heading to set format and designation for individual column.

Number of columns 25

Text Qualifier <None> ☐ Remove

☐ Keep target column format

☒ Remove leading zeroes from numbers

☐ Force Rows to same size by filling missing value

☐ Column Width Preview (Click and drag edge of column header to resize columns)

Custom Date Format <None>

Custom Time Format <None>

Numeric Separator 1,000.00

Add Sparklines Yes(if less than 50 columns)

V (T&N)	U (V) (T&N)	W (V) (T&N)	X (V) (T&N)	Y (V) (T&N)
45127E-14	-3,3779E-14	-3,40531E-14	3,69606E-6	39
45127E-14	-3,3779E-14	-3,40531E-14	3,69606E-6	39
62539E-14	-3,66653E-14	-3,65715E-14	3,70018E-6	40
7519E-14	-3,66701E-14	-3,75622E-14	3,70224E-6	42
7406E-14	-3,67361E-14	-3,62972E-14	3,68782E-6	47
69569E-14	-3,6782E-14	-3,65866E-14	3,69812E-6	56
65169E-14	-3,69191E-14	-3,68988E-14	3,70018E-6	69
64655E-14	-3,64322E-14	-3,74515E-14	3,69606E-6	84
7256E-14	-3,69268E-14	-3,67231E-14	3,69812E-6	97
70389E-14	-3,71024E-14	-3,59251E-14	3,70018E-6	111
56317E-14	-3,6504E-14	-3,60733E-14	3,70018E-6	121
50041E-14	-2,54704E-14	-2,72675E-14	3,67546E-6	120

8. On Data Selection, just leave Partial import to None and click Next – the data should be correctly displayed in the window below, just like in the last step. Then go Next .

Partial Import None

From Column 1 To 0 Skip Columns 0 Read Columns 0

From Row 1 To 0 Skip Rows 0 Read Rows 1

Non-numeric data in a numeric field Read as text

A (V) (T&N)	B (V) (D)	C (V) (Tm)	D (V) (T&N)	E (V) (T&N)
1	19/11/2013	266:23	0,015	0,23441
2	19/11/2013	266:23	0,015	0,23441
3	19/11/2013	267:19	55,661	0,23472
4	19/11/2013	268:14	111,308	0,24939
5	19/11/2013	269:10	166,923	0,28559
6	19/11/2013	270:05	222,553	0,33459
7	19/11/2013	271:01	278,185	0,41449
8	19/11/2013	271:57	333,816	0,49907
9	19/11/2013	272:52	389,465	0,58428
10	19/11/2013	273:48	445,112	0,65887
11	19/11/2013	274:44	500,774	0,71879
12	19/11/2013	275:39	556,437	0,76904
13	19/11/2013	240:35	612,085	0,81367
14	19/11/2013	241:31	667,7	0,85705
15	19/11/2013	242:26	723,316	0,9098
16	19/11/2013	243:22	778,978	0,97378
17	19/11/2013	244:18	834,61	1,03683

9. On Save Filters, leave everything as it is, unless you want to save this

import filter for a next time. Click **Finish**.

Now you have two worksheets, one with M/z data, the other with the actual MS curves.

To make future worksheet reference easier, I renamed the worksheets with the respective names "mz sheet", "ms data". To do the same, right-click a worksheet tab on the bottom, "Name and Comments..." and fill the "Short Name" field.



	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)
Long Name						
Units						
Comments						
F(x)=						
Sparklines						
1	Datablock 0	Analog Input [V]				
2	'0/0'	[V] TC	min:	0.23441	max:	8.54384
3	Datablock 1	Ion Current [A]				
4	'1/0'	2 min:	-2.3045E-14	max:	7.54705E-13	
5	'1/1'	12 min:	-3.38069E-14	max:	1.20491E-14	
6	'1/2'	14 min:	1.68903E-13	max:	3.98264E-12	
7	'1/3'	15 min:	-3.20437E-14	max:	1.54455E-12	
8	'1/4'	16 min:	6.96484E-14	max:	2.06829E-12	
9	'1/5'	18 min:	-7.16411E-15	max:	4.31659E-14	
10	'1/6'	28 min:	8.48202E-13	max:	2.08033E-12	
11	'1/7'	30 min:	1.51461E-13	max:	4.36167E-13	
12	'1/8'	31 min:	-3.55389E-14	max:	8.21005E-15	
13	'1/9'	42 min:	-3.7694E-14	max:	-7.51887E-15	
14	'1/10'	43 min:	-3.74612E-14	max:	3.30935E-14	
15	'1/11'	44 min:	-3.22126E-14	max:	1.21587E-13	
16	'1/12'	45 min:	-3.75118E-14	max:	8.46162E-14	
17	'1/13'	46 min:	-3.59657E-14	max:	-1.62815E-14	
18	'1/14'	58 min:	-3.71239E-14	max:	-4.52501E-15	
19	'1/15'	59 min:	-3.7519E-14	max:	1.19628E-14	
20	'1/16'	73 min:	-3.71024E-14	max:	-1.42418E-14	
21	'1/17'	91 min:	-3.75622E-14	max:	-1.78932E-14	
22	Datablock 2	Analog Input [mbar]				
23	'2/0'	AI 1	min:	3.63425E-6	max:	4.22764E-6
24	Datablock 3	Float Var. []				
25	'3/0'	Temp [°C]	min:	39	max:	1452
26						
27	Cycle	Date	Time	ReTime[s]	'0/0'	'1/0'
28	1	19/11/2013	09:50:23.01	0.015	0.23441	-4.01502E-15
29	2	19/11/2013	09:50:23.01	0.015	0.23441	-4.01502E-15
30	3	19/11/2013	09:51:18.66	55.661	0.23472	-1.60586E-14
31	4	19/11/2013	09:52:14.30	111.308	0.24939	-1.72305E-14
32	5	19/11/2013	09:53:09.92	166.923	0.28559	-1.59787E-14

	A(X)	B(Y)	C(Y)	D(Y)	E(Y)	F(Y)	G(Y)	H(Y)	I(Y)	J(Y)
Long Name	Cycle	Date	Time	ReTime[s]	'0/0'	'1/0'	'1/1'	'1/2'	'1/3'	'1/4'
Units										
Comments										
F(x)=										
Sparklines										
1	1	19/11/2013	266.23	0.015	0.23441	-4.01502E-15	-1.77078E-14	3.16359E-13	-2.22537E-14	1.24057E-13
2	2	19/11/2013	266.23	0.015	0.23441	-4.01502E-15	-1.77078E-14	3.16359E-13	-2.22537E-14	1.24057E-13
3	3	19/11/2013	267.19	55.661	0.23472	-1.60586E-14	-3.04259E-14	3.05827E-13	-2.81147E-14	1.15784E-13
4	4	19/11/2013	268.14	111.308	0.24939	-1.72305E-14	-3.24716E-14	3.07468E-13	-2.95648E-14	1.16719E-13
5	5	19/11/2013	269.10	166.923	0.28559	-1.59787E-14	-3.24532E-14	3.05755E-13	-3.18105E-14	1.10384E-13
6	6	19/11/2013	270.05	222.553	0.33459	-1.76831E-14	-3.38069E-14	3.03437E-13	-3.16278E-14	1.1715E-13
7	7	19/11/2013	271.01	278.185	0.41449	-1.70443E-14	-3.25024E-14	3.08316E-13	-3.20437E-14	1.17971E-13
8	8	19/11/2013	271.57	333.816	0.48907	-1.8495E-14	-3.24101E-14	3.00758E-13	-3.05478E-14	1.07569E-13
9	9	19/11/2013	272.52	389.465	0.58428	-1.7769E-14	-3.22245E-14	3.07359E-13	-3.09377E-14	1.19047E-13
10	10	19/11/2013	273.48	445.112	0.65887	-2.3045E-14	-3.12191E-14	3.04119E-13	-3.07255E-14	1.17341E-13
11	11	19/11/2013	274.44	500.774	0.71879	-1.34026E-14	-3.28112E-14	3.09409E-13	-2.84043E-14	1.12810E-13
12	12	19/11/2013	275.39	556.437	0.76904	-7.37815E-15	-3.20597E-14	3.12775E-13	-2.2633E-14	1.16392E-13
13	13	19/11/2013	240.35	612.085	0.81387	-3.33125E-15	-3.13307E-14	3.14447E-13	-1.66297E-14	1.13199E-13
14	14	19/11/2013	241.31	667.7	0.85705	-1.68108E-15	-3.06531E-14	3.17041E-13	-1.1653E-14	1.15477E-13
15	15	19/11/2013	242.26	723.316	0.9098	8.8839E-16	-2.99781E-14	3.21972E-13	-4.27881E-15	1.19216E-13
16	16	19/11/2013	243.22	778.978	0.97378	-6.005E-16	-2.90485E-14	3.24711E-13	3.20446E-15	1.16354E-13
17	17	19/11/2013	244.18	834.61	1.03683	2.12603E-15	-2.92614E-14	3.29083E-13	1.02303E-14	1.12432E-13
18	18	19/11/2013	245.13	890.287	1.10362	5.05978E-15	-2.859E-14	3.29458E-13	1.05663E-14	1.15934E-13
19	19	19/11/2013	246.09	945.918	1.16728	5.69251E-15	-2.97839E-14	3.24581E-13	1.22779E-14	1.09476E-13
20	20	19/11/2013	247.04	1001.55	1.22246	6.6174E-15	-2.84457E-14	3.24231E-13	1.41242E-14	1.11472E-13
21	21	19/11/2013	248.00	1057.24	1.27309	6.16862E-15	-2.81908E-14	3.1733E-13	1.2655E-14	1.12228E-13
22	22	19/11/2013	248.56	1112.87	1.31803	1.02724E-14	-2.86008E-14	3.15808E-13	1.37961E-14	1.09708E-13
23	23	19/11/2013	249.51	1168.52	1.36766	1.41284E-14	-2.84103E-14	3.16762E-13	1.05888E-14	1.07114E-13
24	24	19/11/2013	250.47	1224.18	1.4229	1.61197E-14	-2.83991E-14	3.11669E-13	1.34446E-14	1.05271E-13
25	25	19/11/2013	251.43	1279.84	1.47783	1.53088E-14	-2.81487E-14	3.11362E-13	1.26339E-14	1.07345E-13
26	26	19/11/2013	252.38	1335.45	1.53889	2.26762E-14	-2.78393E-14	3.03697E-13	1.50824E-14	1.08367E-13
27	27	19/11/2013	253.34	1391.11	1.58789	3.22888E-14	-2.80248E-14	3.05174E-13	1.83354E-14	1.0853E-13
28	28	19/11/2013	254.30	1446.72	1.65292	4.22103E-14	-2.69212E-14	3.05427E-13	2.24047E-14	1.13193E-13
29	29	19/11/2013	255.25	1502.35	1.7041	5.00289E-14	-2.54983E-14	3.05693E-13	2.88262E-14	1.08925E-13
30	30	19/11/2013	256.21	1559.03	1.75404	6.05523E-14	-2.6125E-14	3.10922E-13	3.55058E-14	1.1276E-13
31	31	19/11/2013	257.17	1613.73	1.80741	6.33115E-14	-2.52149E-14	3.01834E-13	4.14554E-14	1.14063E-13
32	32	19/11/2013	258.12	1669.41	1.85859	6.77893E-14	-2.62309E-14	3.10436E-13	4.62842E-14	1.18852E-13
33	33	19/11/2013	259.08	1725.07	1.91696	7.06243E-14	-2.4359E-14	3.14671E-13	5.53112E-14	1.15059E-13
34	34	19/11/2013	260.04	1780.75	1.97251	6.93469E-14	-2.46477E-14	3.12594E-13	6.29995E-14	1.20038E-13
35	35	19/11/2013	260.59	1836.43	2.0315	6.73743E-14	-2.39839E-14	3.13653E-13	6.73589E-14	1.17664E-13
36	36	19/11/2013	261.55	1892.11	2.08237	5.98748E-14	-2.40557E-14	3.10882E-13	7.39515E-14	1.19244E-13
37	37	19/11/2013	262.51	1947.8	2.1373	5.82595E-14	-2.24065E-14	3.12893E-13	8.24638E-14	1.17948E-13
38	38	19/11/2013	263.45	2003.5	2.18693	5.55978E-14	-2.10131E-14	3.15591E-13	8.98063E-14	1.15048E-13
39	39	19/11/2013	264.42	2059.18	2.24217	5.37044E-14	-2.13031E-14	3.1499E-13	9.75074E-14	1.14343E-13
40	40	19/11/2013	265.38	2114.85	2.29879	5.41937E-14	-1.94182E-14	3.20991E-13	1.1428E-13	1.17647E-13

1.2.2 Import TG data in .txt format

This is a bit shorter than the MS import but it is the same idea.

1. Create a new worksheet and switch to it.
2. Reach **File > Import > Import Wizard** and browse the desired file.
3. Filter the file the same way as for the MS file (headers and column numbers)

1.2.3 Import baseline data in .txt format

The steps are the same than the TG import in paragraph 1.2.2 since the files are formatted in the same way.

1.3 Preliminary treatments

You can rearrange the columns of your worksheets the way you want, delete some of the useless information, put names, units, comments etc...

The following steps treat the data to prepare the TGMS plots.

1.4 Place the M/z labels on MS columns

1. Switch to the "mz sheet" worksheet.
2. Create a new column by right-clicking on the empty gray space in the worksheet and selecting `Add new column`.
3. Right-click on the new column header and select `Set column values...`.
4. On the text area, type the following :

```
"M/z = "+col(M/z)$
```

Now the new column should have proper labels.

5. Delete the meaningless labels such as "M/z = Ion current", select the block of cells with the right label, right-click on it and select `Copy` (or press `Ctrl+C`).
6. Go to the "ms data" worksheet, select the leftmost columns with ms data (you can find it with the cycle number), right-click on it at the row "Long Name" and click `Paste transpose`.

The MS columns should now be properly labeled.

1.5 Calculate the relative intensity on mz sheet

1.5.1 Polynomial regression of the temperature curve in TG data

Since temperature vs. time is not given in the MS data, it is needed to whether fit a curve, whether interpolate the data, to get new temperature points corresponding to MS time points.

Assuming the temperature growth is more or less I chose to fit a degree one polynomial in this case.

1.5.2 Baseline mass loss data interpolation and subtraction⁴

If the exports are correct, with the same number of points, just skip this step.

The time points for TG and baseline may not be the same. If it is the case, we will want to interpolate the baseline mass loss data in order to get the correct values to subtract from TG ones, since the baseline data does not follow a predictable model.

The fit must only consider the points where the temperature grows – approximately – linearly, therefore it must omit all points from segment 2 and 3. The temperature increase shows some variations at the beginning, until a stabilized growth settles. Usually, this variation becomes marginal around $T = 200^\circ\text{C}$.

⁴ This is only needed if the TG and baseline data don't have the same measurement points. If they have been exported from Proteus with the same settings, please ignore this part.

2 Origin scripting for automated plots

To reduce the time spent on overly repetitive tasks, I produced a LabTalk – Origin's scripting language – file run by Origin to execute the procedure detailed above in section 1.

2.1 Scripts installation

2.1.1 Automatic installation

Go to the following address:

<https://github.com/sylvain-kern/tgmsplot-script>

and reach for the `setup.exe` file in the `setup` folder. Download it and run it⁵. The setup creates a `tgmsplot-script` folder in the Origin files directory and puts the script files in it. When installing, verify the destination folder, by default it is

```
C:\Program Files\OriginLab\Origin2016
```

⁵ Do not worry if Windows freaks out and thinks it is a virus, I do not have an authentication certificate indeed, so I can not guarantee to Windows that my program is safe (do not worry, it actually is).

but it can change with your version of Origin, so check your software version and where the program files are stored.

2.1.2 Manual installation

Download the folder that contains the source files on the project repository:

<https://github.com/sylvain-kern/tgmsplot-script>.

Place the `tgmsplot-script` in the following folder (check that this folder is the right for your software files):

```
C:\ProgramFiles\OriginLab\Origin2016\
```

If you have a different version of Origin, it may not be
'...\$\'backslash \$Origin2016',
but whatever your version is.

2.1.3 Button groups installation⁶

For more information about this step, check <https://www.originlab.com/doc/Origin-Help/UserDef-Custom-Toobar-Button>.

⁶ The button bitmap :



1. On Origin, go to `View > Toolbars` or press `Ctrl+T`. Go to the `Button groups` tab. Click `New`.
2. Choose a name for the button group.
3. Select "4" for the number of buttons.
4. For the bitmap, and browse for the file located at:

```
C:\ProgramFiles\OriginLab\Origin2016\tgmsplot-script\button-b
↪ itmap\bitmap.bmp
```

5. Then, right-click on the buttons that appear on the right pane, and assign them to the script files, respectively :

- `import-ms.ogs`
- `import-tg.ogs`
- `plot-vs-time.ogs`
- `plot-vs-temp.ogs`

6. Drag and drop the buttons in your favourite toolbar on Origin.

2.2 Usage

2.2.1 Using buttons

If the buttons are installed, just click on them to use the program.

2.2.2 Using the `run.file` command

Open the command window –this icon  on the right of the top toolbar. Then run the following command:

```
run.file("C:\ProgramFiles\Origin2016\tgmsplot-script\<file>")
```

A file browser window appears, select the file you want to load.

To import only the MS data, run the following in the command window:⁷ you want to load. Click `Ok` then do the same for the TG and baseline files.

```
run.file("C:\Program
↪ Files\Origin2016\tgmsplot-script\import-ms.ogs")
```

The same goes for TG and BL data:

```
run.file("C:\Program
↪ Files\Origin2016\tgmsplot-script\import-tg.ogs")
```

```
run.file("C:\Program
↪ Files\Origin2016\tgmsplot-script\import-bl.ogs")
```

Then, execute the plot program:

```
run.file("C:\Program Files\Origin2016\tgmsplot-script\plot.ogs")
```

⁷ Note that the script will NOT work if the file name contains accents or fancy characters.

The MS curves are not to scale on the *y* axis, which is not ticked. The TGMS plot is only meant to give a qualitative overview and not precise quantitative information.

2.3 Issues

In progress ...

3 Merge several Origin projects : the *Append* function

To compare several experiments imported in separated Origin projects, it is possible to merge the `.opj` files with the following procedure :

1. open a new Origin project ;
2. go on `File > Append` and select the first project you want to import ;
3. repeat the last step for the other project to append.

If the temperature increase and the number of points are the same, it is possible to copy/paste the desired data on one single worksheet and plot it directly.