

PROCEDURE

1

TO PLOT MASS SPECTROSCOPY AND THERMOGRAVIMETRY DATA FROM NETZSCH DISPSAV AND PROTEUS IN ORIGIN SOFTWARE

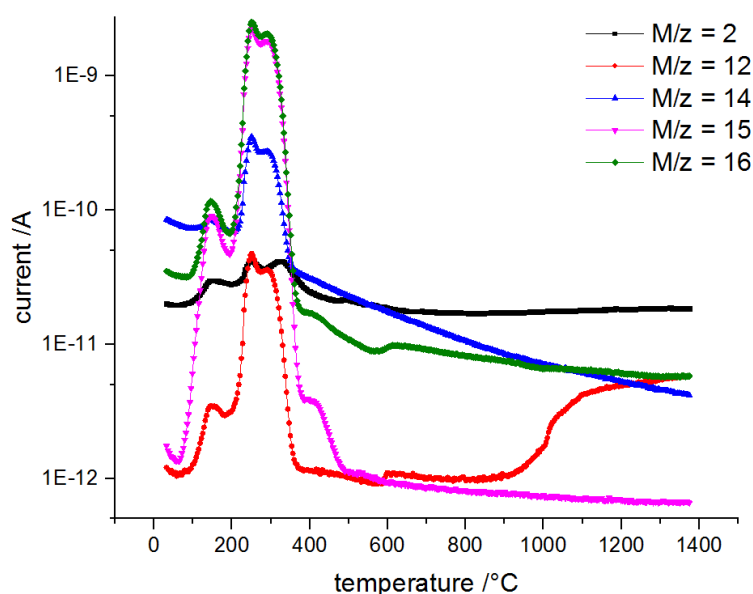
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January 18, 2021

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.

All source files can be found at . . . 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 quickly² get TGMS plots from data collected in the different Netzsch pieces of software, using Origin.

² The manual procedure is actually quite long and repetitive, so there is an Origin script presented in section 2.

This is a visual overview of the procedure explained below.

figures/overview.png

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 points³. The number of points must be exactly the same as in the .asc file exported from Dispsav. Check that the maximum time matches too.

³ 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

3. 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
☐ Line number start from bottom
 Number of subheader lines: 0
☐ Auto determine header lines

Column Label Assignment from Subheader Lines
 Short Names: <None> Comments: <None> to 0
 Long Names: <None> 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

```

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
011 Datablock 0 Analog Input [V]
012 '0/0' [V] TC min: 0.234409 max: 8.54384
013 Datablock 1 Ion Current [A]
014 '1/1' 2.00 min: -2.3045E-014 max: 7.54705E-013
015 '1/1' 12.00 min: -3.38069E-014 max: 1.20491E-014
016 '1/2' 14.00 min: 1.68903E-013 max: 3.98264E-013
017 '1/3' 15.00 min: -3.20437E-014 max: 1.54455E-012
018 '1/4' 16.00 min: 6.96464E-014 max: 2.06829E-012
019 '1/5' 18.00 min: 7.4644E-014 max: 1.94450E-014
  
```

Cancel << Back **Next >>** Finish

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

Then, click Next.

4. 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

5. 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

6. 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 4 Apply

Column Designations

<Unchanged> Apply

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

Number of columns 6 Apply

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) Add Column Delete Column

Custom Date Format <None> Apply

Custom Time Format <None> Apply

Numeric Separator 1,000.00

Add Sparklines Yes(if less than 50 columns)

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:

Cancel << Back Next >> Finish

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 None

From Column 1 To 0 Skip Columns 0 Read Columns 0

From Row 1 To 0 Skip Rows 0 Read Rows 1

Apply

Non-numeric data in a numeric field Read as text





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:

Cancel << Back Next >> Finish

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

this import filter for a next time. Click Finish.

Now your worksheet should look like this:⁴

	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-13
7	'1/3'	15	min:	-3,20437E-14	max:	1,54455E-12
8	'1/4'	16	min:	6,96464E-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	RelTime[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

⁴ It is possible that Origin creates another empty worksheet with the same name as the one you created, and I don't know why. You can just delete it by right-clicking on it > Delete.

To import the second MS piece of data, see the following steps.

1. Create a new worksheet by right-clicking a worksheet tab on the bottom, "Add".
2. Open File > Import > Import Wizard or press Ctrl+3.
3. On the Import Wizard - Source window, select the MS data file you saved. Make sure the data type ASCII is selected, and click Next.
4. 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. This time, put the Number of subheader lines at 1, and Long Names at 1 too.

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 0.580775 -1.77405E-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>

☐ 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 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.

Your second worksheet should look like this.

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-13			
7	'1/3'	15 min: -3.20437E-14	max: 1.54455E-12			
8	'1/4'	16 min: 6.96464E-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: -3.75119E-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	RelTime[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	-1.60588E-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										
Units										
Comments										
F(x)=										
Sparklines										
1	1	19/11/2013	09:50:23	0.015	0.23441	-4.01502E-15	-1.77079E-14	3.16359E-13	-2.22537E-14	1.24097E-13
2	2	19/11/2013	09:50:23	0.015	0.23441	-4.01502E-15	-1.77079E-14	3.16359E-13	-2.22537E-14	1.24097E-13
3	3	19/11/2013	09:51:18	55.661	0.23472	-1.60588E-14	-3.04259E-14	3.05827E-13	-2.81147E-14	1.15784E-13
4	4	19/11/2013	09:52:14	111.308	0.24939	-1.72305E-14	-3.24710E-14	3.07468E-13	-2.95645E-14	1.18719E-13
5	5	19/11/2013	09:53:09	166.923	0.28559	-1.59787E-14	-3.24532E-14	3.08755E-13	-3.18109E-14	1.10384E-13
6	6	19/11/2013	09:53:09	222.553	0.33459	-1.76531E-14	-3.38069E-14	3.03437E-13	-3.16278E-14	1.17151E-13
7	7	19/11/2013	09:53:09	278.185	0.41449	-1.70443E-14	-3.25024E-14	3.09316E-13	-3.20437E-14	1.17871E-13
8	8	19/11/2013	09:53:09	333.816	0.48907	-1.64655E-14	-3.24191E-14	3.09755E-13	-3.05478E-14	1.07859E-13
9	9	19/11/2013	09:53:09	389.465	0.56828	-1.77696E-14	-3.22245E-14	3.07359E-13	-3.09377E-14	1.19047E-13
10	10	19/11/2013	09:53:09	445.112	0.65887	-2.3045E-14	-3.21291E-14	3.04119E-13	-3.07255E-14	1.17341E-13
11	11	19/11/2013	09:53:09	500.774	0.71879	-1.34928E-14	-3.28132E-14	3.09409E-13	-2.84843E-14	1.12819E-13
12	12	19/11/2013	09:53:09	556.437	0.78904	-7.37815E-15	-3.20597E-14	3.12775E-13	-2.2633E-14	1.16392E-13
13	13	19/11/2013	09:53:09	612.085	0.81367	-3.33125E-15	-3.13307E-14	3.14447E-13	-1.68207E-14	1.13199E-13
14	14	19/11/2013	09:53:09	667.7	0.85705	-1.68108E-15	-3.06631E-14	3.17941E-13	-1.1553E-14	1.16477E-13
15	15	19/11/2013	09:53:09	723.316	0.8996	8.8630E-16	-2.99781E-14	3.21972E-13	-4.27881E-15	1.15216E-13
16	16	19/11/2013	09:53:09	778.978	0.93738	-6.005E-16	-2.90485E-14	3.24711E-13	-3.20446E-15	1.16354E-13
17	17	19/11/2013	09:53:09	834.61	1.03683	2.12603E-15	-2.92814E-14	3.29083E-13	1.02303E-14	1.12432E-13
18	18	19/11/2013	09:53:09	890.287	1.10362	5.05878E-15	-2.8586E-14	3.29458E-13	1.05663E-14	1.15834E-13
19	19	19/11/2013	09:53:09	945.918	1.16728	5.69251E-15	-2.97839E-14	3.24581E-13	1.22779E-14	1.09476E-13
20	20	19/11/2013	09:53:09	1001.58	1.22346	8.66174E-15	-2.84467E-14	3.24231E-13	1.41242E-14	1.11472E-13
21	21	19/11/2013	09:53:09	1057.24	1.27309	9.16862E-15	-2.81906E-14	3.1733E-13	1.2656E-14	1.12228E-13
22	22	19/11/2013	09:53:09	1112.87	1.31803	1.02724E-14	-2.86008E-14	3.15808E-13	1.37961E-14	1.09708E-13
23	23	19/11/2013	09:53:09	1168.52	1.36766	1.41284E-14	-2.94103E-14	3.16762E-13	1.05988E-14	1.07114E-13
24	24	19/11/2013	09:53:09	1224.18	1.4229	1.61167E-14	-2.83991E-14	3.11659E-13	1.34444E-14	1.05271E-13
25	25	19/11/2013	09:53:09	1279.84	1.47783	1.53086E-14	-2.81487E-14	3.11332E-13	1.26339E-14	1.07345E-13
26	26	19/11/2013	09:53:09	1335.45	1.53889	2.26782E-14	-2.78393E-14	3.03697E-13	1.50824E-14	1.08367E-13
27	27	19/11/2013	09:53:09	1391.11	1.59799	3.22886E-14	-2.80246E-14	3.05174E-13	1.83356E-14	1.08535E-13
28	28	19/11/2013	09:53:09	1446.72	1.65926	4.22103E-14	-2.69212E-14	3.05427E-13	2.24047E-14	1.13193E-13
29	29	19/11/2013	09:53:09	1502.35	1.7041	5.00289E-14	-2.54893E-14	3.05693E-13	2.88262E-14	1.09825E-13
30	30	19/11/2013	09:53:09	1558.03	1.75404	6.05523E-14	-2.6125E-14	3.10922E-13	3.55059E-14	1.1276E-13
31	31	19/11/2013	09:53:09	1613.73	1.80741	6.33115E-14	-2.52149E-14	3.01834E-13	4.14454E-14	1.14693E-13
32	32	19/11/2013	09:53:09	1669.41	1.85859	6.77693E-14	-2.62309E-14	3.10438E-13	4.62842E-14	1.18852E-13
33	33	19/11/2013	09:53:09	1725.07	1.91698	7.06243E-14	-2.4359E-14	3.14871E-13	5.53112E-14	1.15505E-13
34	34	19/11/2013	09:53:09	1780.75	1.97251	6.93469E-14	-2.46477E-14	3.12584E-13	6.20909E-14	1.20038E-13
35	35	19/11/2013	09:53:09	1836.43	2.0315	6.73743E-14	-2.38839E-14	3.13653E-13	6.73589E-14	1.17846E-13
36	36	19/11/2013	09:53:09	1892.11	2.08237	5.98744E-14	-2.40557E-14	3.10882E-13	7.39515E-14	1.19244E-13
37	37	19/11/2013	09:53:09	1947.8	2.1375	5.92559E-14	-2.24056E-14	3.12893E-13	8.24638E-14	1.17848E-13
38	38	19/11/2013	09:53:09	2003.5	2.18693	5.55978E-14	-2.10131E-14	3.15581E-13	8.89063E-14	1.15048E-13
39	39	19/11/2013	09:53:09	2059.18	2.24217	5.37044E-14	-2.13031E-14	3.1496E-13	9.75074E-14	1.14343E-13
40	40	19/11/2013	09:53:09	2114.85	2.29679	5.41937E-14	-1.94182E-14	3.22991E-13	1.1428E-14	1.17847E-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. Plot

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

1.5 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 PID controller for the furnace is well adjusted, the temperature increase in the furnace should be linear so I chose to fit a degree one polynomial in this case.

1.5.2 Baseline mass loss data interpolation and subtraction⁵

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.

1.6 Plotting graphs

1.6.1 For TG

1.6.2 For MS

1.6.3 Plot TGMS graph

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

Download the folder that contains the source files here Place the tgmsplot-script in the following folder:

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

2.2 Usage

Using buttons


installbuttons

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 $T = 200\text{ }^{\circ}\text{C}$.

⁵ 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.

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

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\main.ogs")
```

This will sequentially import MS,⁶ TG and BL data, and will draw the graphs.⁷

A file browser window appears, select the MS file⁸ you want to load. Click Ok then do the same for the TG and baseline files.

Then choose the plot type you want, and if needed, the different M/z corresponding curves to plot. The data is now plotted.

Partial data imports

To import only the MS data, run the following in the command window:

```
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")
```

2.2.1 Script and execution details

The source folder contains the following files:

⁶ It works for MS bargraphs too.

⁷ To do separate MS or TG importations, or just plot, see the title below.

⁸ 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.

<code>changelinlog.ogs</code>	changes the y axis on the current to linear or log;
<code>import-bl.ogs</code>	imports baseline data;
<code>import-ms.ogs</code>	imports MS data, whether from 'regular' or bargraph formattings, directly plots if it is from bargraph;
<code>import-tg.ogs</code>	imports tg data;
<code>main.ogs</code>	main execution file, executes all the imports and plot.ogs;
<code>plot.ogs</code>	asks the user what to plot, then plots it;
<code>plot-ms-temp</code>	plots MS current <i>vs.</i> temperature;
<code>plot-ms-time</code>	plots MS current <i>vs.</i> time;
<code>plot-tg</code>	plots TG mass loss <i>vs.</i> temperature;
<code>plot-tgms</code>	plot MS and TG data on separate layers of the same graph, works only if everything is correctly imported –it is advised to execute it only after <code>main.ogs</code> has been executed.

I recommend using `main.ogs` rather than the individual separate files, as some dependency issues may appear.

2.2.2 *Button groups*

`in progress`

create new project unlocks access to the buttons

2.3 *Issues*

`in progress`

Bargraph data format not supported.

Not very robust.

Scripts dependance –only main is advised for execution.