

Leading Thermal Analysis -

Identify ... the Next Stage (from Proteus® 8.0)

 Enlarged Database (> 2000 db entries available)
Combined and Simultaneous Signals (TGA+DSC, TGA+*c*-DTA[®], STA)

Dr. A. Schindler, 10.09. 2018

Use, Applications and Benefits of Identify







Archiving/Searching "Data Mining"



K

ETZS

ГН

Identify makes interpretations:

easier

faster

more significant

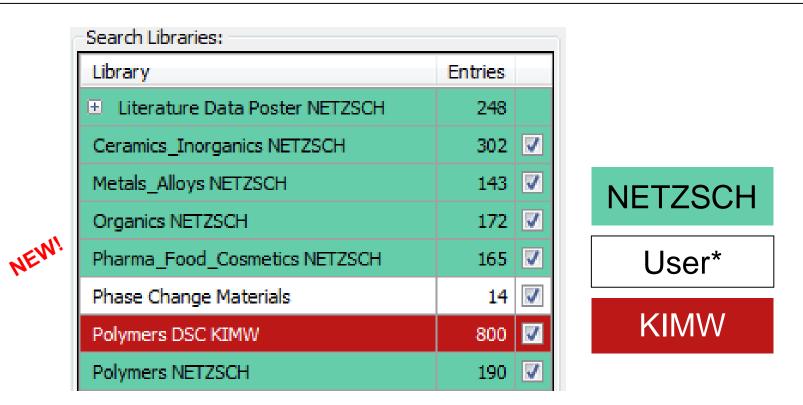


01 Database Content (09/2018)

Identify: Database Status 2018 (Proteus® 8.0)



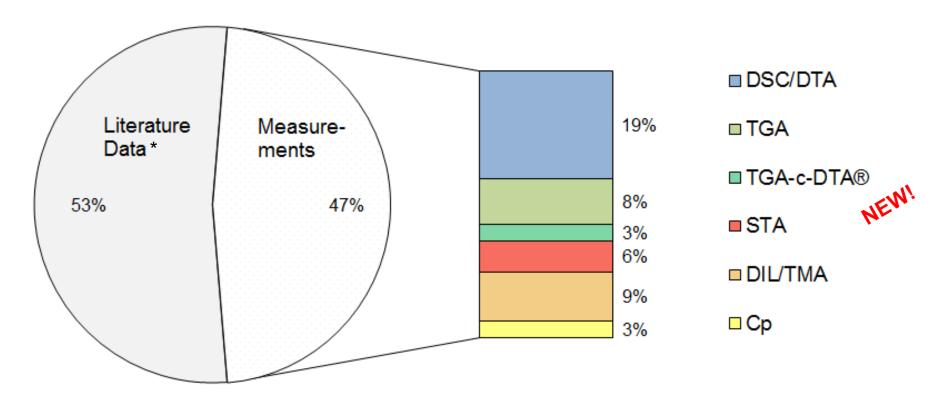
More than 2000 db entries available!



Database entries*: 1220 NETZSCH + 800 KIMW optional

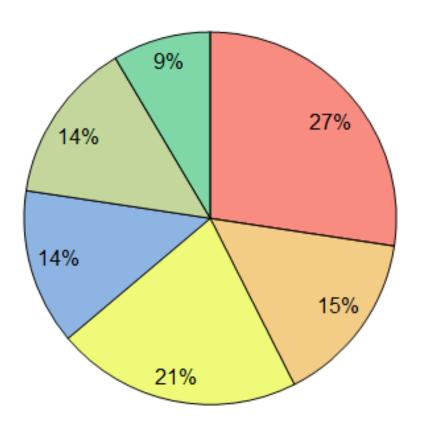
*Expandable without limits. Such libraries can be shared with several other users at the same time in the computer network.

Identify: NETZSCH Database Contents 2018 (~1220 entries) NETZSCH Distribution regarding measurement types:



* Most of such entries contain several properties (T_g , T_m , α , c_p , mass changes) at once!

Identify: NETZSCH Database Contents 2018 (~1220 entries) **NETZSCH** Distribution regarding materials:



Ceramics/Inorganics
Metals/Alloys
Polymers
Pharma/Food/Cosmetics
Organics
Chemical Elements



Proteus[®] 7.1 + higher: **The (optional) KIMW Database for DSC on Polymers**

- **DSC** measurements on
 - 800 commercially available polymers
- NET 151 polymer types.
 - suppliers, trade names
 - filler contents, colors

Results:								
Measurement/Literature Data	Similarity [%] 📼 📥	Class	Similarity [%] 🔻 🔺					
PA6_Akulon_F223-D_DSC	94,17	PA6	81,51					
PA6_Ultramid_B3K_DSC	92,99	E PBT	52,16 19,76 =					
PA6_Domamid_A1-001-N1-N	92,33	PA66	10,96					
PA6_Aquamid_6AV_DSC	91,35	E PET	6,74					
PA6_Durethan_B30S_DSC	90,94	ETFE	3,39					
PBT_Celanex_2300_GV1-10	81,30	I LCP	1,00					
PBT_Crastin_S620_F20_DSC PA6_vernetzt_Betalink_Mast	73,96 71,40	₽ PP	0,19					
PAG_Vernetzt_betailnK_Mast	/1,40	🖬 TPU	0,06 👻					

Search Libraries:					
Library	Entries				
🗄 Literature Data Poster NETZSCH	248				
Ceramics_Inorganics NETZSCH	302				
Metals_Alloys NETZSCH	143				
Organics NETZSCH	172				
Pharma_Food_Cosmetics NETZSCH	165				
Polymers DSC KIMW	800	V			
Polymers NETZSCH	190				

1.1.1



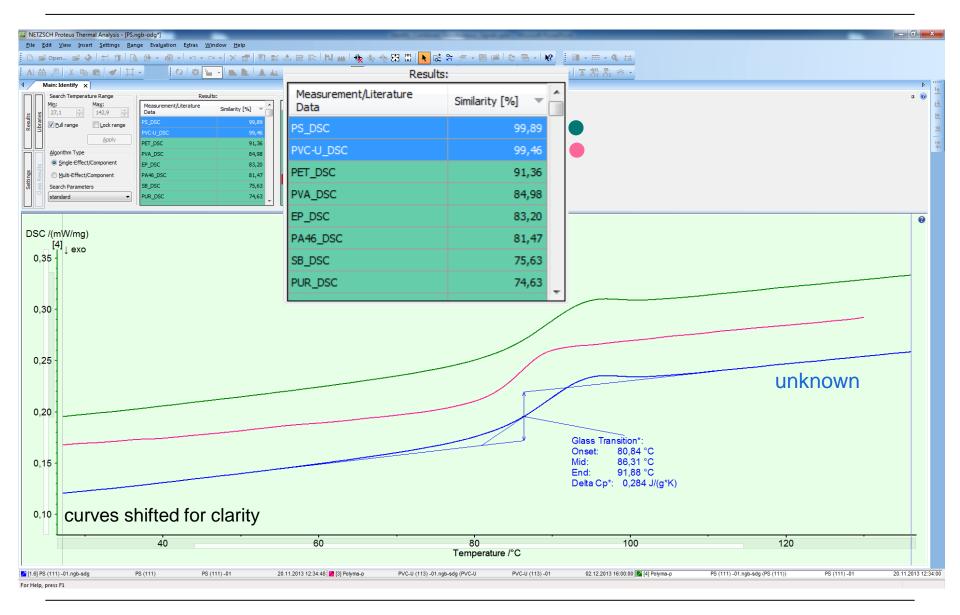




02 Combined and Simultaneous Signals

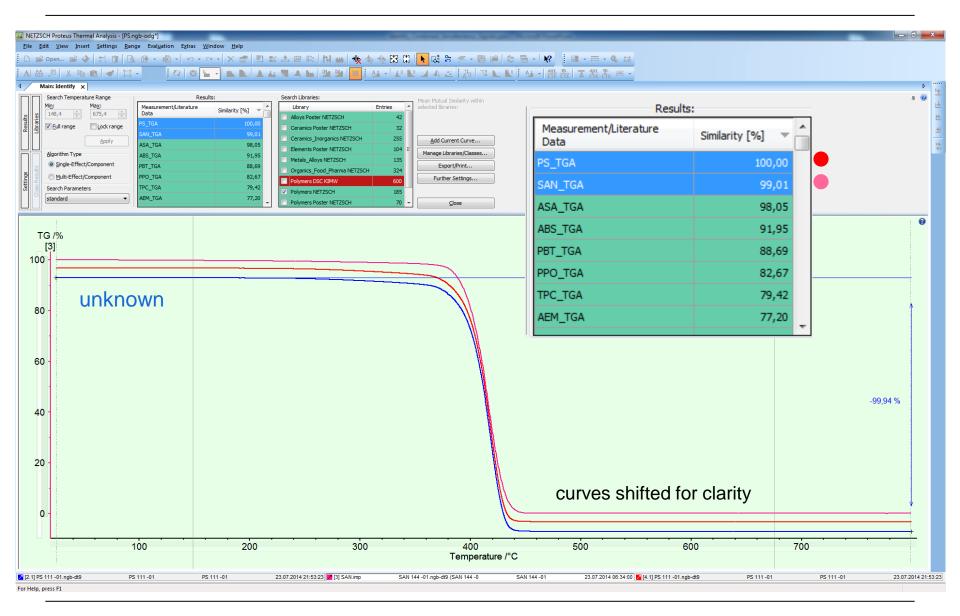
Problem: Multiple Interpretations of DSC Signals

Example: We can unfortunately not distinguish PS from PVC-U via DSC



Problem: Multiple Interpretations of TGA Signals

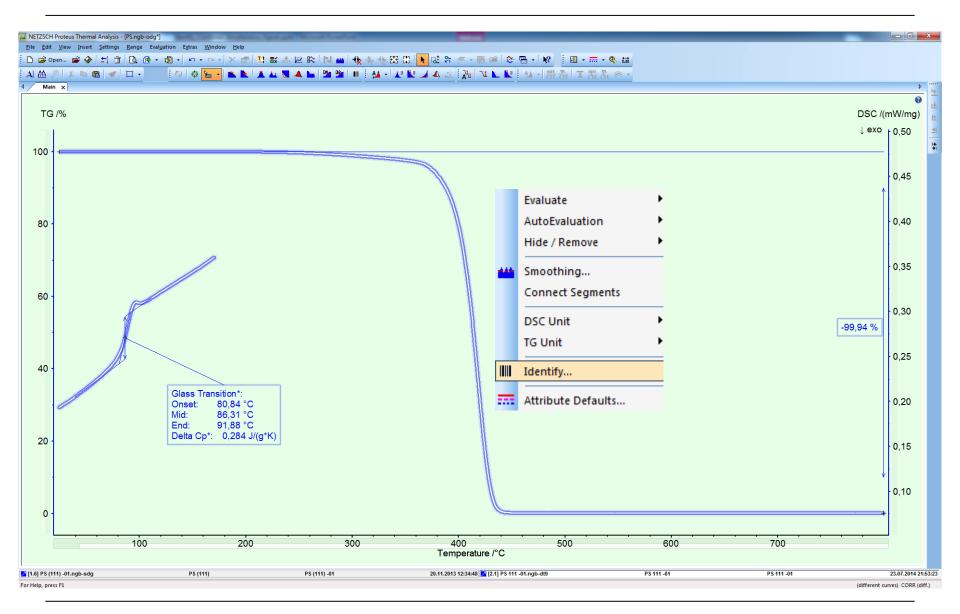
Example: And we can unfortunately also not distinguish PS from SAN via TGA





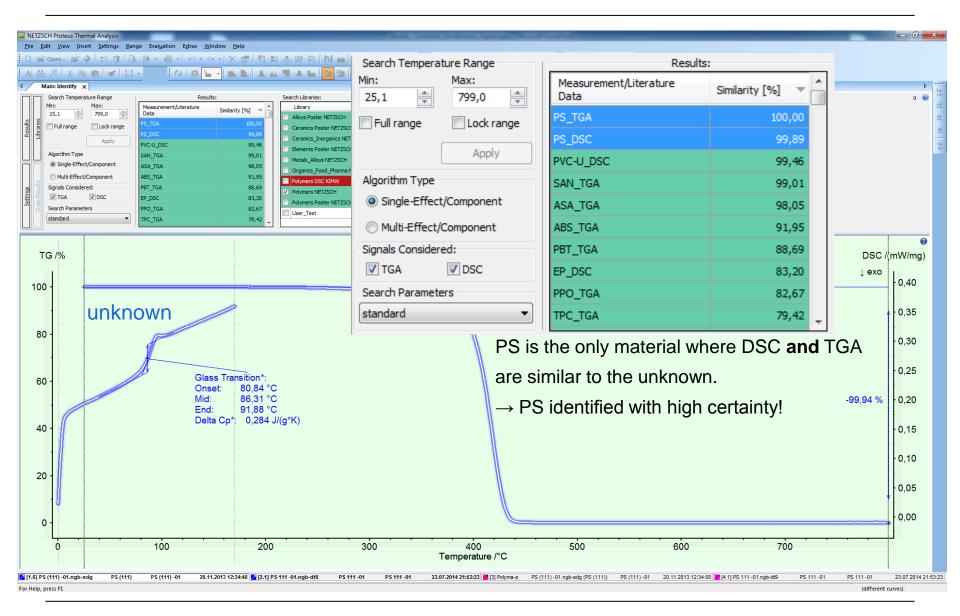
Solution: Combine (independent!) DSC and TGA signals

Select DSC+TGA with Ctr-button and left mouse and call Identify (right mouse button)



Solution: Combine (independent!) DSC and TGA

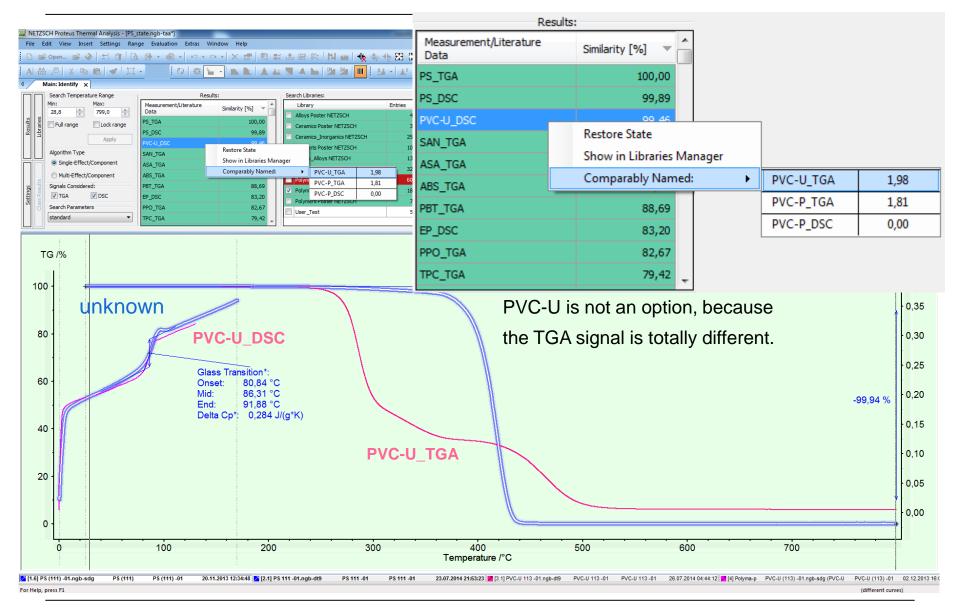
In Identify, search for TGA+DSC in combination, or consider either TGA or DSC



Solution: Combine (independent!) DSC and TGA

In Identify, search for TGA+DSC in combination, or consider either TGA or DSC

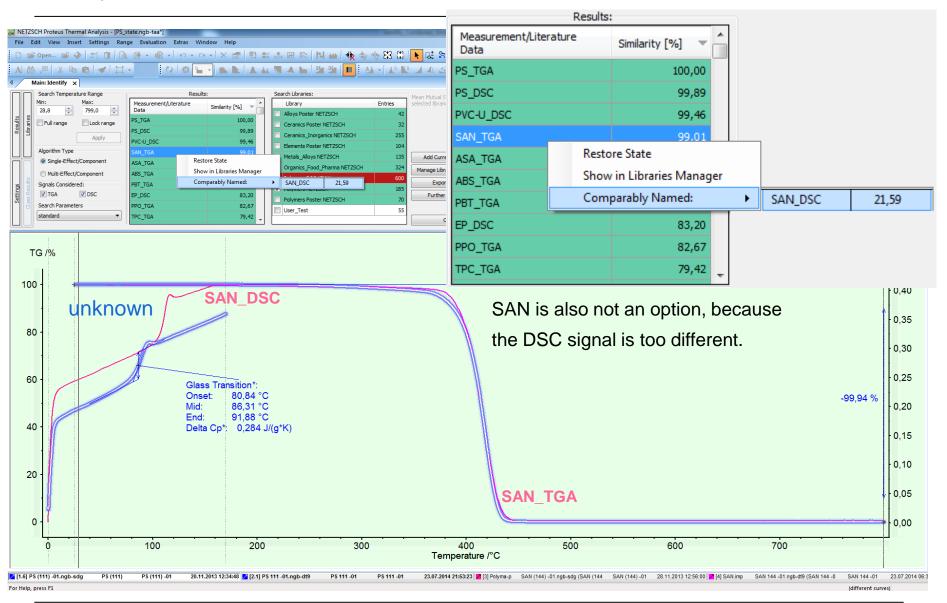




Identify | A. Schindler | 2018

Solution: Combine (independent!) DSC and TGA

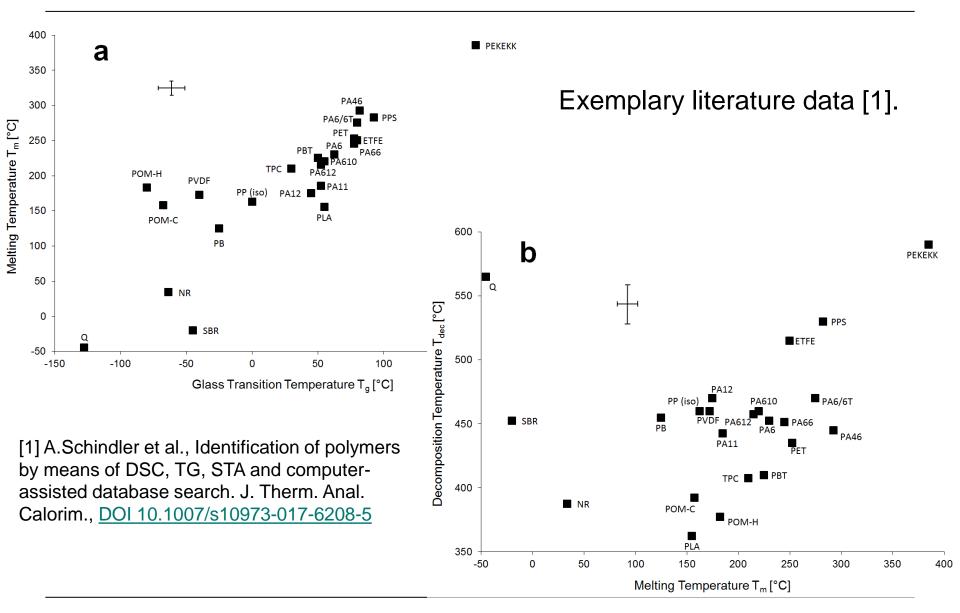
In Identify, search for TGA+DSC in combination, or consider either TGA or DSC





Let's have a look at further cases

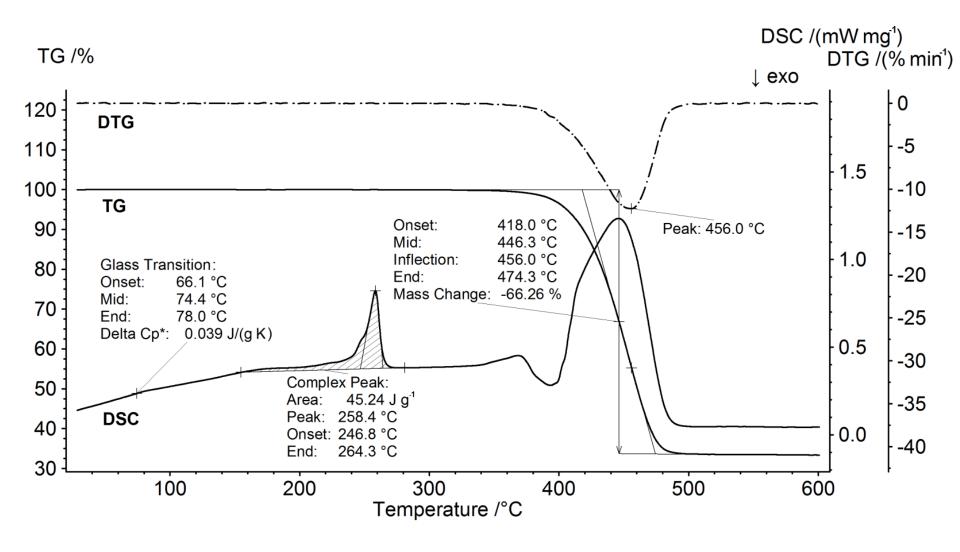
Consideration of DSC and TGA will in many cases improve the situation of multiple interpretations!



STA measurement on "PA66-GF30_STA" (see ref. [1])



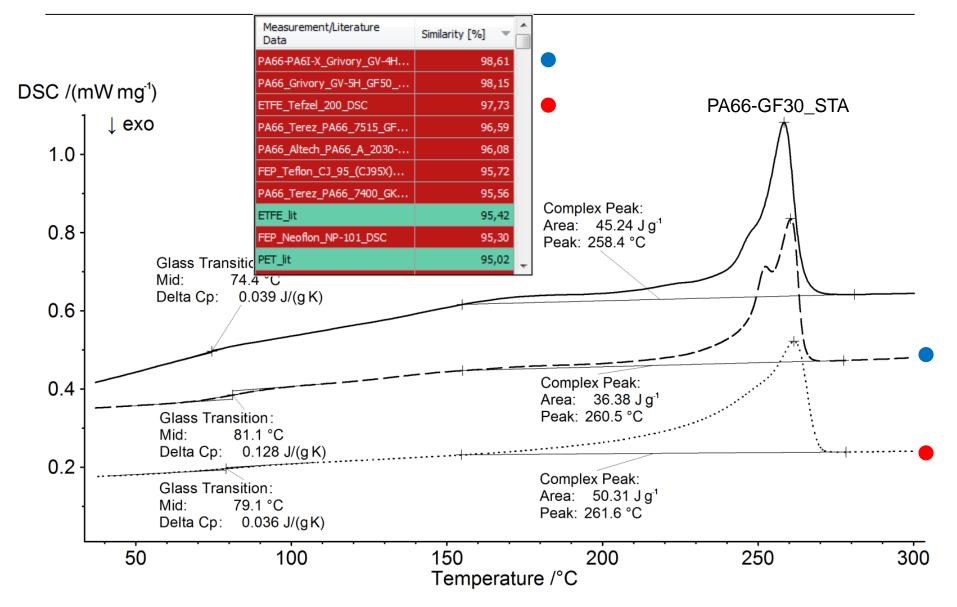
STA 449 **F3** Jupiter[®], steel furnace.



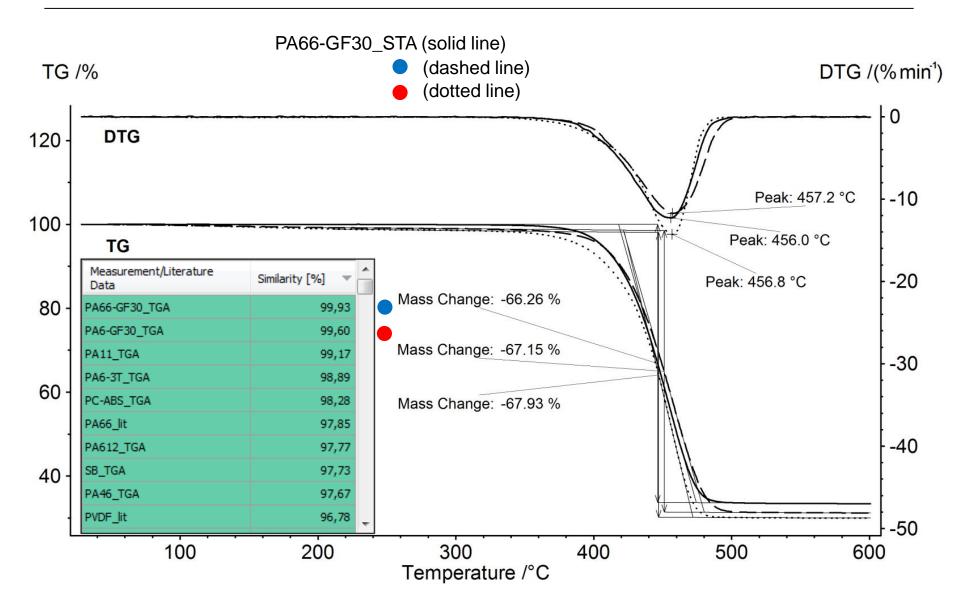
Identify on "PA66-GF30_STA" (see ref. [1])

Just considering the DSC signal \rightarrow No definite identification!





Just considering the TGA signal \rightarrow Again no definite identification!





In this example, PA66 is the only material with a high similarity regarding, both, DSC and TGA.

This can most easily be seen when only the library "NETZSCH Polymer Poster" is selected. These database entries contain DSC *and* TGA properties that are considered in combination!

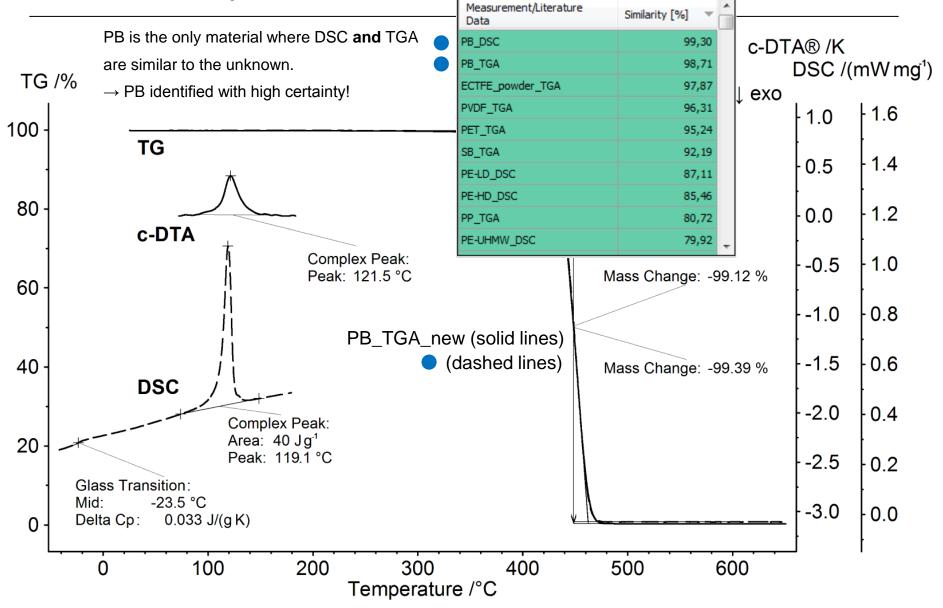
 \rightarrow PA66 is best hit, other materials are discriminated.

Measurement/Literature Data	Similarity [%] 🔍	11 ×
PA66_lit	94,29	
PA6-6T_lit	87,84	
PET_lit	86,92	
ETFE_lit	75,87	
FEP_lit	72,04	
(HBA, HNA)-LCP_lit	64,84	
EP_lit	64,79	
PF_lit	62,61	
PA6_lit	59,44	
PVAL_lit	58,71	÷

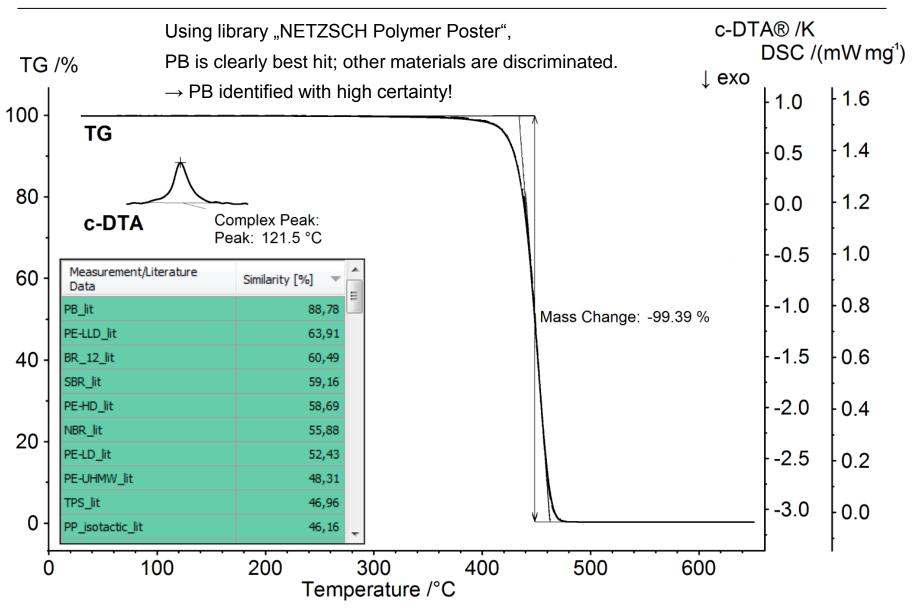
TGA measurement on "PB_TGA_new" (see ref. [1])

TG 209 F1 Libra®. Identify can consider TGA+c-DTA®





TG 209 *F1 Libra*[®]. *Identify* can consider TGA+*c*-*DTA*[®]





TGA-*c*-*DTA*[®] \rightarrow TGA(-*c*-*DTA*[®]) but also DSC and STA are found by *Identify*

- DSC \rightarrow DSC but also TGA-*c*-DTA[®] and STA are found by *Identify*
- STA \rightarrow STA, DSC, TGA, TGA-*c*-*DTA*[®] are found by *Identify*



AB	DSC	TGA	STA	TGA- <i>c-DTA</i> ®	DIL	TMA	C _p
DSC	\checkmark		\checkmark	\checkmark			
TGA		\checkmark	\checkmark	\checkmark			
STA	\checkmark	\checkmark	$\checkmark\checkmark$	$\checkmark\checkmark$			
TGA- <i>c-DTA</i> ®	\checkmark	\checkmark	\checkmark	$\checkmark\checkmark$			
DIL					\checkmark	\checkmark	
ТМА					\checkmark	\checkmark	
C _p							\checkmark

Remarks:

- A, B: measurements or literature data ("unknown" is always a measurement).
- DSC can also be DTA.
- //: two signal types can be identified in combination or just one of the signal types.

N ETZ5EH





- More than 2000 db entries are available!
- Identify can now incorporate: Combined signals (TGA+DSC indep. and TGA-*c-DTA®*) Simultaneous signals (TGA+DSC = STA)
- This makes material identification more definite!
- The contents of this presentation is published: A.Schindler et al., Identification of polymers by means of DSC, TG, STA and computer-assisted database search, J. Therm. Anal. Calorim., <u>DOI 10.1007/s10973-017-6208-5</u>