

Supporting Information**Effect of Adding 5-Aminotetrazole to a Modified U.S. Army Terephthalic Acid White Smoke Composition****Johann Glück,¹ Thomas M. Klapötke,^{1*} Anthony P. Shaw^{2**}**¹ *Department of Chemistry, Ludwig-Maximilian University Butenandtstraße 5-13 (D), 81377 Munich, Germany*² *U.S. Army RDECOM-ARDEC, Pyrotechnics Technology Division, Picatinny Arsenal, New Jersey, 07806, USA**E-mails: *tmk@cup.uni-muenchen.de; **anthony.p.shaw.civ@mail.mil***Table 1.** Transmittance (555 nm) over time for each formulation

	Pellet 1	Pellet 2	Pellet 3	Pellet 4	Average transmittance (555 nm) over time^a	Standard deviation
1 (79)	0.56257	0.62138	0.56954	0.5848	0.585	0.026
2 (82)	0.51710	0.55267	0.57401	0.48019	0.531	0.041
3 (347)	0.20015	0.19131	0.23536	0.23591	0.216	0.023
4 (350)	0.23167	0.22645	0.21456	0.24005	0.228	0.011

Annotation: a = average of collected transmittance values at 555 nm over time for all pellets

The plots show the transmittance (555 nm) over time for each formulation. The y-axis shows the transmittance [%], the x-axis gives the time [s]. The exact mass of each pellet [g] is depicted in each graph (e.g. 1.9913 g, 2.0350 g, 2.0800 g, 2.0941 g in Figure 1).

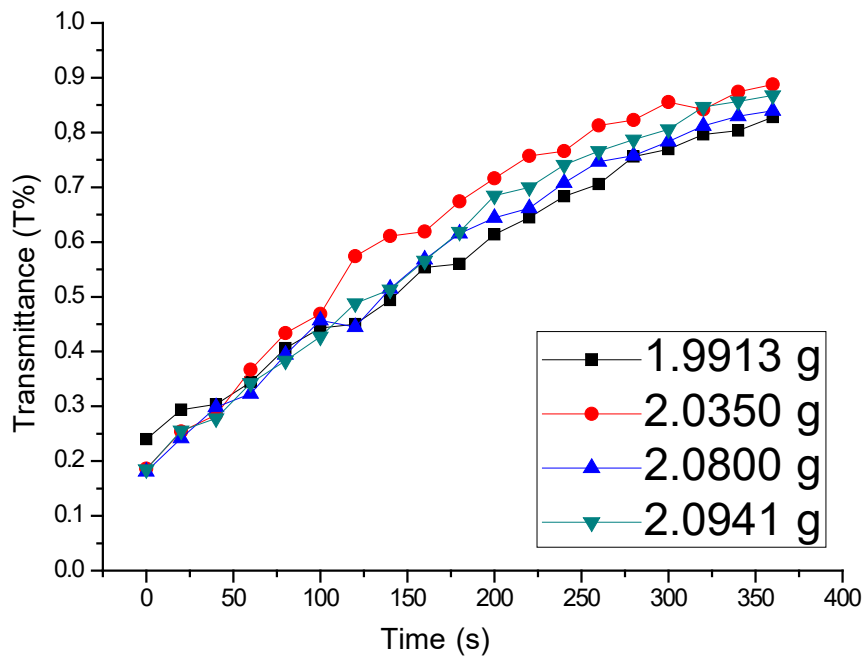


Figure 1. Transmittance (555 nm) over time of formulation 1

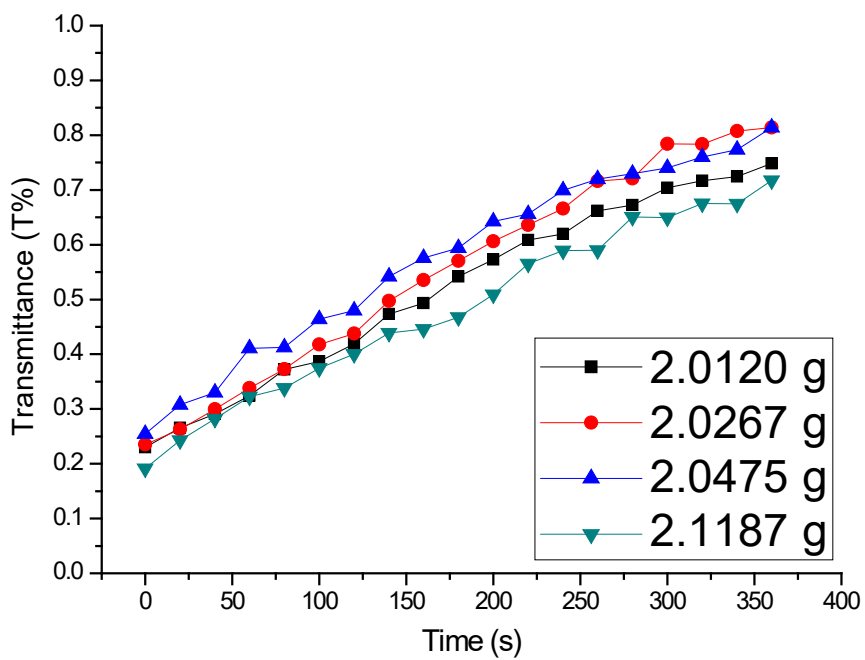


Figure 2. Transmittance (555 nm) over time of formulation 2

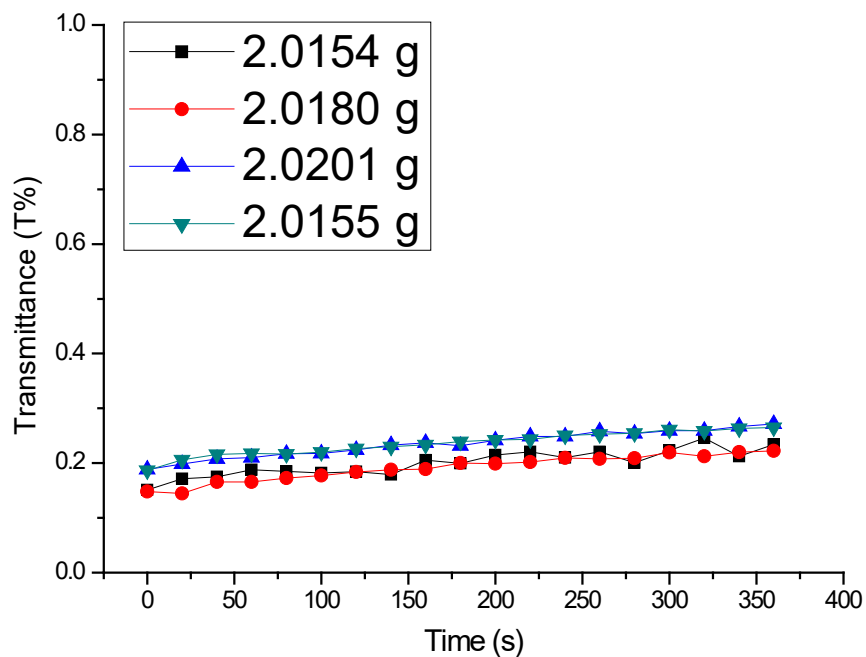


Figure 3. Transmittance (555 nm) over time of formulation 3

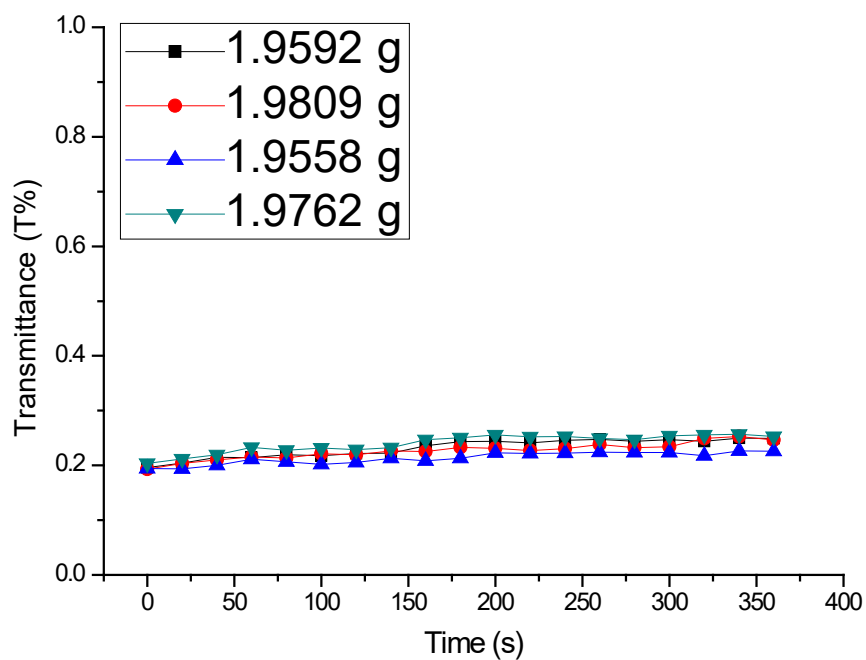


Figure 4. Transmittance (555 nm) over time of formulation 4

Table 2. Averaged burning time of tested formulations

Formulation	Burning time [s]	Standard deviation [s]
1	28	1
2	33	3
3	28	1
4	26	1

Determination of the yield factor

The experimental setup was described earlier in following journal [A]:

[A] Glück, J.; Klapötke, T. M.; Rusan, M.; Shaw, A. *Propellants Explos. Pyrotech.* **2017**, *42*, 131.

Table 3. Yield factor of tested formulations

Formulation	Yield factor	Standard deviation	Relative humidity [%]
1	0.274	0.028	66
2	0.309	0.053	61
3	0.237	0.014	61
4	0.229	0.039	63

Annotation: Yield factor = mass of aerosol/mass of pyrotechnical payload

The quantification of the aerosol revealed that formulation **1** and **2** produced more aerosol compared to the sugar-free formulations. Since the recorded transmittance values show a better performance for formulation **3** and **4**, it may be concluded that the either a higher degree of dispersion or different resulting combustion products are responsible for this behavior. A higher amount of aerosol, neglecting the resulting particle size or degree of dispersion, is therefore no guarantee for a better performance.

Differential Thermal Analysis (DTA) of tested formulations (Figure 5-8):

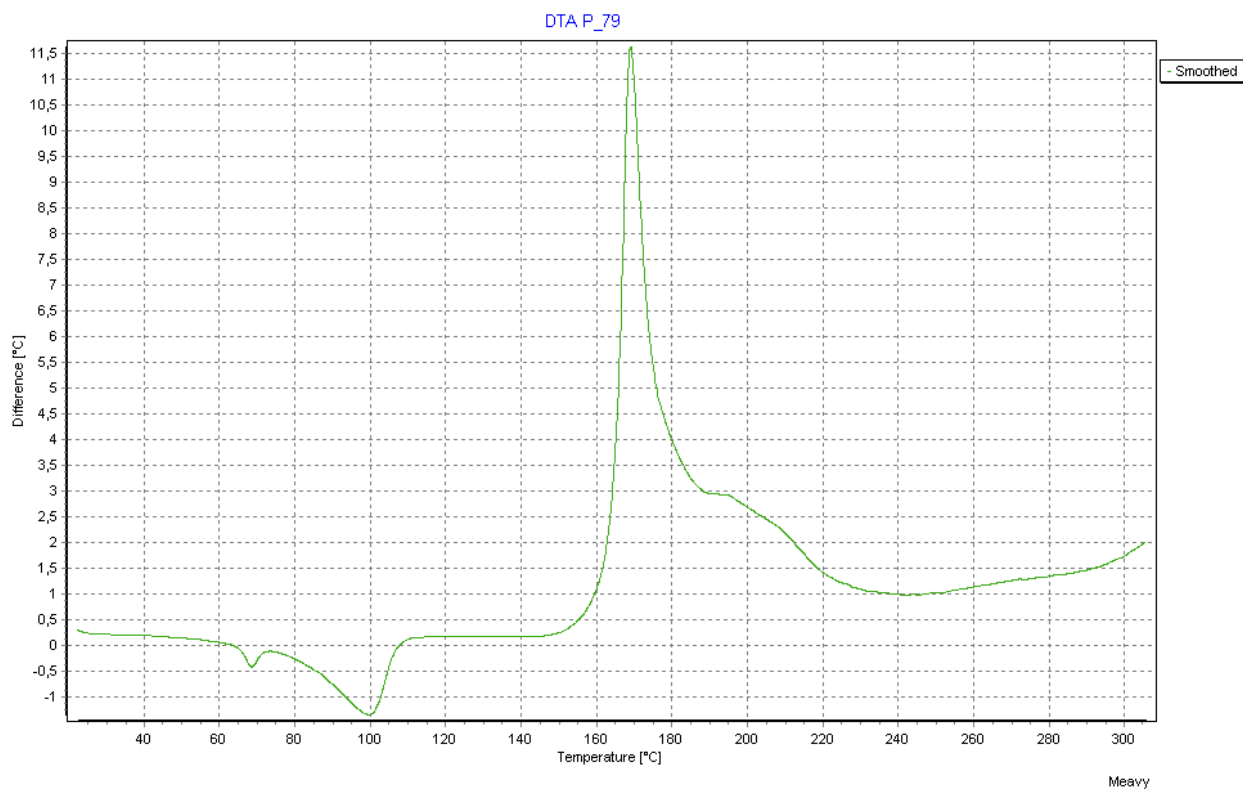


Figure 5. DTA (5 °C/min) of formulation 1

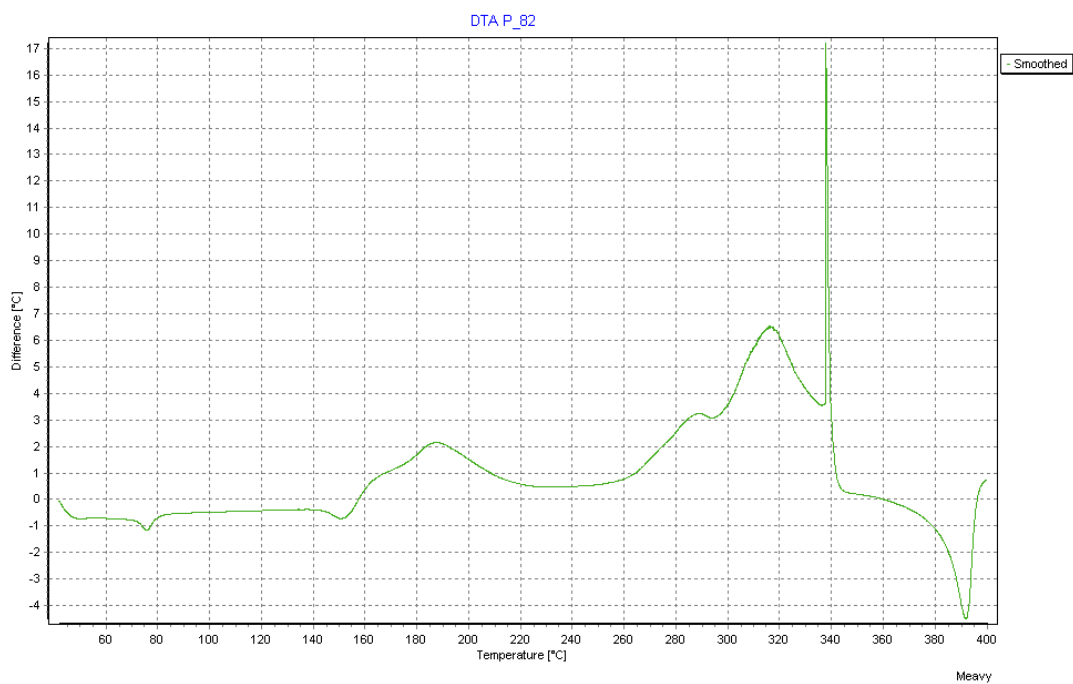


Figure 6. DTA (5 °C/min) of formulation 2

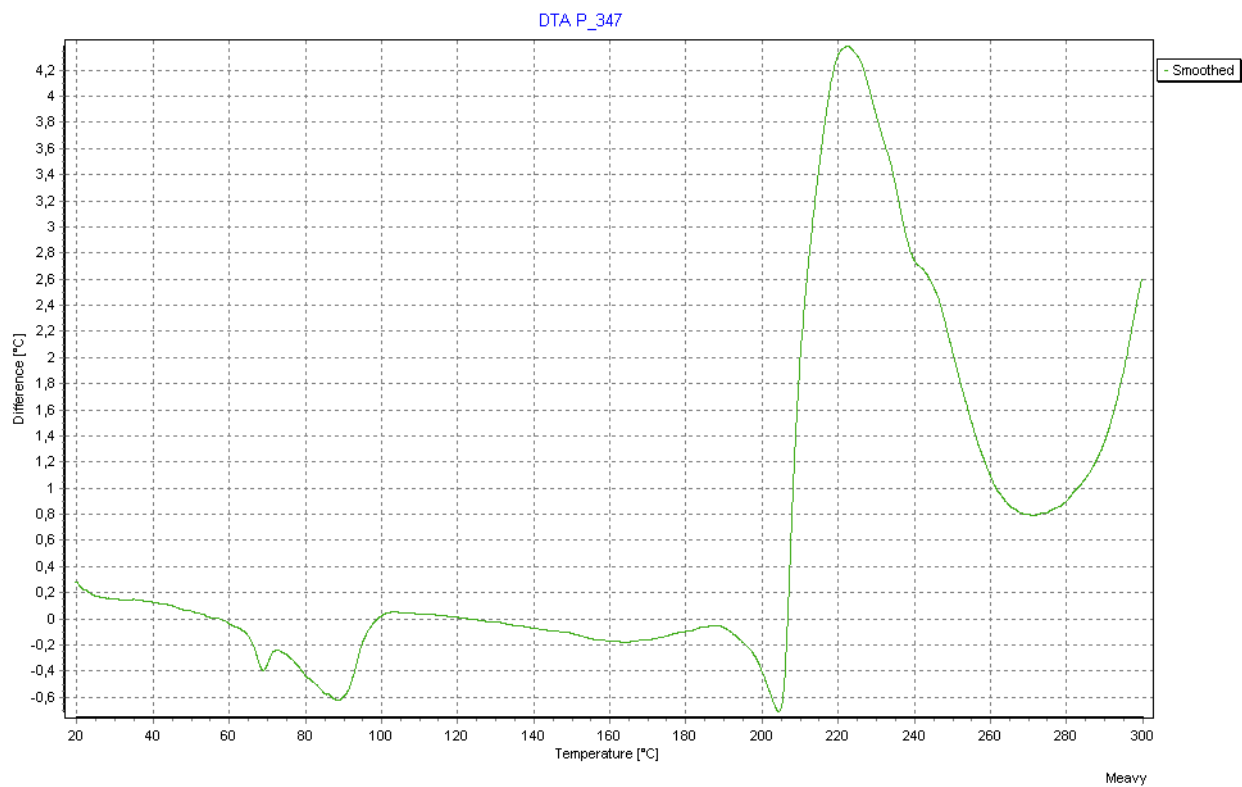


Figure 7. DTA (5° C/min) of formulation 3

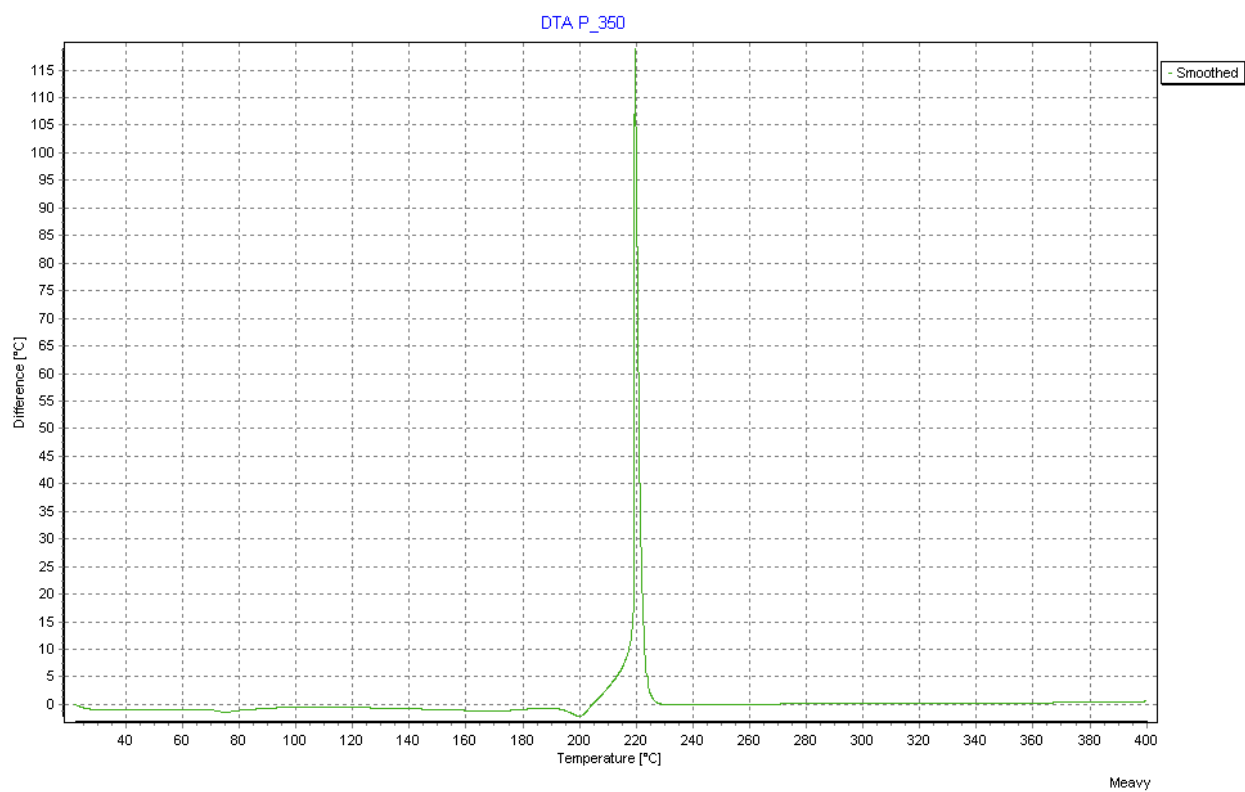


Figure 8. DTA (5° C/min) of formulation 4

All DTA graphs showed an endothermic peak in the range of 60-80 °C which might be correlated to stearic acid (see Figure 14). Formulation 1 and 2 (see Figures 5 and 6) showed an exothermic peak for sucrose in the range of 160-200 °C. In contrast, formulation 3 and 4 (see Figures 7 and 8) did not contain this peak. The exothermic peak at 220 °C can be correlated to 5-aminotetrazole (see Figure 10). The DTA of terephthalic acid (TA) showed no decomposition point, but a strong endothermic behavior starting from 330 °C (see Figure 12).

Differential Thermal Analysis (DTA) of single components (Figures 9-16):

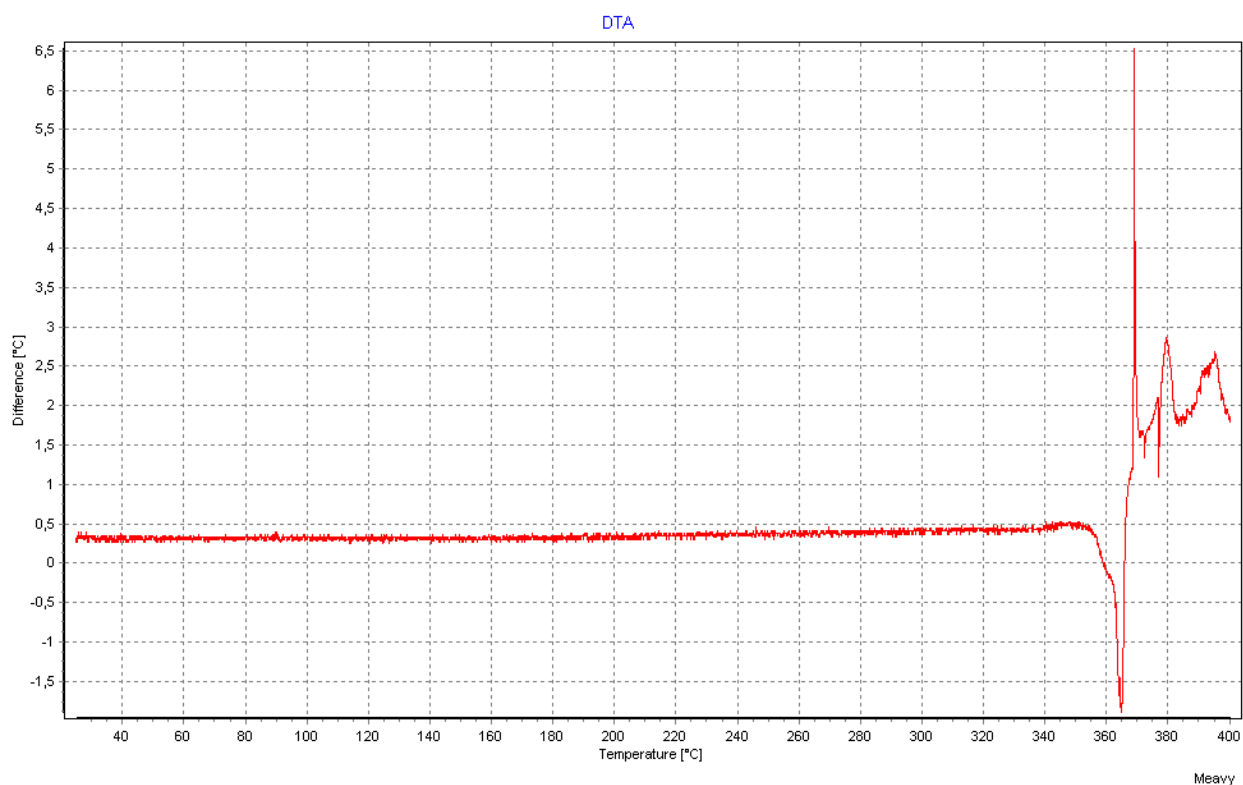


Figure 9. DTA (5 °C/min) of KClO₃

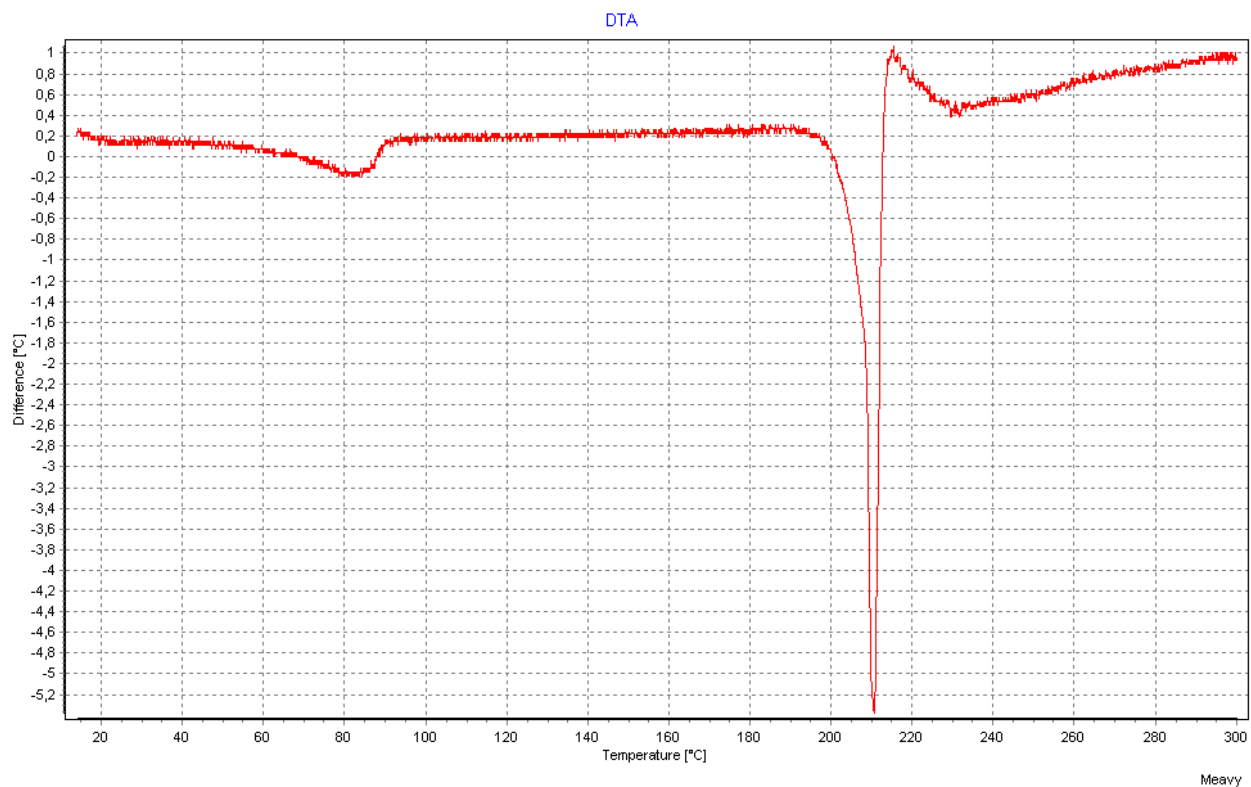


Figure 10. DTA (5 °C/min) of 5-aminotetrazole

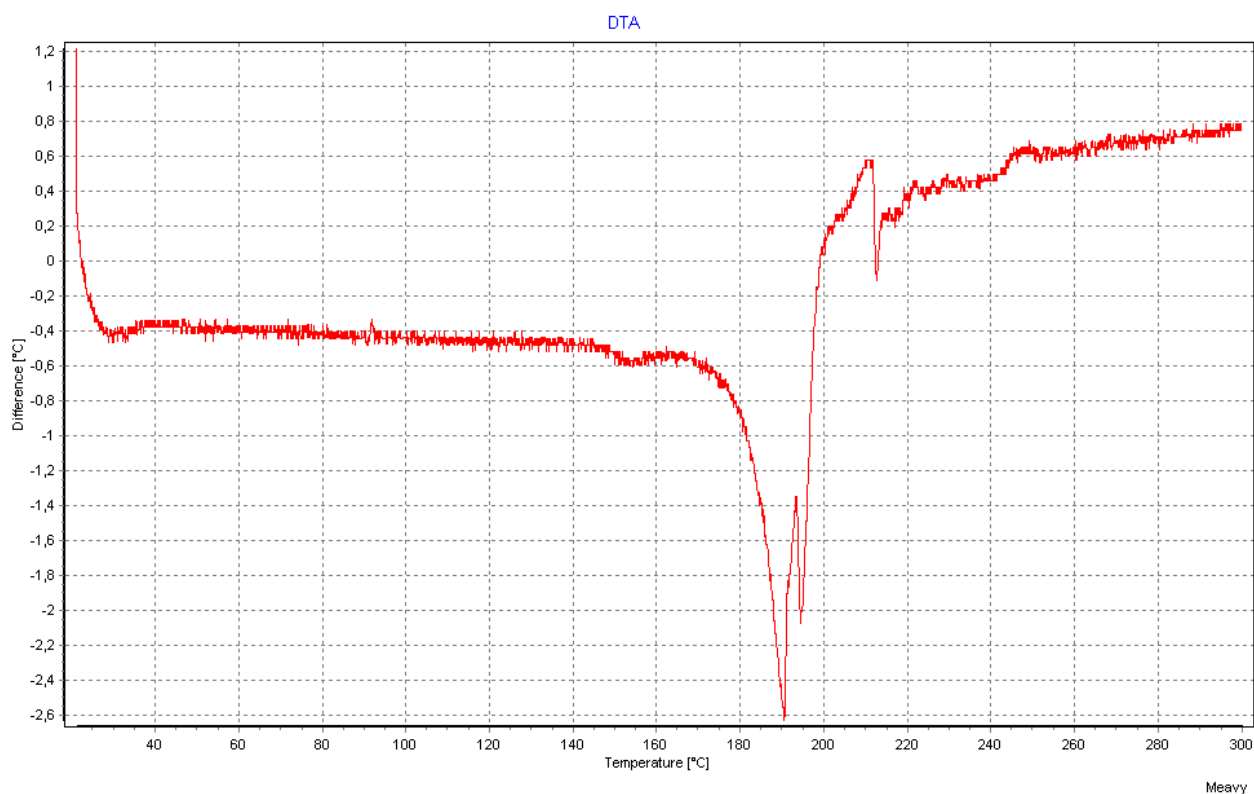


Figure 11. DTA (5 °C/min) of sucrose

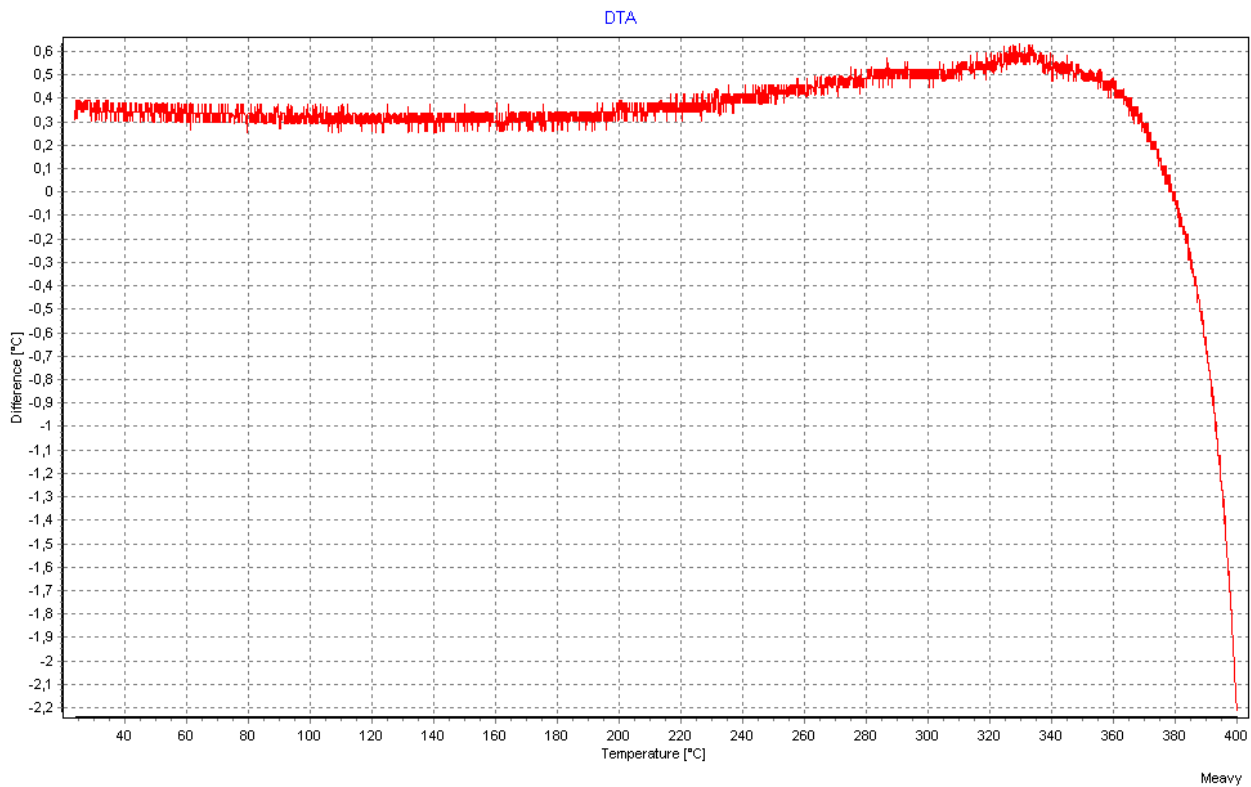


Figure 12. DTA (5 °C/min) of terephthalic acid

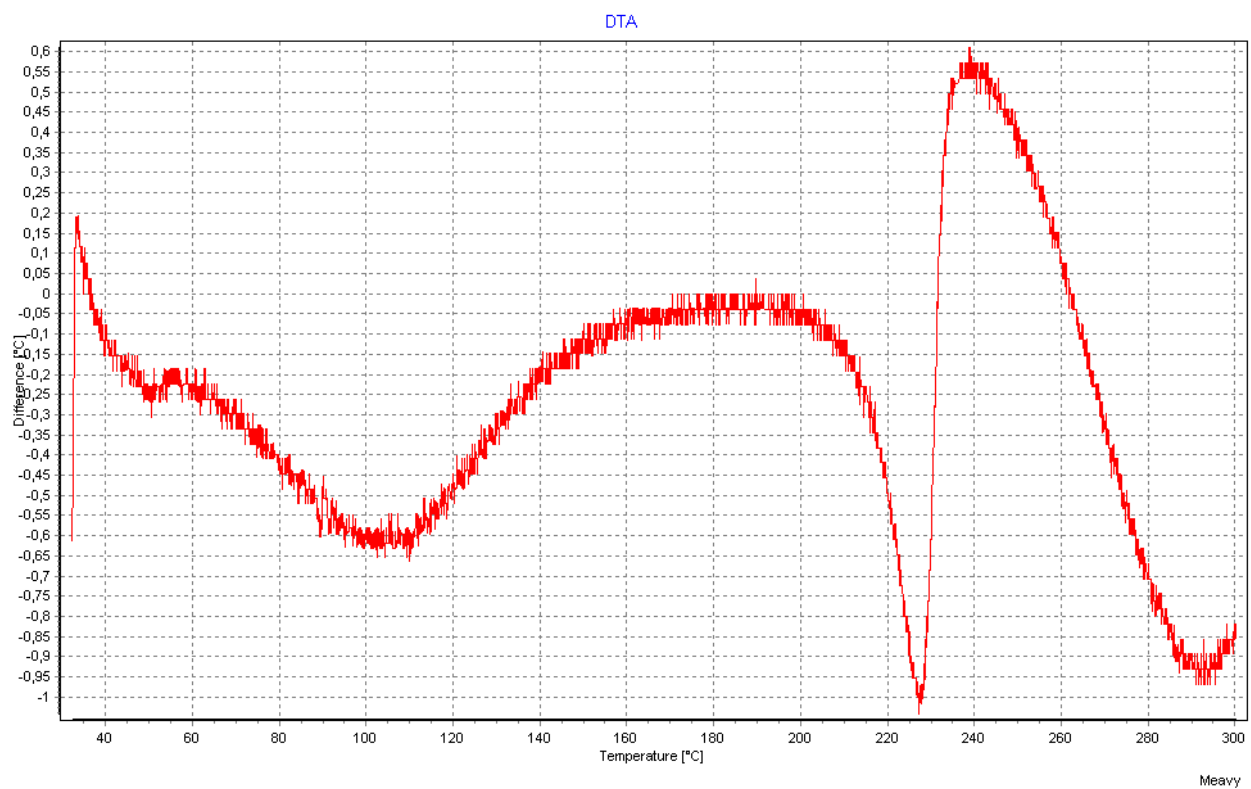


Figure 13. DTA (5 °C/min) of PVA

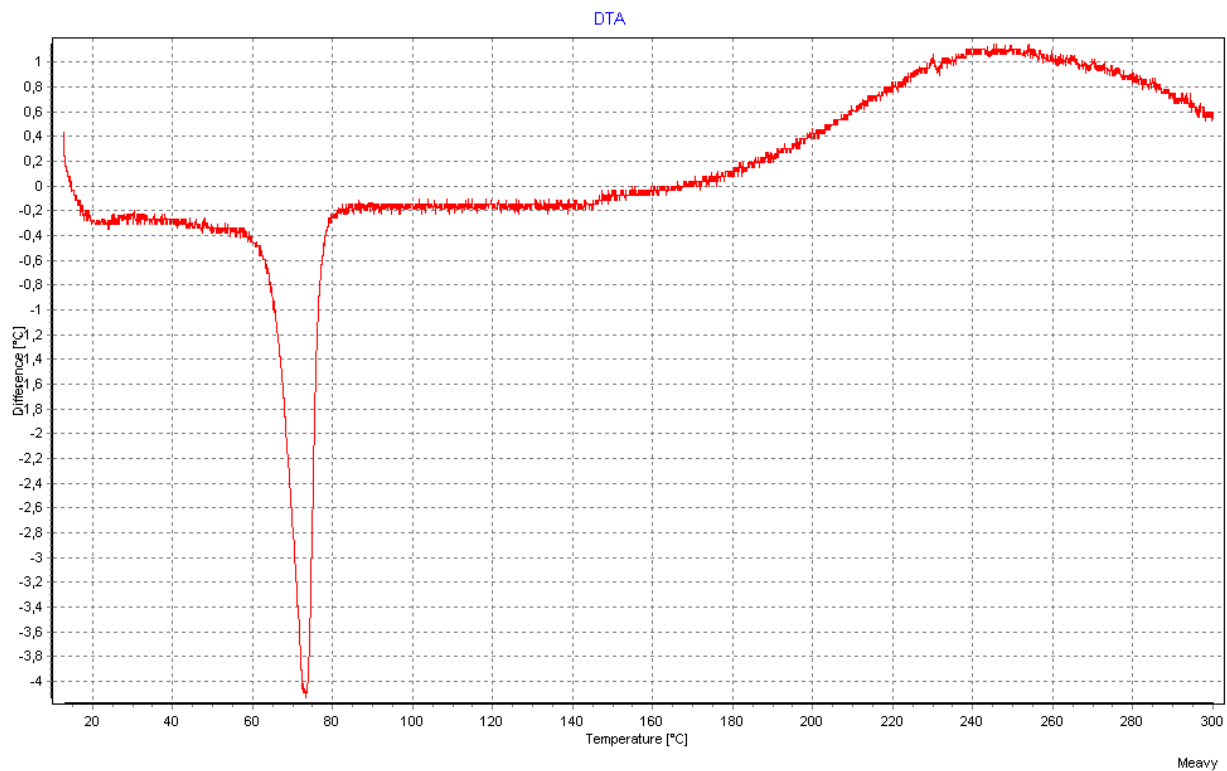


Figure 14. DTA (5 °C/min) of stearic acid

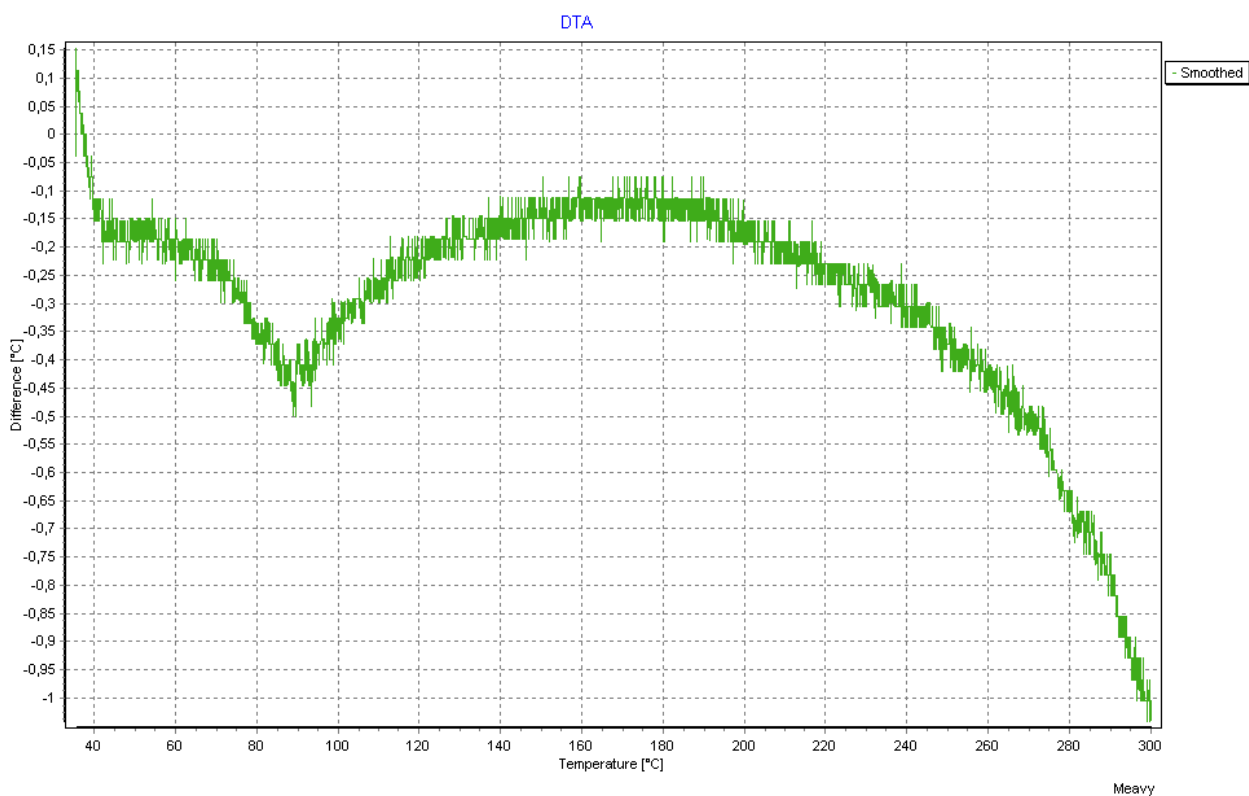


Figure 15. DTA (5 °C/min) of MCHP

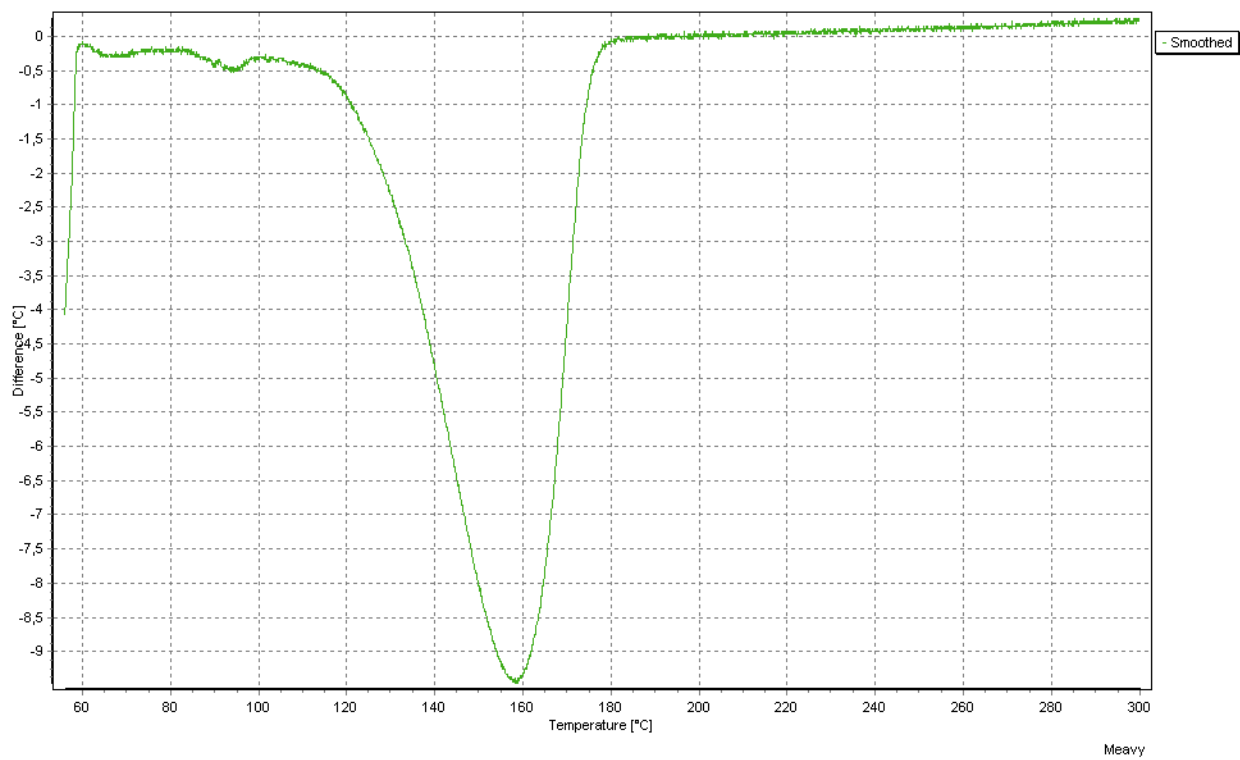


Figure 16. DTA (5 °C/min) of NaHCO₃, measurement started at elevated temperatures (60 °C), no decomposition before 60 °C