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Supplementary Material

Preparation and Characterization of Copper(II) and Nickel(II) Complexes with *N*-Benzyliminodiacetamide Derivatives

Iminodiacetamide Complexes of Cu^{II} and Ni^{II}

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Table S1. Crystal parameters, data collection and refinement details for **2**, **5** and **13**.

	2	**5**	**13**
Molecular formula	$C_{24}H_{26}CuN_8O_{10}$	$C_{22}H_{28}Cl_2CuN_8O_{10}$	$C_{28}H_{42}Cl_2N_{10}NiO_{12}$
M_r	658.13	698.96	840.31
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P\,2_1/n$	$P\,2_1/n$	$P\,2_1/c$
Crystal data:			
a / Å	8.5414(2)	8.3965(9)	9.7868(4)
b / Å	19.3423(4)	19.0459(15)	18.3765(6)
c / Å	9.5184(2)	9.7242(9)	11.0019(3)
α / °	90	90	90
β / °	107.546(3)	107.896(11)	96.978(4)
γ / °	90	90	90
V / Å^3	1499.39(6)	1479.8(2)	1964.00(12)
Z	2	2	2
ρ_{calc} / g cm^{-3}	1.458	1.569	1.421
λ(MoK_α) / Å, graphite monochromator	0.71073	0.71073	0.71073
T / K	296(2)	296(2)	296(2)
Crystal dimension / mm^3	0.51 × 0.47 × 0.43	0.22 × 0.17 × 0.13	0.82 × 0.22 × 0.21
μ / mm^{-1}	0.795	0.985	0.699
$F(000)$	670	702	876
θ range/ °	4.23-25	4.1-25	4.2-24.99
hkl range	-10, 10; -23, 23; -11, 11	-9, 7; -22, 20; -11, 11	-11, 8; -21, 21; -13, 13

Number of measured reflections	17963	9186	12250
Number of independent reflections	2627	2588	3443
Number of reflections with $I > 4\sigma(I)$	2529	1805	2280
Number of parameters	197	208	246
$\Delta\rho_{max}$, $\Delta\rho_{min}$ / e Å^{-3}	0.609, -0.239	0.445, -0.259	0.534, -0.381
$R[F^2>4\sigma(F^2)]$	0.0371	0.0358	0.0420
$wR(F^2)$	0.1107	0.0918	0.1160
Goodness of fit, *S*	0.888	0.956	0.942

Table S2. Thermal analysis data for complexes **1-8** under nitrogen atmosphere.

Complex	Temperature range (°C)	Mass loss (%); observed / calculated	Assignment	Observed residue at 600 °C (%)
1	Step 1: 25-120	1.6 / 1.4	½ water molecule	28.6
	Step 2: 120-600	69.9 / 89.1	incomplete degradation	
2	200-600	71.3 / 90.3	incomplete degradation	28.7
3	Step 1: 50-140	5.8 / 5.2	2 water molecules	26.2
	Step 2: 140-600	67.9 / 85.7	incomplete degradation	
4	Step 1: 25-130	2.8 / 2.5	1 water molecule	30.9
	Step 2: 130-600	66.3 / 88.7	incomplete degradation	
5	200-600	65.6 / 90.9	incomplete degradation	34.4
6	Step 1 : 25-170	5.4 / 4.9	2 water molecules	30.7
	Step 2: 170-600	63.6 / 86.5	incomplete degradation	
7	Step 1 : 50-150	5.8 / 5.1	2 water molecules	25.6
	Step 2: 150-600	68.7 / 85.9	incomplete degradation	
8	Step 1 : 50-180	5.0 / 4.4	2 water molecules	32.2
	Step 2: 180-600	62.9 / 87.9	incomplete degradation	

Table S3. Thermal analysis data for complexes **1-8** under oxygen atmosphere.

Complex	Temperature range (°C)	Mass loss (%); observed / calculated	Assignment	Residue at 600 °C (%)	
				Observed	Calculated for CuO
1	Step 1: 25-130 Step 2: 170-550	1.3 / 1.4 87.6 / 89.1	½ water molecule 2 ligand molecules + 2 nitrate ions	11.3	11.9
2	200-470	87.5 / 90.3	2 ligand molecules + 2 nitrate ions	12.7	12.1
3	Step 1: 25-150 Step 2: 150-460	5.9 / 5.2 83.1 / 85.7	1 water molecule 2 ligand molecules + 2 nitrate ions	11.4	11.5
4	Step 1: 50-160 Step 2: 170-600	2.5 / 2.5 86.3 / 88.7	1 water molecule 2 ligand molecules + 2 nitrate ions	11.5	11.1
5	200-600	89.2 / 90.9	2 ligand molecules + 2 nitrate ions	11.0	11.3
6	Step 1 : 50-170 Step 2: 170-600	5.4 / 4.9 84.1 / 86.5	2 water molecules 2 ligand molecules + 2 nitrate ions	10.9	10.8
7	Step 1 : 50-140 Step 2: 160-540	5.8 / 5.1 68.7 / 85.9	2 water 2 ligand molecules + 2 nitrate ions	11.3	11.3
8	Step 1 : 70-180 Step 2: 180-600	4.7 / 4.4 85.8 / 87.9	2 water 2 ligand molecules + 2 nitrate ions	9.8	9.6

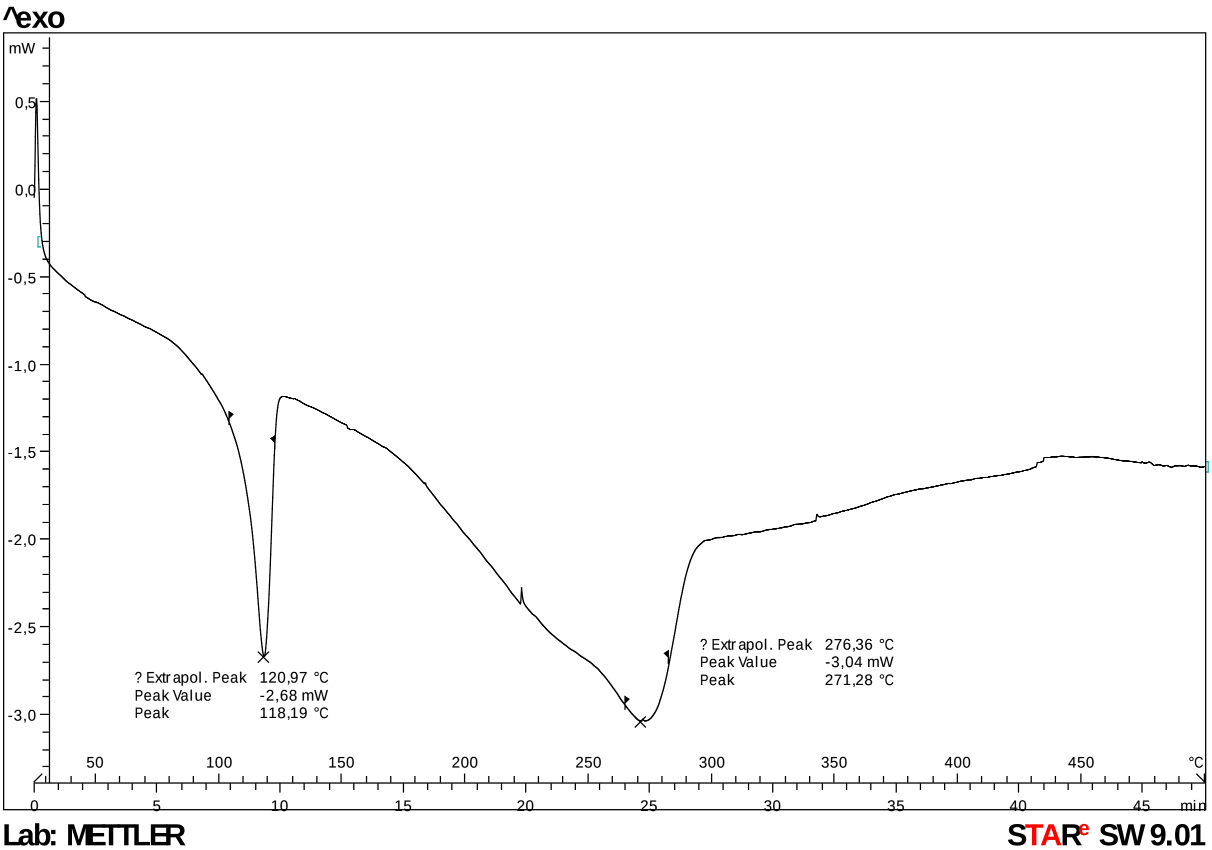
Table S4. Thermal analysis data for complexes **9-16** under nitrogen atmosphere.

Complex	Temperature range (°C)	Mass loss (%); observed / calculated	Assignment	Observed residue at 600 °C (%)
9	Step 1: 50-110	2.6 / 2.7	1 water molecule	26.6
	Step 2: 110-600	70.9 / 88.6	incomplete degradation	
10	Step 1: 25-110	6.3 / 5.2	2 water molecules	26.5
	Step 2: 110-600	67.2 / 86.2	incomplete degradation	
11	Step 1: 25-150	3.0 / 2.7	1 water molecule	28.5
	Step 2: 150-600	68.7 / 88.6	incomplete degradation	
12	250-600	63.9 / 91.6	incomplete degradation	36.2
13	Step 1: 90-160	16.3 / 17.3	2 DMF molecules	25.0
	Step 2: 160-600	58.8 / 75.7	incomplete degradation	
14	Step 1 : 50-160	5.8 / 4.9	2 water molecules	33.6
	Step 2: 160-600	60.6 / 87.1	incomplete degradation	
15	Step 1 : 50-150	3.7 / 2.6	2 water molecules	32.5
	Step 2: 150-600	63.8 / 88.7	incomplete degradation	
16	Step 1 : 50-160	5.8 / 4.4	2 water molecules	30.3
	Step 2: 160-600	64.0 / 88.5	incomplete degradation	

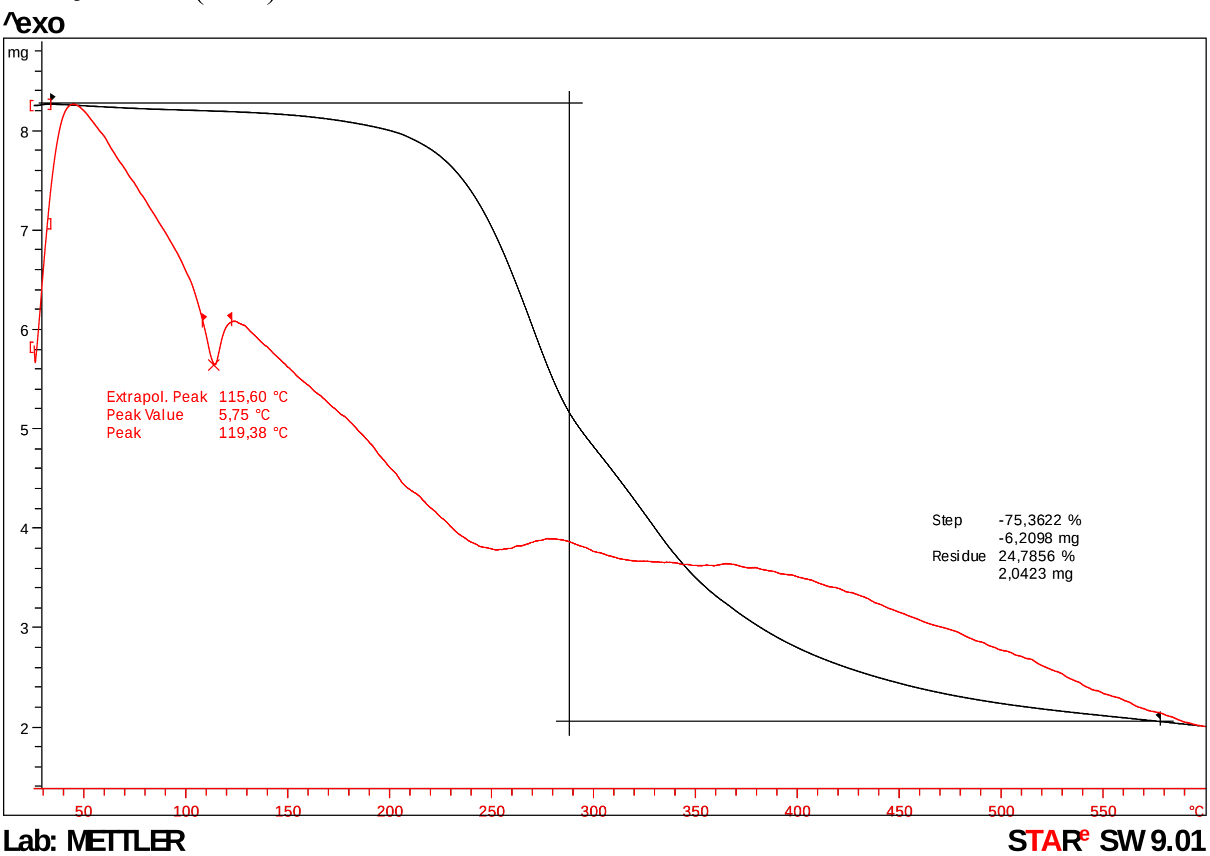
Table S5. Thermal analysis data for complexes **9-16** under oxygen atmosphere.

Complex	Temperature range (°C)	Mass loss (%); observed / calculated	Assignment	Residue at 600 °C (%)	
				Observed	Calculated for NiO
9	Step 1: 50-120 Step 2: 120-600	3.0 / 2.7 87.8 / 88.6	1 water molecule 2 ligand molecules + 2 nitrate ions	9.3	11.1
10	Step 1: 25-120 Step 2: 200-420	6.3 / 5.2 84.1 / 86.2	2 water molecules 2 ligand molecules + 2 nitrate ions	9.9	10.8
11	Step 1: 25-150 Step 2: 150-410	2.7 / 2.7 87.4 / 88.6	1 water molecule 2 ligand molecules + 2 nitrate ions	9.9	11.1
12	200-600	89.8 / 91.6	2 ligand molecules + 2 nitrate ions	10.7	10.7
13	Step 1: 90-160 Step 2: 160-570	15.2 / 17.3 76.0 / 75.7	2 DMF molecules 2 ligand molecules + 2 nitrate ions	9.0	8.9
14	Step 1 : 50-160 Step 2: 160-600	5.6 / 4.9 84.5 / 87.1	2 water molecules 2 ligand molecules + 2 nitrate ions	10.2	10.2
15	Step 1 : 50-150 Step 2: 230-520	3.2 / 2.6 86.0 / 88.7	2 water molecules 2 ligand molecules + 2 nitrate ions	11.1	11.0
16	Step 1 : 50-160 Step 2: 210-550	5.1 / 4.4 85.0 / 88.5	2 water molecules 2 ligand molecules + 2 nitrate ions	10.0	9.1

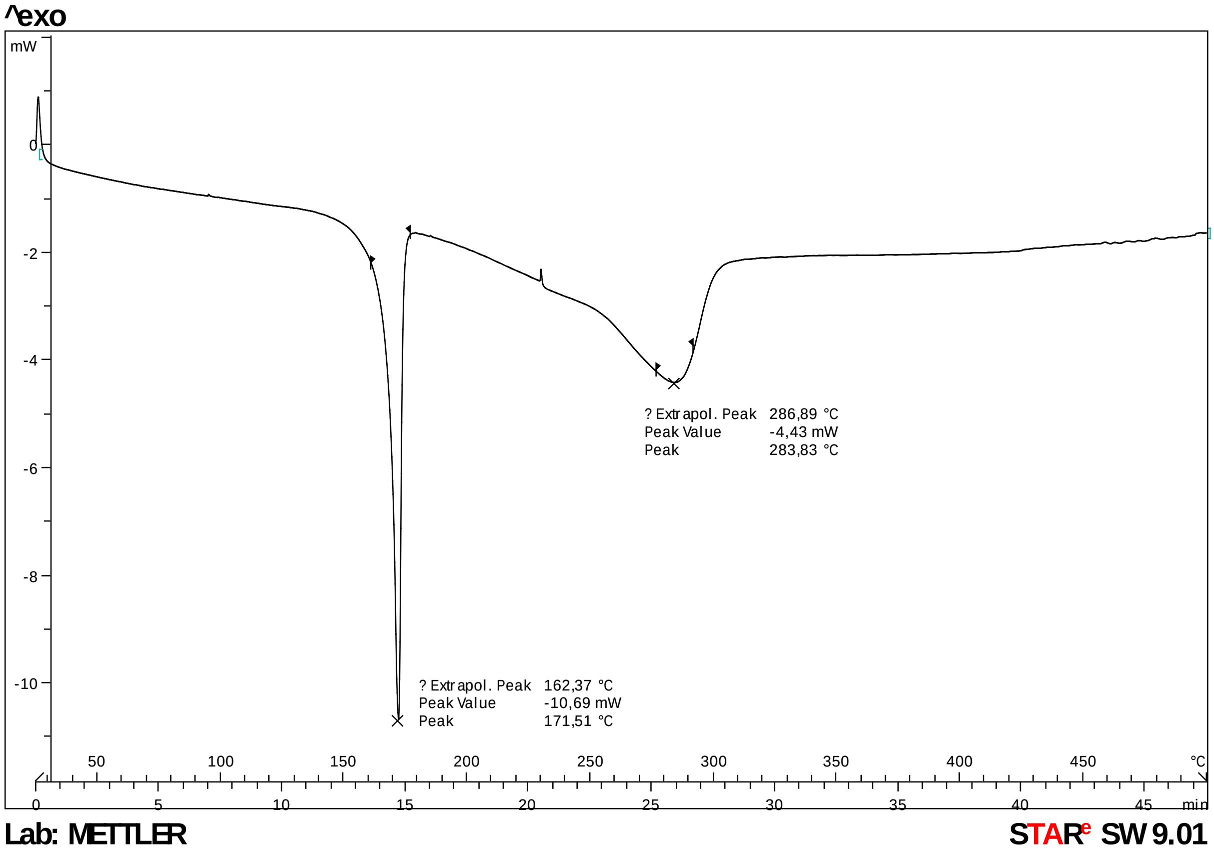
DSC and TGA curves for the ligands, recorded under nitrogen atmosphere



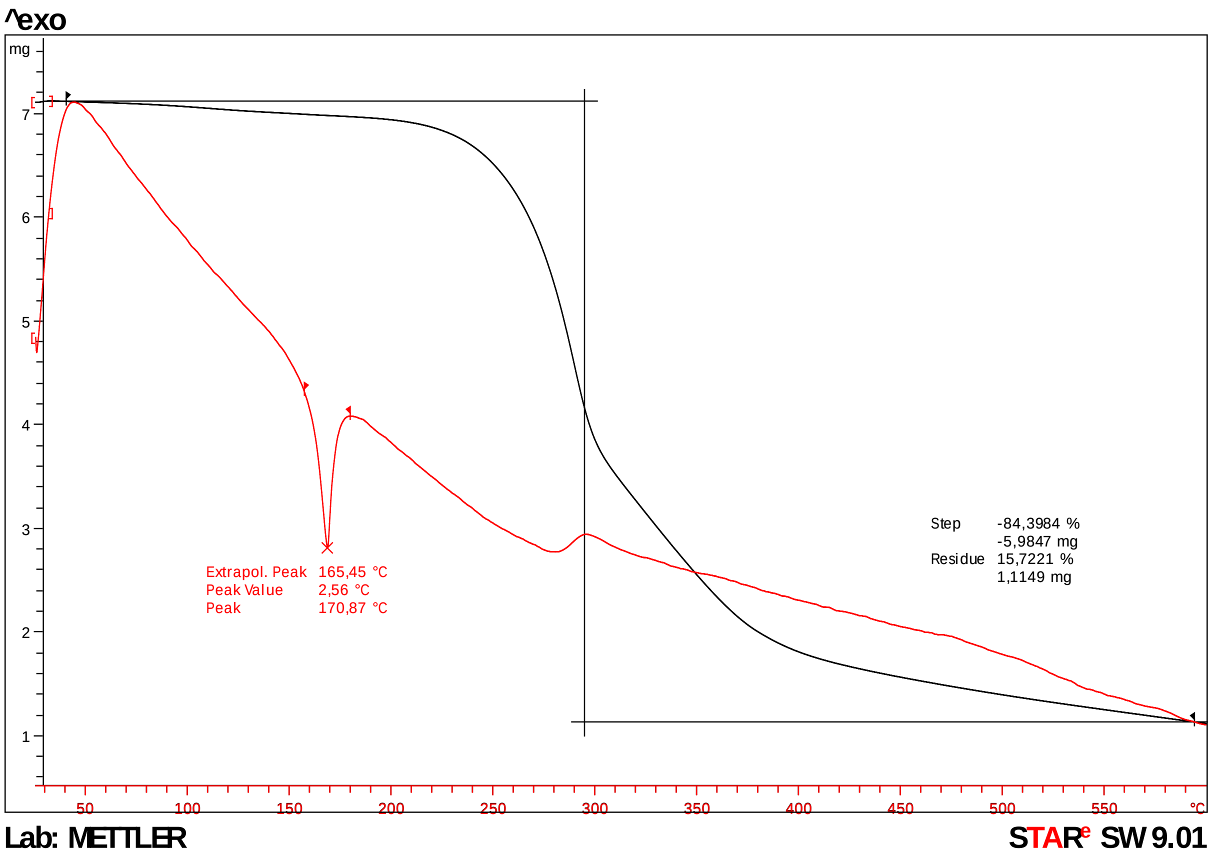
o-CH_3Bnimda (DSC)



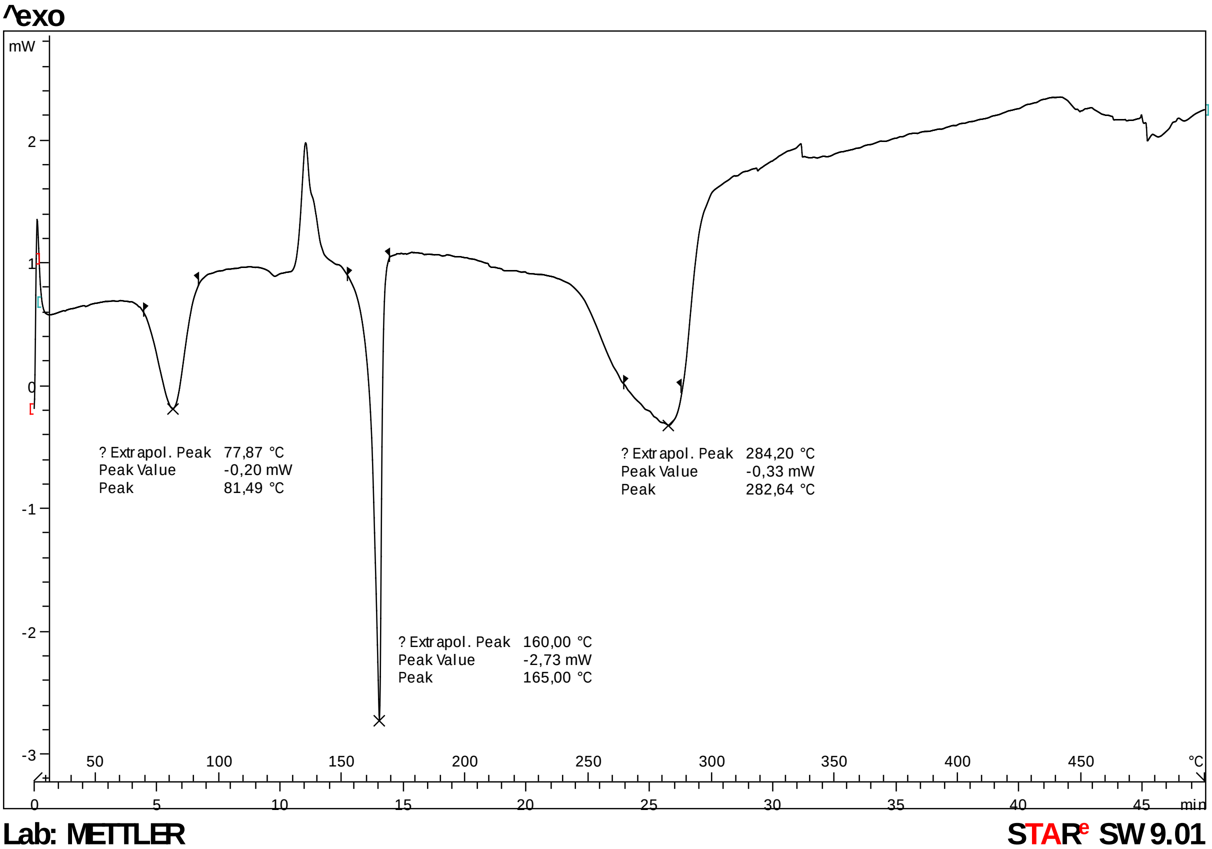
o-CH_3Bnimda (TGA/DTA)



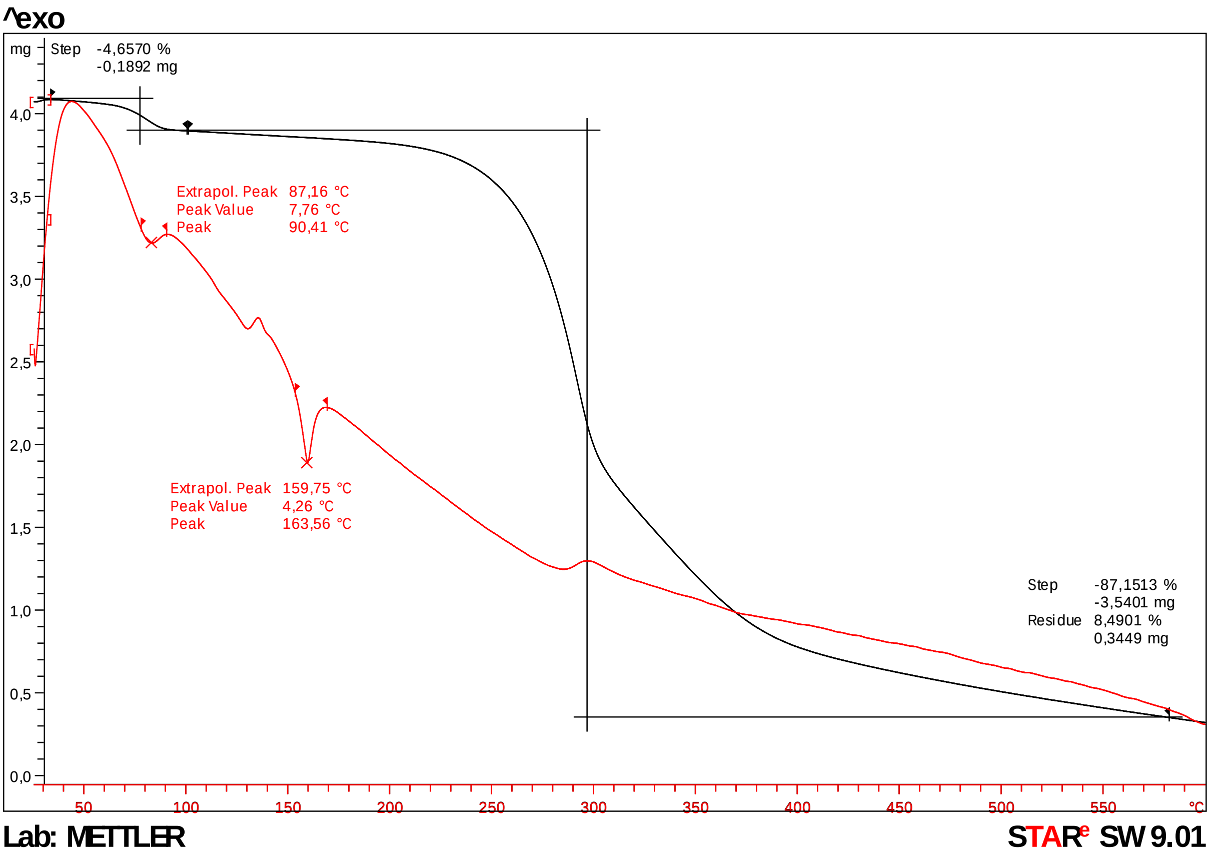
m-CH_3Bnimda (DSC)



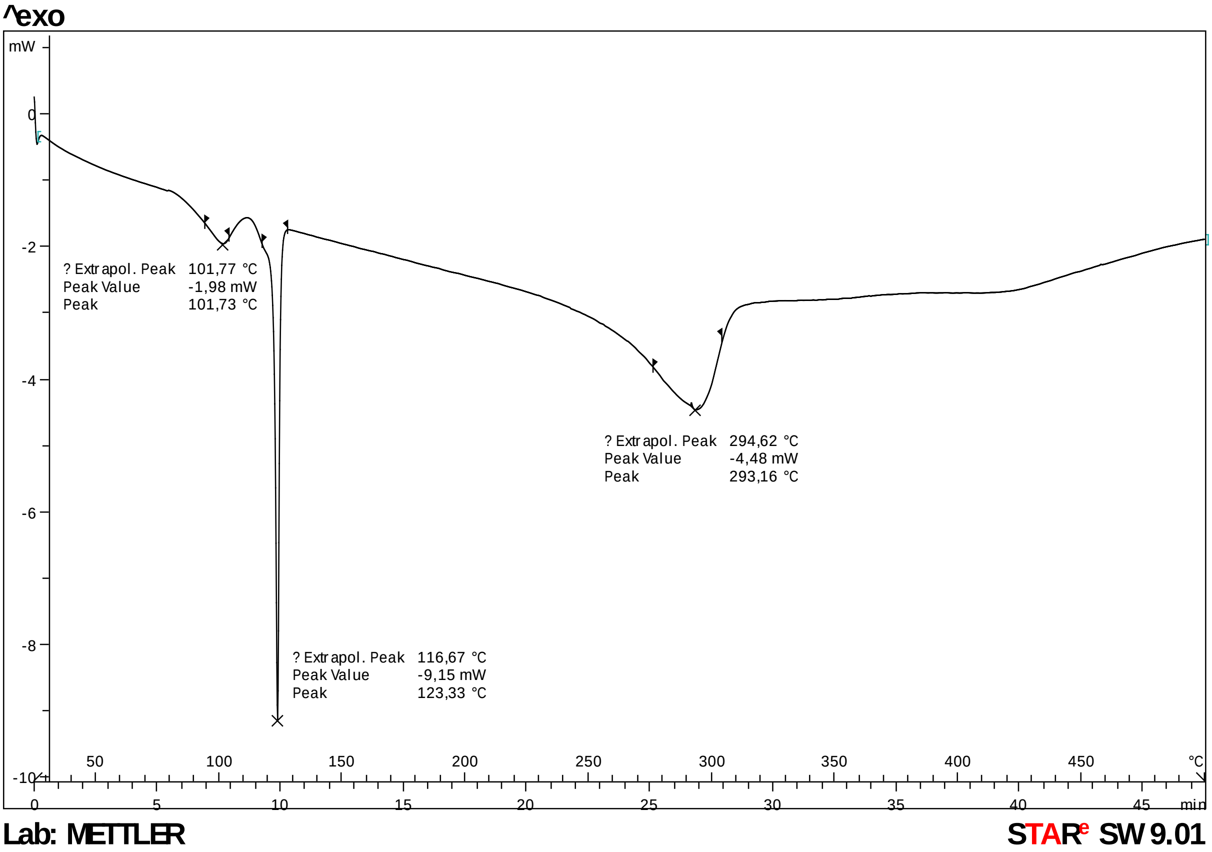
m-CH_3Bnimda (TGA/DTA)



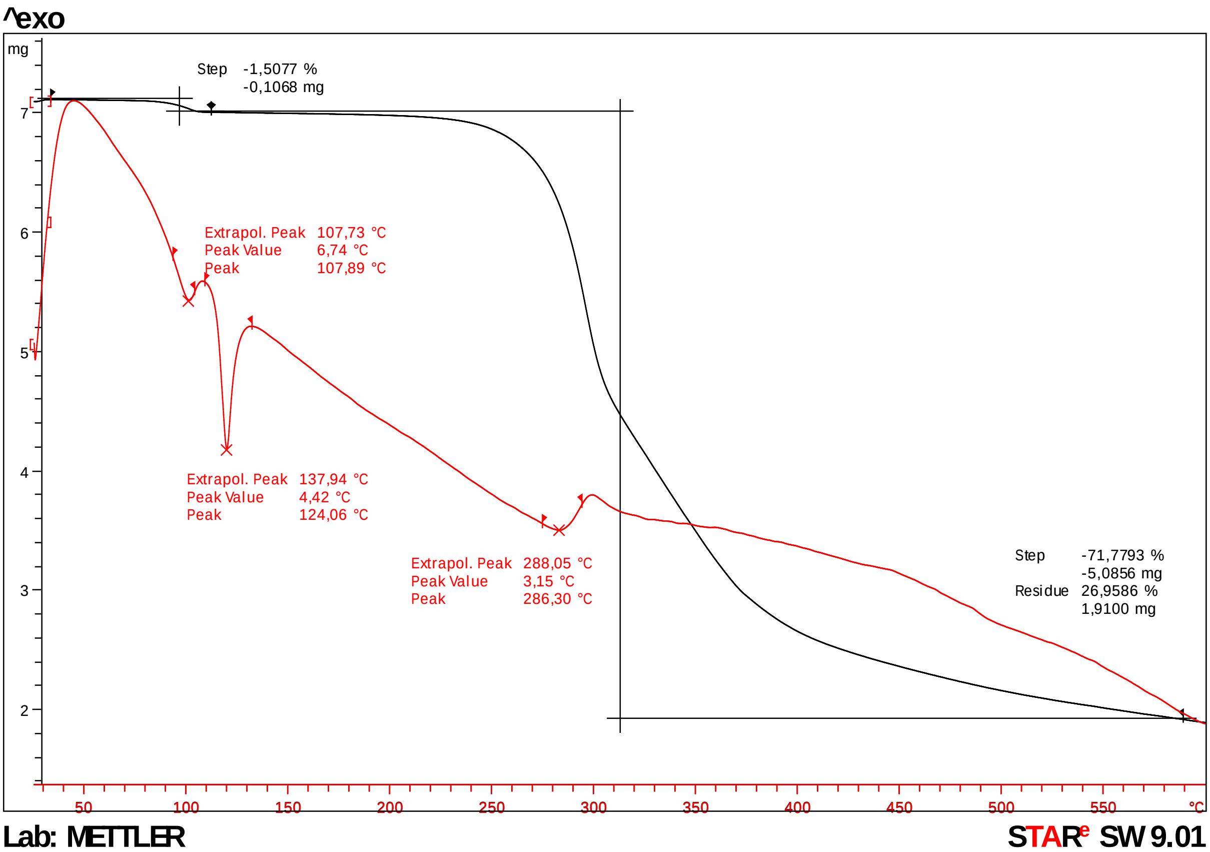
p-CH_3Bnimda · 0.75H_2O (DSC)



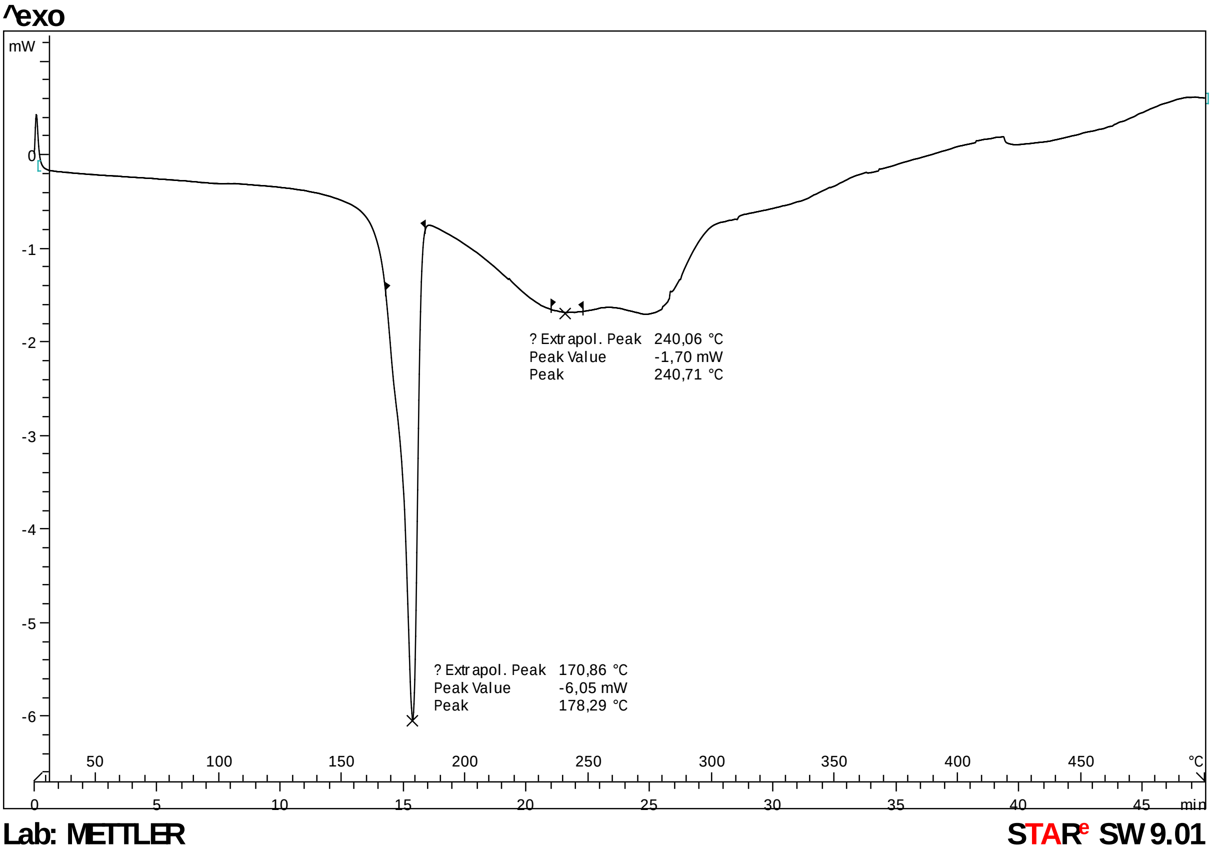
p-CH_3Bnimda · 0.75H_2O (TGA/DTA)



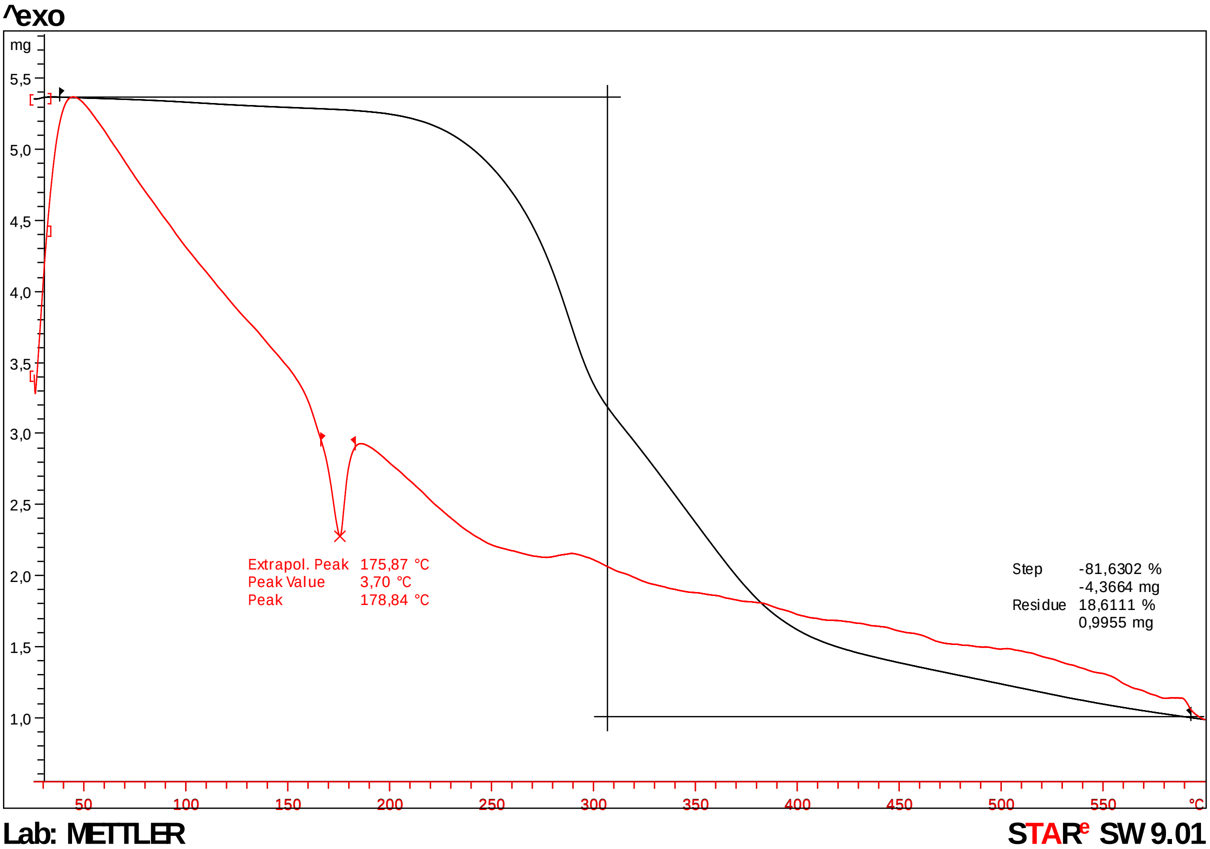
o-ClBnimda (DSC)



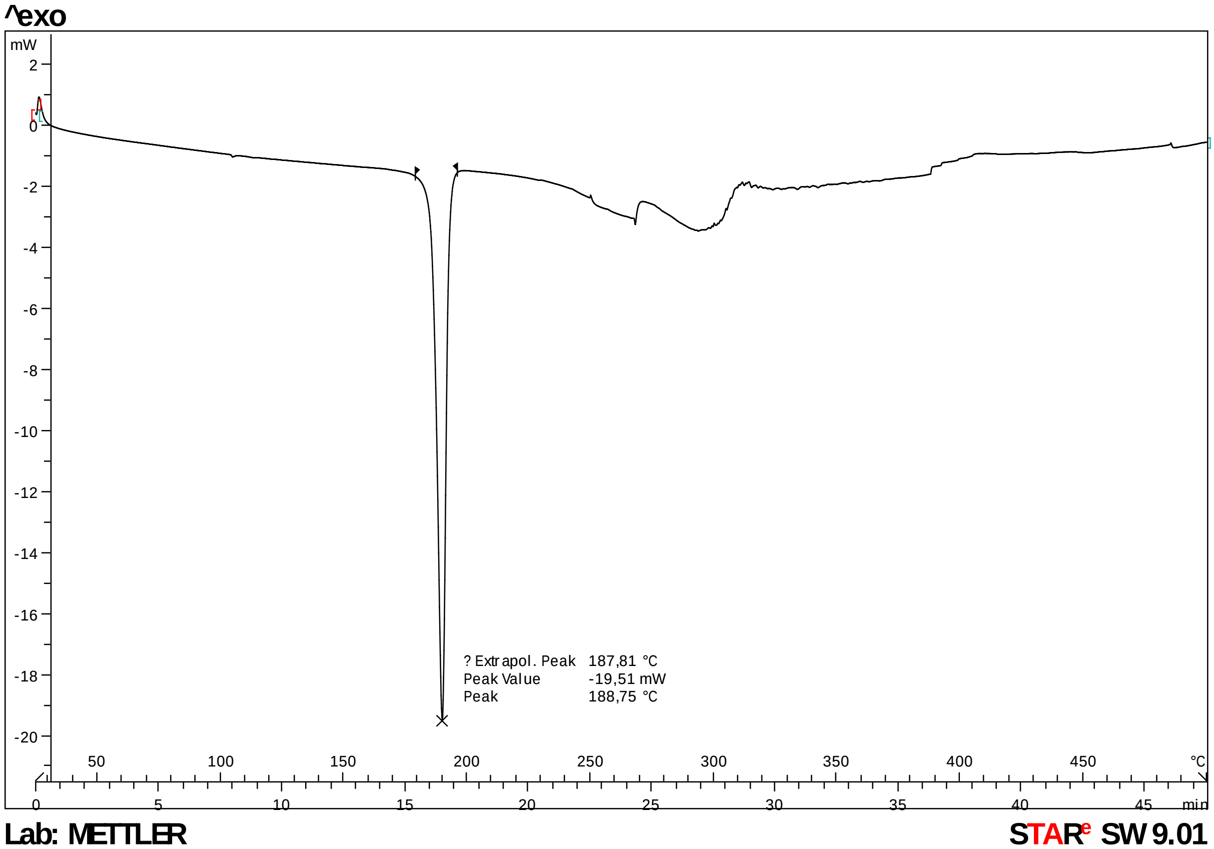
o-ClBnimda (TGA/DTA)



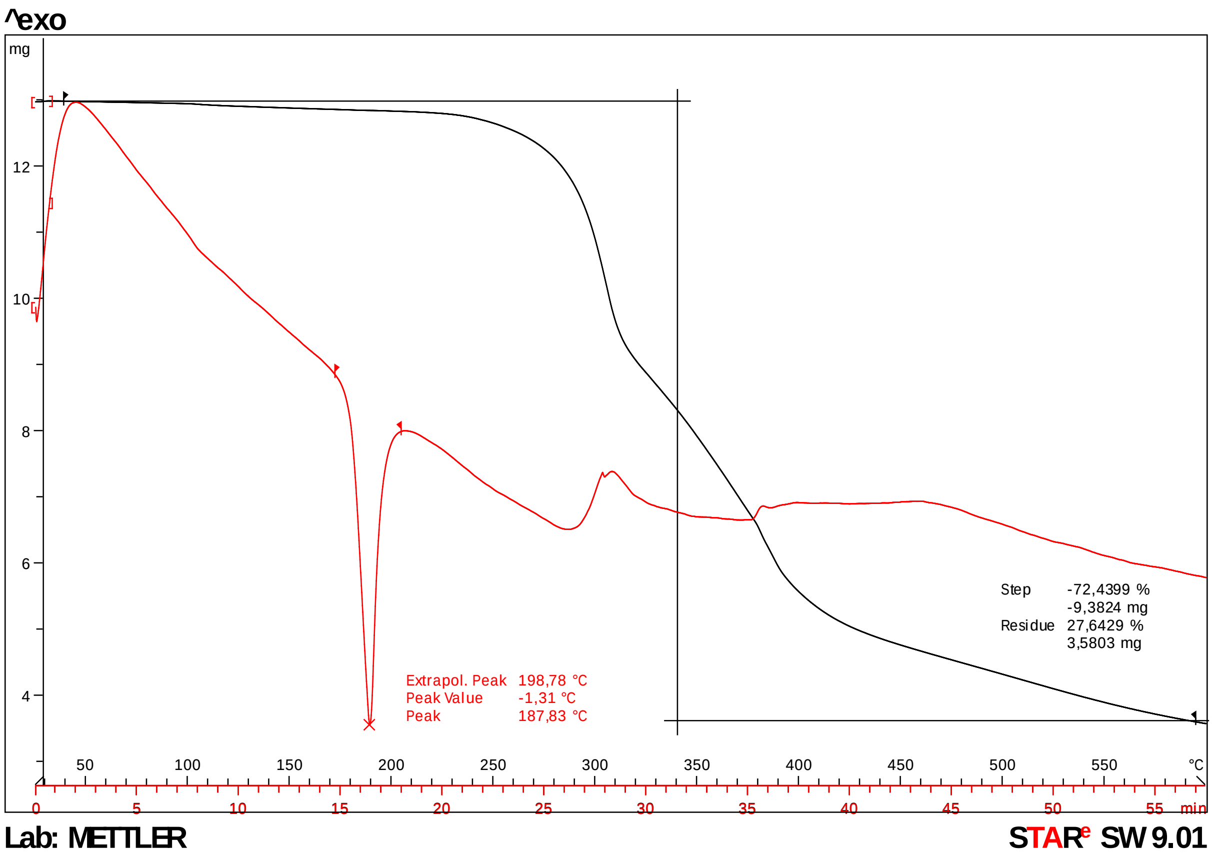
m-ClBnimda (DSC)



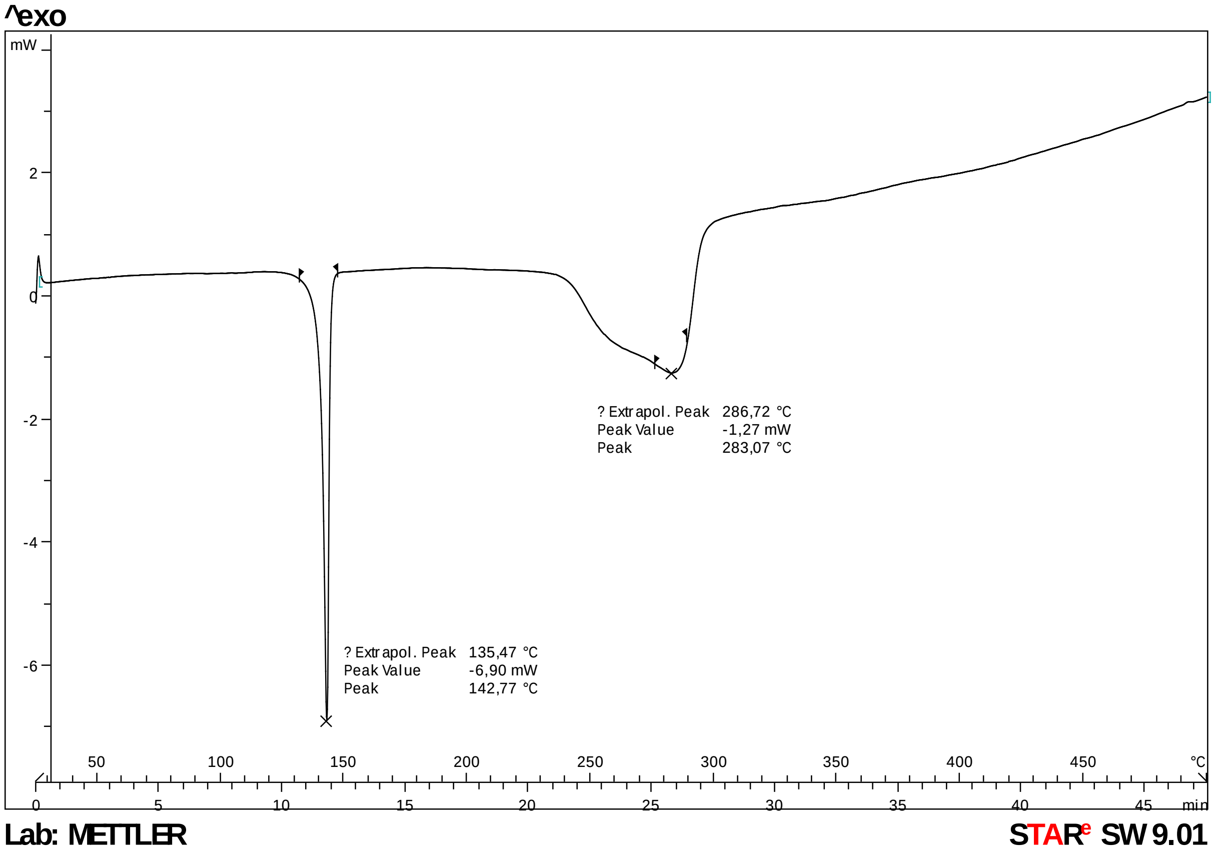
m-ClBnimda (TGA/DTA)



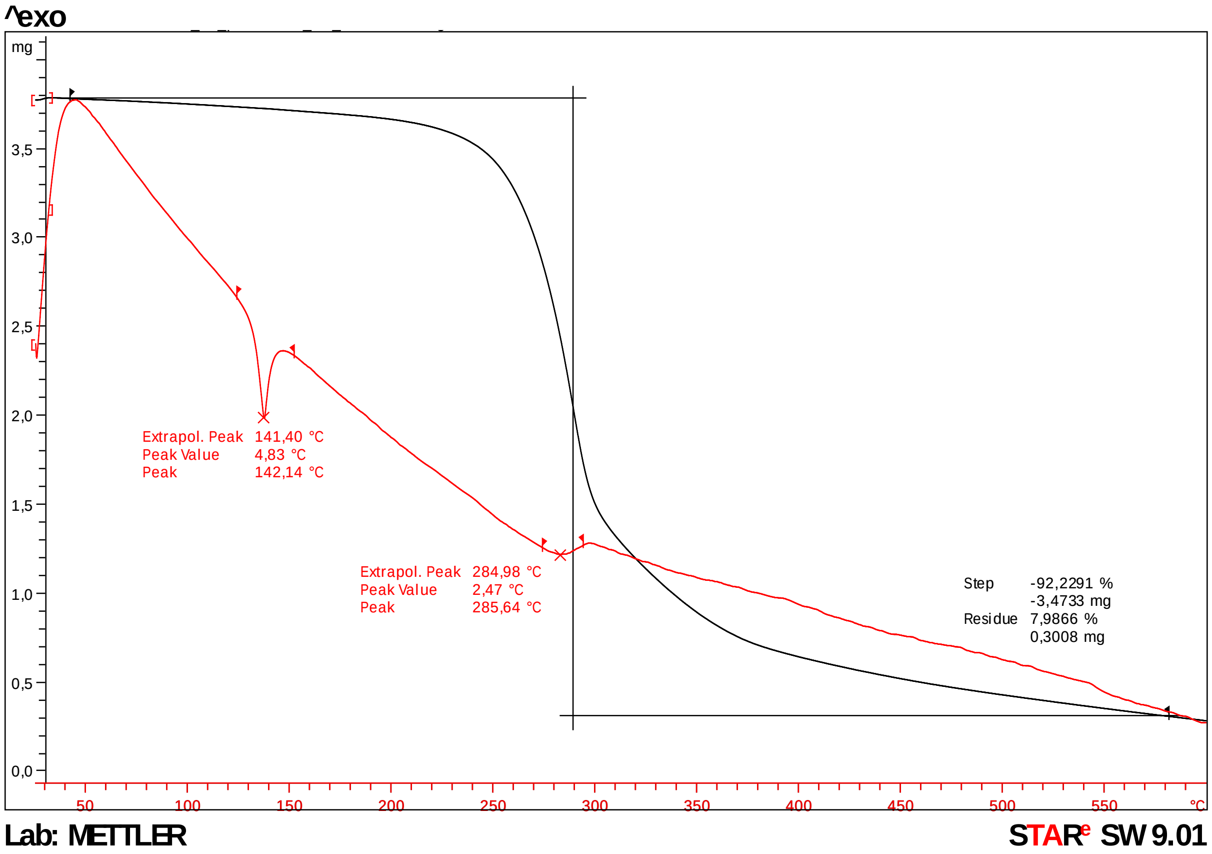
p-ClBnimda (DSC)



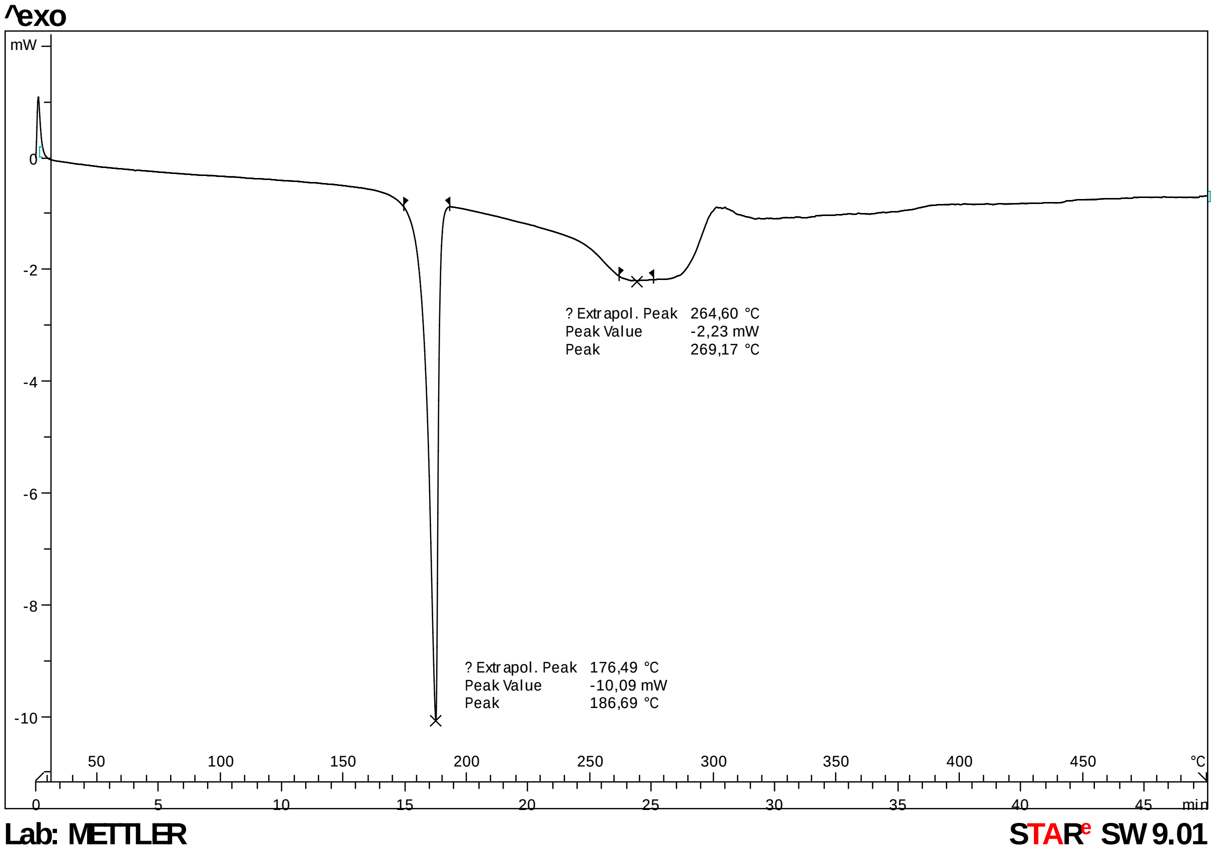
p-ClBnimda (TGA/DTA)



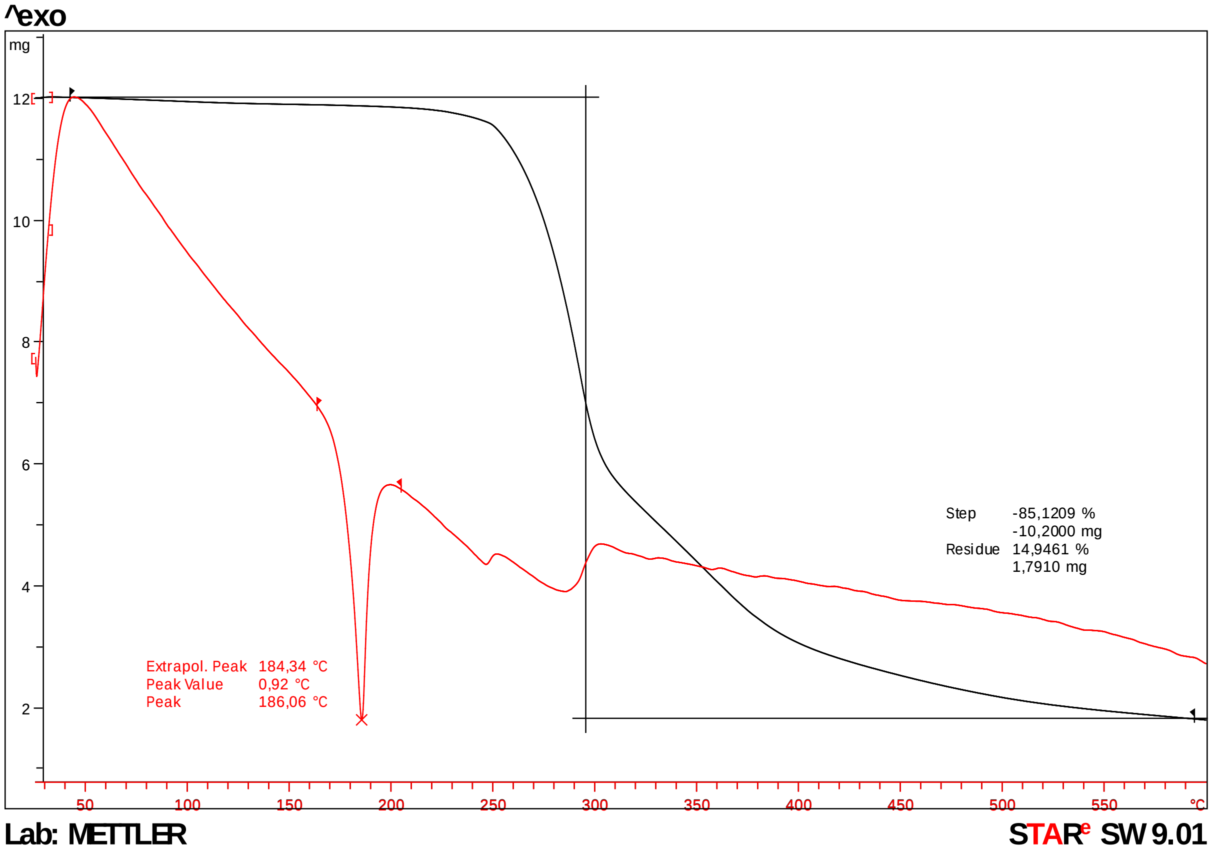
p-FBnimda (DSC)



p-FBnimda (TGA/DTA)

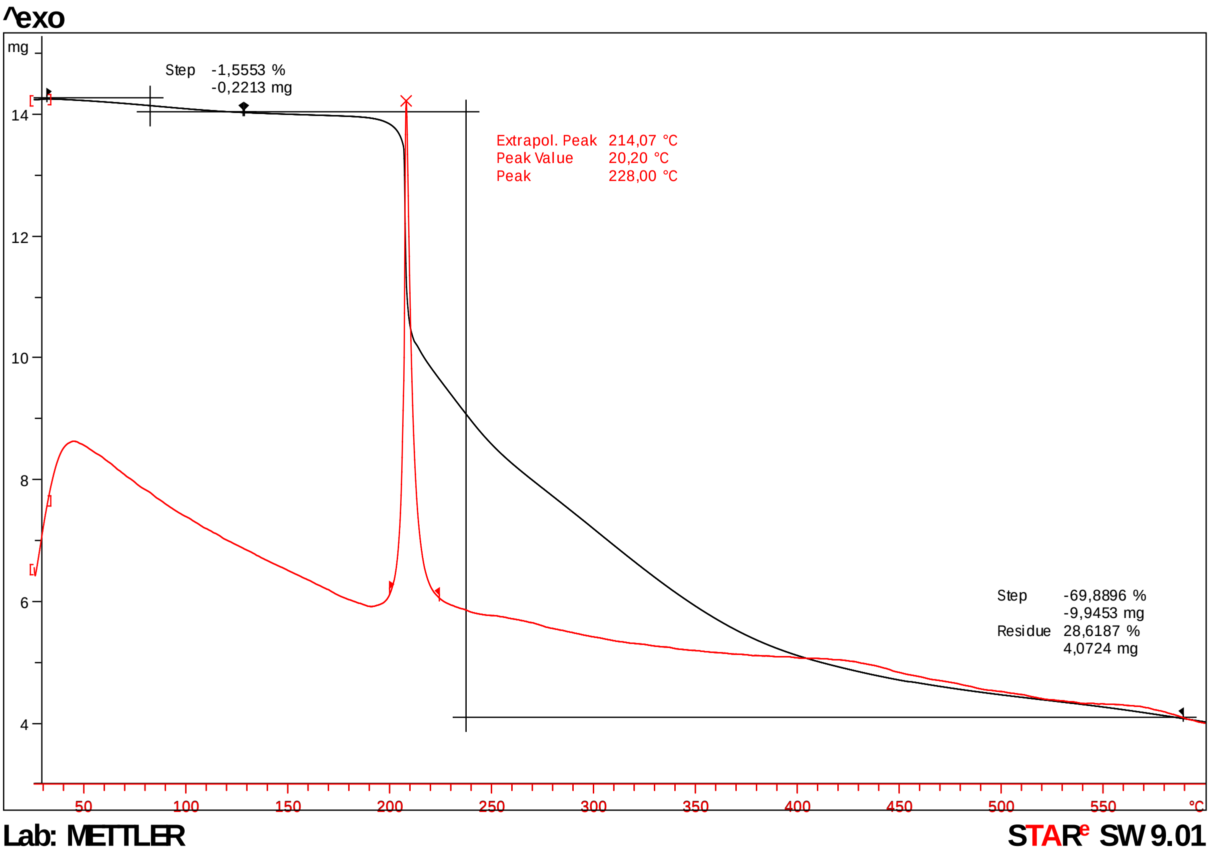


p-BrBnimda (DSC)

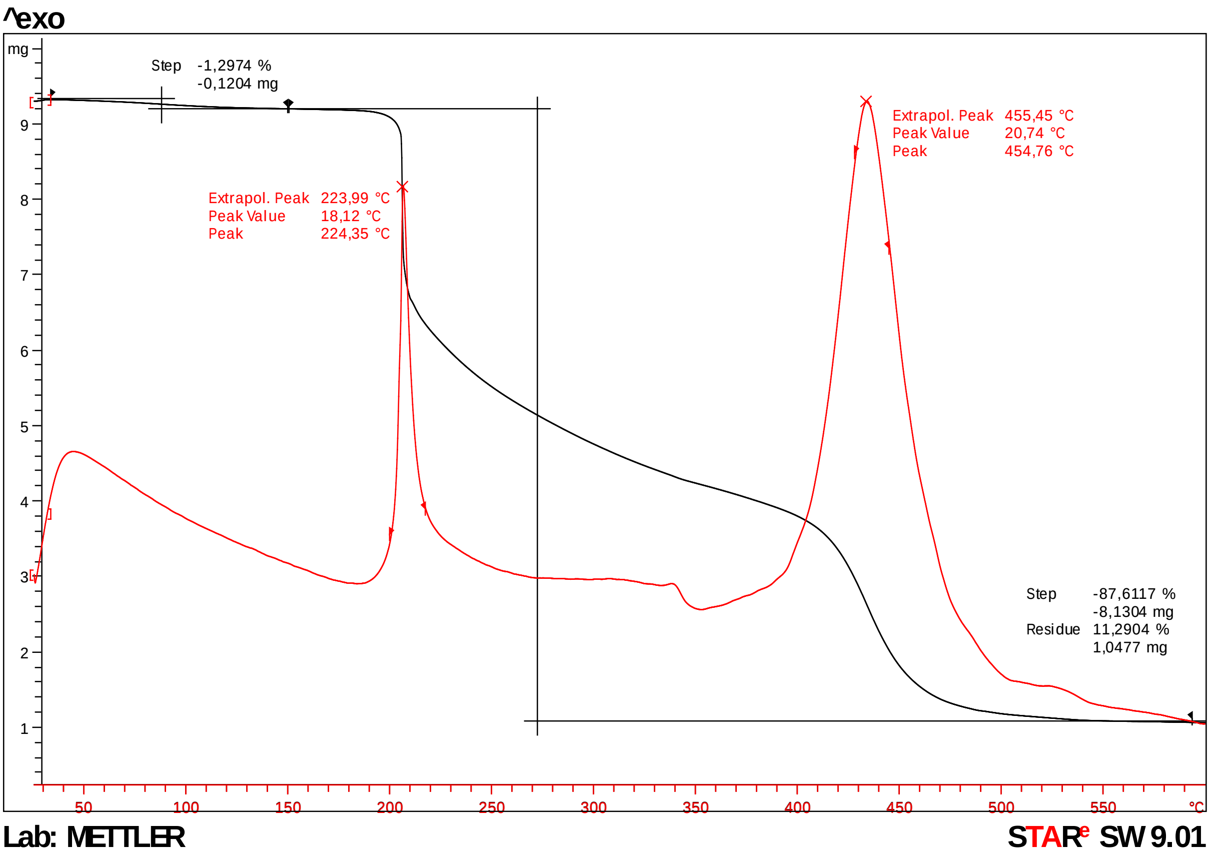


p-BrBnimda (TGA/DTA)

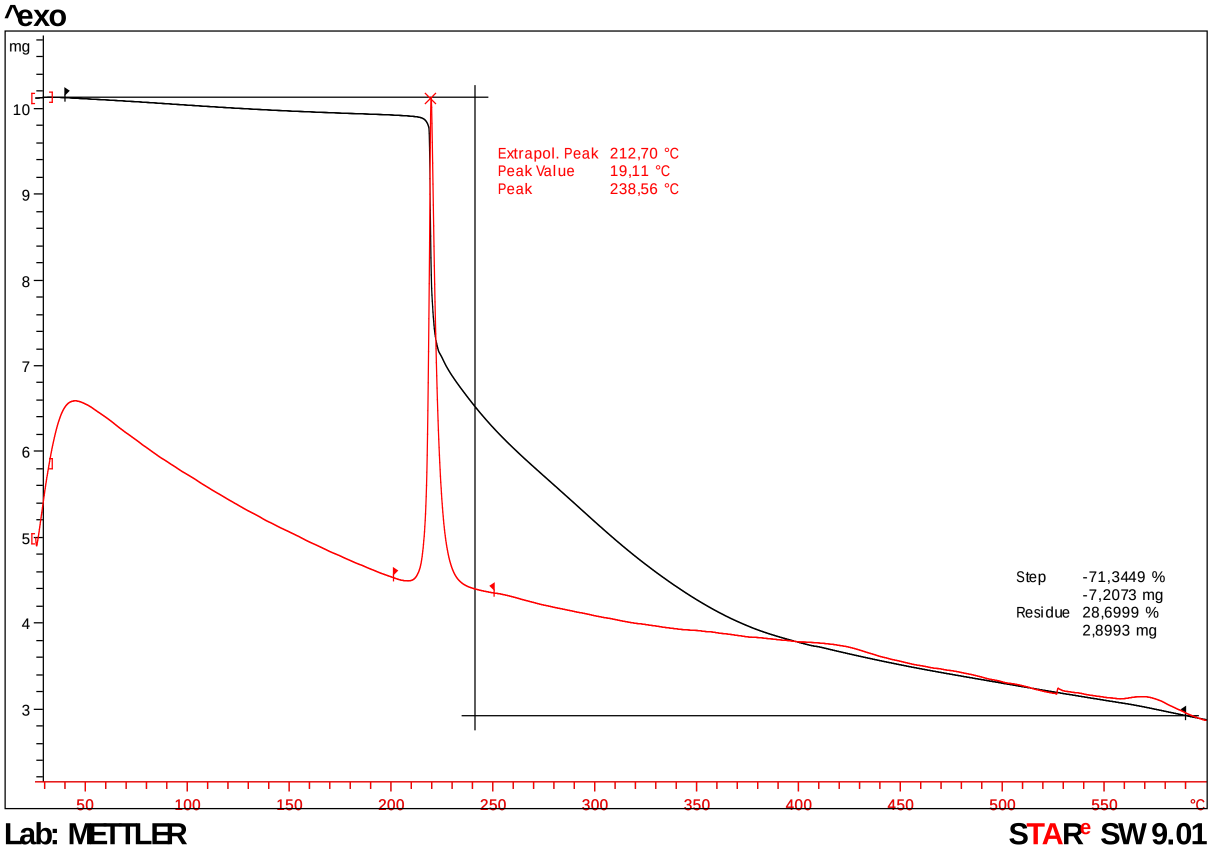
TGA/DTA curves for the complexes, recorded under nitrogen or oxygen atmosphere



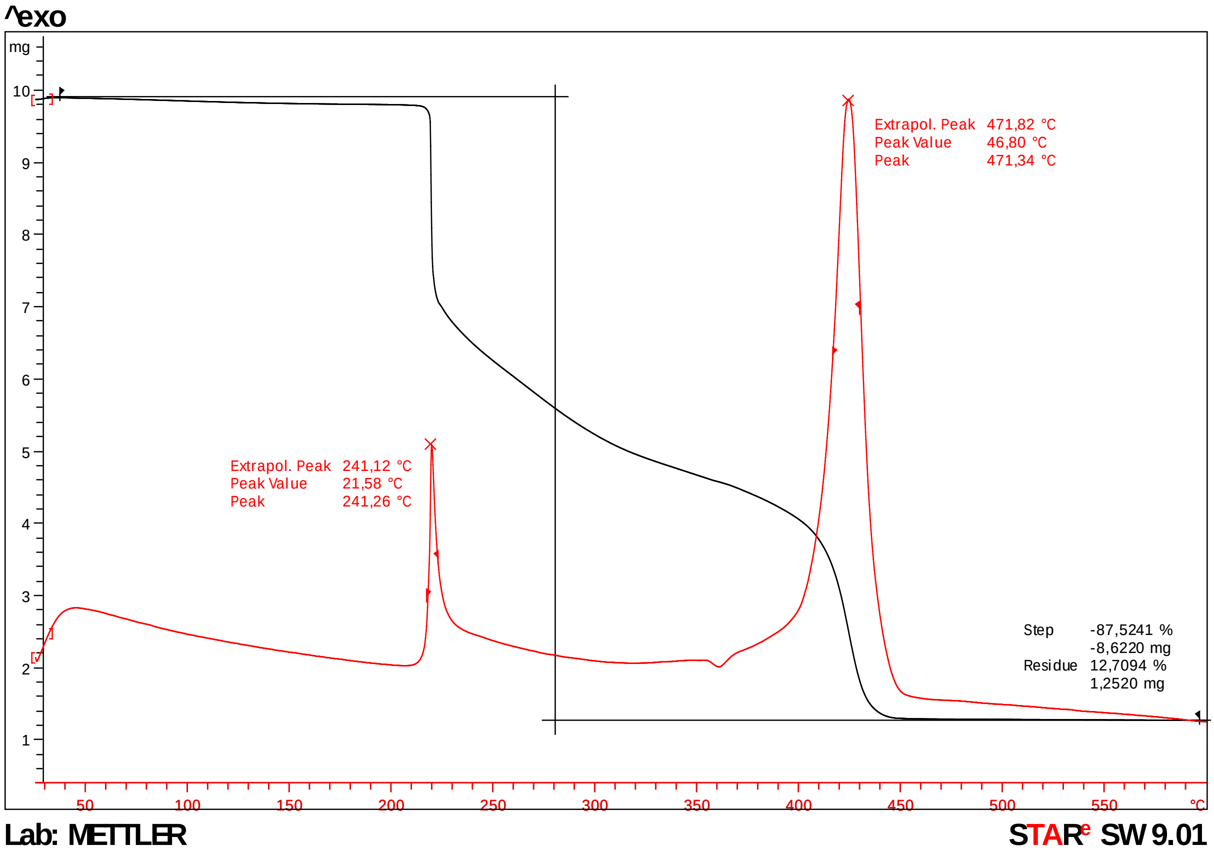
[Cu(*o*-CH_3Bnimda)$_2$](NO_3)$_2$ · ½ H_2O (**1**) (N_2)



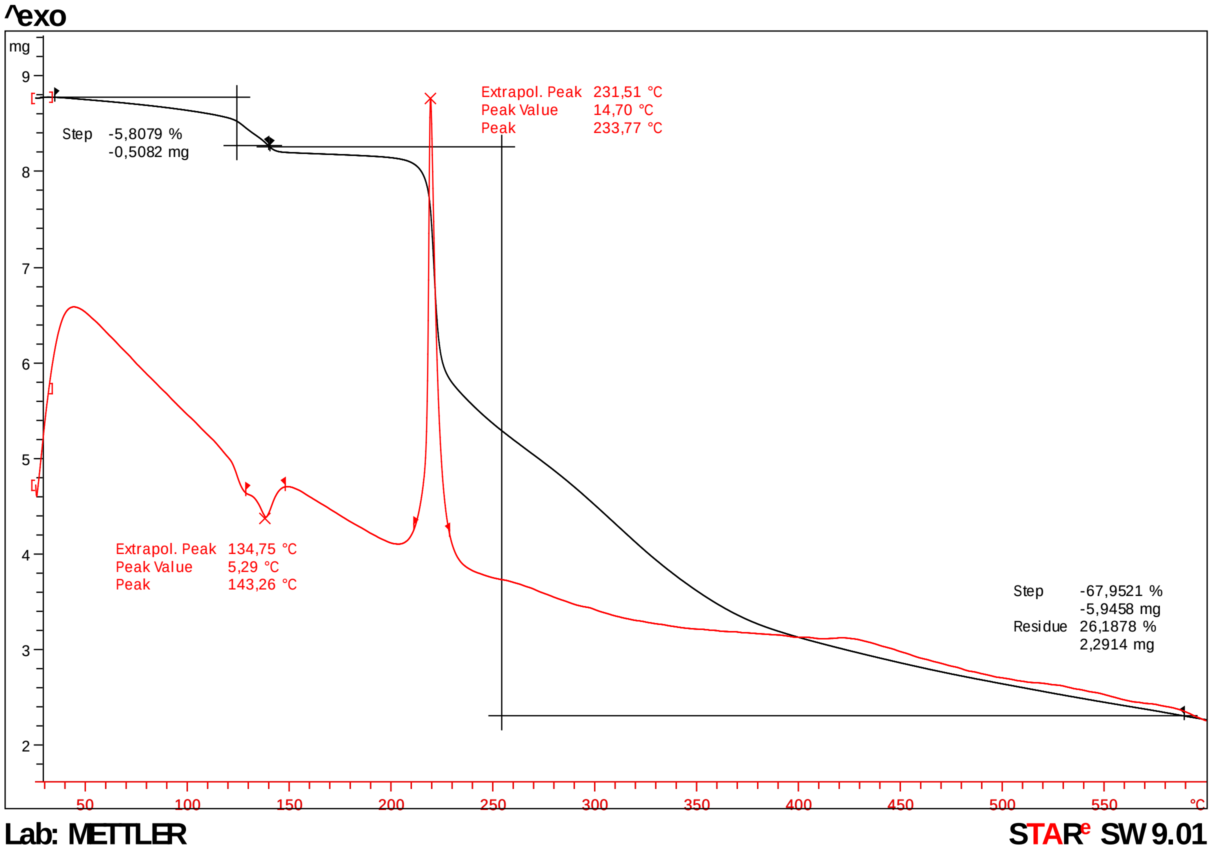
[Cu(*o*-CH_3Bnimda)$_2$](NO_3)$_2$ · ½ H_2O (**1**) (O_2)



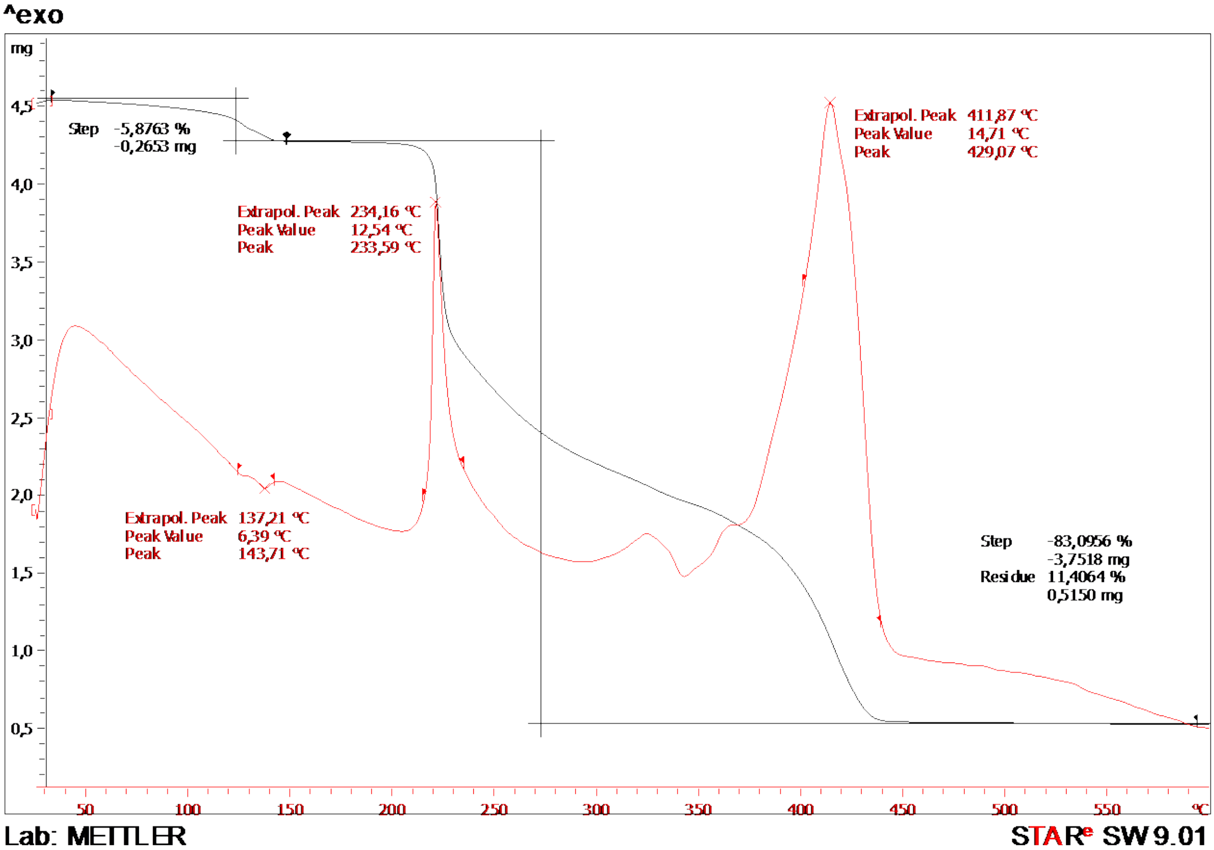
[Cu(*m*-CH_3Bnimda)$_2$](NO_3)$_2$ (**2**) (N_2)



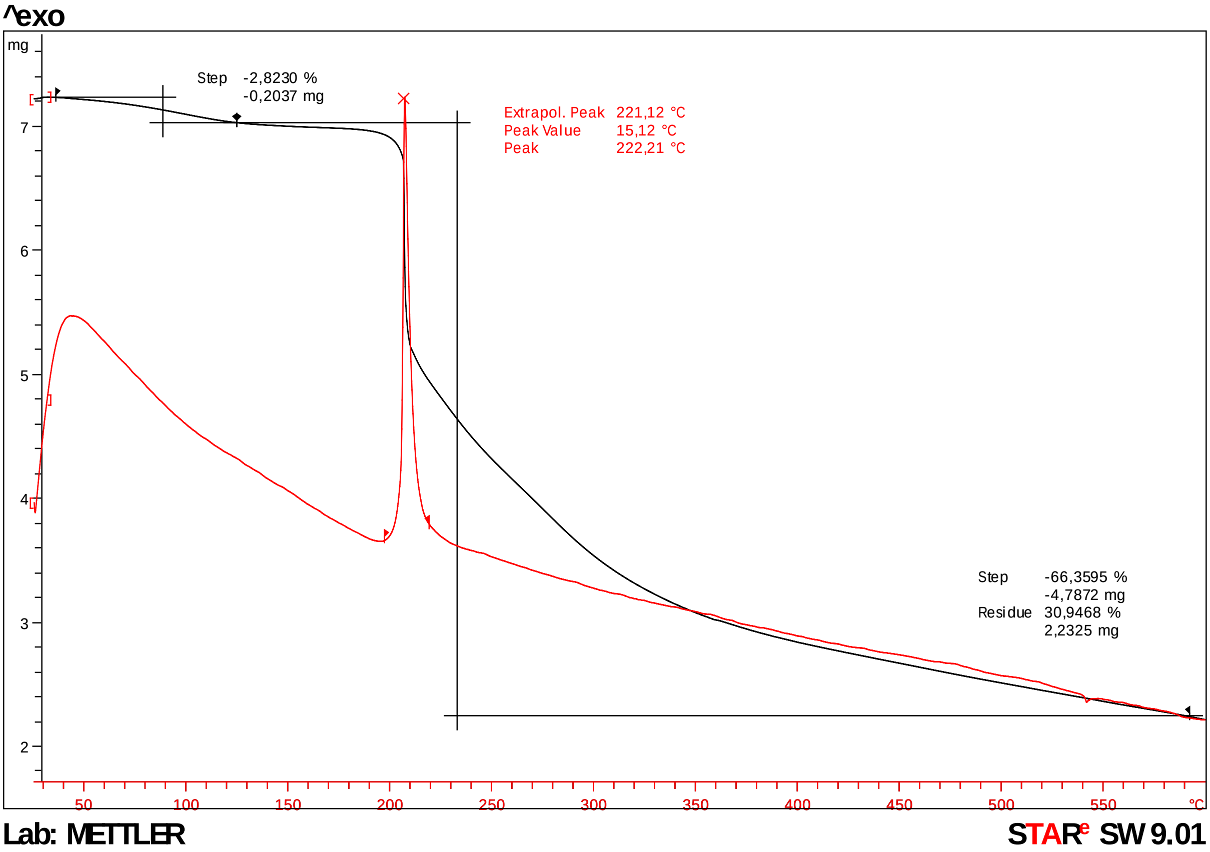
[Cu(*m*-CH_3Bnimda)$_2$](NO_3)$_2$ (**2**) (O_2)



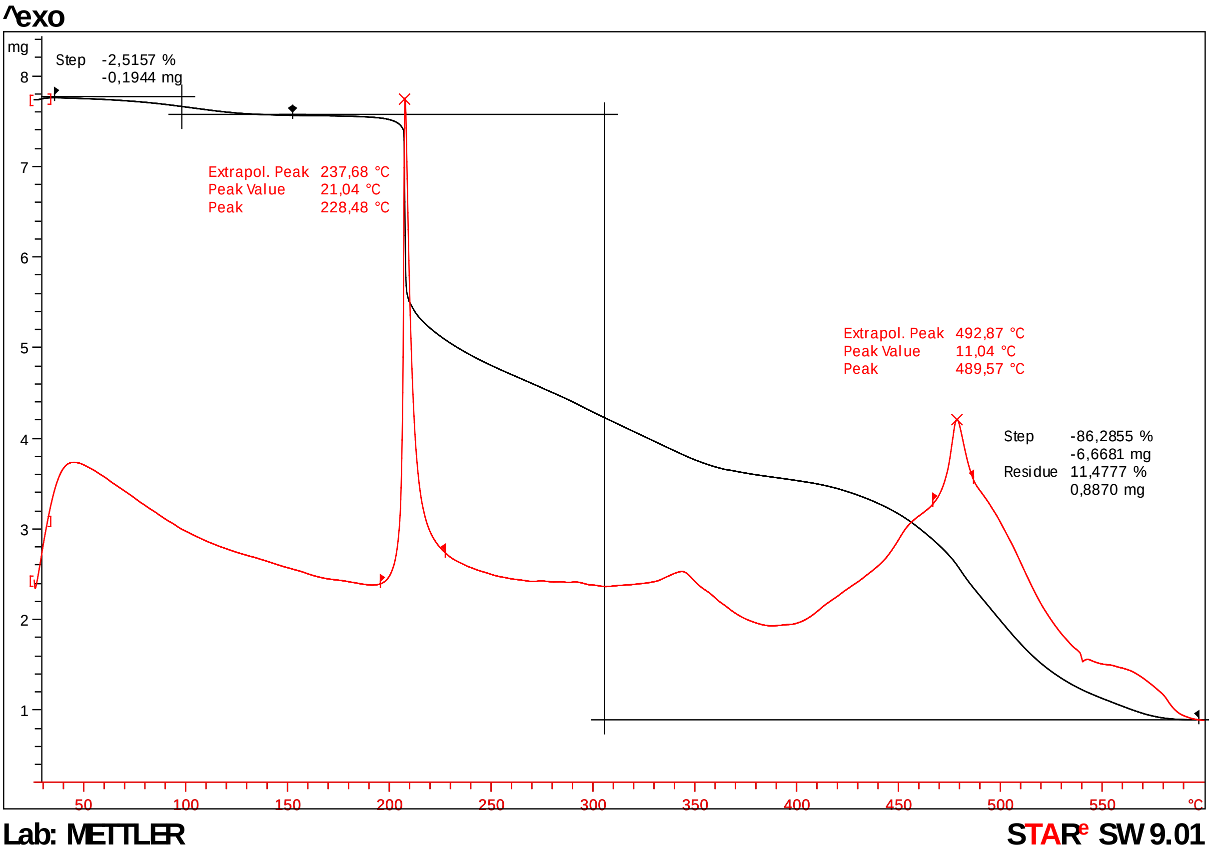
[Cu(*p*-CH_3Bnimda)$_2$](NO_3)$_2$ · $2H_2O$ (**3**) (N_2)



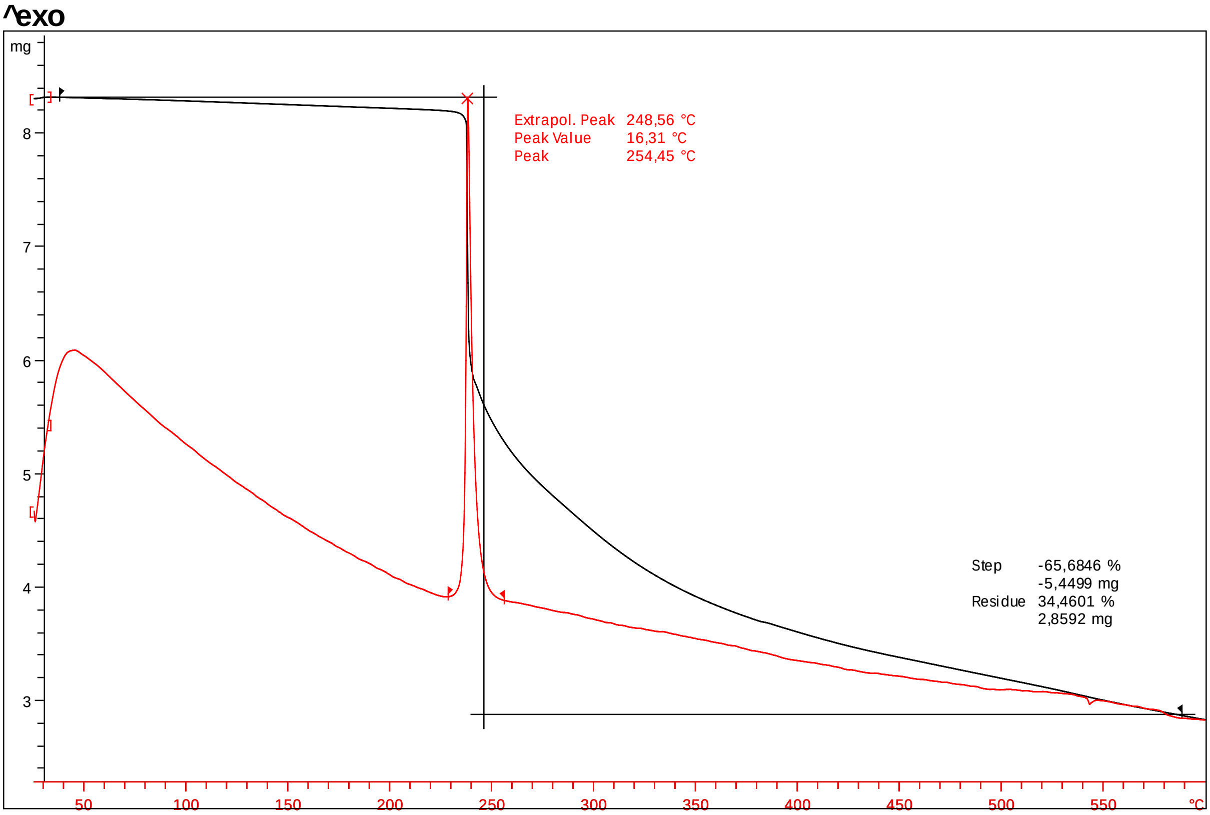
[Cu(*p*-CH_3Bnimda)$_2$](NO_3)$_2$ · $2H_2O$ (**3**) (O_2)



[Cu(*o*-ClBnimda)$_2$](NO$_3$)$_2$ · H$_2$O (**4**) (N$_2$)



[Cu(*o*-ClBnimda)$_2$](NO$_3$)$_2$ · H$_2$O (**4**) (O$_2$)



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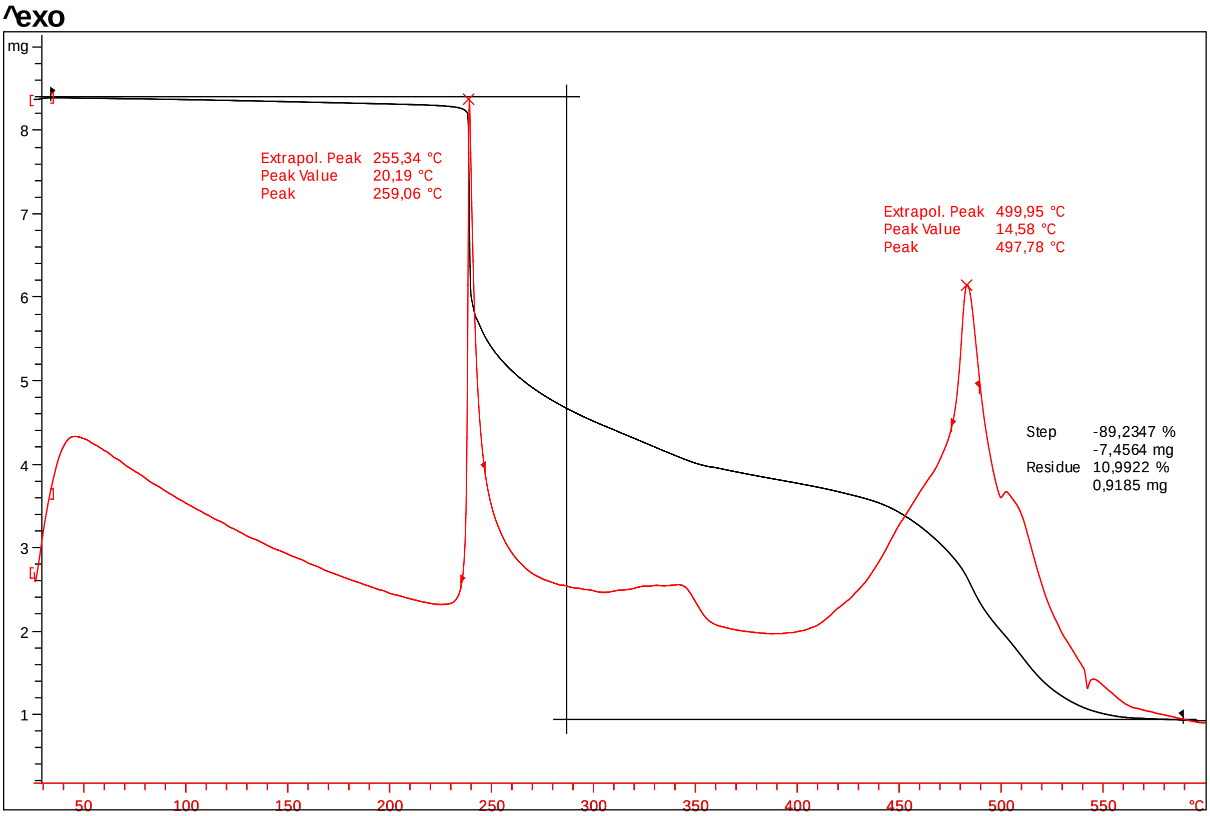
[Cu(*m*-ClBnimda)$_2$](NO$_3$)$_2$ (**5**) (N$_2$)



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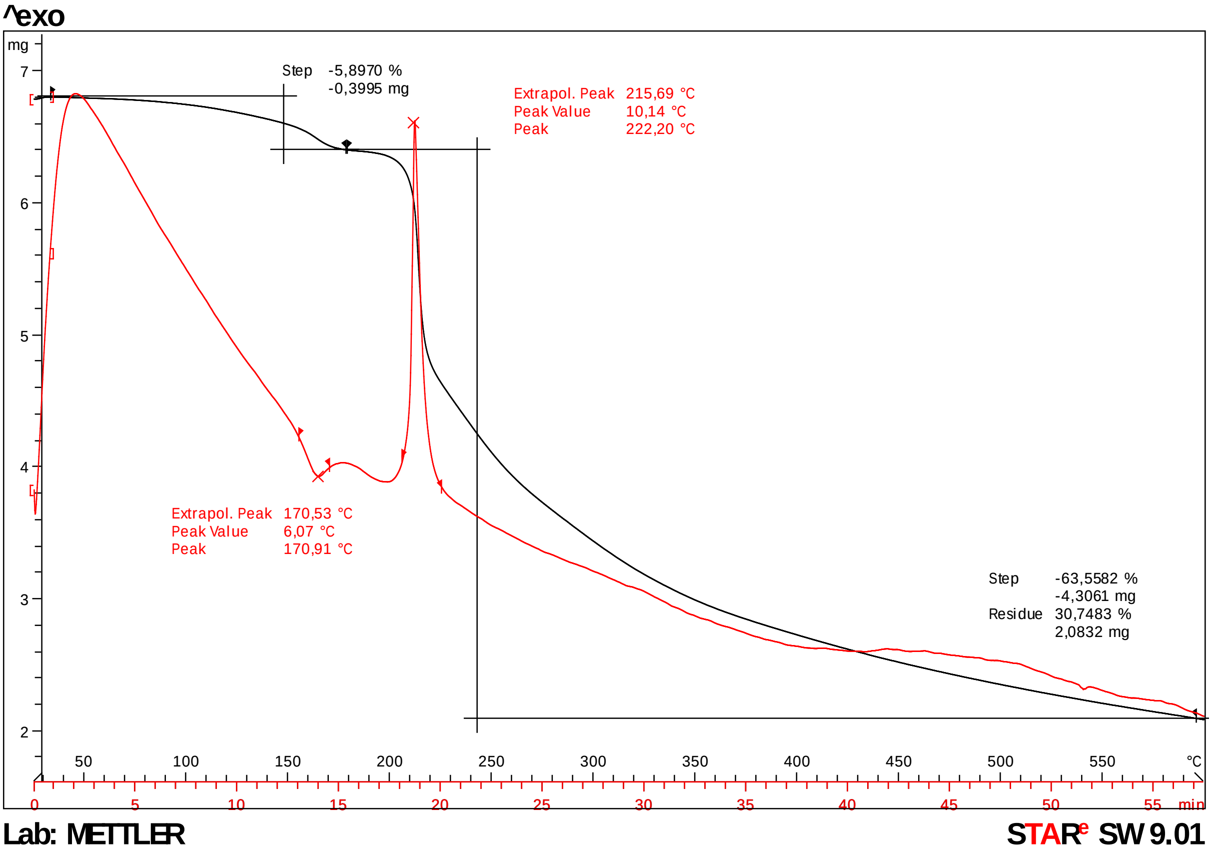
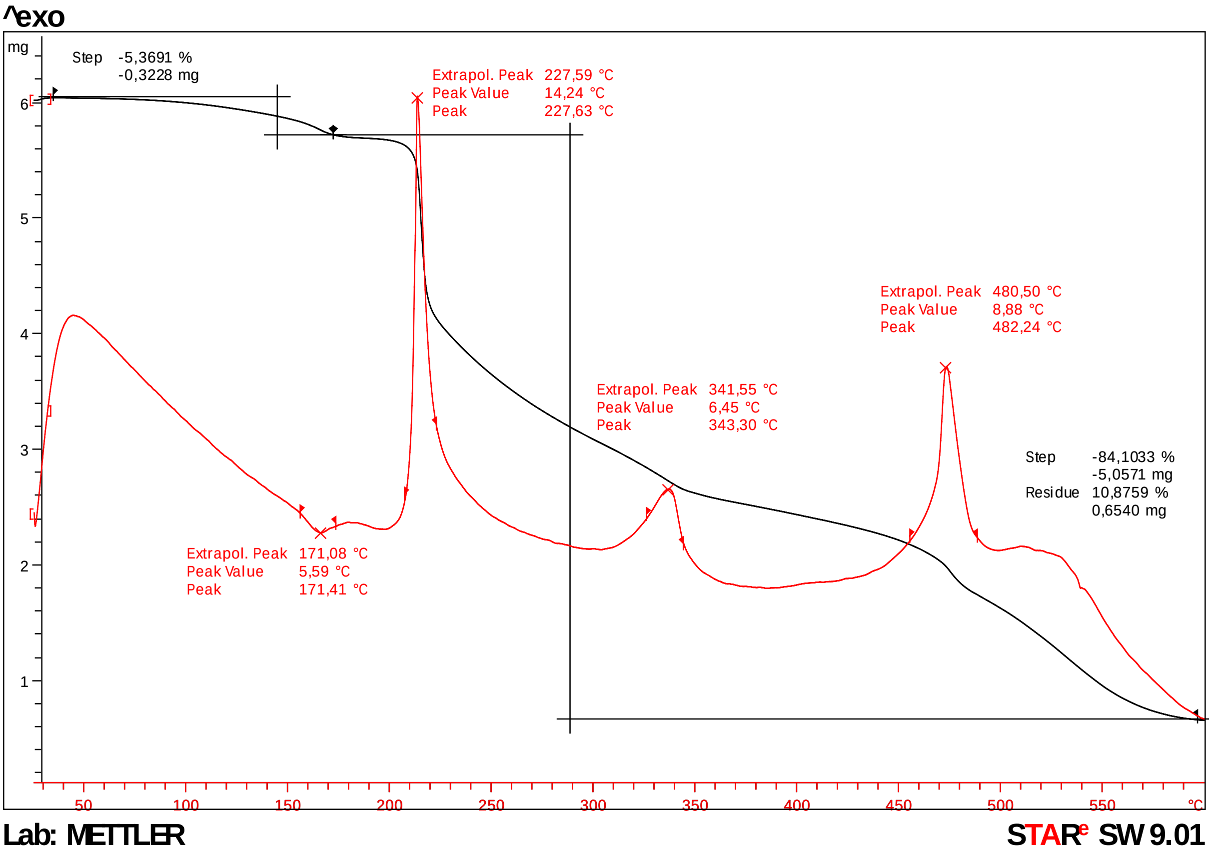
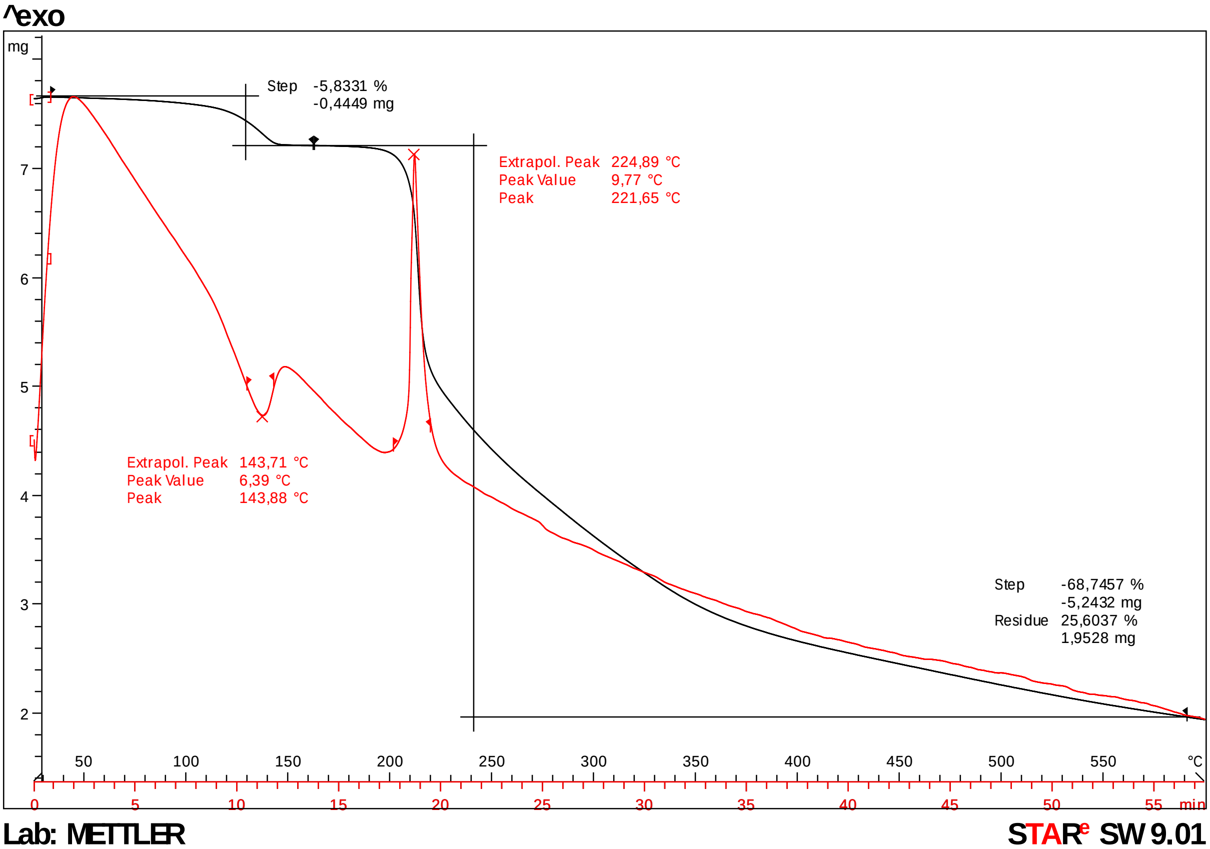
[Cu(*m*-ClBnimda)$_2$](NO$_3$)$_2$ (**5**) (O$_2$)



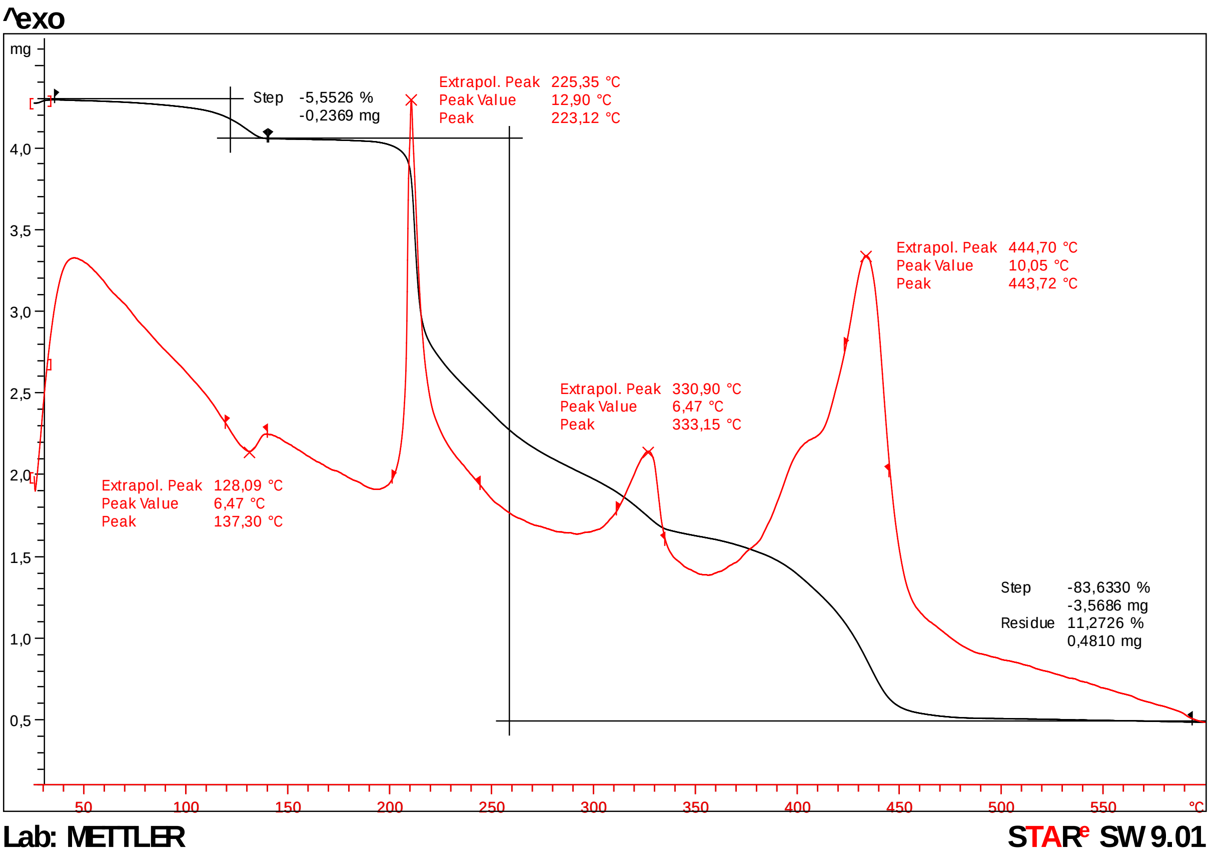
[Cu(*p*-ClBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**6**) (N$_2$)



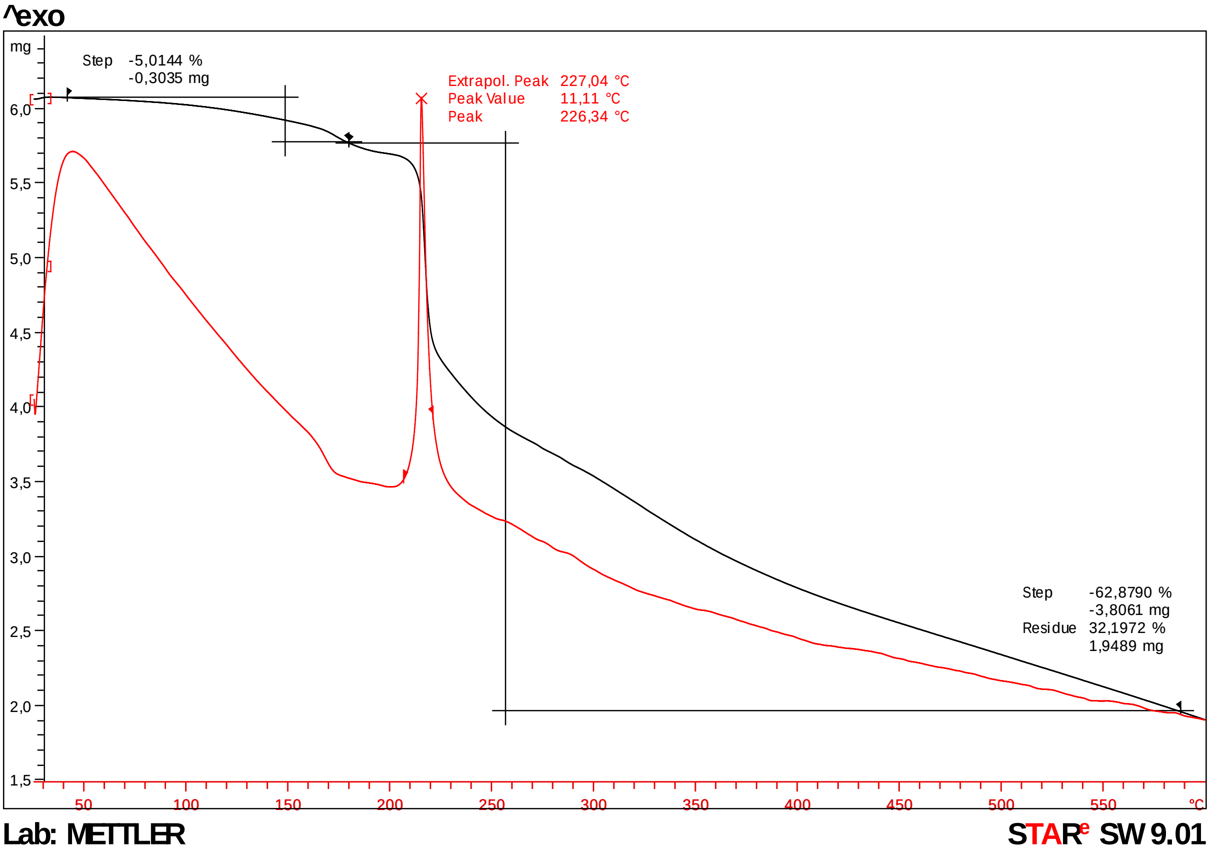
[Cu(*p*-ClBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**6**) (O$_2$)



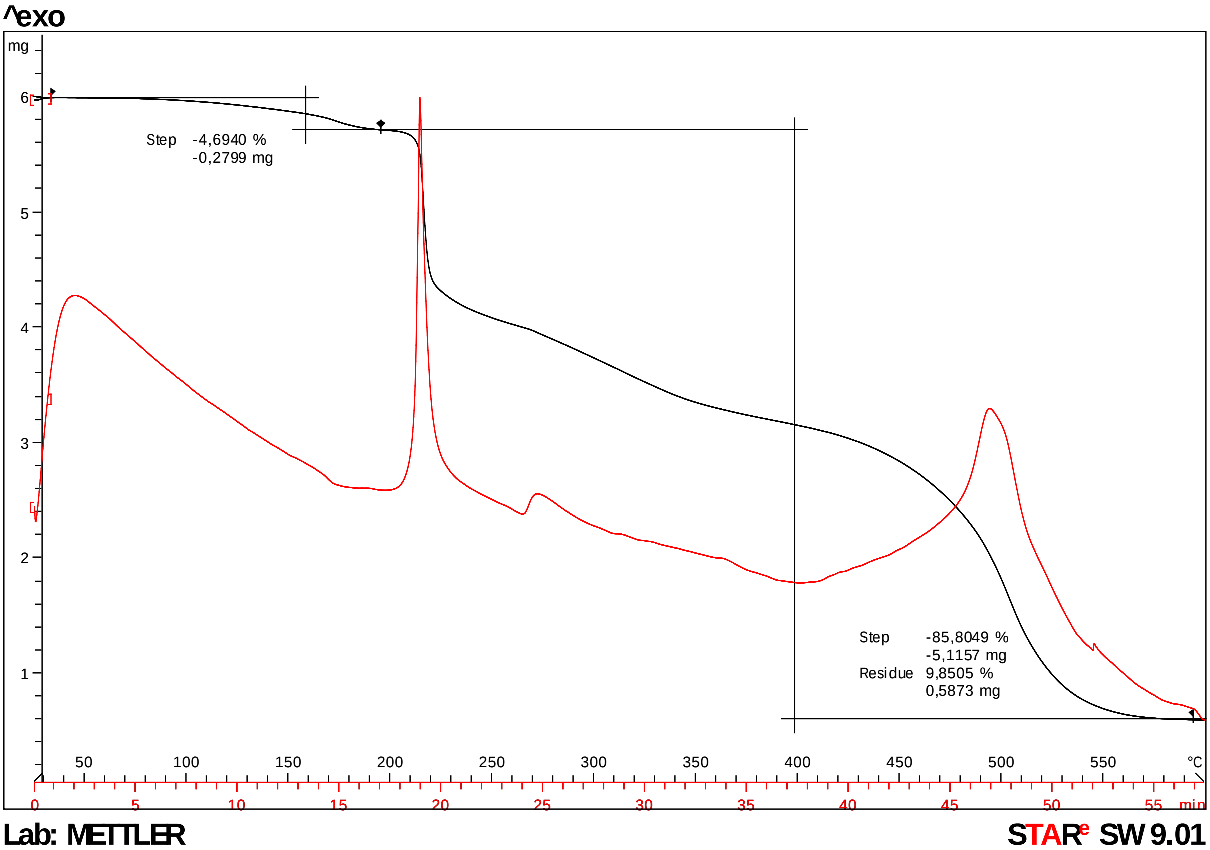
[Cu(*p*-FBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**7**) (N$_2$)



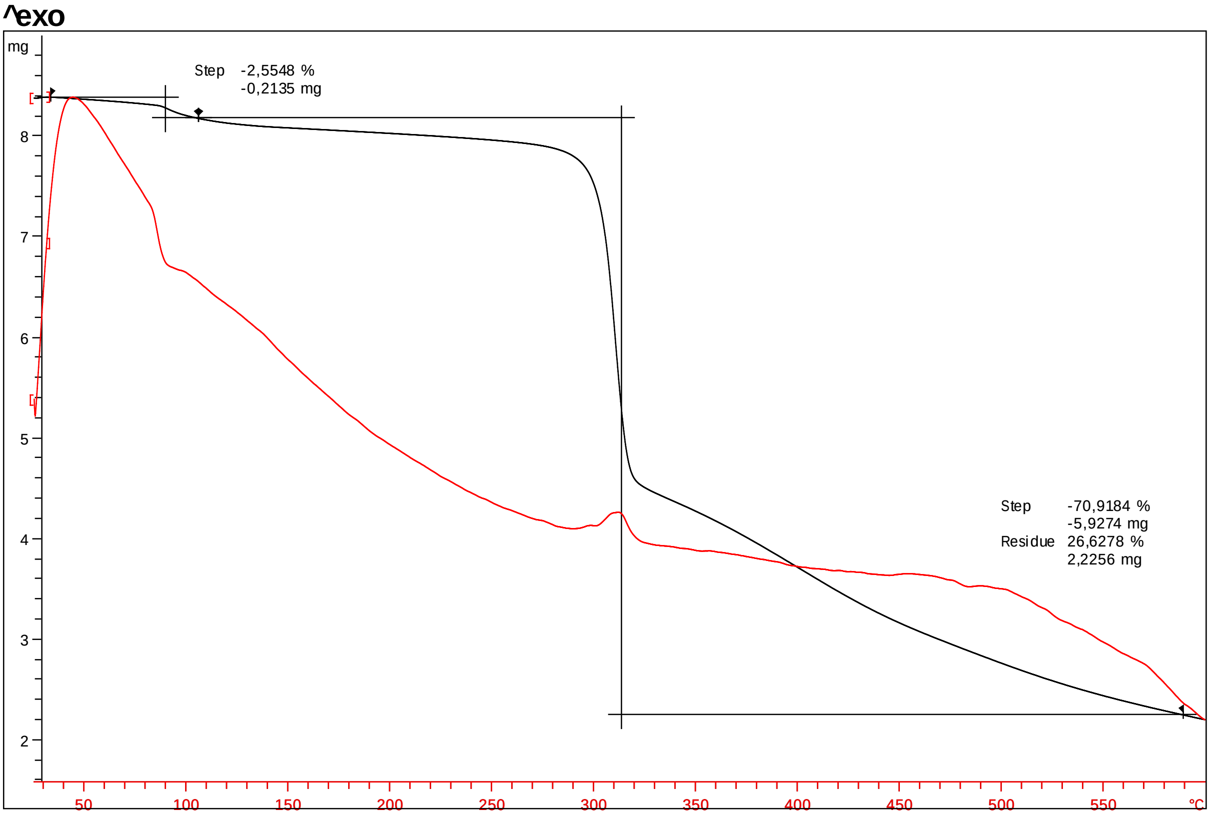
[Cu(*p*-FBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**7**) (O$_2$)



[Cu(p-BrBnimda)$_2$](NO_3)$_2$ · 2H_2O (**8**) (N_2)



[Cu(p-BrBnimda)$_2$](NO_3)$_2$ · 2H_2O (**8**) (O_2)



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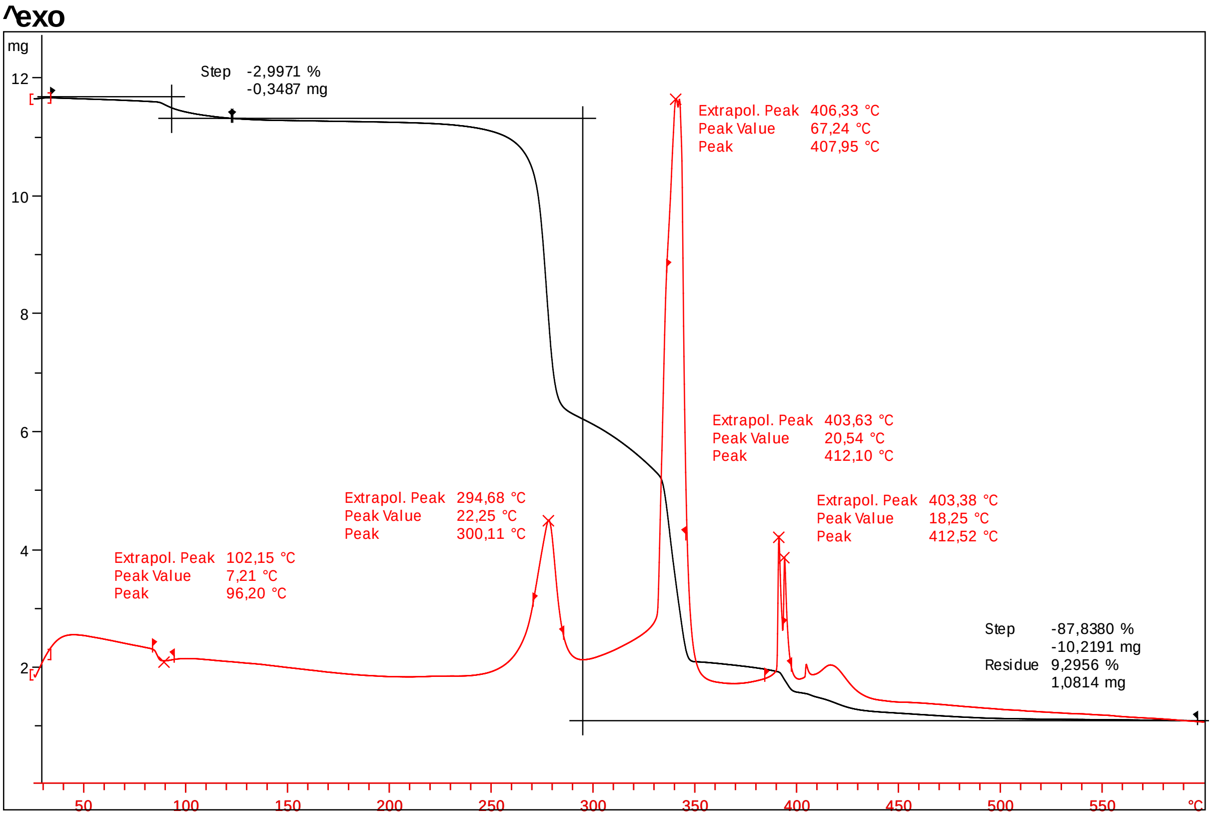
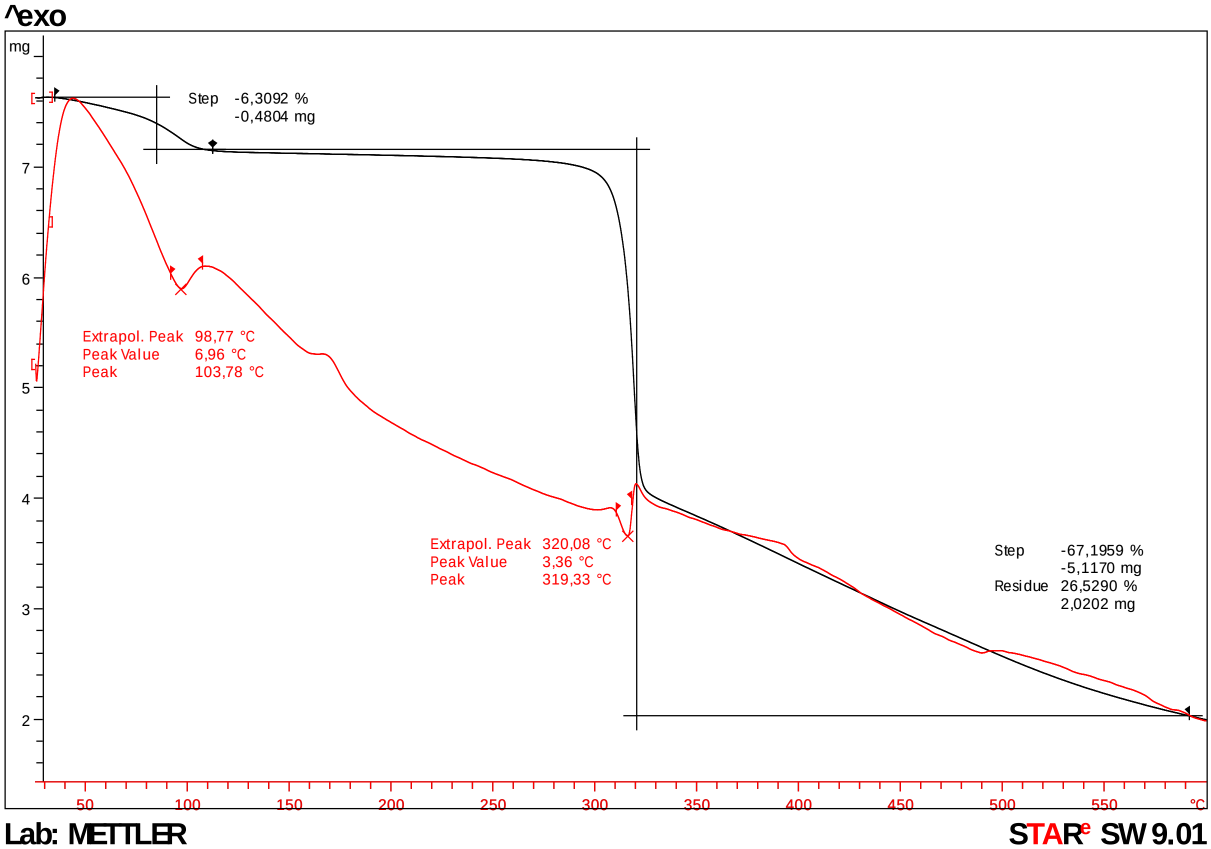
[Ni(o-CH_3Bnimda)$_2$]$(NO_3)_2 \cdot H_2O$ (**9**) (N_2)

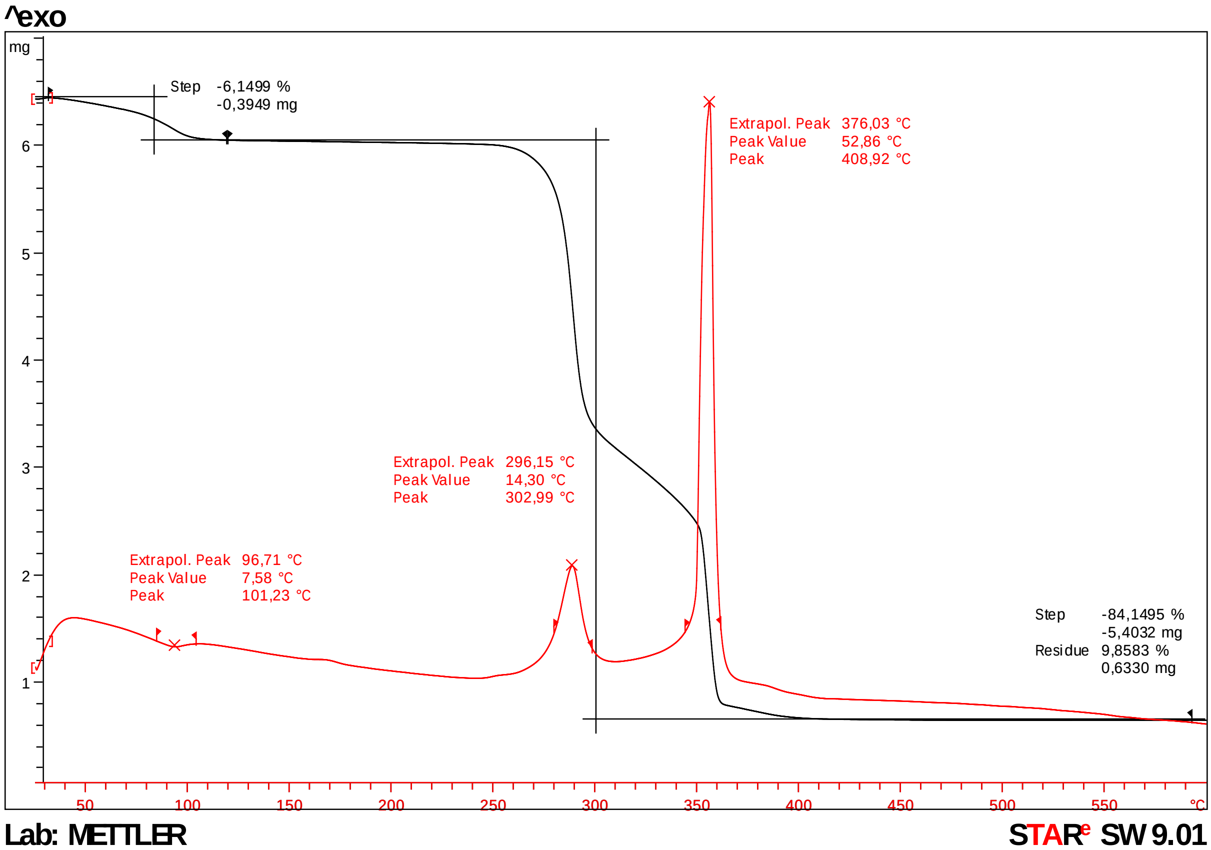


Lab: METTLER STAR^e SW 9.01

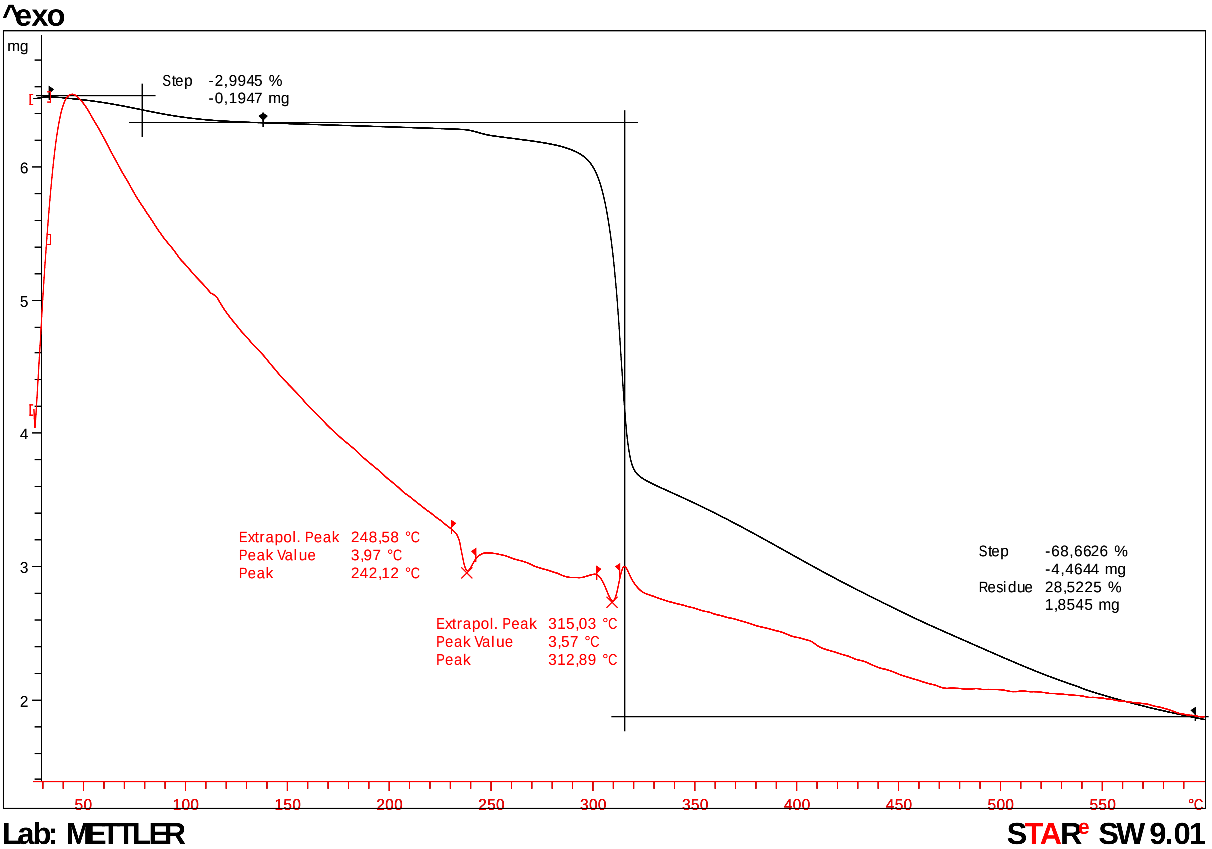
[Ni(o-CH_3Bnimda)$_2$]$(NO_3)_2 \cdot H_2O$ (O_2) (**9**) (O_2)



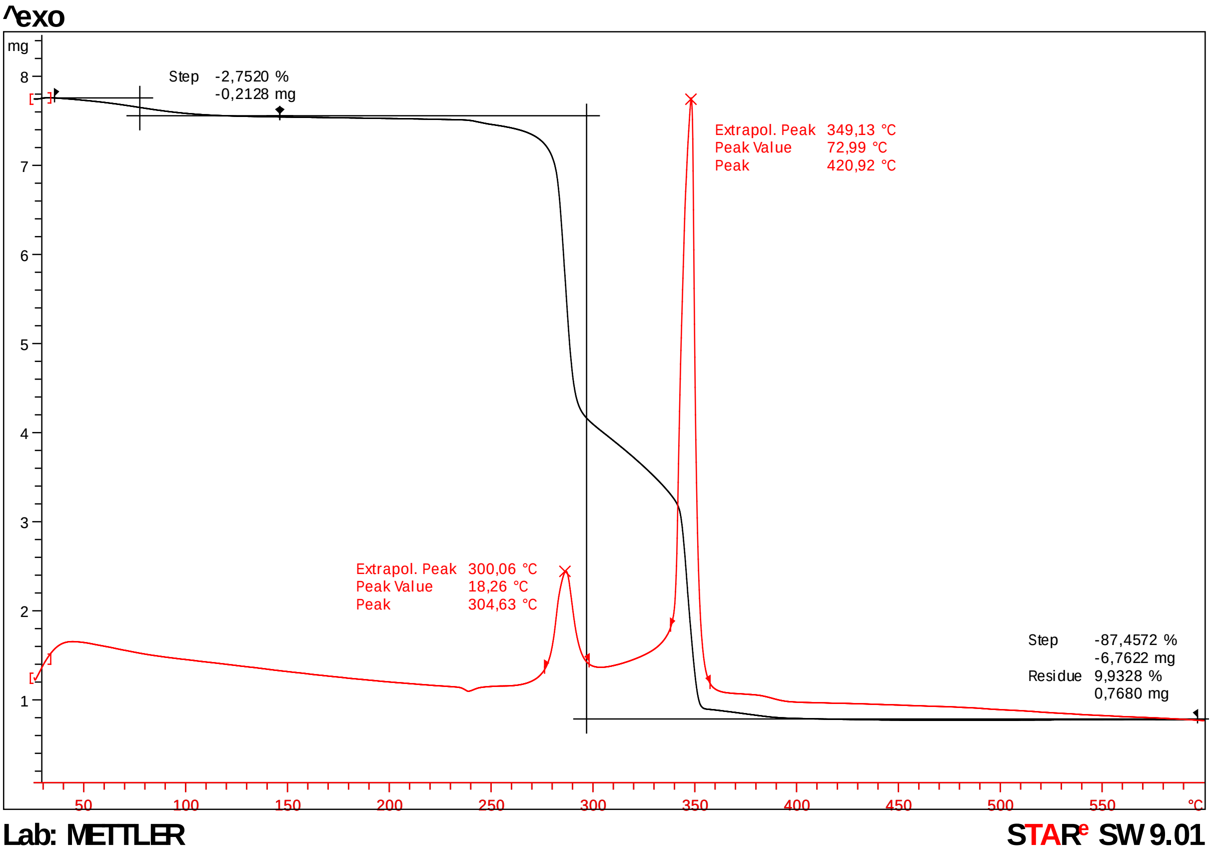
[Ni(*m*-CH$_3$Bnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**10**) (N$_2$)



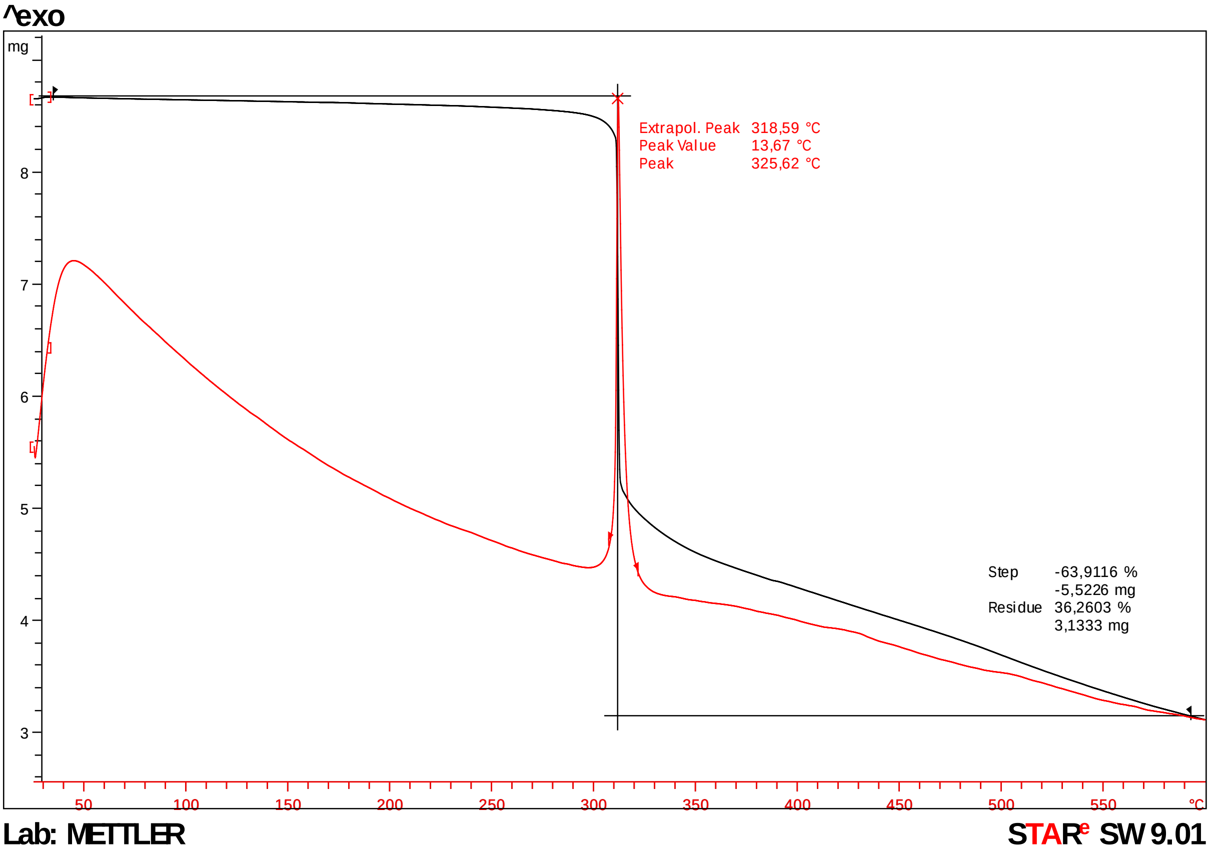
[Ni(*m*-CH$_3$Bnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**10**) (O$_2$)



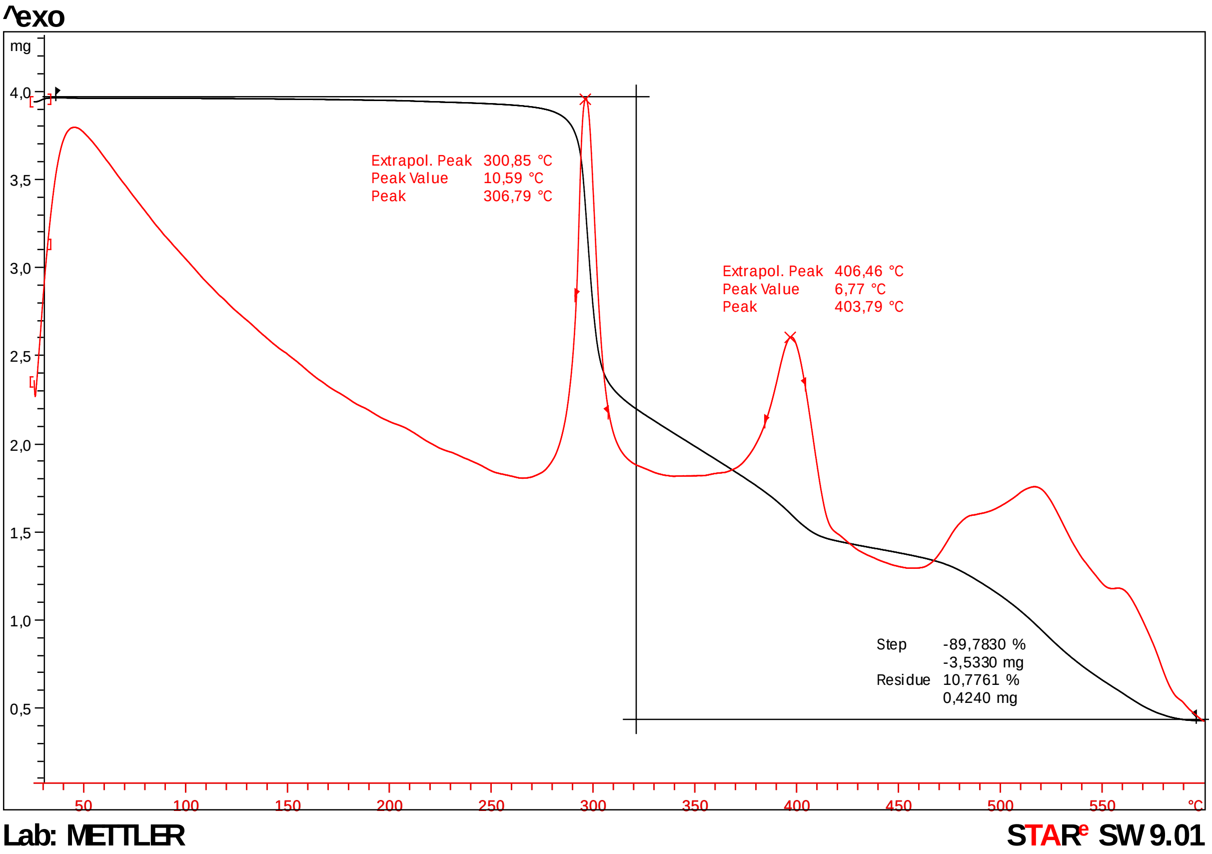
[Ni(*p*-CH_3Bnimda)$_2$](NO_3)$_2$ · H_2O (**11**) (N_2)



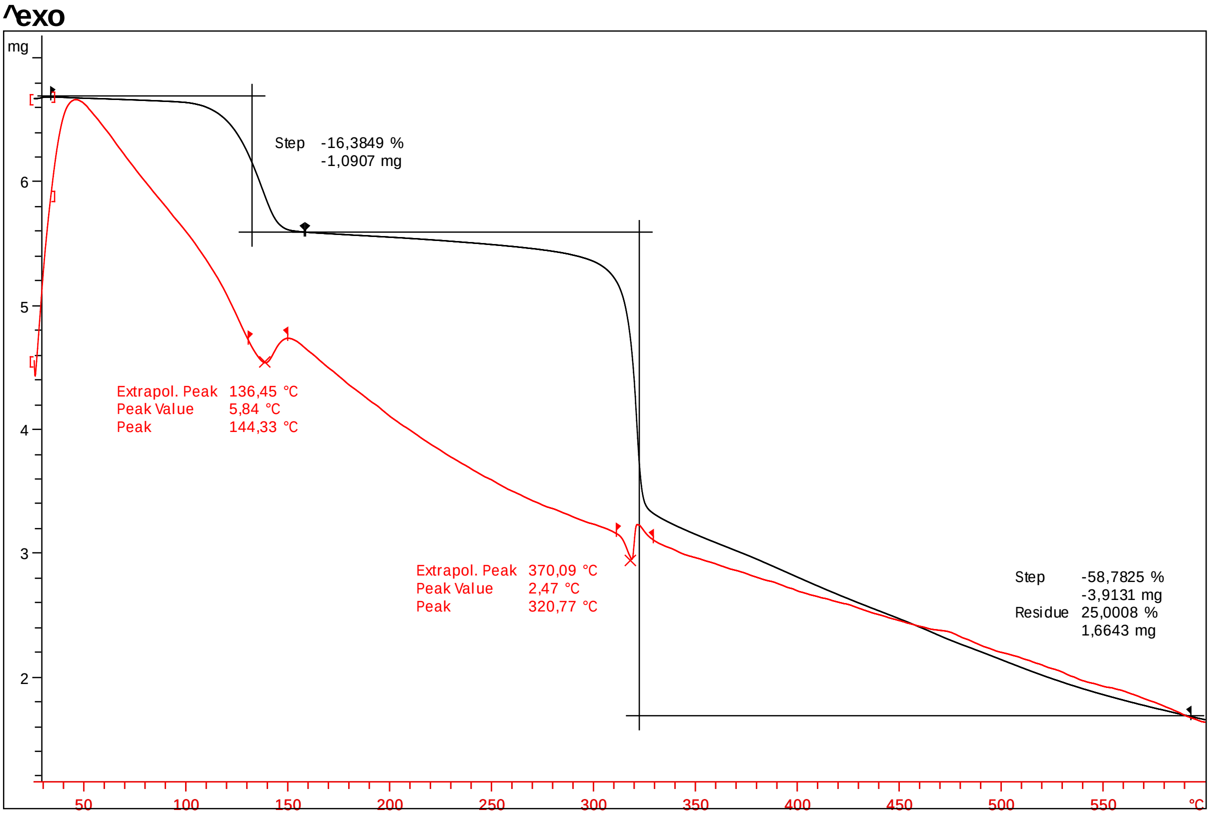
[Ni(*p*-CH_3Bnimda)$_2$](NO_3)$_2$ · H_2O (**11**) (O_2)



[Ni(*o*-ClBnimda)$_2$](NO$_3$)$_2$ (**12**) (N$_2$)

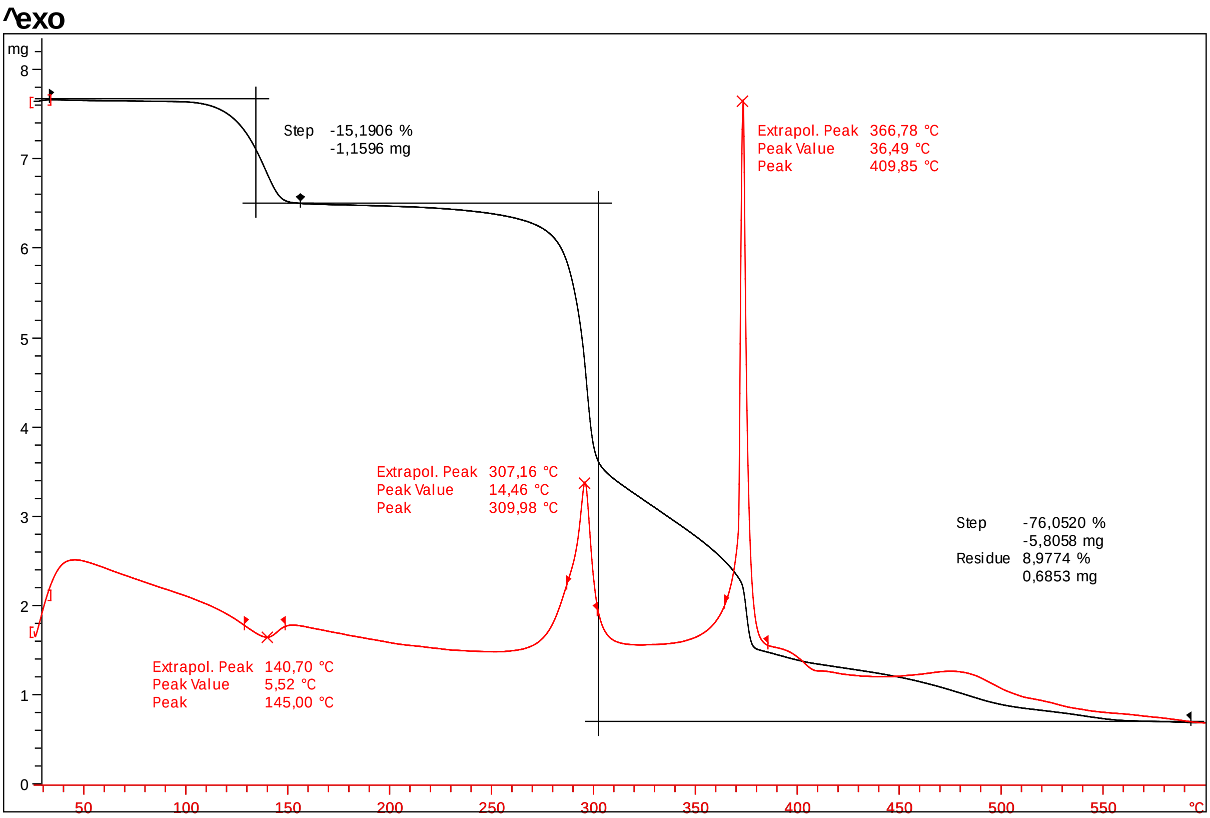


[Ni(*o*-ClBnimda)$_2$](NO$_3$)$_2$ (**12**) (O$_2$)



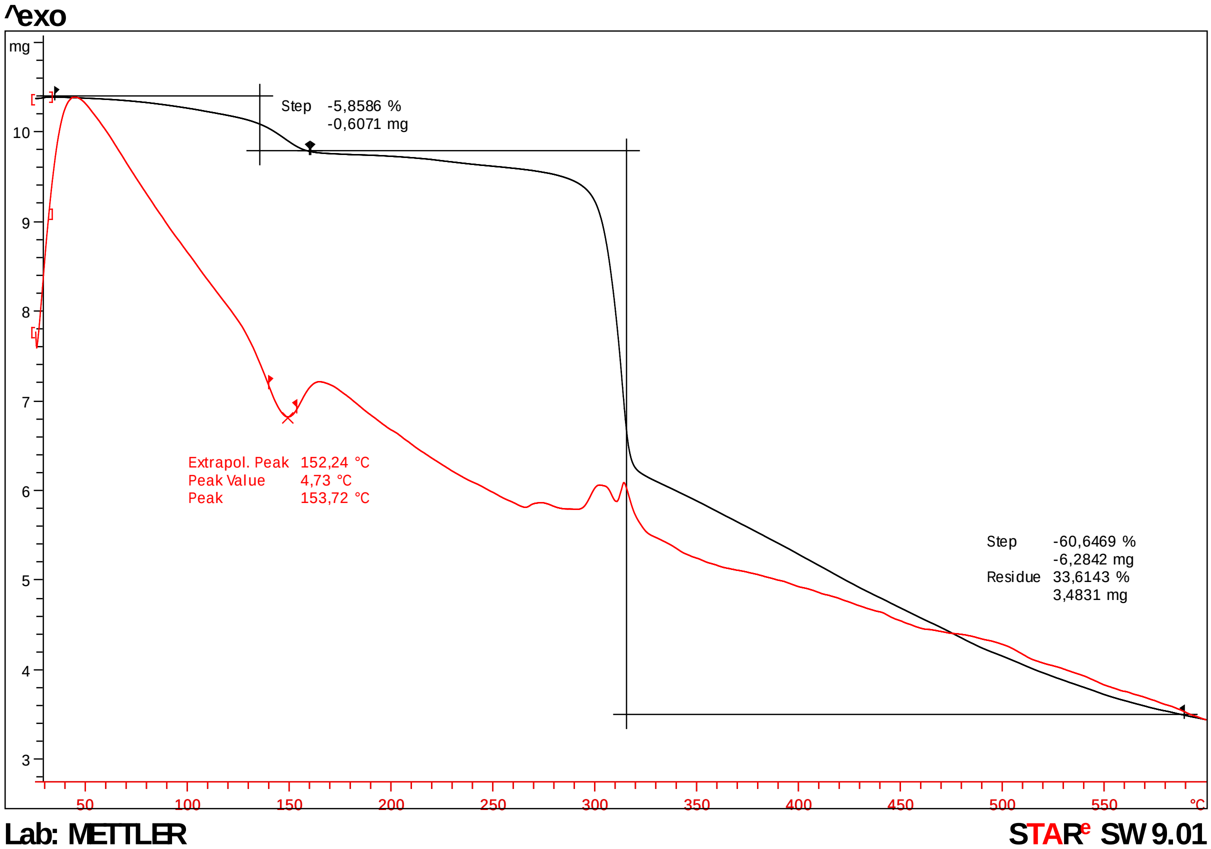
Lab: METTLER STAR^e SW 9.01

[Ni(m-ClBnimda)$_2$](NO$_3$)$_2$ · 2 DMF (**13**) (N$_2$)

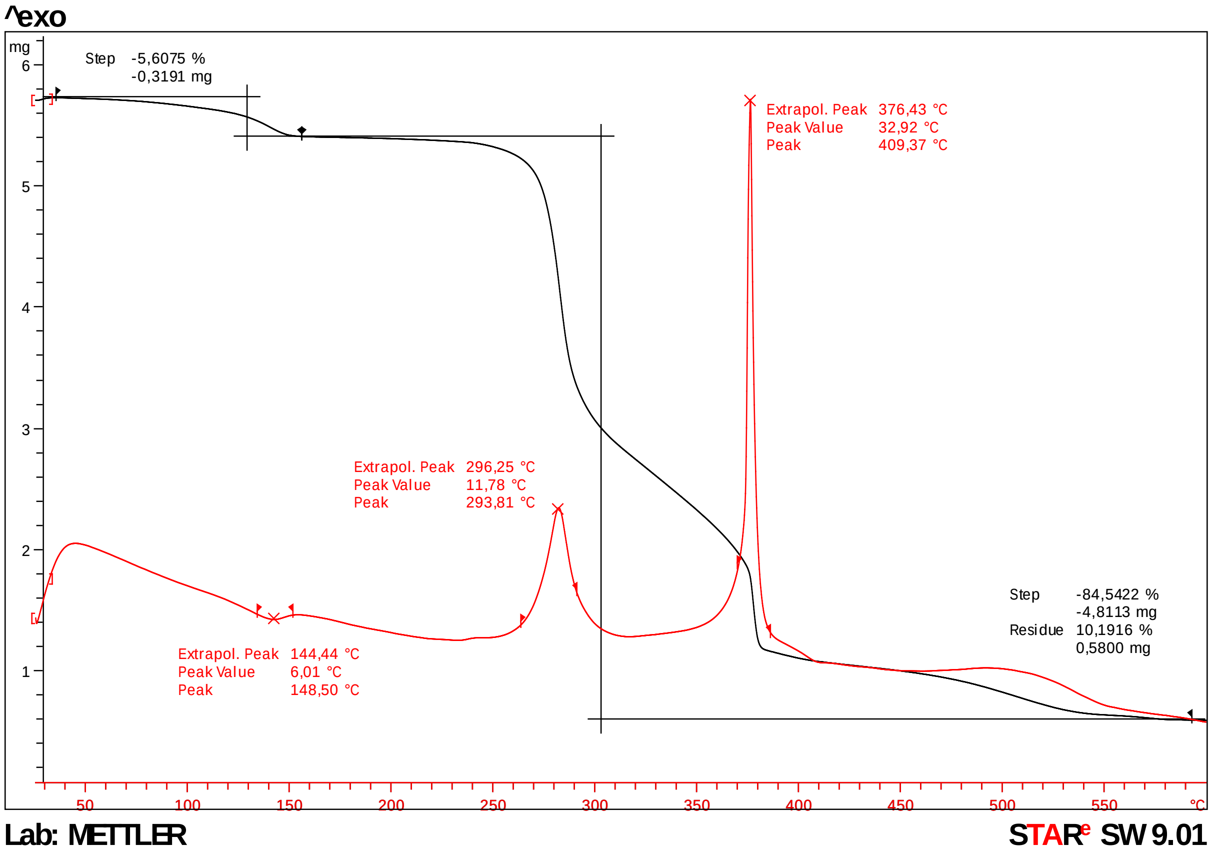


Lab: METTLER STAR^e SW 9.01

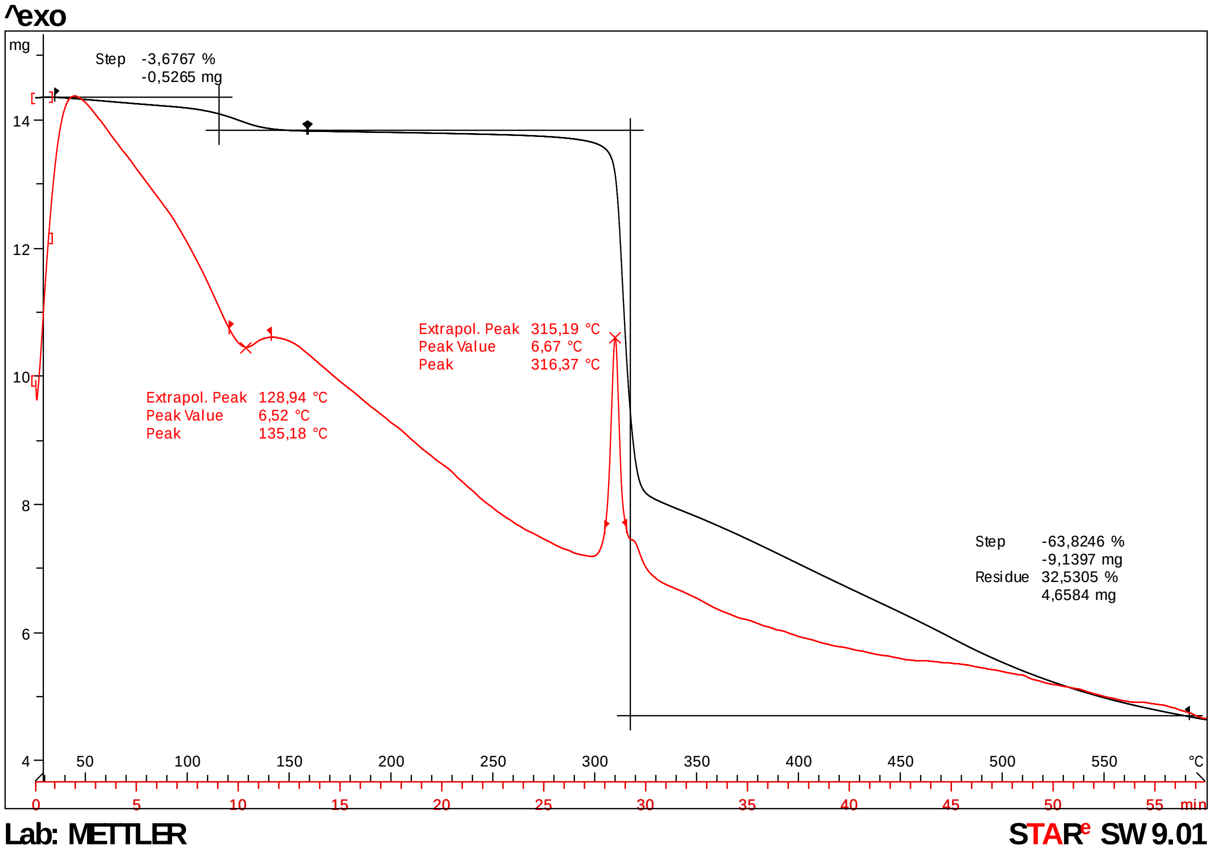
[Ni(m-ClBnimda)$_2$](NO$_3$)$_2$ · 2 DMF (**13**) (O$_2$)



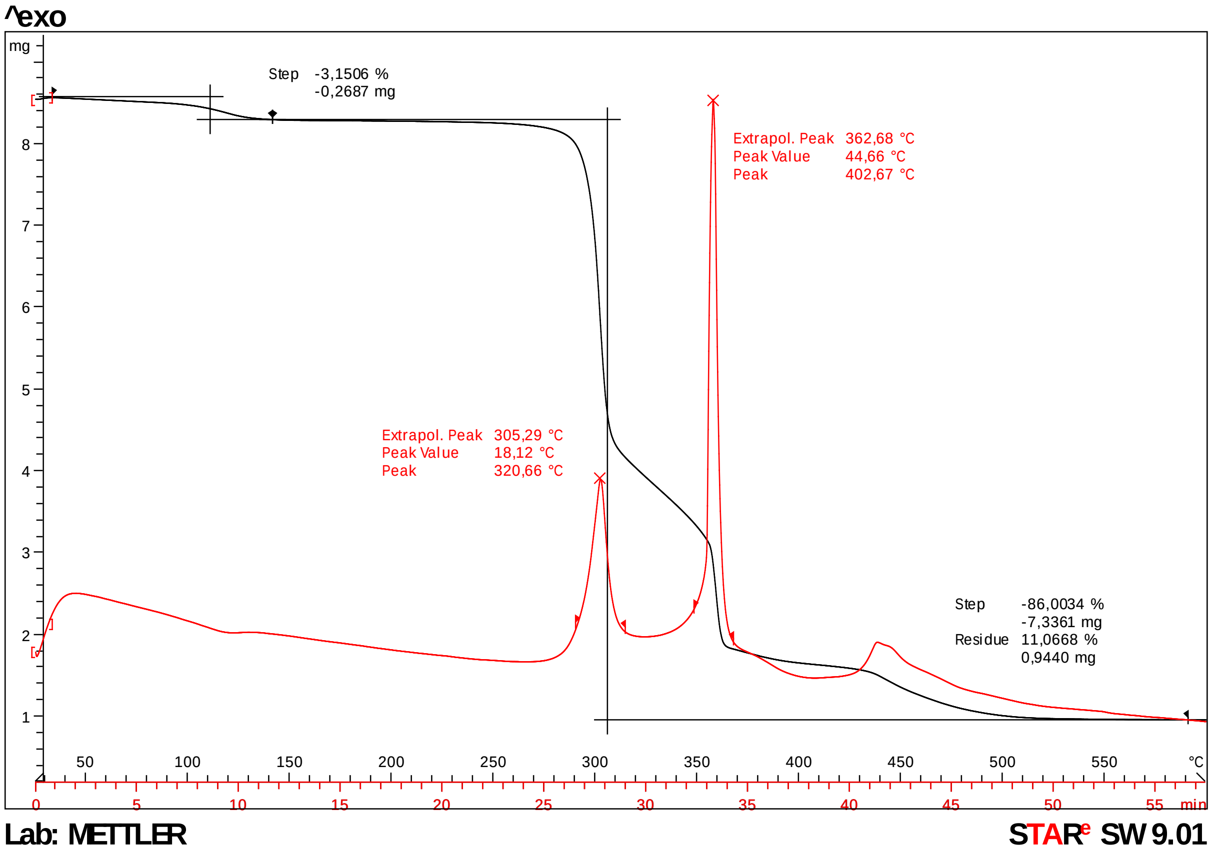
[Ni(*p*-ClBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**14**) (N$_2$)



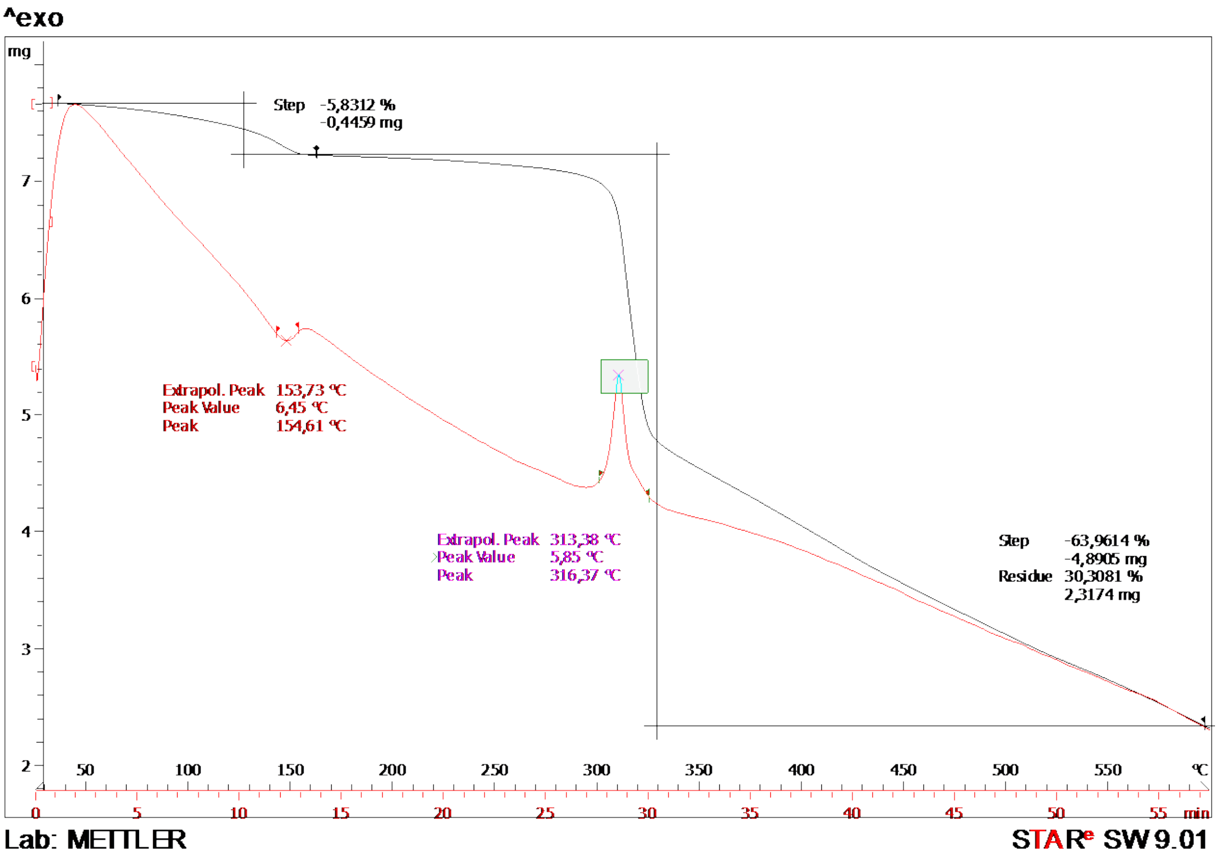
[Ni(*p*-ClBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**14**) (O$_2$)



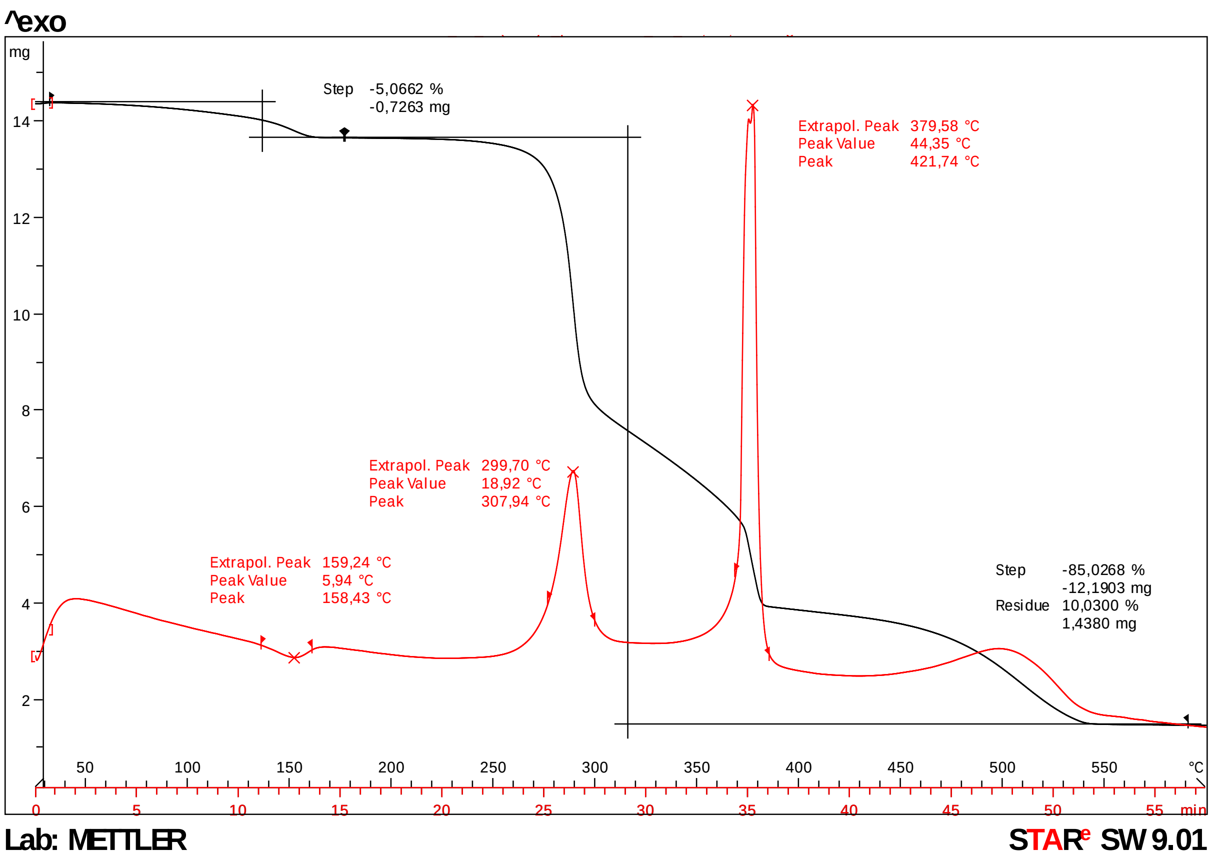
[Ni(*p*-FBnimda)$_2$](NO$_3$)$_2$ · H$_2$O (**15**) (N$_2$)



[Ni(*p*-FBnimda)$_2$](NO$_3$)$_2$ · H$_2$O (**15**) (O$_2$)



[Ni(*p*-BrBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**16**) (N$_2$)



[Ni(*p*-BrBnimda)$_2$](NO$_3$)$_2$ · 2H$_2$O (**16**) (O$_2$)