

Electronic Supplementary Information

N-(Chalcogen)phosphorylated (chalcogen)ureas of Zinc and Cadmium (II): SSPs for 12-16 thin films

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June -2014

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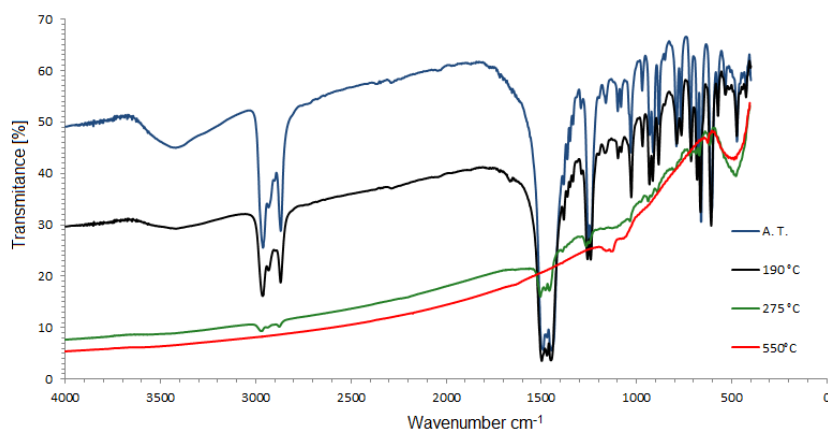


Fig. S1: FTIR spectra at different temperatures for thermolysis of **8**.

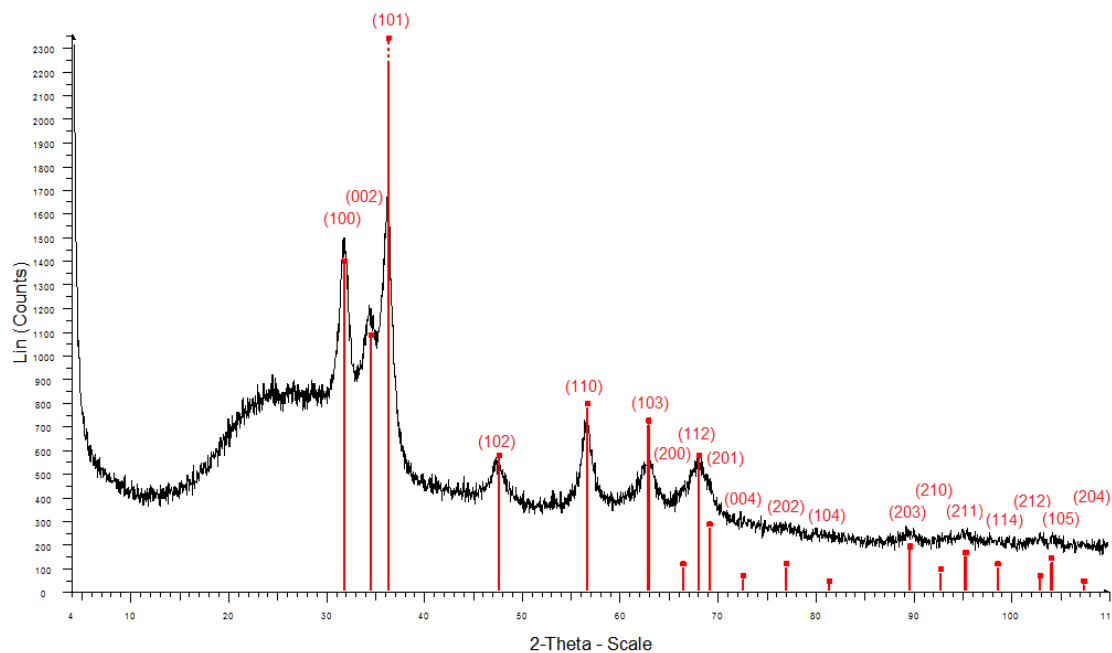


Fig. S2: XRPD pattern for deposit of the compound $\text{Zn}(\text{L}^{\text{S}},\text{O})_2$ (In Air)

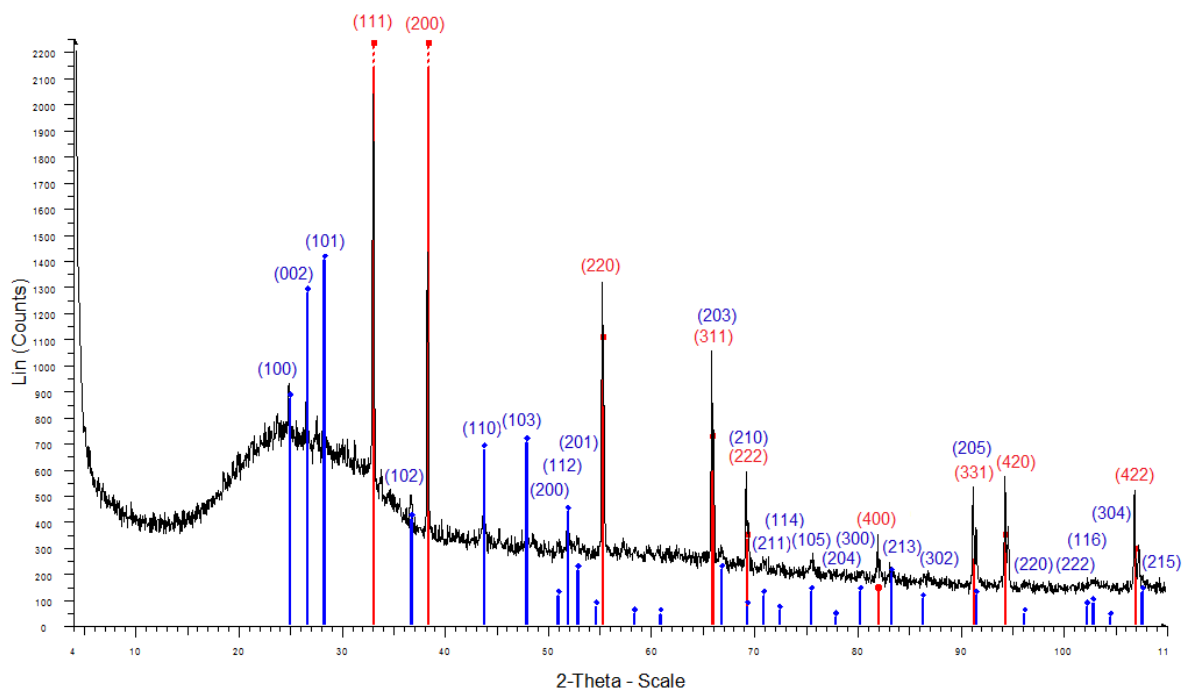


Fig. S3: XRPD pattern for deposit of the compound $\text{Cd}(\text{L}^{\text{S,O}})_2$ (in air)
 Red: cubic CdO, Blue: hexagonal CdS

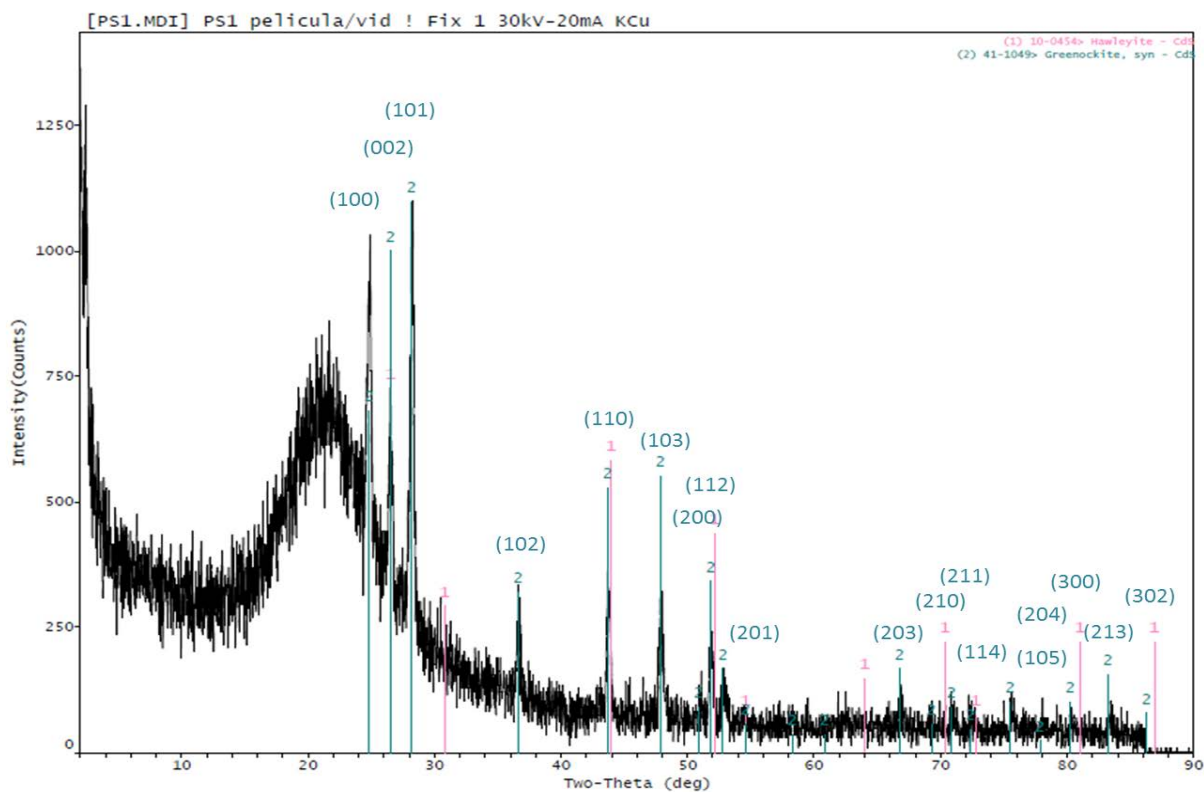
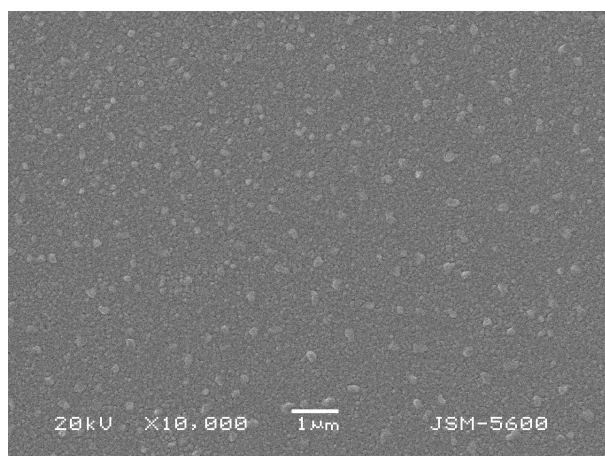
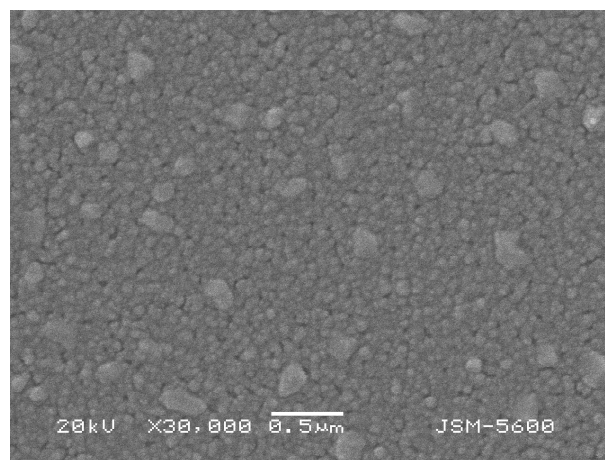


Fig. S4: GAXRD pattern for deposit of the compound $\text{Cd}(\text{L}^{\text{S,O}})_2$ (AACVD)
 hexagonal CdS



a)



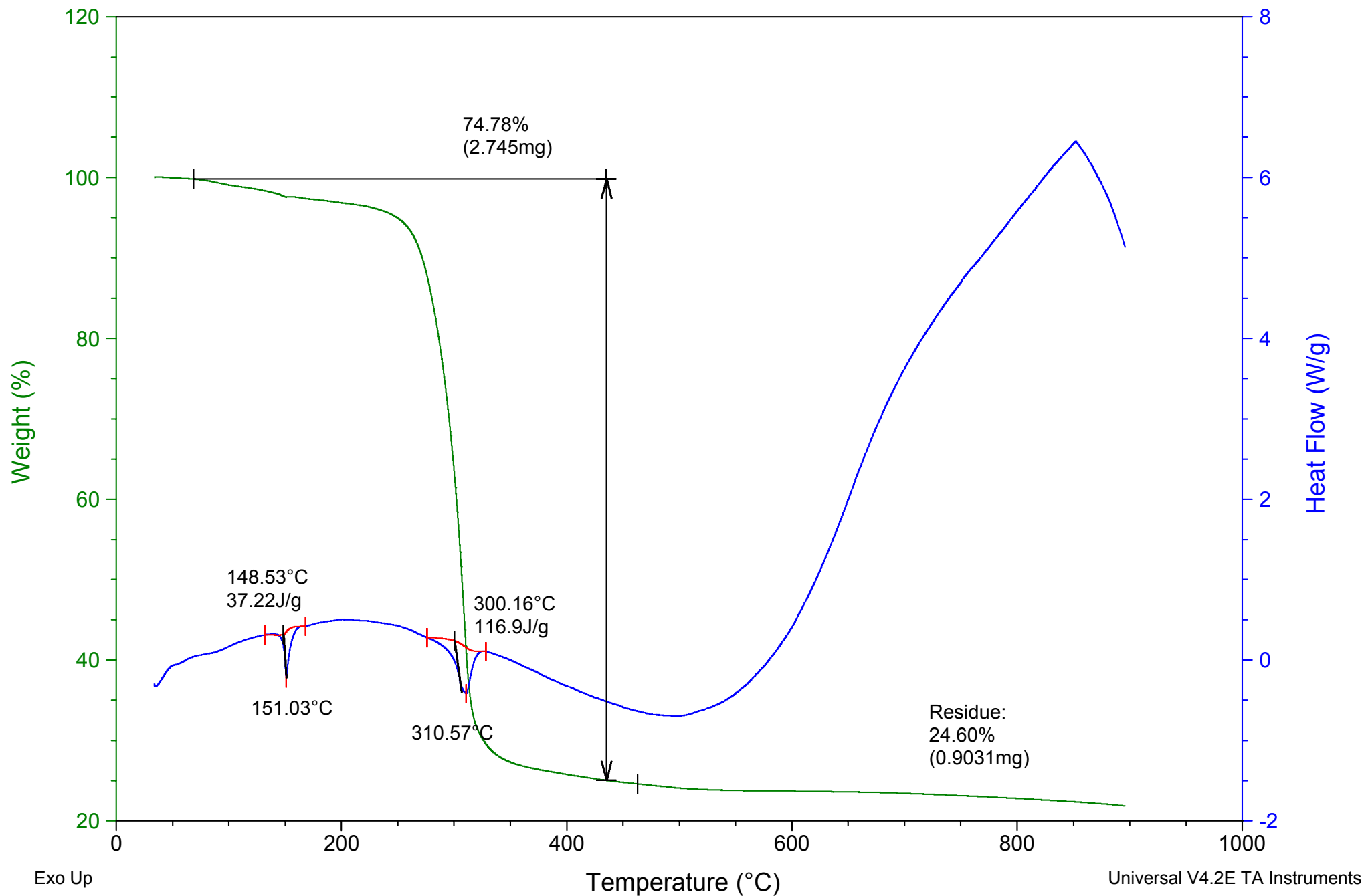
b)

Fig. S5: SEM images of the as-deposited thin film from **14** Cd(L^{O,S})₂ (AACVD).

Sample: Zn (SS) (7)
Size: 3.6710 mg
Method: DSC Heatflow

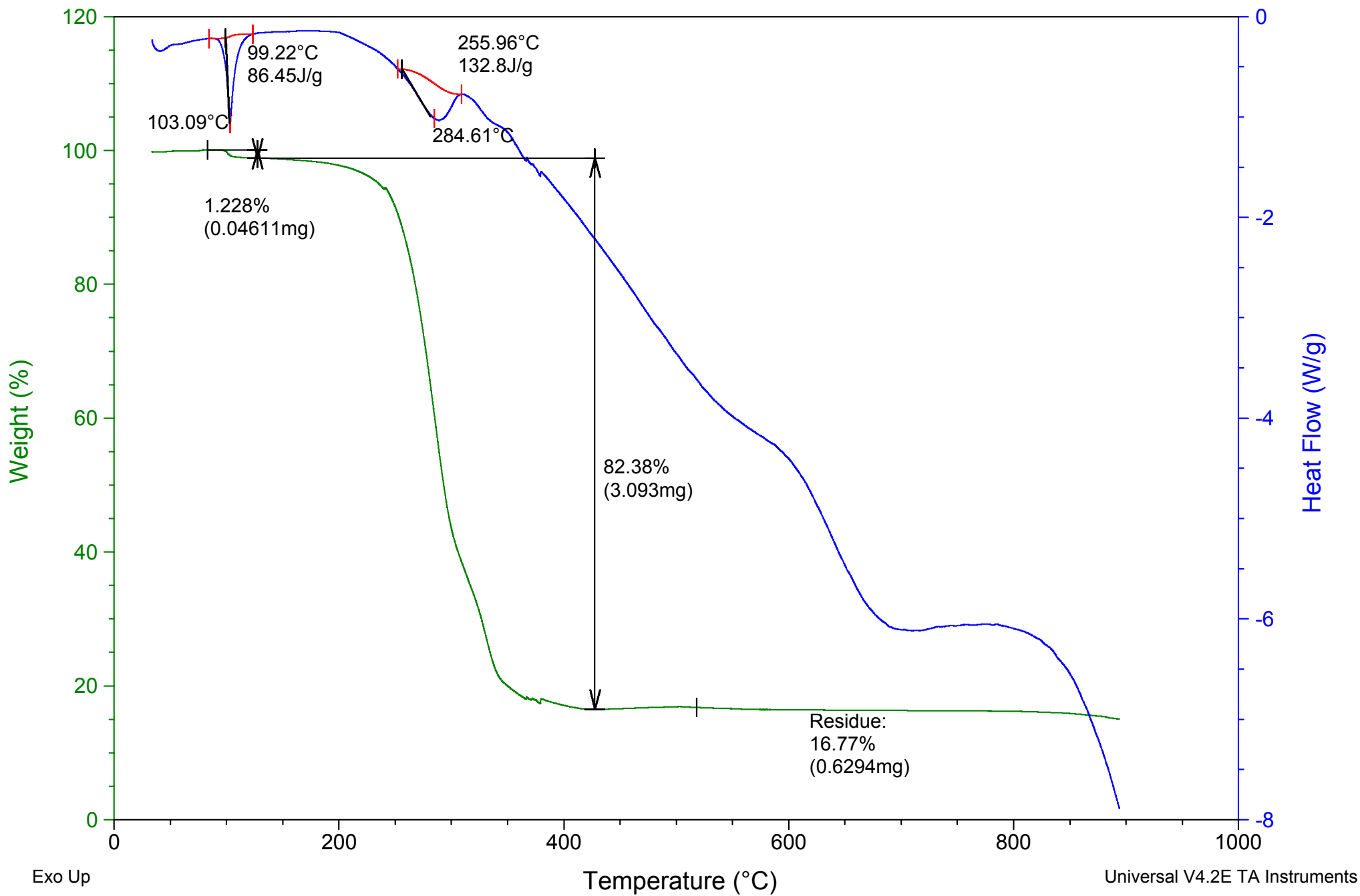
Fig. S6: TGA/DSC ANALYSES FOR COMPLEXES

DSC-TGA



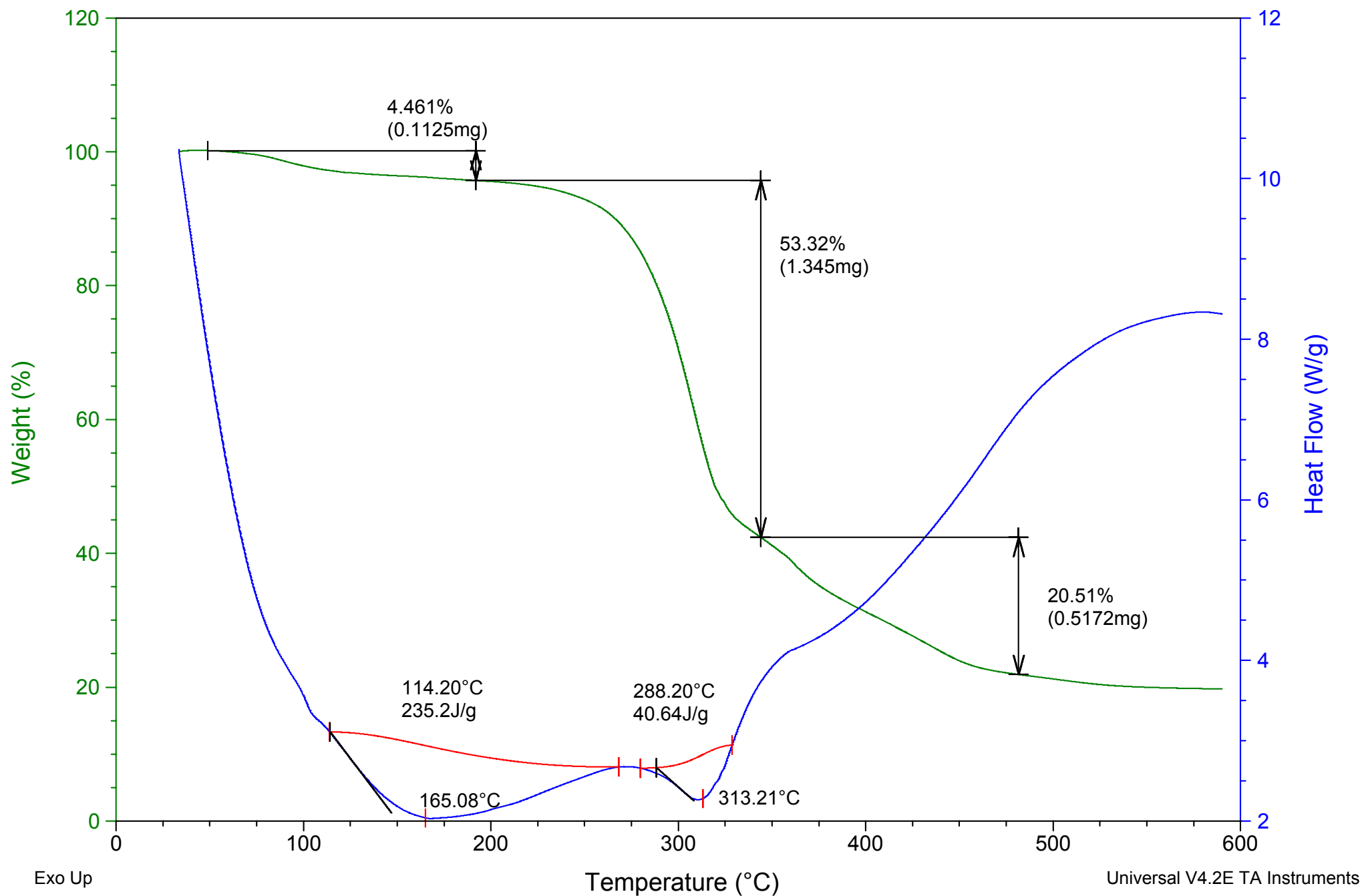
Sample: Zn (SO) (8)
Size: 3.7540 mg
Method: DSC Heatflow

DSC-TGA



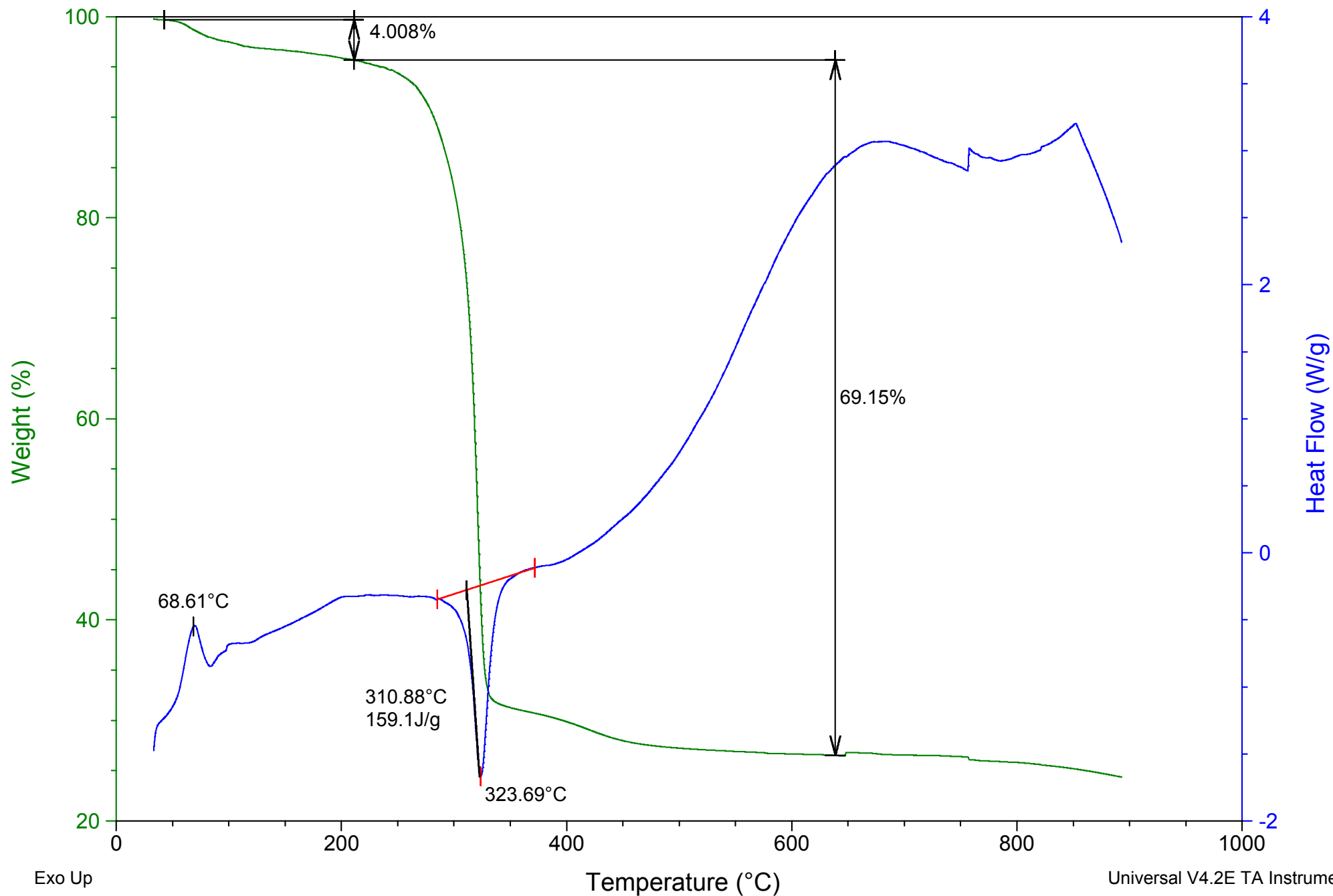
Sample: ZnOS (9)
Size: 2.5220 mg

DSC-TGA



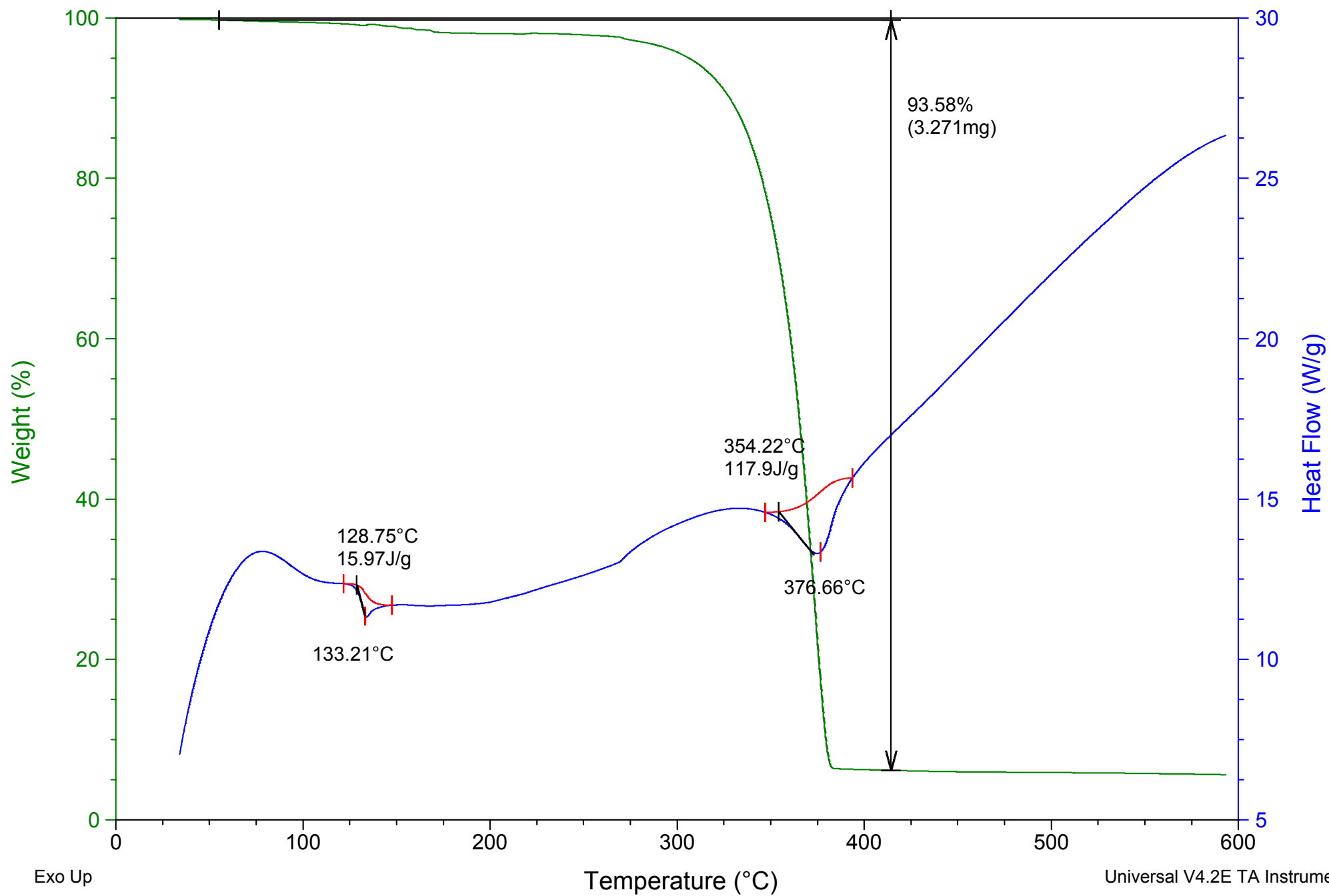
Sample: ZnSeS (**10**)
Size: 3.7250 mg
Method: DSC Heatflow
Comment: ZnSeS

⁸
DSC-TGA



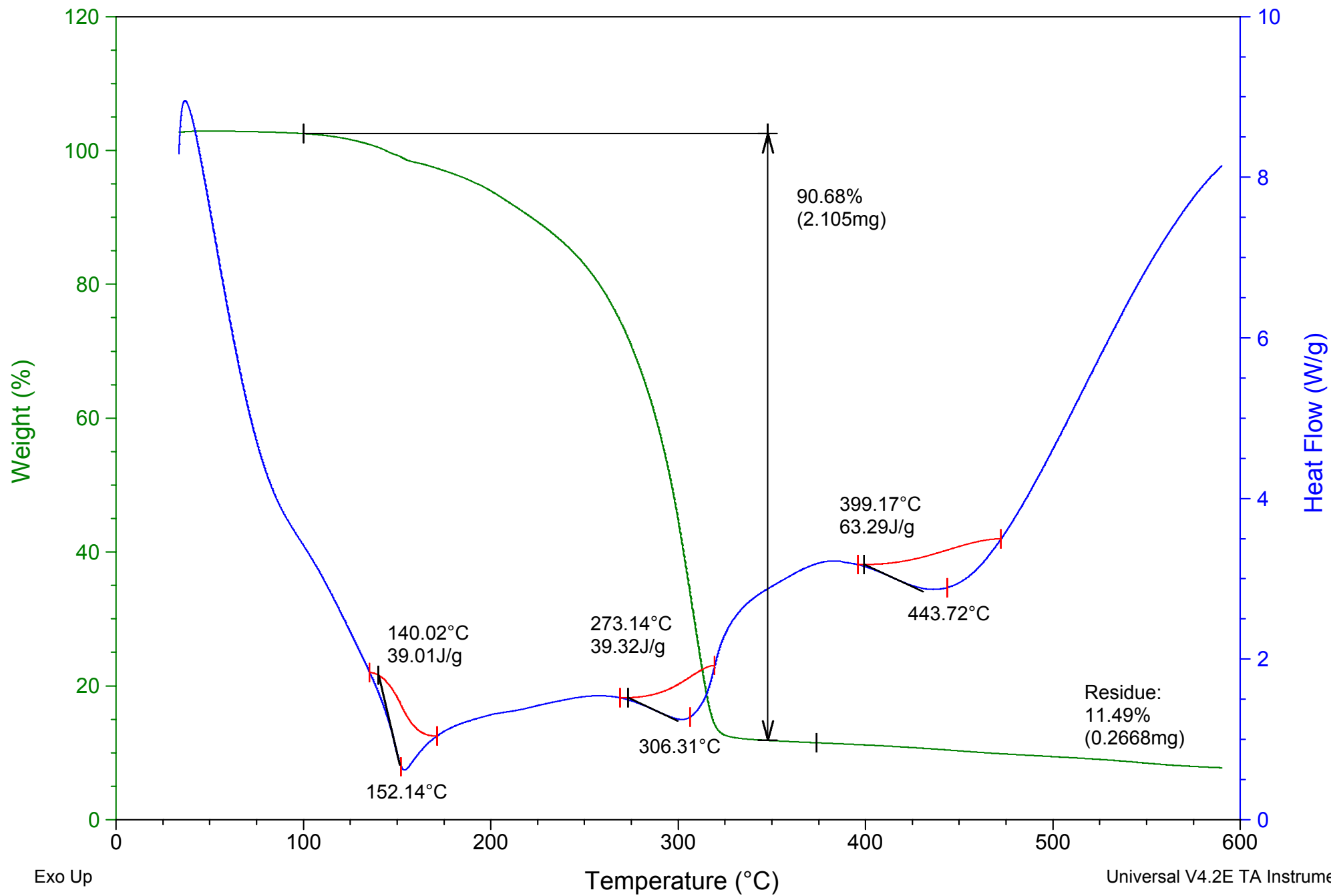
Sample: CdSS (12)
Size: 3.4950 mg

⁹
DSC-TGA



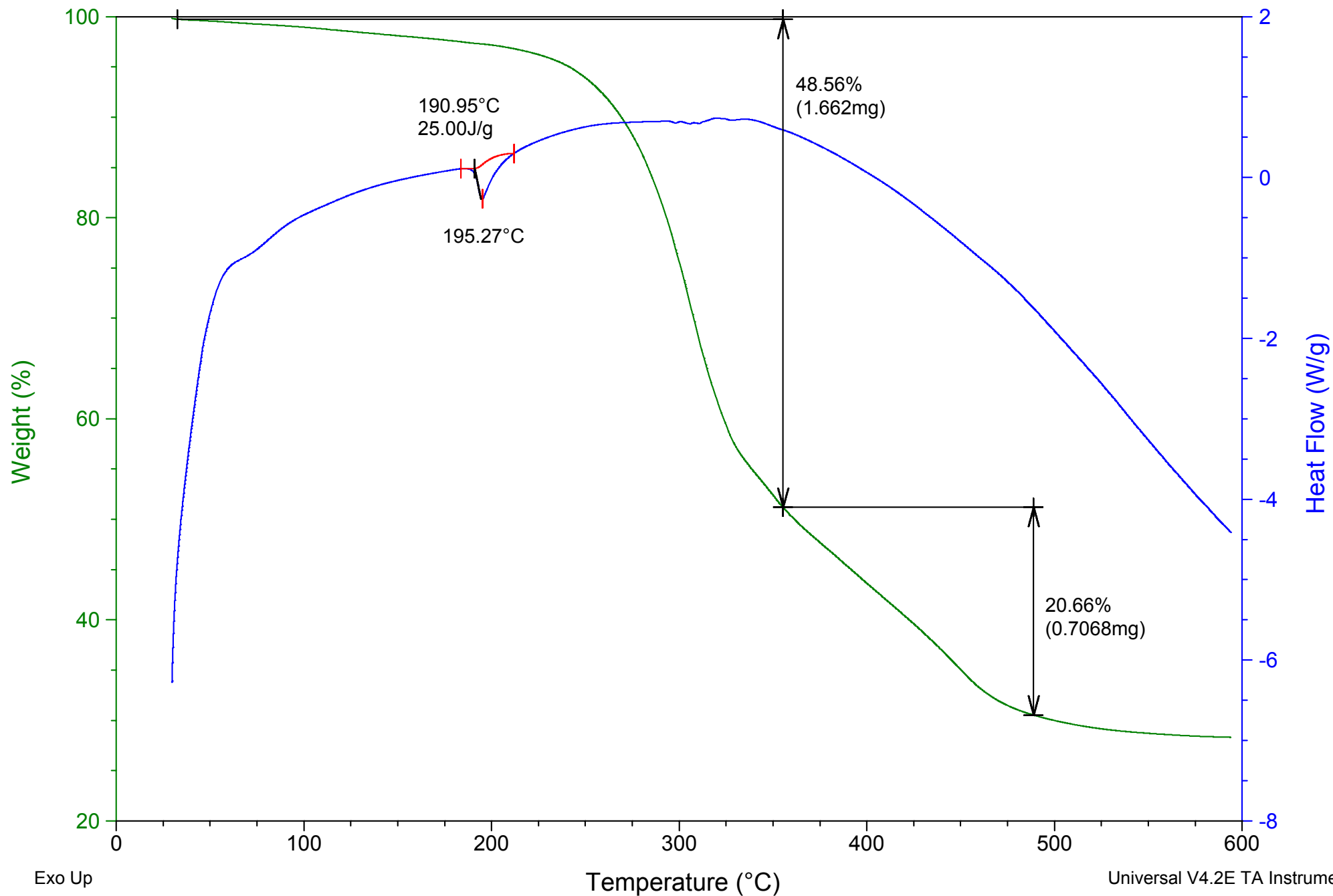
Sample: CdSO (13)
Size: 2.3210 mg

¹⁰
DSC-TGA



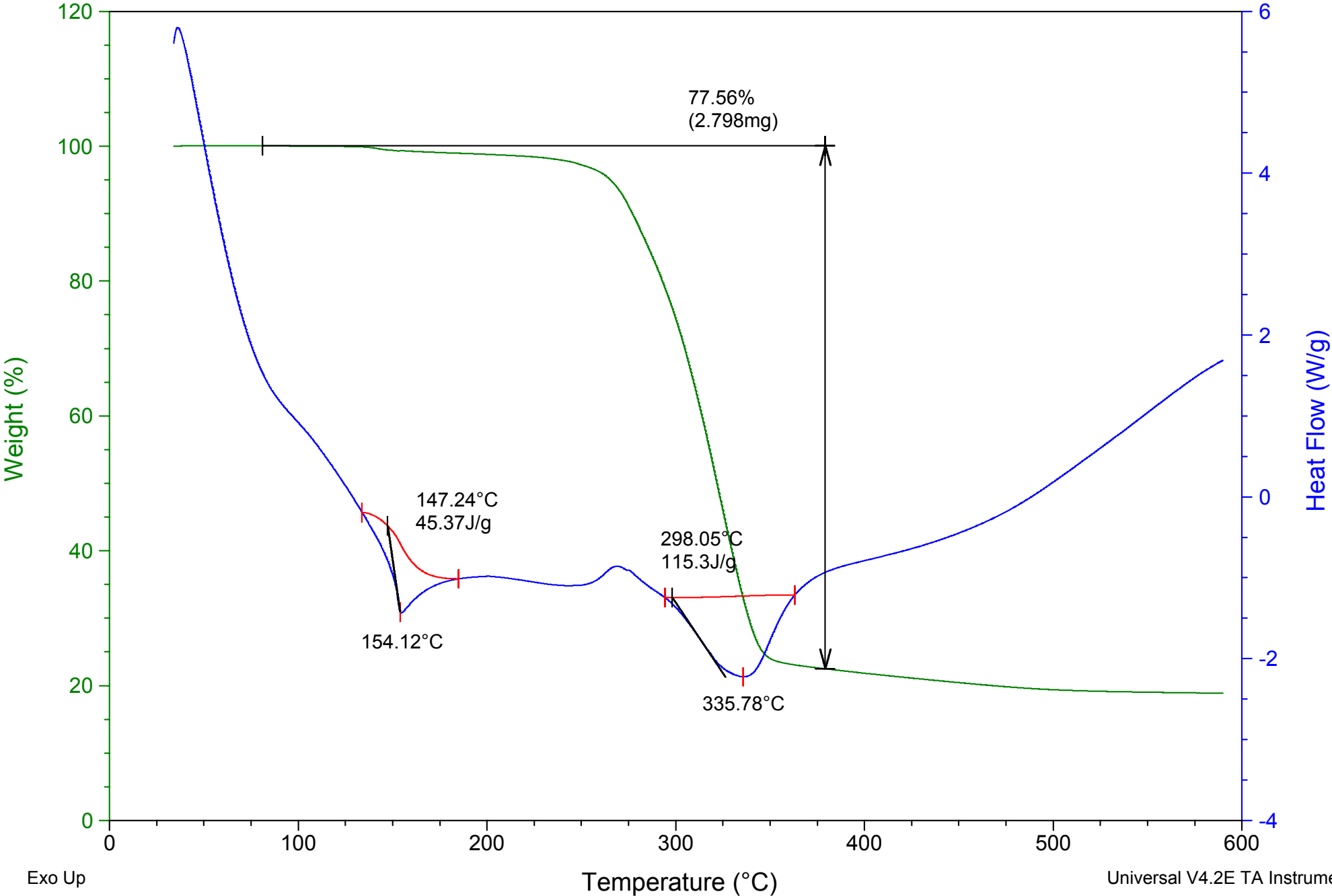
Sample: CdOs (**14**)
Size: 3.4220 mg
Method: DSC Heatflow
Comment: CdOs

¹¹
DSC-TGA



Sample: CdSSe (15)
Size: 3.6070 mg

¹²
DSC-TGA



Sample: CdSeS (16)
Size: 2.4710 mg

¹³
DSC-TGA

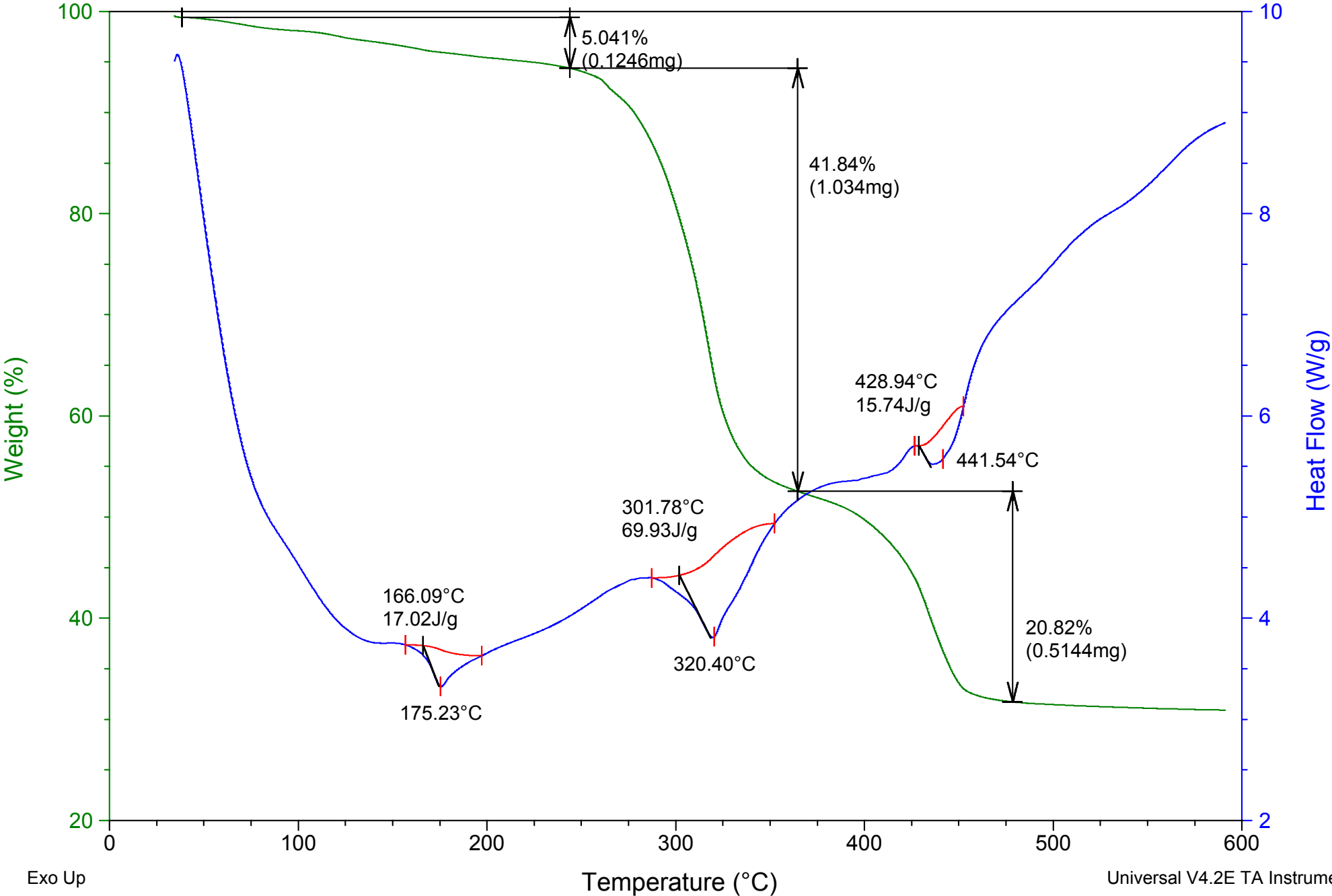


TABLE S1

Compound	1	7	8	11	15
Formula	C ₁₁ H ₂₃ N ₂ PS ₂	C ₂₂ H ₄₄ N ₄ P ₂ S ₄ Zn	C ₂₂ H ₄₄ N ₄ O ₂ P ₂ S ₂ Zn	C ₃₆ H ₄₀ N ₄ P ₂ S ₄ Zn	C ₂₂ H ₄₄ N ₄ P ₂ S ₂ Se ₂ Cd
M [g/mol]	278.40	620.16	588.04	782.09	760.99
Crystal size (mm)	0.36 x 0.23 x 0.22	0.27 x 0.21 x 0.16	0.32 x 0.23 x 0.16	0.24 x 0.14 x 0.12	0.37 x 0.28 x 0.13
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P</i> 21/n	P21/c	P-1	P-1	P-1
ρ_{calc} (g cm⁻³)	1.226	1.324	1.379	1.336	1.599
Z	4	4	2	2	2
<i>a</i> (Å)	11.2004(12)	15.324(3)	10.3217(19)	10.5894(14)	9.689(3)
<i>b</i> (Å)	11.8057(13)	15.069(3)	11.081(2)	13.7850(19)	10.542(3)
<i>c</i> (Å)	11.9727(13)	13.756(3)	13.944(3)	16.051(2)	16.813(5)
α (°)	90.00	90.00	79.689(3).	64.633(2)	102.528(5)
β (°)	107.720(2)	101.624(4)	86.905(3).	73.929(2)	102.781(5)
γ (°)	90.00	90.00	64.540(3)	68.548(2)	101.233(5)
<i>V</i> (Å³)	1508.0(3)	3111.4(11)	1416.2(5)	1950.3(4)	1580.8(8)
μ (mm⁻¹)	0.439	1.179	1.153	0.956	3.244
<i>F</i>(000)	600	1312	624	816	764
Reflections Collected	12173	42582	16515	16255	15385
Unique reflections <i>R</i>_{int}	2766; 0.0349	5483, 0.1954	4463, 0.0381	7111; 0.0352	5562 ,0.0410
<i>R</i>1, w<i>R</i>2 [<i>I</i>>2σ(<i>I</i>)]	0.0373; 0.1032	0.0459; 0.0945	0.0413, 0.1076	0.0365; 0.0694	0.0384, 0.0804
<i>R</i>1, w<i>R</i>2 (all data)	0.0427; 0.1063	0.0704; 0.0968	0.0441, 0.1092	0.0614; 0.0741	0.0550, 0.0920

Correction Methodd	-----	PSI-SCAN	MULTI-SCAN	ANALYTICAL	MULTI-SCAN
GooF	1.000	0.988	1.076	0.841	0.995