Electronic Supplementary Information (ESI)

Acylselenoureato bis(chelates) of lead: Synthesis, Structural characterisation and Microwave-assisted formation of PbSe nano and microstructures

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Content:

Section SI. Thermal analysis

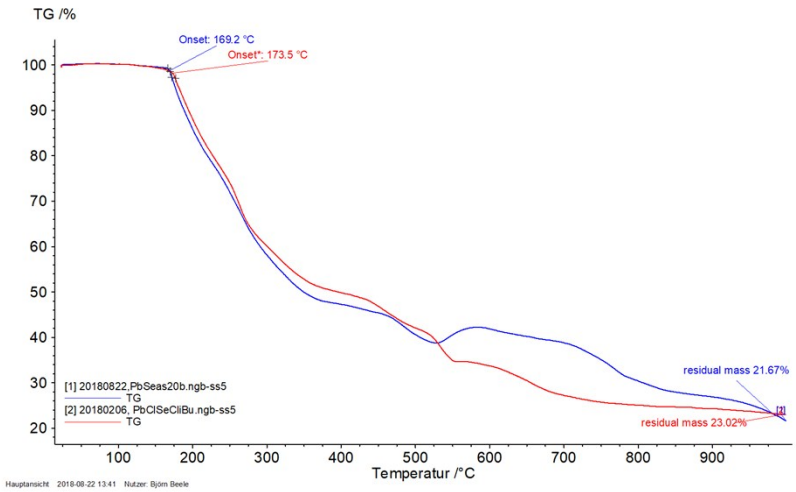

Fig. S1 TGA curves of complexes **1a** (blue) and **3a** (red).

Section SII. Supplementary information on the particle characterization

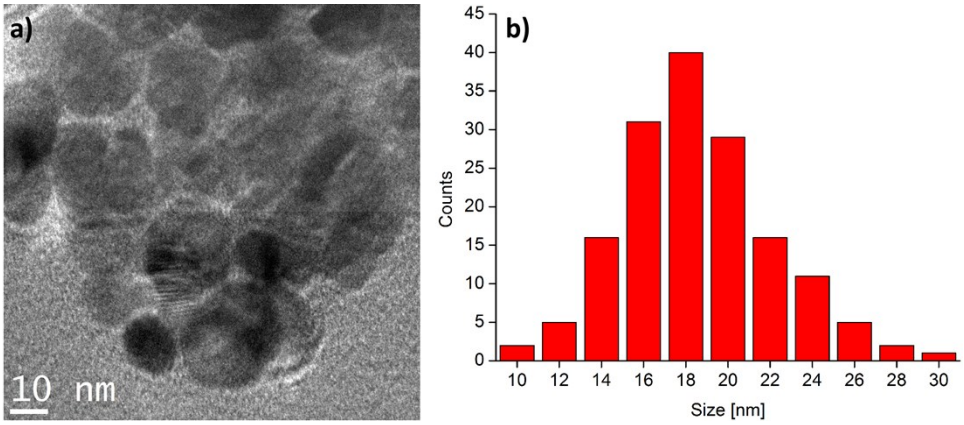

Fig. S2 (a) HR-TEM image and (b) particle-size distribution of the PbSe nanoparticles obtained from the microwave-assisted decomposition of **3a** in a mixture of ODC, TOP and [BMIm][NTf_2], giving an average particle size of 19 + 4 nm.

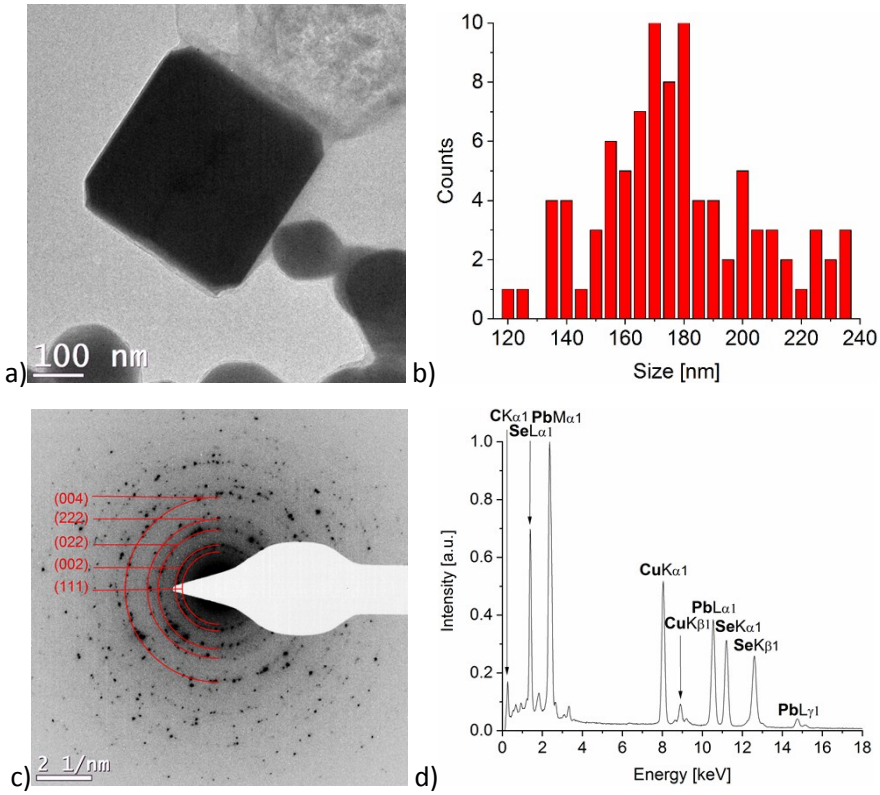

Fig. S3 Additional information on the PbSe particles obtained from the microwave-assisted decomposition of **3a** in [BMIm][NTf_2] at 180 °C: (a) Detailed image of a separated particle with an edge length of 267 nm, (b) particle-size distribution, giving an average diameter of 178 ± 90 nm, (c) SAED and (d) EDX-analysis.

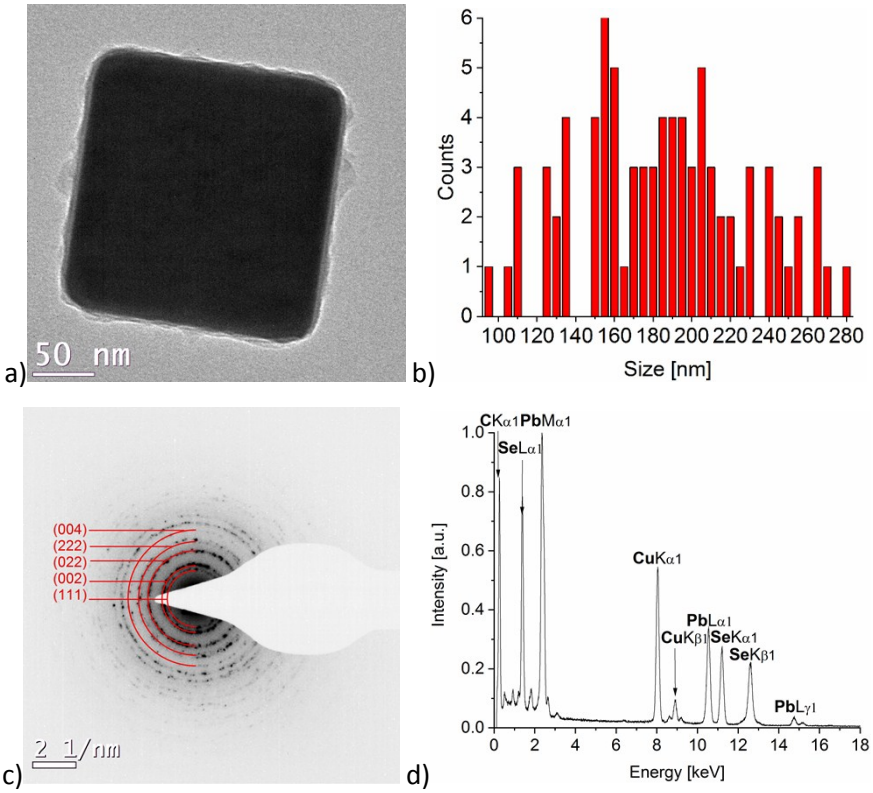

Fig. S4 Additional information on the PbSe particles obtained from the microwave-assisted decomposition of **3a** in [BMIm][NTf_2] at 200 °C: (a) Detailed image of a separated particle with an edge length of 213 nm, (b) particle-size distribution, giving an average diameter of 186 ± 116 nm, (c) SAED and (d) EDX-analysis.

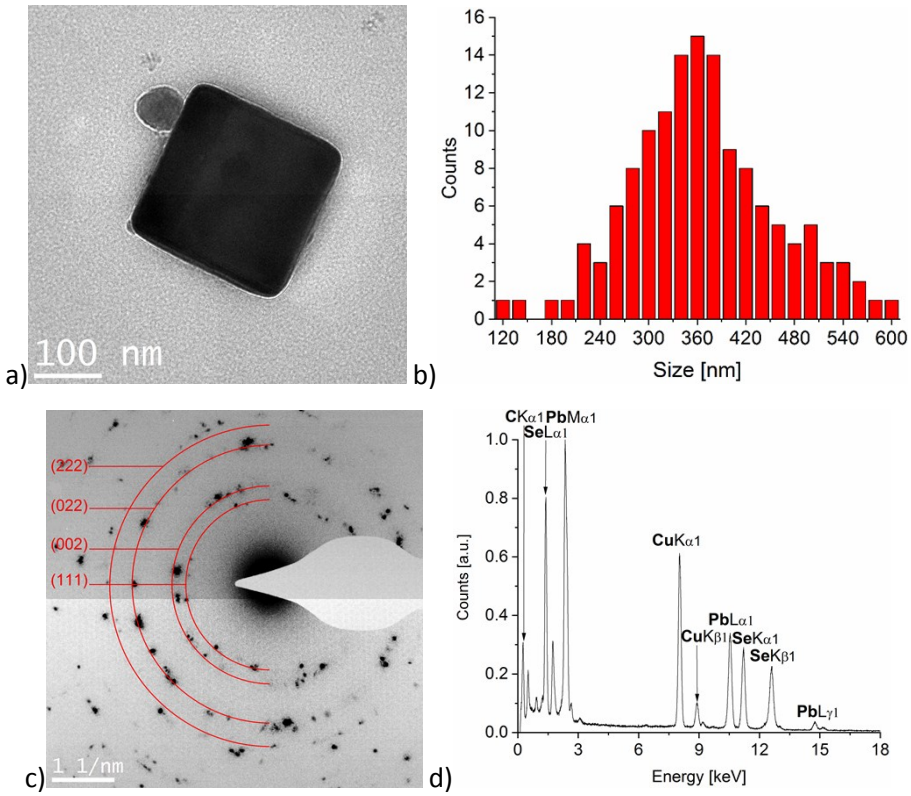

Fig. S5 Additional information on the PbSe particles obtained from the microwave-assisted decomposition of **3a** in [BMIm][NTf_2] in PC (50 vol. %) at 200 °C: (a) Detailed image of a separated particle with an edge length of 411 nm and (b) particle-size distribution, giving an average diameter of 366 ± 90 nm, (c) SAED and (d) EDX-analysis.

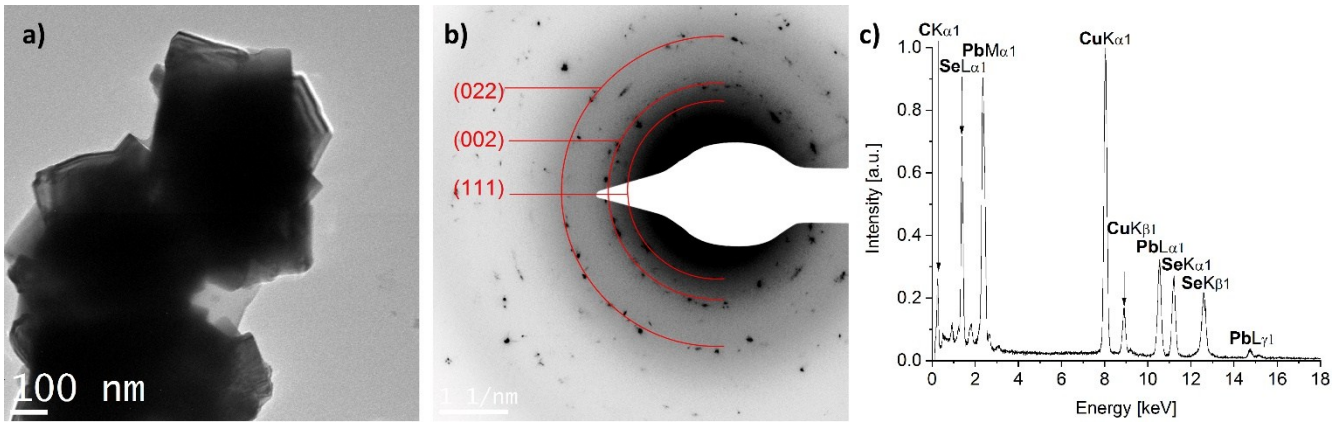

Fig. S6 Additional information on the PbSe particles obtained from the microwave-assisted decomposition of **3a** in PC at 200 °C: (a) Detailed image of an intergrown particle assembly, (b) SAED and (c) EDX-analysis.

Section SIII. Crystallographic and refinement details

Table S1 Crystallographic and refinement details for compounds **2**, **3**, **1a**, **2a** and **3a**.

	2	**3**	**1a**	**2a**	**3a**
Empirical formula	$C_{16}H_{23}ClN_2OSe$	$C_{16}H_{23}ClN_2OSe$	$C_{32}H_{28}N_6O_6PbSe_2$	$C_{26}H_{34}N_4O_2PbSe_2$	$C_{32}H_{44}Cl_2N_4O_2PbSe_2$
Formula weight	373.77	373.77	957.71	799.68	952.72
Crystal system	monoclinic	Triclinic	monoclinic	orthorhombic	orthorhombic
Space group	$P2_1/c$	P-1	$P2_1/n$	Iba2	Iba2
a/Å	10.6871(5)	8.1942(7)	14.1737(2)	20.7267(5)	17.9384(5)
b/Å	15.8440(6)	10.8431(8)	14.1942(2)	13.0349(11)	19.0184(12)
c/Å	10.4873(4)	11.8118(12)	16.5168(2)	10.1701(2)	10.4156(4)
α/°	90.00	64.775(8)	90.00	90.00	90.00
β/°	103.813(4)	69.712(8)	95.0944(16)	90.00	90.00
γ/°	90.00	80.596(6)	90.00	90.00	90.00
Volume/Å^3	1724.43(12)	890.36(13)	3309.79(9)	2747.7(3)	3553.4(3)
Z	4	2	4	4	4
ρ_{calc}mg/mm^3	1.440	1.394	1.922	1.933	1.781
m/mm^{-1}	2.333	2.259	7.350	8.820	6.981
F(000)	768	384	1840	1536	1856
Crystal size/mm^3	0.09×0.07×0.06	0.13×0.12×0.03	0.08×0.03×0.02	0.07×0.04×0.03	0.16×0.02×0.01
2Θ range	6.48 to 58.6°	5.84 to 58.86°	6.2 to 58.82°	6.42 to 58.9°	6.24 to 58.9°
Reflections collected	8277	7450	13648	4251	5214
Indep. reflections (Rint)	3951 (0.0231)	4067 (0.0270)	7523 (0.0266)	2543 (0.0252)	3244 (0.0204)
Data/restraints/parameters	3951/0/192	4067/0/194	7523/0/428	2543/1/162	3244/1/199
Goodness-of-fit on F^2	1.021	1.052	1.036	0.990	1.040
Final R indexes [I>=2σ (I)]	R_1 = 0.0314 wR_2 = 0.0711	R_1 = 0.0320 wR_2 = 0.0661	R_1 = 0.0308 wR_2 = 0.0647	R_1 = 0.0254 wR_2 = 0.0429	R_1 = 0.0238 wR_2 = 0.0465
Final R indexes [all data]	R_1 = 0.0405 wR_2 = 0.0757	R_1 = 0.0389 wR_2 = 0.0699	R_1 = 0.0434 wR_2 = 0.0700	R_1 = 0.0316 wR_2 = 0.0461	R_1 = 0.0299 wR_2 = 0.0489
Largest diff. peak/hole /eÅ^{-3}	0.729/-0.498	0.547/-0.465	1.492/-1.246	0.831/-0.700	0.580/-0.536
CCDC deposition code	1586975	1586977	1586978	1586974	1586976