Supplementary information

Synthesis, electronic structure and physical properties of two new layered compounds, EuFAgSe and EuFAg$_{1-\delta}$Te, featuring the active redox pair Eu^{2+}/Ag^{+}

Igor V. Plokhikh, Alexander A. Tsirlin, Lukas Heletta, Steffen Klenner, Dmitri O. Charkin, Alexey N. Kuznetsov, Andrei V. Shevelkov, Rainer Pöttgen, Arno Pfitzner

Table S1. Selected bond distances in Å and angles in deg. for the M^{2+}F*TCh* (*T* = Cu, Ag; *Ch* = S, Se, Te) fluoride chalcogenides.

	SrFCuS [a]	**SrFCuSe** [a]	**SrFCuTe** [b]	**SrFAgS** [b]	**SrFAgSe** [b]	**SrFAgTe** [b]
d(Sr – F)	2.445(1)	2.476(1)	2.515(1)	2.468(2)	2.503(1)	2.543(1)
d(Sr – Ch)	3.144(2)	3.239(2)	3.427(1)	3.190(3)	3.272(1)	3.456(1)
d(T – Ch)	2.430(2)	2.531(2)	2.671(1)	2.699(5)	2.761(1)	2.871(1)
α_2(SrFSr)	108.00(2)	110.26(4)	115.32(7)	108.88(5)	112.64(5)	117.1(1)
α_4(SrFSr)	110.21(2)	109.08(4)	106.63(3)	110.67(5)	107.91(2)	105.79(5)
α_2(ChTCh)	108.95(5)	106.75(5)	105.39(5)	97.50(1)	97.92(4)	98.19(5)
α_4(ChTCh)	109.73(5)	110.85(5)	111.55(3)	115.77(1)	115.54(2)	115.39(3)
	BaFCuS [b]	**BaFCuSe** [b]	**BaFCuTe** [b]	**BaFAgS** [b]	**BaFAgSe** [b]	**BaFAgTe** [c]
d(Ba – F)	2.607(1)	2.620(1)	2.652(1)	2.626(1)	2.642(1)	2.668(1)
d(Ba – Ch)	3.305(2)	3.387(1)	3.561(1)	3.337(2)	3.422(1)	3.586(1)
d(T – Ch)	2.464(3)	2.565(1)	2.694(1)	2.679(2)	2.753(1)	2.879(1)
α_2(BaFBa)	104.50(4)	108.01(3)	113.25(3)	107.69(2)	110.65(3)	116.15(1)
α_4(BaFBa)	112.01(2)	110.21(3)	107.61(3)	110.37(1)	108.88(1)	106.24(1)
α_2(ChTCh)	107.4(1)	111.44(3)	110.62(3)	104.65(8)	104.22(5)	103.69(1)
α_4(ChTCh)	113.6(2)	108.50(3)	108.90(3)	111.93(4)	112.16(2)	112.43(1)
	EuFCuS [a]	**EuFCuSe** [a]	**EuFCuTe** [c]	**EuFAgS**	**EuFAgSe**	**EuFAg$_{1-\delta}$Te**
d(Eu – F)	2.465(2)	2.488(2)	2.520(1)	-	2.508(1)	2.540(1)
d(Eu – Ch)	3.134(2)	3.223(2)	3.393(1)	-	3.250(1)	3.424(1)
d(T – Ch)	2.434(1)	2.521(1)	2.666(1)	-	2.758(1)	2.881(1)
α_2(EuFEu)	106.44(5)	109.21(5)	114.40(1)	-	111.85(2)	115.87(1)
α_4(EuFEu)	111.01(5)	109.60(5)	107.06(1)	-	108.29(1)	97.30(1)
α_2(ChTCh)	108.46(2)	107.15(3)	105.27(1)	-	97.73(3)	105.96(1)
α_4(ChTCh)	109.98(2)	110.64(3)	111.61(1)	-	115.64(2)	116.75(2)

[a]E. Motomitsu, H. Yanagi, T. Kamiya, M. Hirano, H. Hosono Synthesis, structure and physical properties of layered semiconductors *M*CuF*Ch* (*M* = Sr, Eu, *Ch* = S, Se). *J. Solid State Chem.* **2006**, *179*, 1668.

[b]D. O.Charkin, A. V. Urmanov, S. M. Kazakov. Preparation and crystal structures of novel LaOAgS-type copper and silver fluoride chalcogenides. *J. Alloys Compd.* **2012**, *516*, 134.

[c]O. Janka, T. Schleid. CuEuFTe und AgBaFTe: Zwei neue Münzmetall(I)-Fluorid-Telluride mit unterschiedlichen M^{2+}-Kationen. *Z. Anorg. Allg. Chem.* **2008**, *634*, 2048.

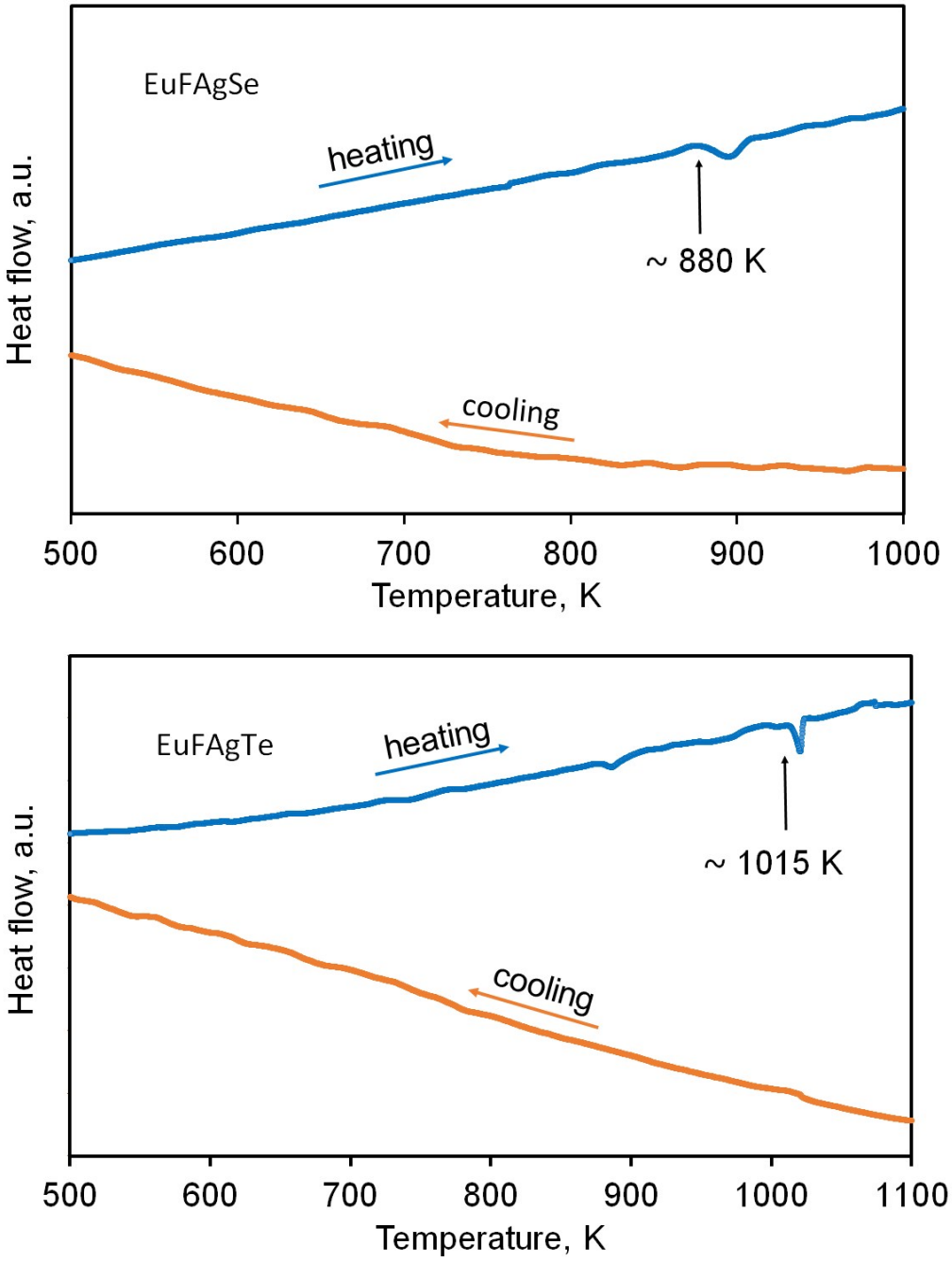

Figure S1. Differential thermal analysis plots for EuFAgSe and EuFAgTe.

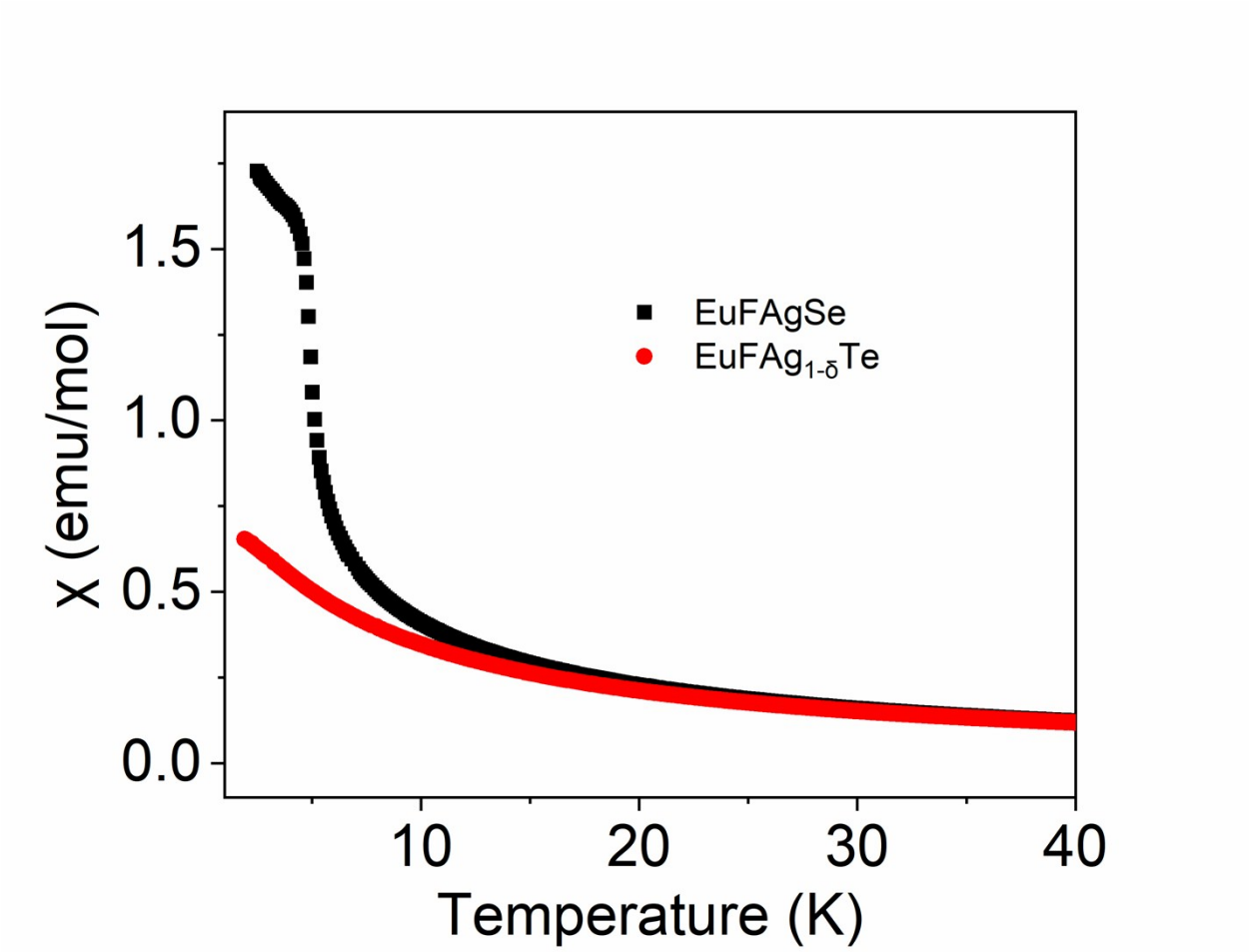

Figure S2. Magnetic susceptibility curves for EuFAgSe and $EuFAg_{1-\delta}Te$ measured in 0.01 T field.