Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supplementary Information for:

Synthesis, structural characterisation and thermoelectric properties of $Bi_{1-x}Pb_xOCuSe$

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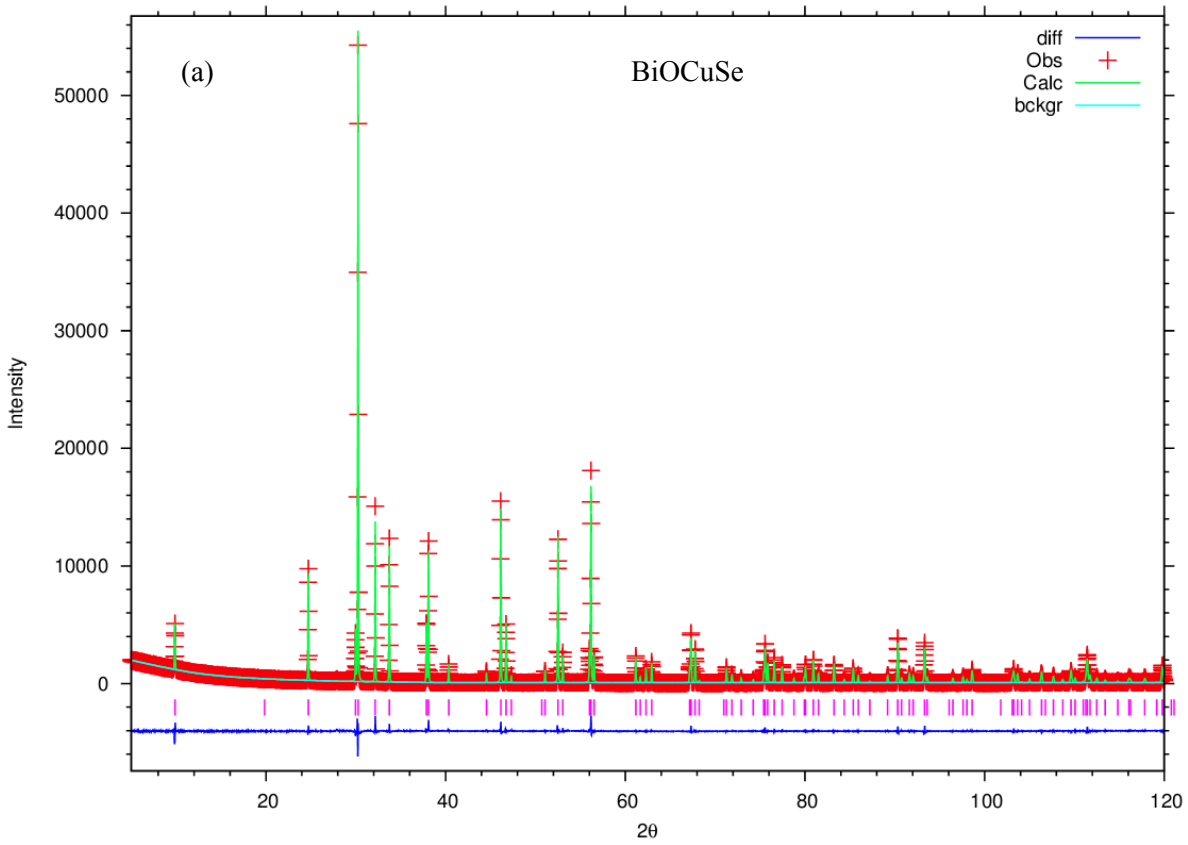

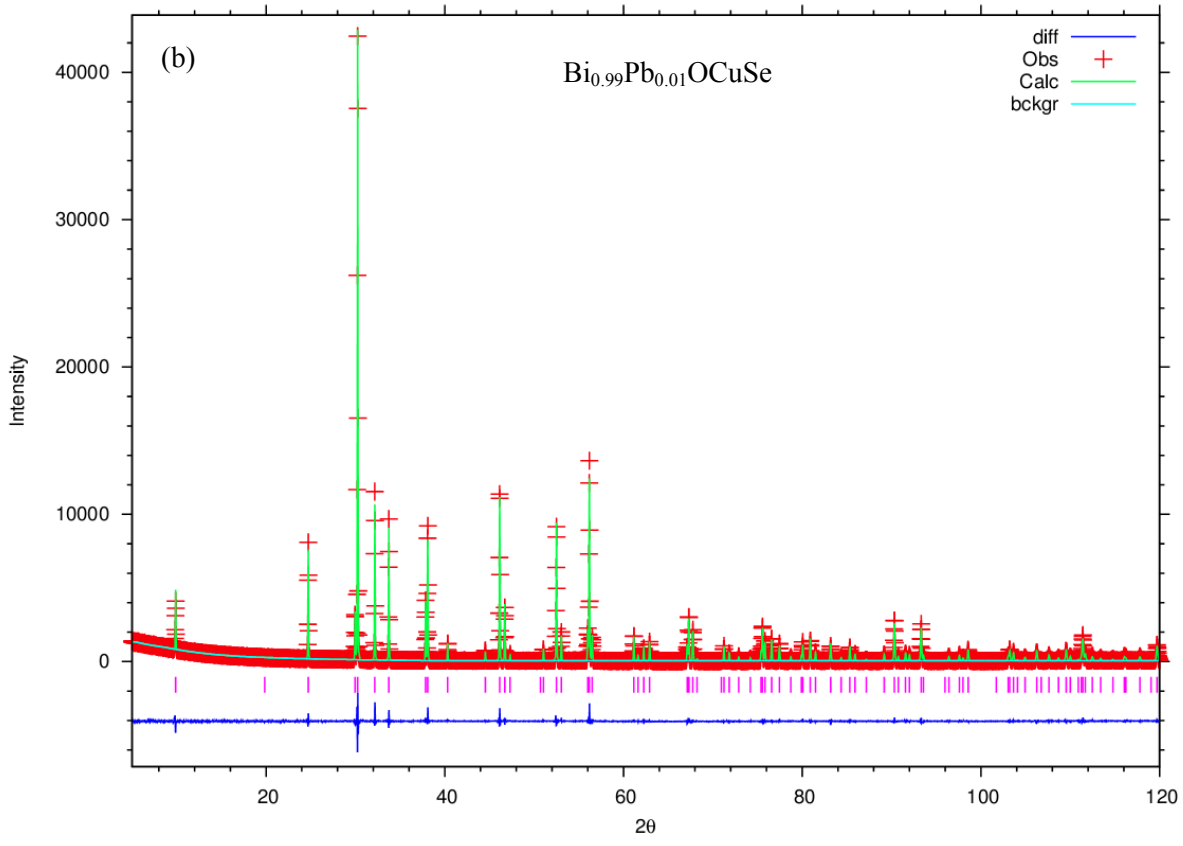

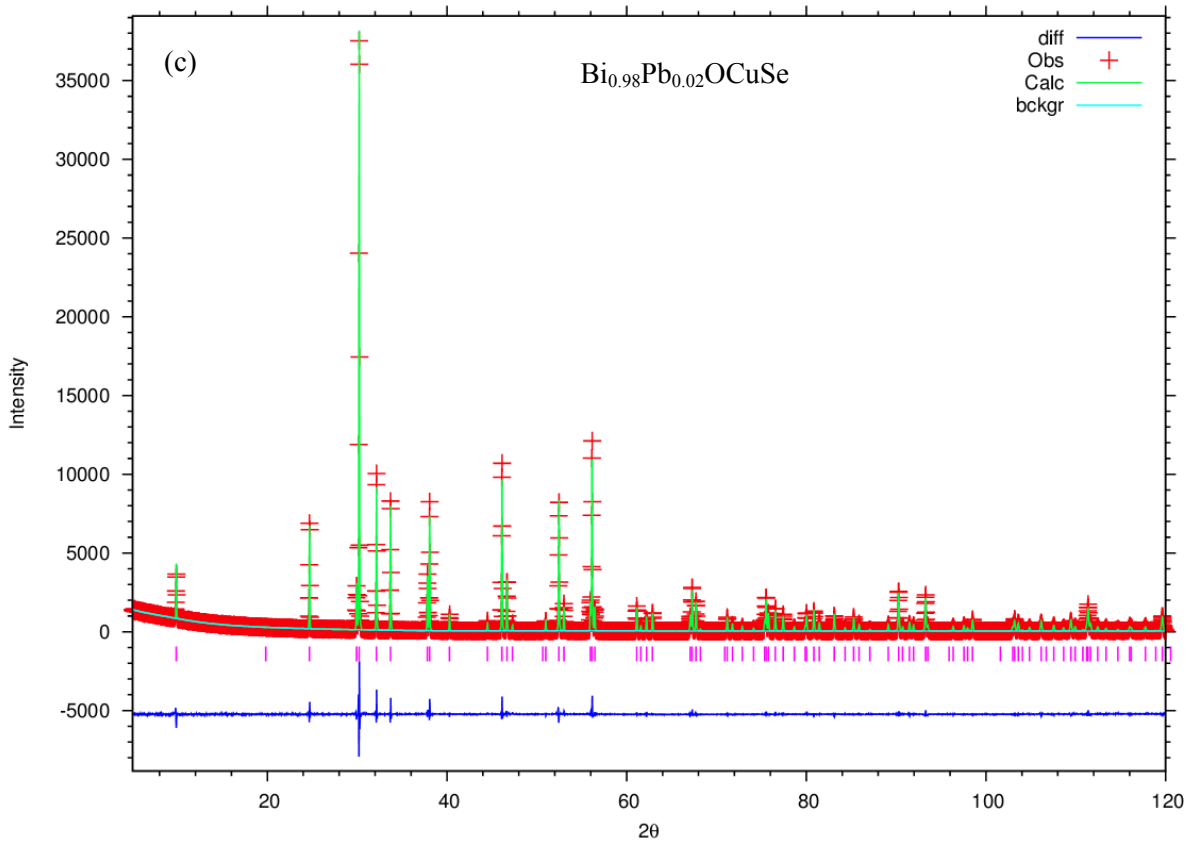

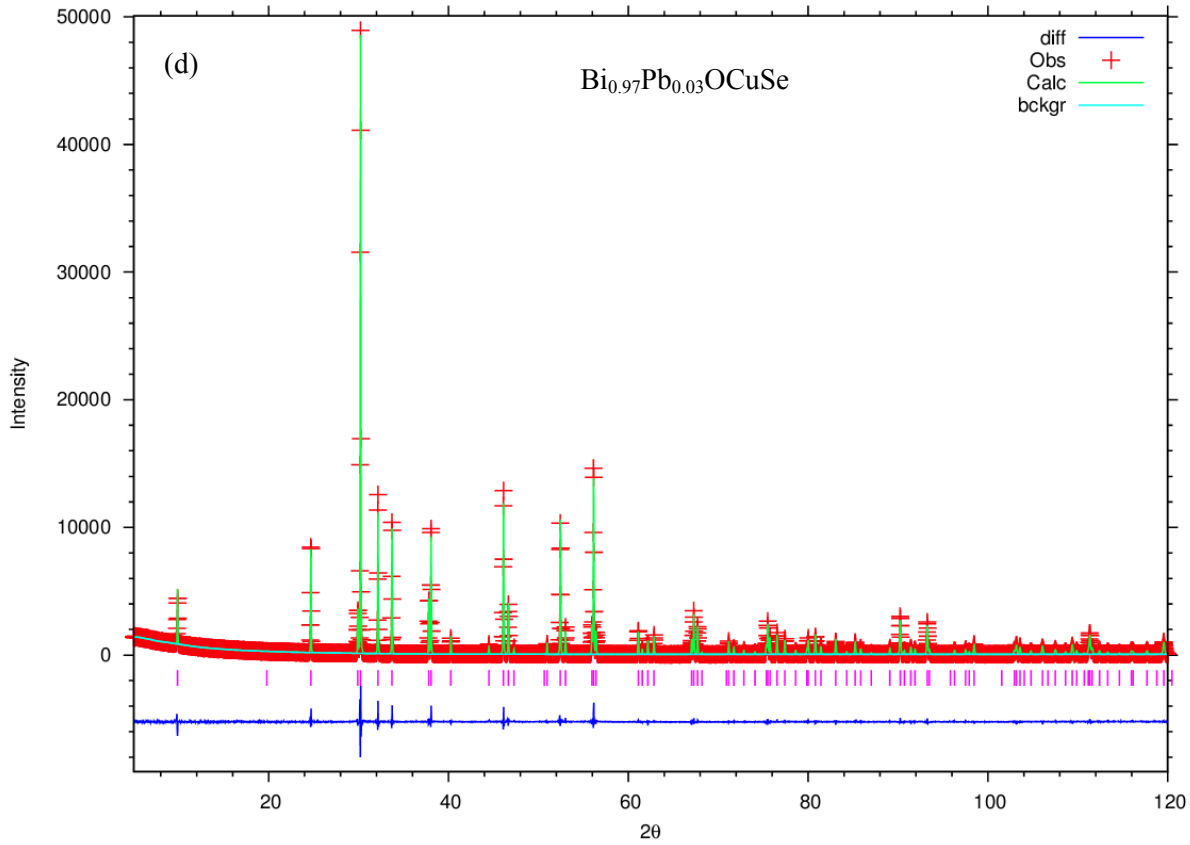

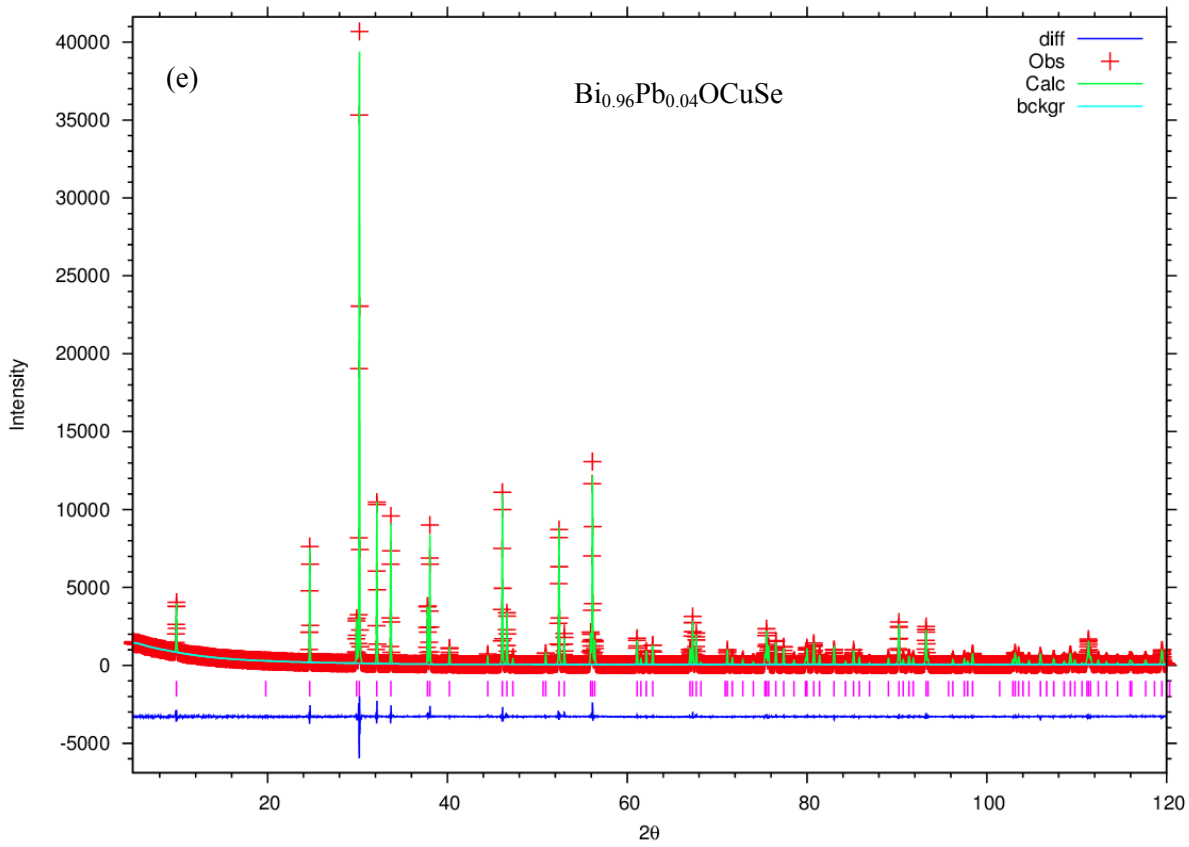

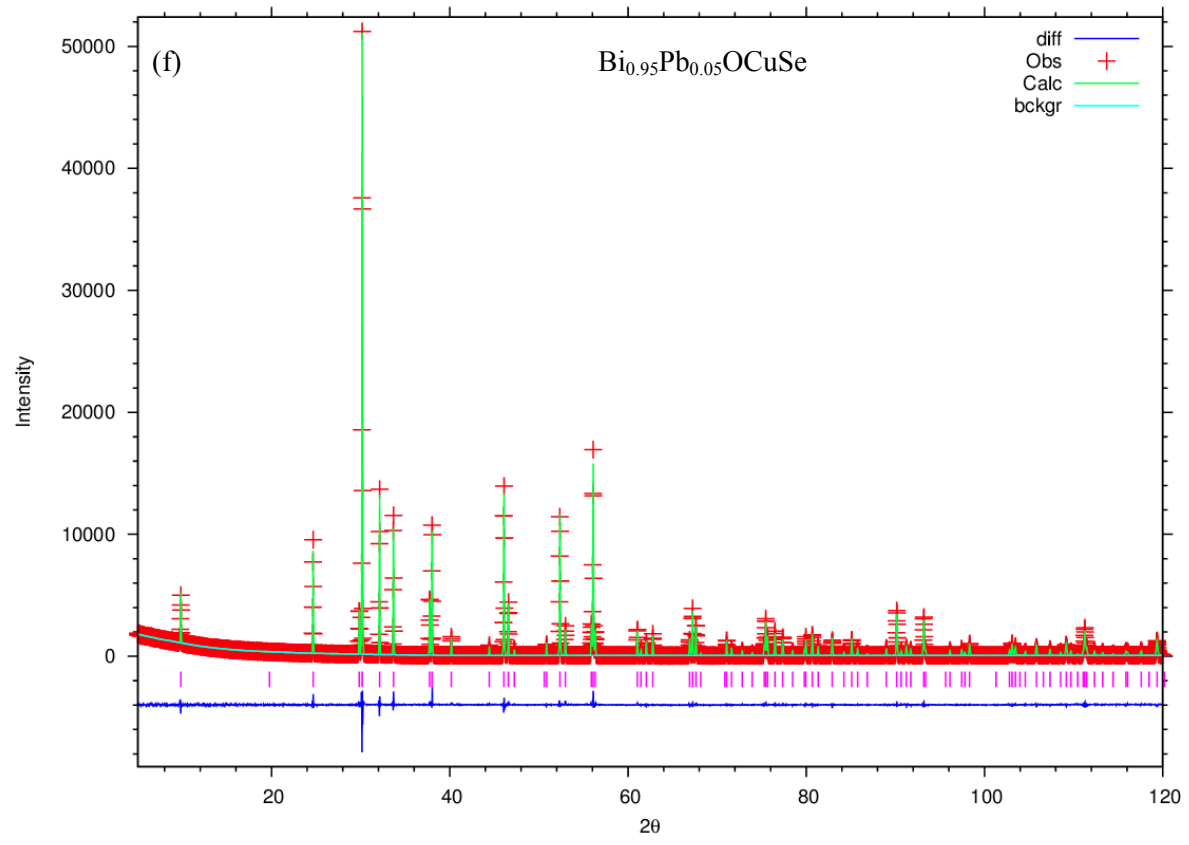

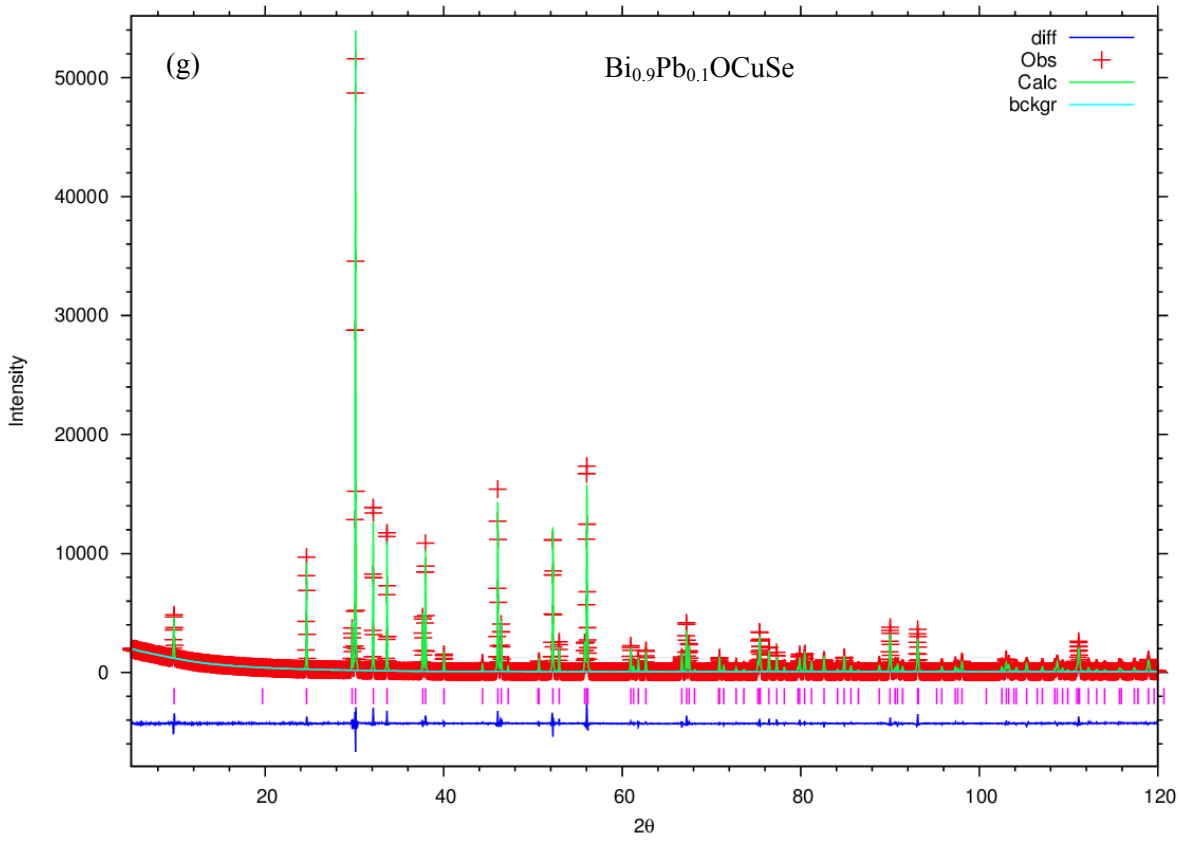

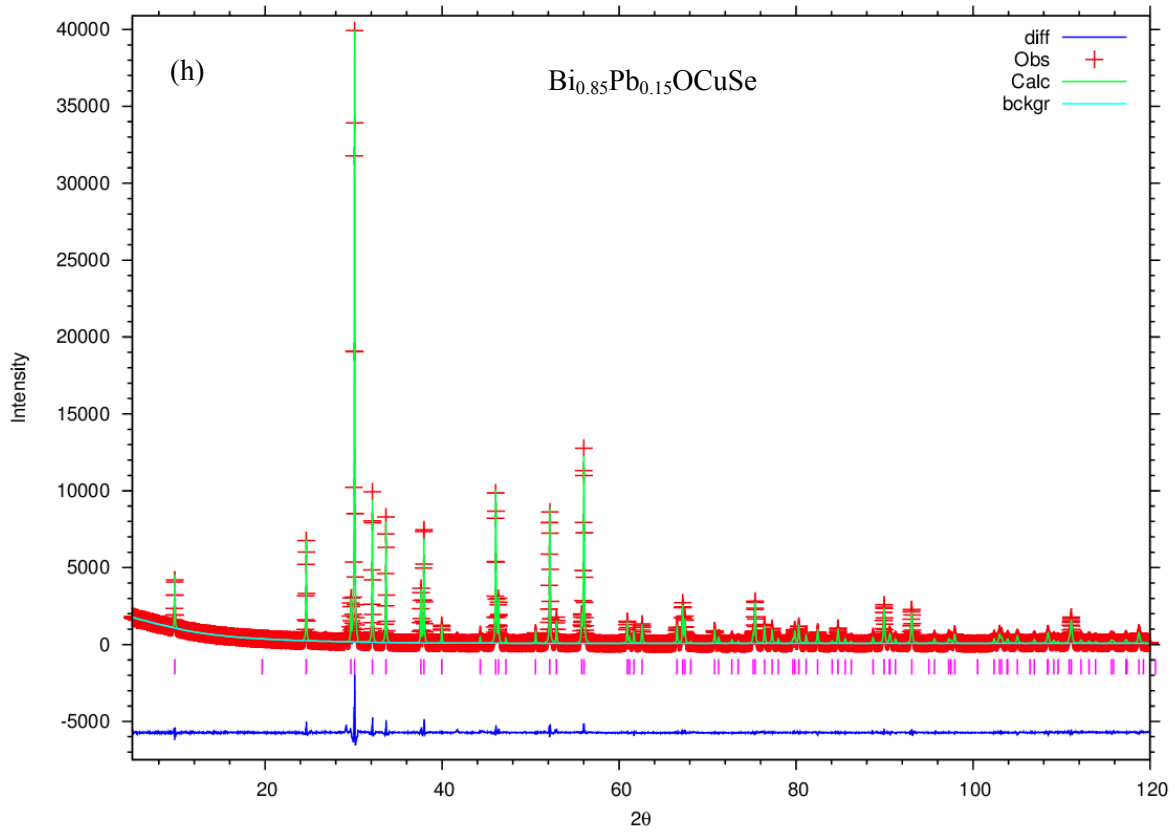

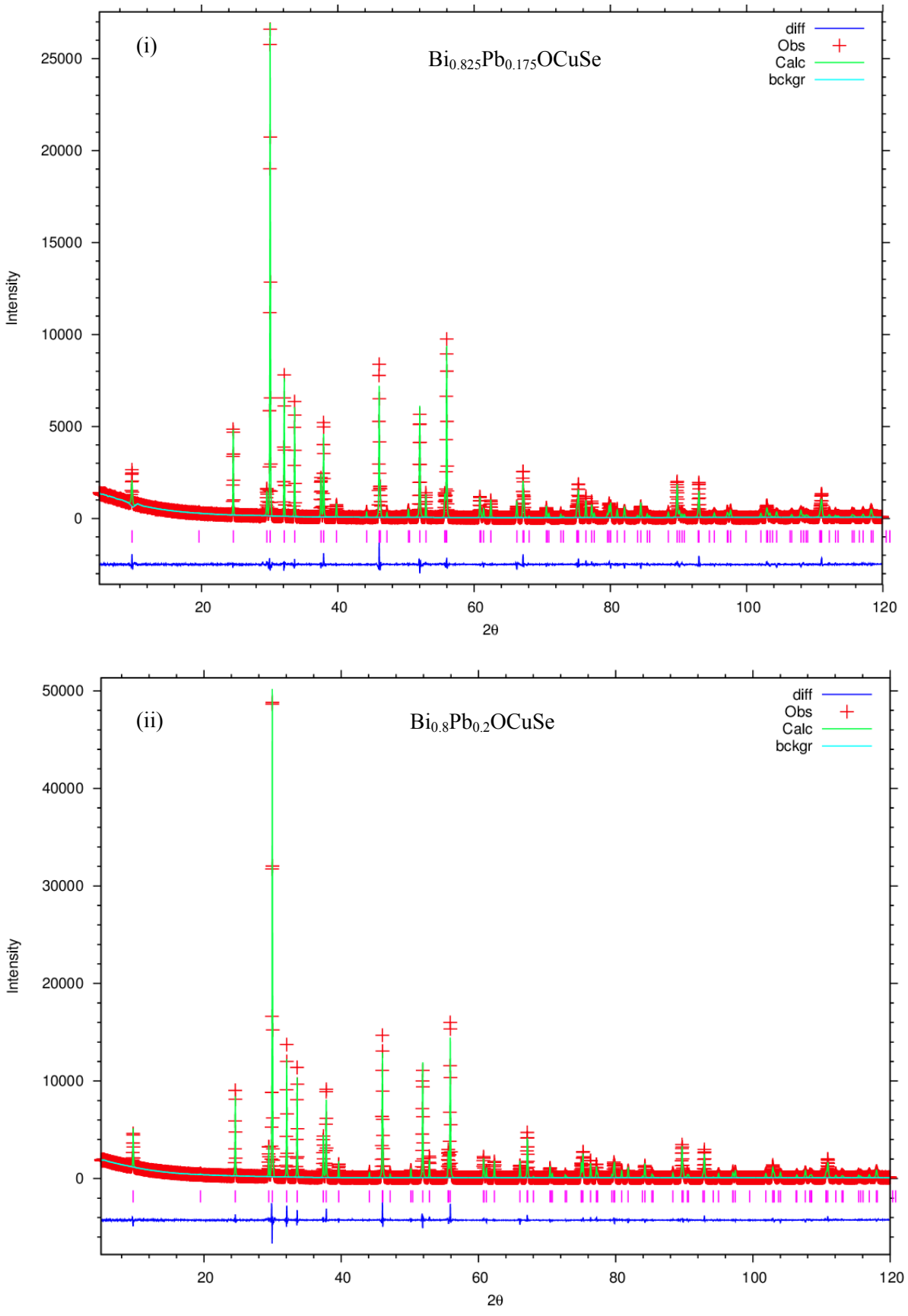

Figure S1. Rietveld refinements using power diffraction data for $Bi_{1-x}Pb_xOCuSe$ ($0 \leq x \leq 0.20$)

Table S1. Final refined parameters for $Bi_{1-x}Pb_xOCuSe$ ($0 \le x \le 0.20$). Site occupancy factors for Bi and Pb were fixed at the stoichiometric composition.

		x in $Bi_{1-x}Pb_xOCuSe$				
		0.0	0.01	0.02	0.03	0.04
	a/Å	3.93026(2)	3.930768(9)	3.931174(23)	3.932024(15)	3.932706(9)
	c/Å	8.93193(5)	8.937858(35)	8.943021(60)	8.948463(47)	8.955914(38)
Bi/Pb[a]	z	0.14021(6)	0.140052(62)	0.139915(67)	0.139790(66)	0.139572(65)
	B/Å^2	0.0012(2)	0.00229(27)	0.00125(20)	0.00402(18)	0.00198(18)
O[b]	B/Å^2	0.0034(22)	0.00484(237)	0.00335(254)	0.00804(259)	0.00656(254)
Cu[c]	B/Å^2	0.0104(5)	0.01129(57)	0.00988(62)	0.01286(62)	0.01074(60)
Se[a]	z	0.67555(15)	0.675253(156)	0.674829(168)	0.674371(165)	0.674700(165)
	B/Å^2	0.0011(4)	0.00221(37)	0.00138(42)	0.00399(40)	0.0028(40)
R_{wp}/%		8.980	9.979	10.380	10.340	10.040

		x in $Bi_{1-x}Pb_xOCuSe$				
		0.05	0.10	0.15	0.175	0.20
	a/Å	3.933238(13)	3.93629(2)	3.93719(3)	3.938811(28)	3.93867(2)
	c/Å	8.962312(41)	8.99652(7)	9.01514(9)	9.056079(91)	9.07746(8)
Bi/Pb[a]	z	0.139456(61)	0.13855(8)	0.1381(8)	0.137249(81)	0.13707(8)
	B/Å^2	0.0010(17)	0.0027(2)	0.0015(2)	0.00606(50)	0.0054(2)
O[b]	B/Å^2	0.00688(245)	0.007(2)	0.003(28)	0.00451(317)	0.004(30)
Cu[c]	B/Å^2	0.00946(56)	0.01(7)	0.0083(7)	0.01222(91)	0.0116(7)
Se[a]	z	0.674063(155)	0.67191(19)	0.6712(2)	0.669303(226)	0.66793(19)
	B/Å^2	0.00114(37)	0.0019(5)	0.0013(5)	0.00329(5)	0.0055(5)
R_{wp}/%		9.450	11.710	10.410	11.460	10.750

[a]Bi/Pb and Se on 2(*c*) (1/4, 1/4, z); [b]O on 2(*a*) (3/4, 1/4, 0); [c]Cu on 2(*b*) (3/4, 1/4, 1/2).

Table S2. Selected bond lengths and angles for $Bi_{1-x}Pb_xOCuSe$ ($0 \leq x \leq 0.20$).

Sample $Bi_{1-x}Pb_xOCuSe$	Bond length			Bond angle		
	Bi-O (Å)	Bi-Se (Å)	Cu-Se (Å)	O-Bi-O (deg.)	Se-Cu-Se (deg.)	Se-Cu-Se (deg.)
x=0	2.33024(28)	3.2298(7)	2.5140(8)	114.984(22)	102.83(5)	112.893(25)
x=0.01	2.33016(0)	3.23273(1)	2.51323(1)	115.014(0)	102.891(0)	112.858(0)
x=0.02	2.33005(32)	3.2361(9)	2.5115(9)	115.041(25)	103.00(5)	112.799(28)
x=0.03	2.33023(32)	3.2397(8)	2.5100(9)	115.066(24)	103.12(5)	112.735(28)
x=0.04	2.33003(31)	3.2403(8)	2.5129(9)	115.112(24)	103.01(5)	112.797(27)
x=0.05	2.33017(29)	3.2448(8)	2.5102(9)	115.126(23)	103.15(5)	112.719(26)
x=0.10	2.3296(4)	3.2642(10)	2.5031(11)	115.307(28)	103.68(6)	112.443(33)
x=0.15	2.3302(4)	3.2711(10)	2.5015(11)	115.303(28)	103.76(7)	112.40(4)
X=0.175	2.3288(4)	3.2922(11)	2.4937(11)	115.486(31)	104.33(7)	112.1(4)
x=0.20	2.3294(4)	3.3000(10)	2.4904(11)	115.431(29)	104.52(6)	112.003(33)

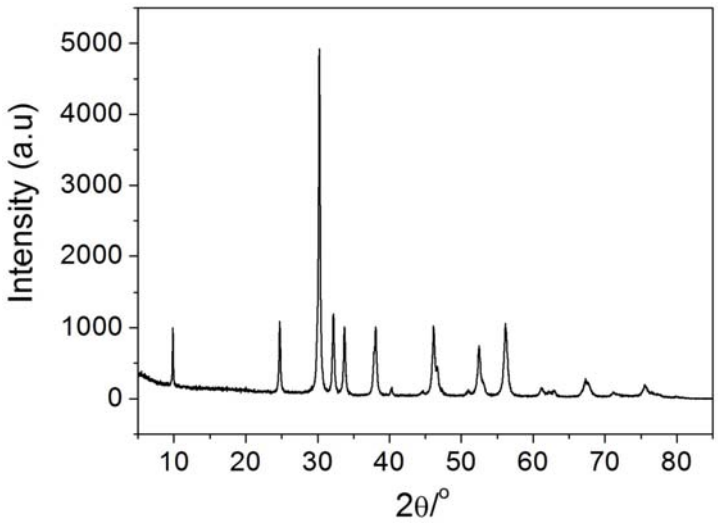

Figure S2. Powder diffraction pattern of a hot-pressed $Bi_{0.95}Pb_{0.05}OCuSe$ sample, showing the marked broadening of the diffraction peaks.