Crystal structures and electronic properties in 3d transition metal doped SrRuO₃.

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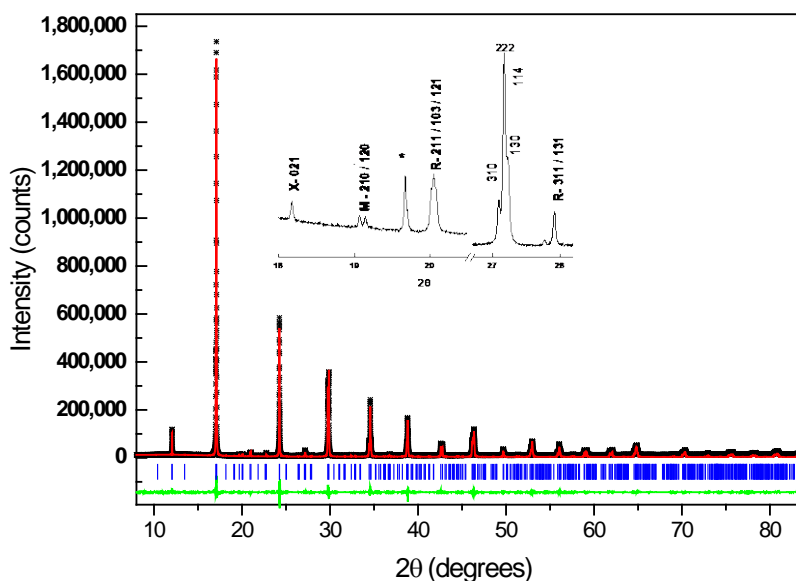E-mail. Brendan.Kennedy@Sydney.edu.au

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Figure S1a. Observed (black symbols), calculated (red line) and difference (green line) S-XRD profiles for $SrRu_{0.8}Ni_{0.2}O_3$ at room temperature. The structure was refined in space group *Pbnm*. A small amount of NiO (0.43 wt %) marked by * is evident in the inset.
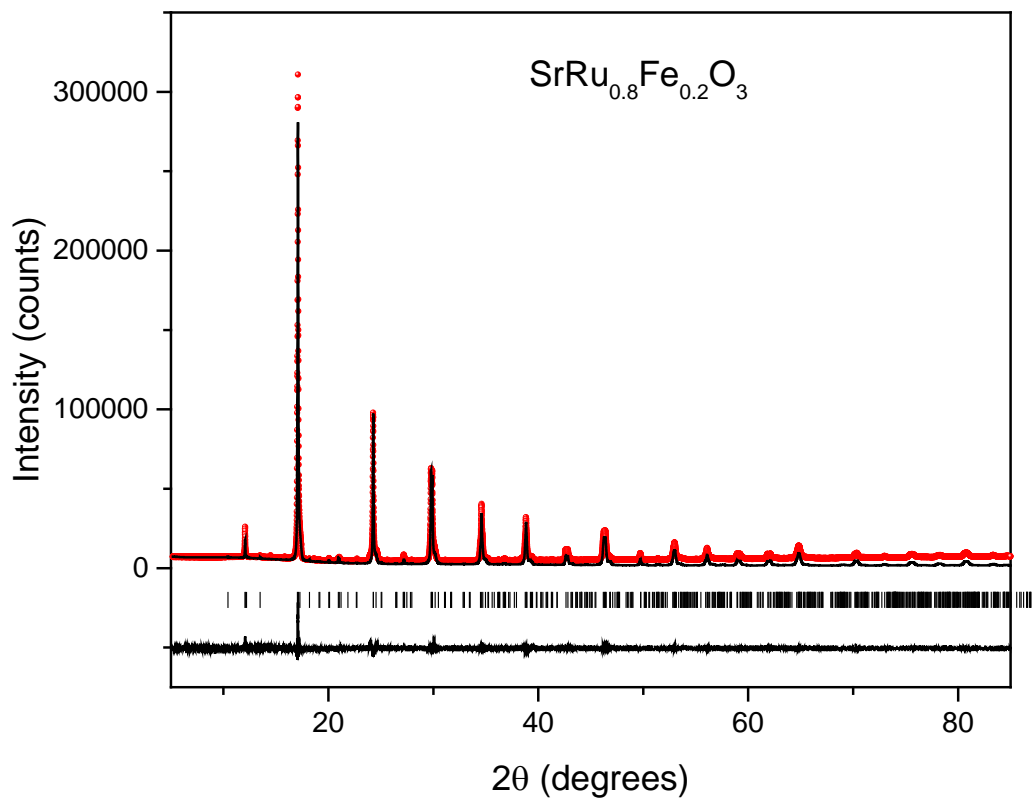

Figure S1b Observed (black symbols), calculated (red line) and difference (green line) S-XRD profiles for $SrRu_{0.8}Fe_{0.2}O_3$ at room temperature. The structure was refined in space group *Pbnm*.
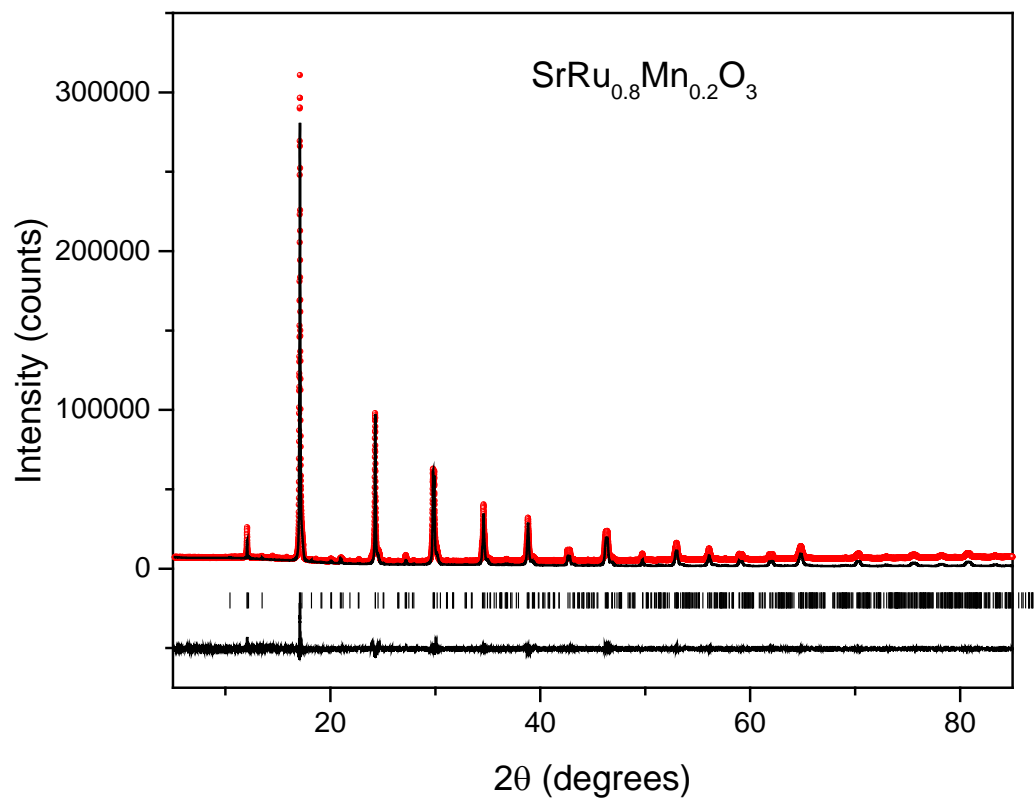
Figure S1c Observed (black symbols), calculated (red line) and difference (green line) S-XRD profiles for SrRu$_{0.8}$Fe$_{0.2}$O$_3$ at room temperature. The structure was refined in space group *Pbnm*.
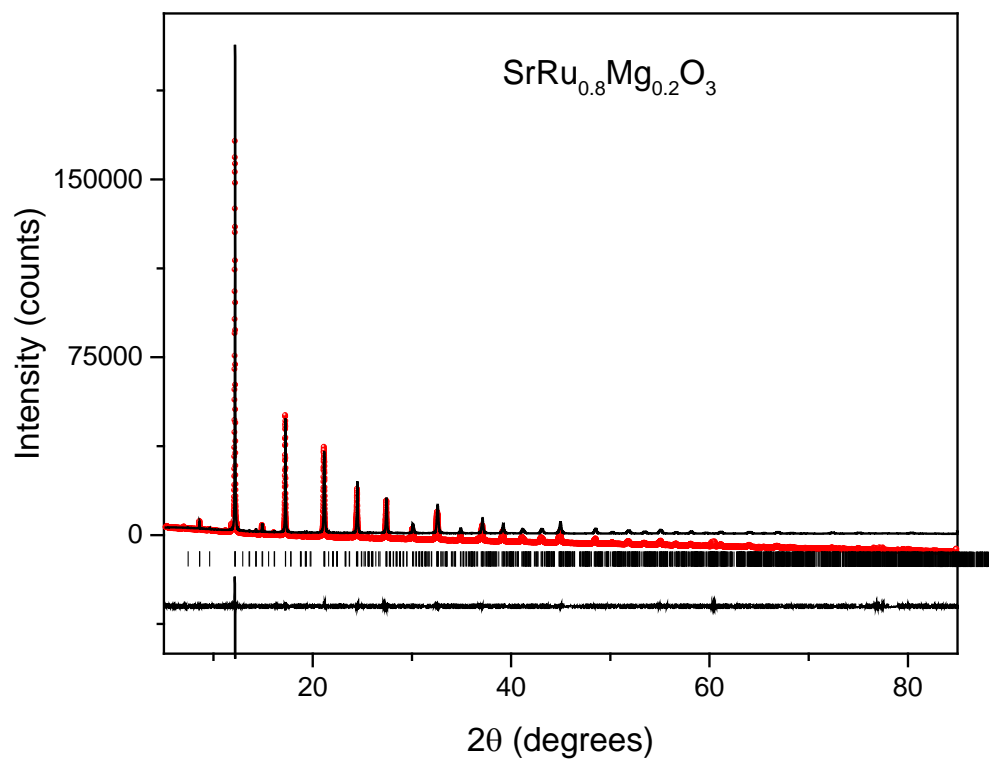
Figure S1d Observed (black symbols), calculated (red line) and difference (green line) S-XRD profiles for $SrRu_{0.8}Mg_{0.2}O_3$ at room temperature. The structure was refined in space group *Pbnm*.
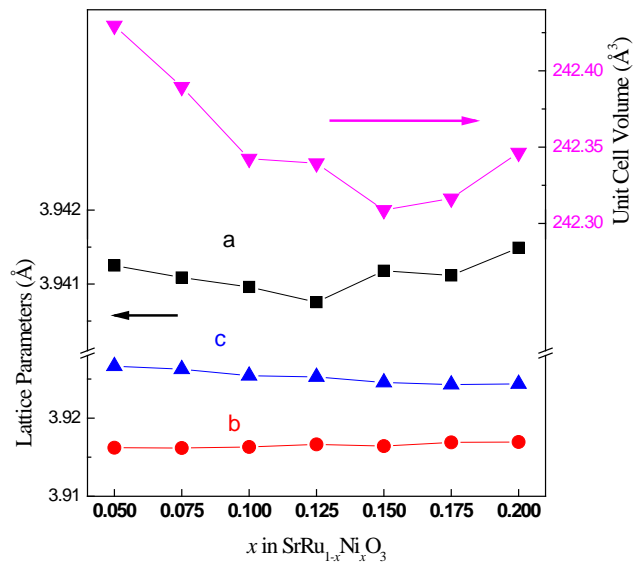
Figure S2. Composition dependence of the unit cell volume (upper), and lattice parameters (lower) from SXRD refinements for SrRu$_{1-x}$Ni$_x$O$_3$. All the parameters are normalised (a/$\sqrt{2}$, b/$\sqrt{2}$, c/2) with respect to the cubic cell for comparison.

Table S1. Refined structural parameters for $SrRu_{1-x}Ni_xO_3$ at room temperature from S-XRD analysis ($\lambda = 0.82544$Å; space group *Pbnm*.)

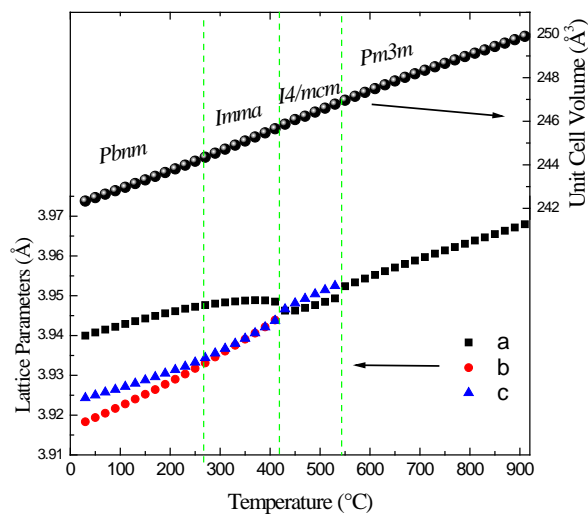| $x =$	0.05	0.075	0.1	0.125	0.15	0.175	0.2
tolerance factor *(t)*	0.9951	0.9956	0.9961	0.9966	0.9971	0.9976	0.9981
a (Å)	5.57378(2)	5.57354(2)	5.57336(1)	5.57307(2)	5.57367(1)	5.57359(2)	5.57411(2)
b (Å)	5.53838(2)	5.53833(2)	5.53850(1)	5.53898(2)	5.53866(1)	5.53934(2)	5.53941(2)
c (Å)	7.85334(3)	7.85252(3)	7.85088(2)	7.85055(3)	7.84912(2)	7.84857(3)	7.84875(4)
vol ($Å^3$)	242.430(2)	242.393(8)	242.393(2)	242.339(1)	242.308(1)	242.317(2)	242.348(2)
R_p (%)	4.35	4.29	3.77	3.83	3.99	4.33	5.33
R_{wp} (%)	5.83	5.82	5.07	4.95	5.28	6.08	8.03
χ^2	31.67	31.97	21.05	19.86	23.47	33.64	69.25
Ru/Ni-O1 Å)	1.9893(10)	1.9874(8)	1..9843(5)	1.9850(6)	1.9836(5)	1.9887(7)	1.9824(8)
Ru/Ni-O2 (Å)	1.950(4)	1.958(4)	1.963(4)	1.959(4)	1.969(4)	1.968(5)	1.957(6)
Ru/Ni-O2 (Å)	2.006(4)	2.000(4)	1.991(4)	1.994(4)	1.984(4)	1.981(5)	1.996(6)
BVS (Ru)	4.03	4.03	4.05	4.06	4.05	4.06	4.06
BVS (Zn)	2.48	2.48	2.49	2.50	2.49	2.49	2.50
Oh distortion	4.21×10^{-4}	2.27×10^{-4}	1.09×10^{-4}	1.69×10^{-4}	0.37×10^{-4}	0.56×10^{-4}	2.00×10^{-4}
(+) Oh tilting (°)	4.43	4.61	3.96	3.97	3.83	3.75	3.61
(-) Oh tilting (°)	8.18	8.12	7.85	7.75	7.83	7.79	7.72

Figure S3. Temperature dependence of the, appropriately scaled, lattice parameters and unit cell volume for $SrRu_{0.8}Co_{0.2}O_3$ as obtained from SXRD measurements.
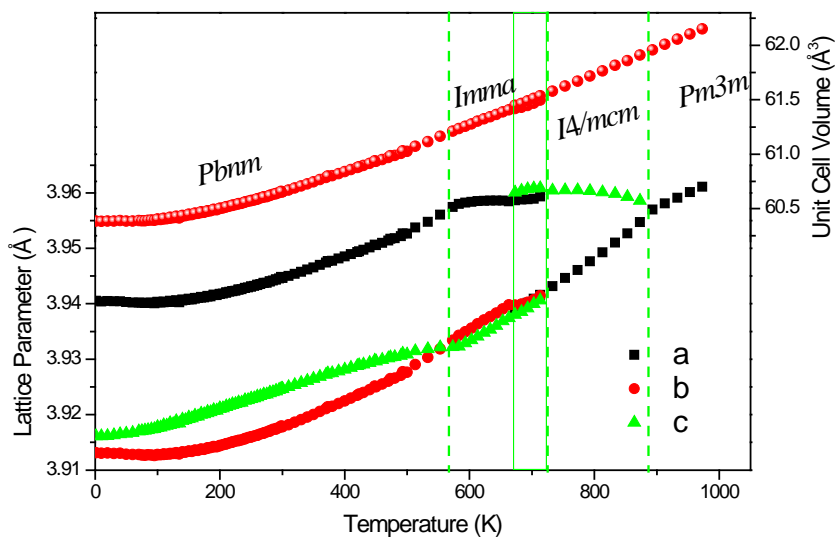

Figure S4. Temperature dependence of the, appropriately scaled, lattice parameters and unit cell volume for $SrRu_{0.9}Cu_{0.1}O_3$ as obtained from SXRD measurements and ND measurement (low temperature region). The hatched region is where the two-phases co-exist.

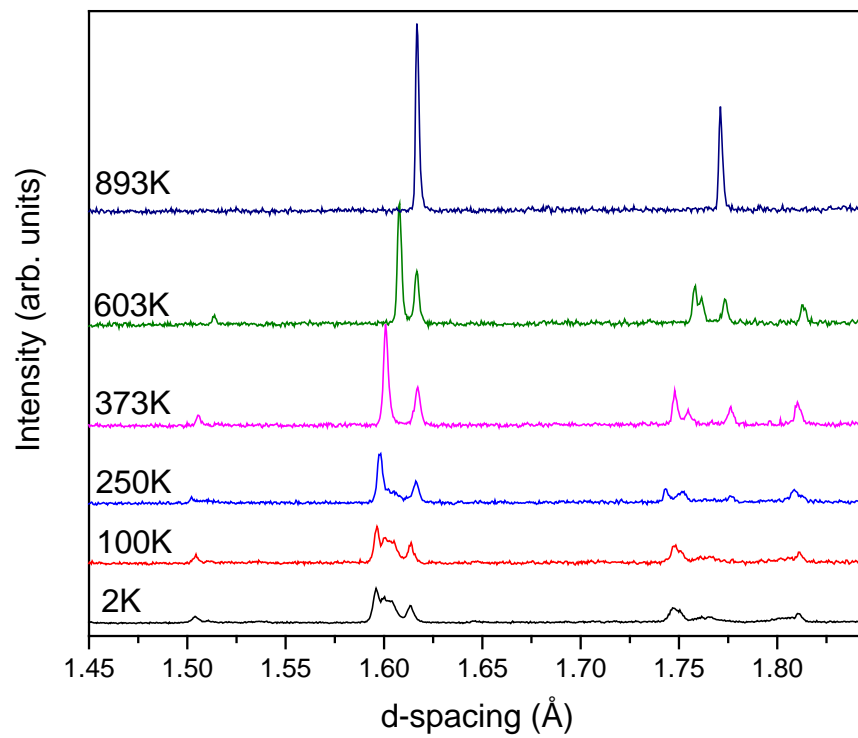Figure S5 Portions of the neutron diffraction profiles for $SrRu_{0.8}Cu_{0.2}O_3$ as a function of temperature.