

Stabilising the Orthorhombic Perovskite Structure in SrIrO₃ through Chemical Doping. Synthesis, Structure and Magnetic Properties of SrIr_{1-x}Mg_xO₃.

Ilyas Qasim and Brendan J. Kennedy*

School of Chemistry, the University of Sydney, Sydney, NSW 2006 Australia

Maxim Avdeev

Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW
2234, Australia

Supplementary information:

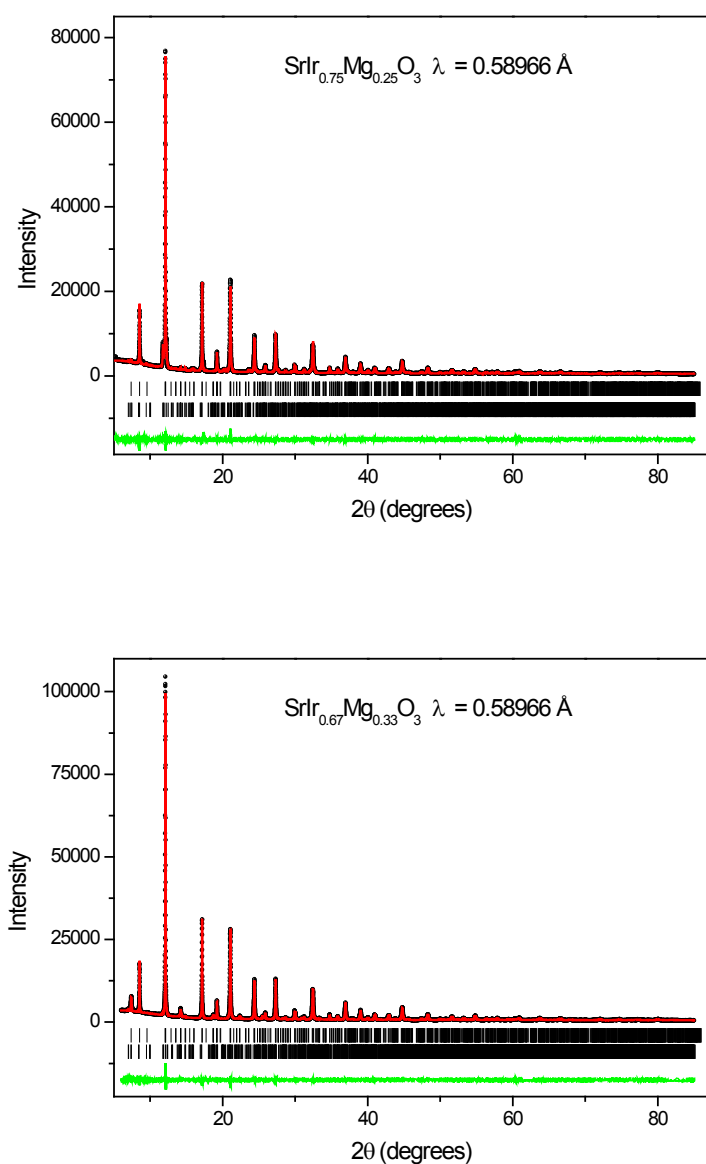


Figure 1. Observed, calculated and difference SXRD pattern for $\text{SrIr}_{0.75}\text{Mg}_{0.25}\text{O}_3$ and $\text{SrIr}_{0.67}\text{Mg}_{0.33}\text{O}_3$ measured at room temperature. The upper set of markers are from the orthorhombic *Pnma* phase and the lower set of markers are due to the poorly crystalline 6H- SrIrO_3 type material.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{iso}}(\text{\AA}^2)$	N
Sr	0.0253(2)	0.5041(12)	0.25	1.10(1)	1
Mg	0	0	0	0.65(0)	0.33
Ir	0	0	0	0.65(0)	0.66
O1	0.1388(16)	0.0019(84)	0.25	1.50(12)	1
O2	0.2768(22)	0.2379(29)	0.0055(9)	1.50(12)	1

Table S1. Refined structural parameters for $\text{SrIr}_{0.67}\text{Mg}_{0.33}\text{O}_3$ from synchrotron X-ray diffraction data. $a = 5.59782(11)$ $b = 5.57185(11)$ $c = 7.89182(18)\text{\AA}$

R_p 6.03 R_{wp} 8.67 R_{exp} GOF 9.50 R_{Bragg} 10.85

Atom	<i>x</i>	<i>y</i>	<i>z</i>	Biso	N
Sr	0.0012(10)	0.5061(7)	0.25	1.37(1)	1.0
Mg	0	0	0	0.68(1)	0.25
Ir	0	0	0	0.68(1)	0.75
O1	-0.1605(18)	-0.0843(21)	0.25	0.22(8)	1.0
O2	0.2193(15)	0.2794(16)	0.0238(11)	0.22(8)	1.0

Table S1. Refined structural parameters for $\text{SrIr}_{0.75}\text{Mg}_{0.25}\text{O}_3$ from synchrotron X-ray diffraction data. $a = 5.59811(9)$ $b = 5.56910(9)$ $c = 7.89056(15)\text{\AA}$

R_p 4.46 R_{wp} 6.58 R_{exp} GOF 5.41 R_{Bragg} 6.16

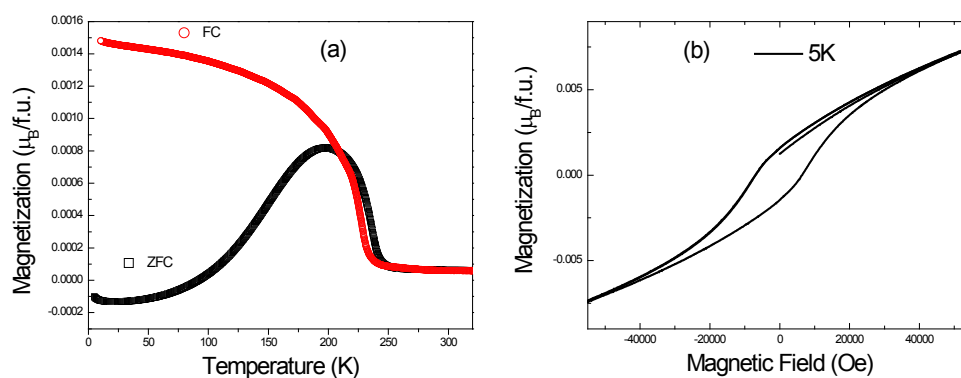


Figure 2. (a) Temperature dependence of magnetization for $\text{SrIr}_{0.75}\text{Mg}_{0.25}\text{O}_3$ samples recorded with an applied magnetic field of 1000 Oe (b) the hysteresis loop at 5 K.

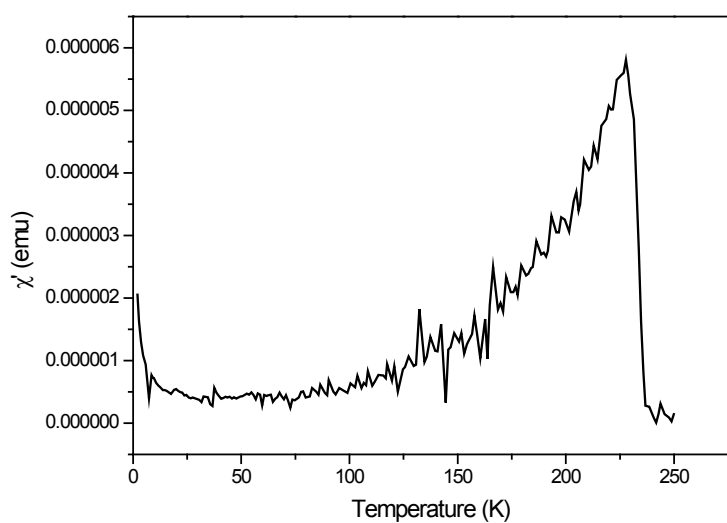


Figure S3. Temperature dependence of real part of ac susceptibility for $\text{SrIr}_{0.67}\text{Mg}_{0.33}\text{O}_3$ measured at 1000 Hz.

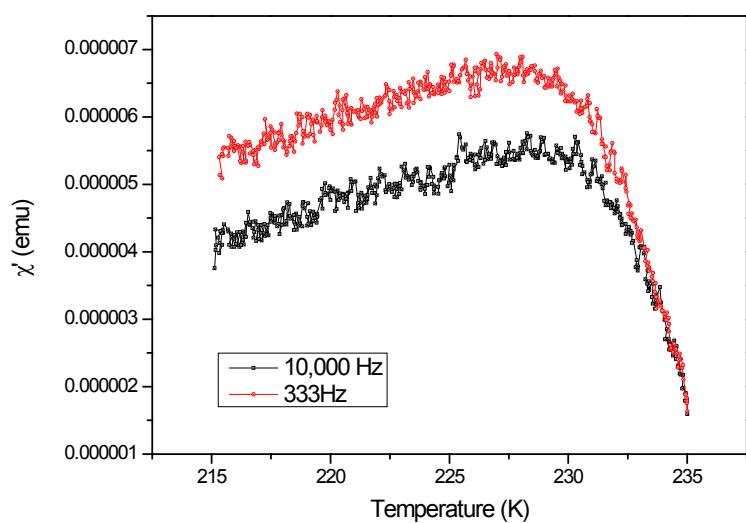


Figure S4. Temperature dependence of real part of ac susceptibility for $\text{SrIr}_{0.67}\text{Mg}_{0.33}\text{O}_3$ measured at different frequencies.