



	Experiment title: Variation of the Magnetic and Superconducting Properties of $\text{Gd}_{2-x}\text{Ce}_x\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ with the Crystal	Experiment number: HE1419
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Report:

Three $\text{Gd}_{2-x}\text{Ce}_x\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ samples ($x = 0.5$, as prepared and after high pressure oxygenation, and $x = 0.7$) have been investigated by synchrotron X-ray diffraction. Samples were contained in 0.5 mm borosilicate capillaries and a wavelength of 0.40027 Å was used. Excellent fits were obtained for all samples using the tetragonal $I4/mmm$ structural model. Disordered rotations and tilts of the RuO_6 octahedra were evidenced as previously observed in $\text{RuSr}_2\text{GdCu}_2\text{O}_8$ ¹. These were modelled by splitting the oxygen sites of the RuO_6 octahedra as shown in Table 1.

Table 1. Refined Atomic Parameters for $\text{Gd}_{2-x}\text{Ce}_x\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ ²

Atom	Occupancy		Sample (x)		
			0.5 (asp)	0.5 (hpo)	0.7
Ru	1.00	$U_{\text{iso}} (\text{Å}^2)$	0.0034(2)	0.0048(1)	0.0053(1)
Sr	1.00	z	0.07832(3)	0.07854(3)	0.07841(2)
		$U_{\text{iso}} (\text{Å}^2)$	0.0084(2)	0.0081(1)	0.0081(1)
Gd/Ce	1.00	z	0.20470(2)	0.20488(2)	0.20514(2)

		$U_{\text{iso}} (\text{\AA}^2)$	0.0083(1)	0.0054(1)	0.0038(1)
Cu	1.00	z	0.14398(4)	0.14373(4)	0.14367(3)
		$U_{\text{iso}} (\text{\AA}^2)$	0.0060(2)	0.0018(2)	0.0024(1)
O(1)	0.25	x	0.021(6)	0.033(3)	0.046(2)
		z	0.0692(2)	0.0687(2)	0.0685(2)
		$U_{\text{iso}} (\text{\AA}^2)$	0.0187(7)	0.0179(6)	0.0125(4)
O(2)	1.00	z	0.1498(2)	0.1481(2)	0.1483(1)
		$U_{\text{iso}} (\text{\AA}^2)$	0.0187(7)	0.0179(6)	0.0125(4)
O(3)	0.50	x	0.125(2)	0.134(2)	0.130(2)
		$U_{\text{iso}} (\text{\AA}^2)$	0.0187(7)	0.0179(6)	0.0125(4)
O(4)	n	$U_{\text{iso}} (\text{\AA}^2)$	0.0187(7)	0.0179(6)	0.0125(4)
		n	0.87(1)	0.95(1)	1.0

It has previously been reported that oxygen vacancies in $\text{Gd}_{2-x}\text{Ce}_x\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ are located on the O(4) site within the GdCeO_2 block³. The fraction of O(4) was refined and its occupancy increases from 0.87 to 0.95 to 1.00 for $\text{Gd}_{1.5}\text{Ce}_{0.5}\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ (asp), $\text{Gd}_{1.5}\text{Ce}_{0.5}\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ (hpo) and $\text{Gd}_{1.3}\text{Ce}_{0.7}\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ respectively. Hence δ decreases with increasing Ce concentration and after high pressure oxygenation. Estimates of the hole-doping of the copper oxide planes have been made from the chemical composition, based on the refined oxygen contents and are in good agreement with the variation of superconductivity; $\text{Gd}_{1.5}\text{Ce}_{0.5}\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ (hpo) and $\text{Gd}_{1.3}\text{Ce}_{0.7}\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ are superconducting ($T_c = 28$ and 30 K respectively), $\text{Gd}_{1.5}\text{Ce}_{0.5}\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ (asp) is not superconducting². The magnetic ordering temperatures of the Ru moments are not a simple function of the doping concentration, but depend on both the Gd/Ce ratio and the oxygen content. Hence in order to obtain the correct electronic phase diagram of $\text{Gd}_{2-x}\text{Ce}_x\text{RuSr}_2\text{Cu}_2\text{O}_{10-\delta}$ it is imperative that the oxygen stoichiometry is well established².

1. A. C. Mclaughlin, W. Zhou, J. P. Attfield, A. N. Fitch and J. L. Tallon, *Phys. Rev. B.*, **60**, 7512 (1999).
2. A. C. Mclaughlin, J. P. Attfield, U. Asaf and I. Felner, *Phys. Rev. B.*, **68**, 014503 (2003).
3. C. S. Knee, B. D. Rainford and M. T. Weller, *J. Mater. Chem.*, **10**, 2445 (2000).