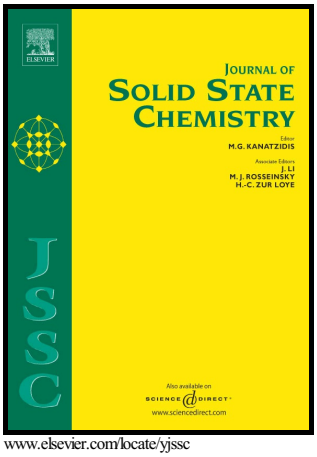

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Evolution of the crystal structure and magnetic properties of $Sr_{2-x}Ca_xCrSbO_6$ with composition

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Abstract

Polycrystalline samples of compositions in the perovskite solid solution $Sr_{2-x}Ca_xCrSbO_6$ (x=0, 0.25. 0.5, 0.75, 1.0, 1.25, 1.50, 1.75, 2.0) were synthesized and characterised by synchrotron x-ray diffraction and SQUID magnetometry. Neutron powder diffraction data were collected on the x=0, 0.25, 0.5, 1.0, 1.5 and 2.0 compositions. It was found that Sr_2CrSbO_6 crystallised in the triclinic $I\bar{1}$ space group. The other compositions were all found to crystallise in the monoclinic space group $P2_1/n$ although $Sr_{1.5}Ca_{0.5}CrSbO_6$ was found to be phase separated into a calcium-deficient and calcium-rich phase, both having the space group $P2_1/n$. Sr_2CrSbO_6 was found to order antiferromagnetically at 12 K and the ordered Cr^{3+} moment was refined to be 2.39(1) μ_B. The antiferromagnetic order was rapidly quenched on doping with Ca and compositions with $x \geq 0.75$ exhibited ferromagnetic order. T_C increased with x to reach a maximum of 14 K at x=2.0, with an ordered moment of 2.56(3) μ_B per Cr^{3+} cation. The tilt angles of the B-site octahedra about [110] and [001] increase from 5.4(1)˚ and 4.6(1)˚ to 13.7(1)˚ and 13.9(1)˚, respectively, across the series; the switch from antiferromagnetism to ferromagnetism occurs when both tilts are at a value of ~8˚.

Graphical Abstract: