Supporting Information

Haravifard et al. 10.1073/pnas.1413318111

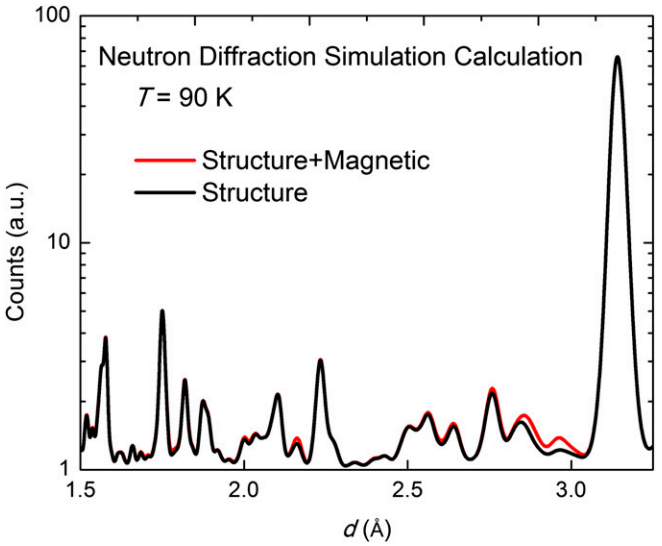

Fig. S1. Neutron diffraction simulation calculations. Using the FULLPROF refinement program (1) and based on the proposed model for the crystal and magnetic structure of SCBO as shown in Fig. 5*B*, we performed computer simulations of the neutron powder diffraction cross-section for the high-pressure, low-temperature antiferromagnetic phase. The comparison between the pure structural (black) and the structural plus magnetic neutron (red) cross-section simulations for $T = 90$ K in the high-pressure phase shows an increased intensity of ~30% for (0 3 0) reflection at $d = 2.9$ Å, in agreement with the (0 3 0) peak observed in the neutron powder diffraction data collected at $T = 90$ K and $P \sim 5.5$ GPa. The calculation considers the decrease of the Cu^{2+} magnetic form factor as function of $|Q|$. As a result of this decrease, no additional magnetic peaks were observed at (0 5 0) and above.

1. Rodriguez-Carvajal J (1993) Recent advances in magnetic structure determination by neutron powder diffraction. *Physica B* 192:55–69.