Correlation between local symmetry breaking, magnetism and Weyl properties in Co3Sn2S2

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Co3Sn2S2 is a newly discovered magnetic Weyl semimetal with a kagome lattice of cobalt ions and has triggered intense interest for rich fantastic phenomena. It was proposed that it exhibits a coexistence of ferromagnetic order and antiferromagnetic order below TC≈ 175 K, followed by a pure ferromagnetic order below TA≈ 5 K. We employed half-polarized neutron technology and confirmed the ferromagnetic order along the c axis below TC≈ 175 K. Using the neutron total scattering, we found that an anomaly in lattice constant a, Co-Sn2-Co bond length, and a striking local symmetry breaking from rhombohedral R-3m to monoclinic Cm co-emerge with the onset of ferromagnetic order below TC. The mismatch of local and long-range crystallographic structures indicates that Co3Sn2S2 becomes an intrinsically lattice disordered system below TC. This provides new insight to the previously puzzling magnetic phase separation and spin glass like state in Co3Sn2S2. Furthermore, our density function theory (DFT) calculation indicates such local symmetry breaking plays a detrimental role in the formation of the Weyl points by breaking mirror symmetries and is expected to induce a broad topological surface band like feature from distorted regions. Our findings highlight the important role that the overlooked local symmetry breaking plays in unveiling the novel interplay between structural complexity, magnetism, and topological properties in Co3Sn2S2.

Figure 1

![Figure 1](Acta Cryst. (2022), A78, a186)