**ABSTRACT**

The interplay between the quantum effects from low-dimensionality and the spin-orbit coupling leads to exotic ground states with unusual excitations. Among the diverse 2D spin systems, the *S* = ½ 2D square lattice has piqued the curiosity of researchers due to its connection with the High-Temperature Superconductivity (HTSC). Studying the Crystal electric field (CEF) and spin-orbit coupling (SOC) effects in a *Jeff*= ½ 2D square lattice magnets is one of the recent fundamental interests in condensed matter physics. While a few transition metal-based square lattice materials exist, the experimental exploration of rare-earth magnetic materials with a perfect 2D square lattice structure is very limited. Herein, we report the structural, magnetic, heat capacity, and electronic structure studies of Bi2REO4Cl (RE = Yb, Er), which constitutes a structurally perfect 2D square lattice with rare-earth magnetic ions. The magnetization and heat capacity data analysis confirms that both the Yb3+ andEr3+  ion hosts the spin-orbit driven *J*eff = ½ state at low temperatures. The Curie-Weiss temperature for the low temperature region in the case of Bi2YbO4Cl and Bi2ErO4Cl come out to be -1 K and -2.1 K, implying the presence of antiferromagnetic (AFM) coupling between the magnetic moments. The heat capacity measurements for Bi2YbO4Cl reveal a broad peak at 0.3 K, suggesting the development of short-range correlations. In contrast, Bi2ErO4Cl exhibits magnetic long-range order at 0.47 K. Our first-principles calculations based on density functional theory provide
further insight into crucial role of spin-orbit coupling and magnetic anisotropy of the spins.