

Supporting Information

KMB₄O₆F₃ (M = Co, Fe): Two-Dimensional Magnetic Fluoroxyborates with Triangular Lattice Directed by Triangular BO₃ Unit

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1. XPS analysis

The compound **1** was characterised by X-ray photoelectron spectroscopy (XPS). The XPS full-scan spectrum confirmed the presence of Co, K, B, F and O elements (Fig. S1a). The Co 2p spectrum exhibits two prominent peaks at 782.4 and 798.3 eV, corresponding to the typical Co²⁺ peaks of Co 2p_{3/2} and Co 2p_{1/2}, respectively, along with two additional satellite peaks centering at 787.4 and 803.8 eV^[1,2]. The peak information in this area coincides with the peak phase of Co²⁺, proved the +2 valence state of Co in the compound **1** (Fig.S1b).

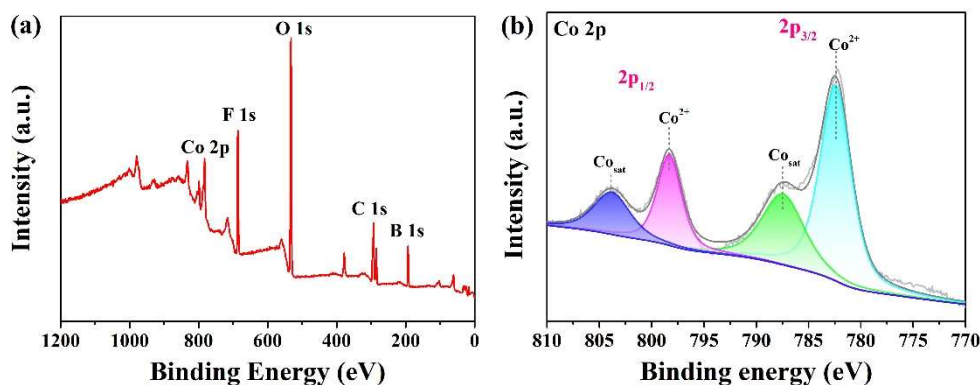


Fig. S1 XPS analysis of compound **1**: (a) full spectrum; (b) high-resolution spectra of Co 2p

2. SEM-EDS and ICP analysis

The Co concentration was both characterised by scanning electron microscope- energy dispersive spectroscopy (SEM-EDS) and inductively coupled plasma optical emission spectroscopy (ICP-

OES). The SEM and EDS spectra of compound **1** showed that the distribution of all elements in the sample is uniform (Fig. S2). And the ratio of K to Co is close to 1:1, which is consistent with the chemical formula $\text{KCoB}_4\text{O}_6\text{F}_3$. Moreover, ICP- OES results show the composition of elements Co 23.4 wt% in compound **1**, which is in good agreement with the theoretical content of 20.0 wt% in the chemical formula $\text{KCoB}_4\text{O}_6\text{F}_3$.

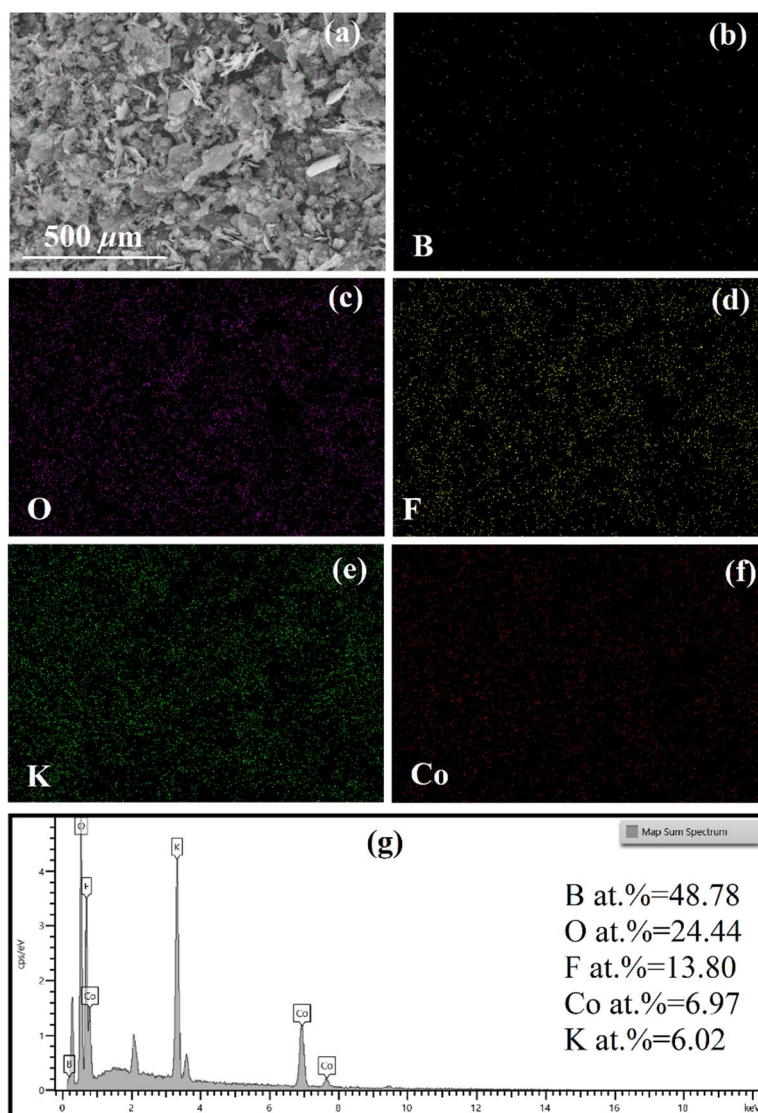


Fig. S2 SEM-EDS analysis of compound **1**: (a) The SEM image; (b)-(f) distribution diagram of element; (g) EDS spectra

References

- [1] B. J. Tan, K. J. Klabunde, and P. M. A. Sherwood, *J. Am. Chem. Soc.*, 1991, 113, 855-861.
- [2] Y. Yang, H. Wan, G. Chen, N. Zhang, J.-H. Li, W. Ma, X.-H. Liu and R.-Z. Ma, *Dalton Trans.*, 2020,49, 10918-10927.