Syntheses, Crystal and electronic Structures, and Characterizations of Quaternary Antiferromagnetic Sulfides: Ba_2MFeS_5 (M= Sb, Bi)

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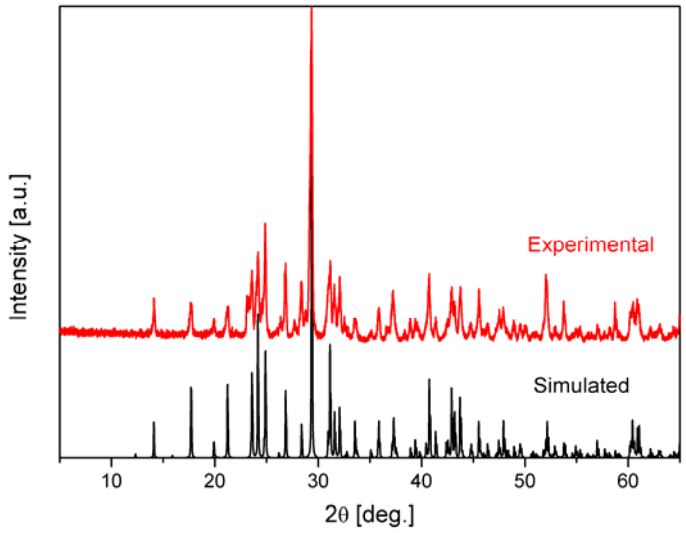
Supporting Information

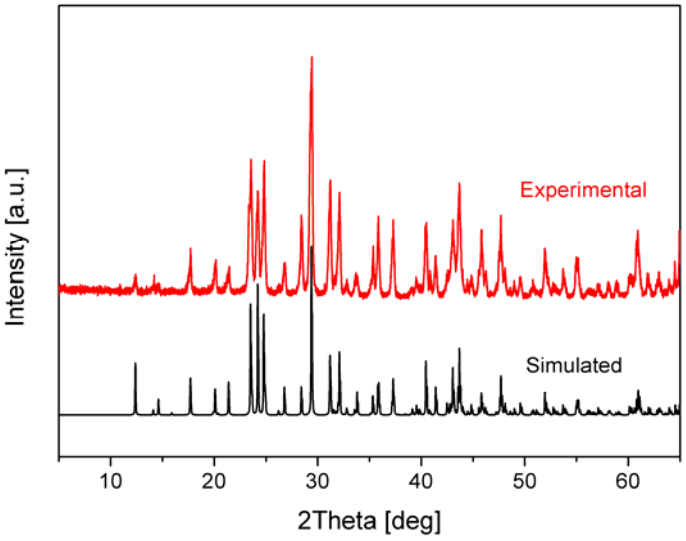
Table S1. The definitions and related state energies (eV) of the special k points for Ba_2SbFeS_5 crystal.

k point	H-VB[a]	L-CB[b]
Γ(0.0, 0.0, 0.0)	–0.00641	1.00872
F(0.0, 0.5, 0.0)	–0.0804	1.01268
Q(0.0, 0.5, 0.5)	–0.10628	1.00526
Z(0.0, 0.0, 0.5)	–0.05219	0.99074
X(0.5, 0.0, 0.5)	–0.01906	1.1073

[a]H-VB, the highest valence band; [b]L-CB, the lowest conduction band.



(a)



(b)

Figure S1. Experimented and simulated X-ray diffraction patterns for polycrystalline Ba_2SbFeS_5 (a) and Ba_2BiFeS_5 (b). (The radiation wavelength of the X-ray is $\lambda = 1.5418$ Å.)

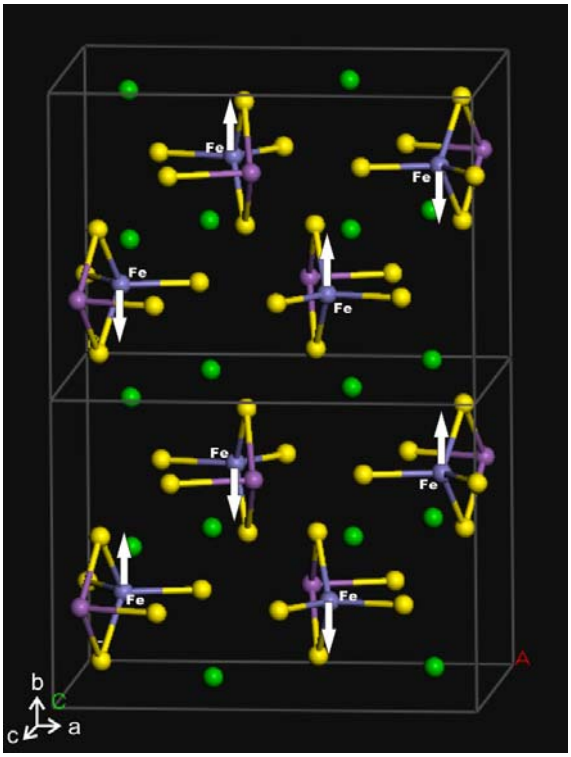


Figure S2. The spin polarization configurations adopted in the band structure calculations for compound Ba_2BiFeS_5.

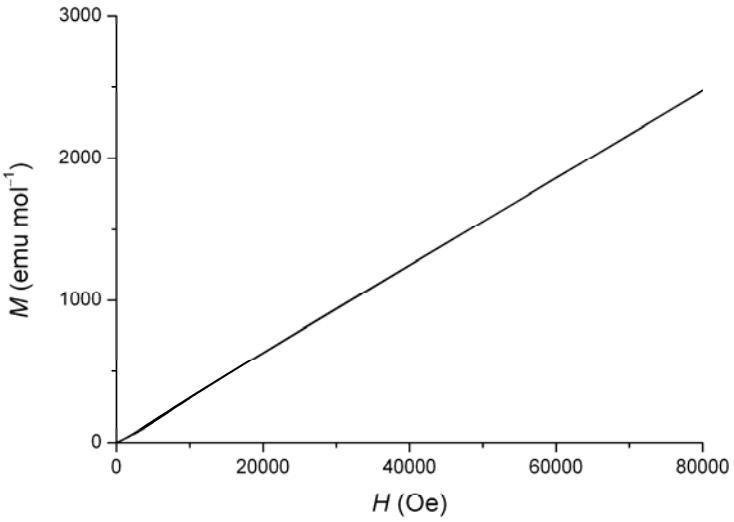


Figure 3. Magnetization (*M*) as a function of magnetic field (*H*) for compound Ba_2BiFeS_5 at T = 2 K.