Supporting Information

A new pnictidehalide with Van Der Waals’ host-guest interactions exhibiting both geometrically spin frustration and resistive humidity sensitivity

Si-Yan Peng,*a,b Liu-Sai Yang,a Ming-Shui Yao,b and Le-Shu Yu,a

a School of Chemistry and Environmental Science, Shangrao Normal University, Shangrao, Jiangxi 343001, P. R. China.
b State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China.
* To whom correspondence should be addressed: E-mail: psypsy524@126.com.

Figure S1. Simulated and experimental (~300 K) XRD powder patterns of 1.
**Figure S2.** TGA spectrum of 1

**Figure S3.** UV diffuse reflectance spectrum of 1 at room temperature. The minor absorptions below 2.20 eV can be ascribed to intraband transition in the valence band or conduction band.
Figure S4. Magnetic loop of 1 at 2K

Figure S5. View of spin configurations of phase I and II along the c direction.