

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.

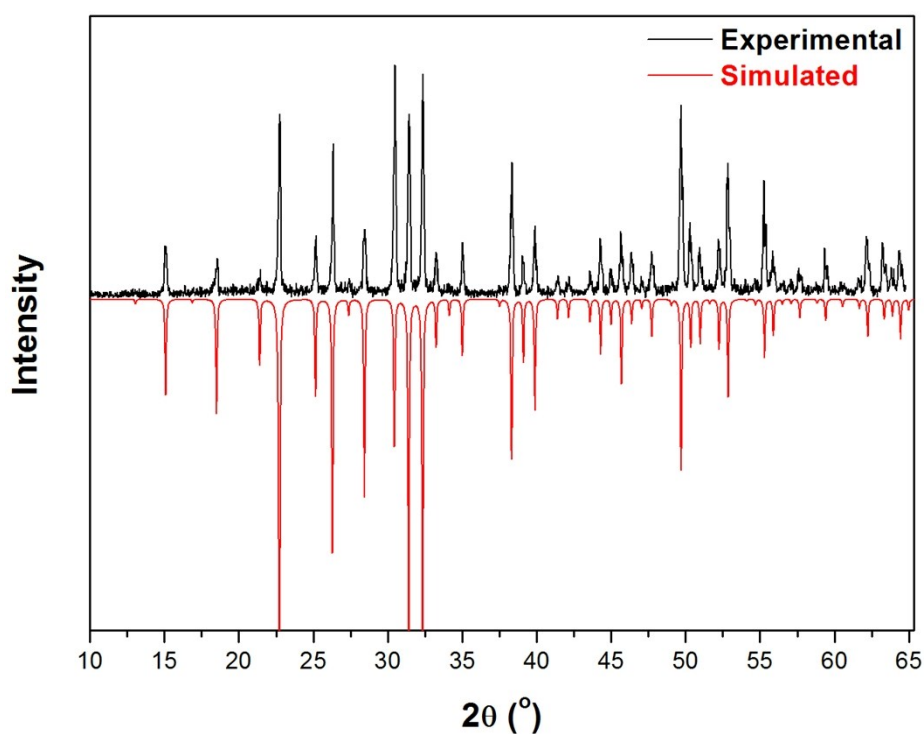


Figure S1. Simulated and experimental (~300 K) XRD powder patterns of **1**.

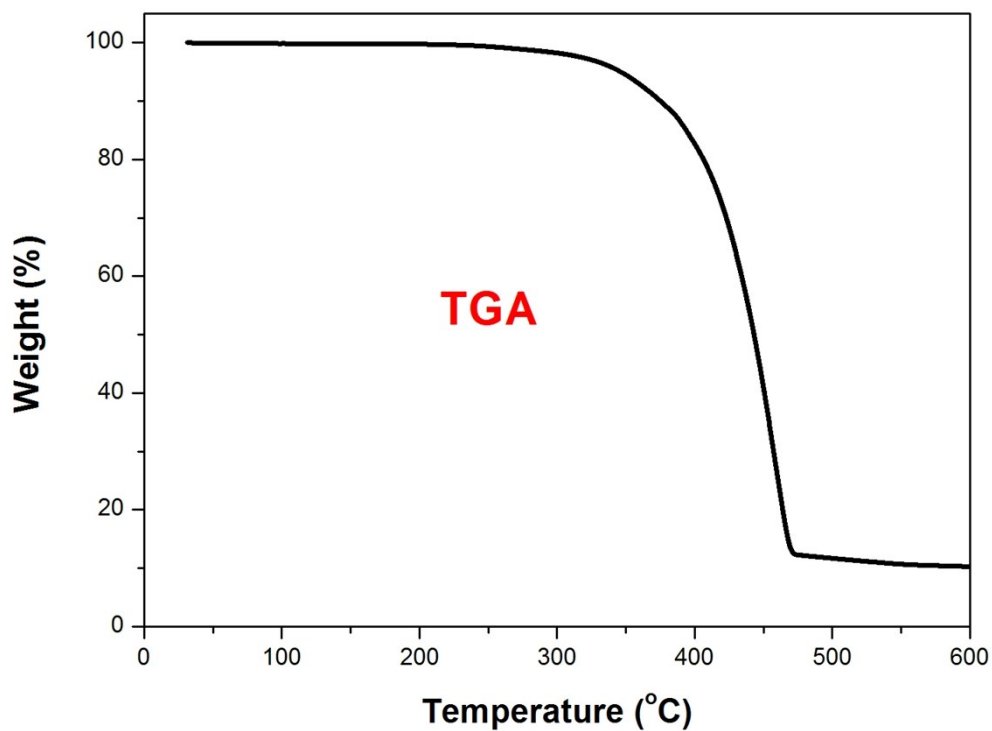


Figure S2. TGA spectrum of **1**

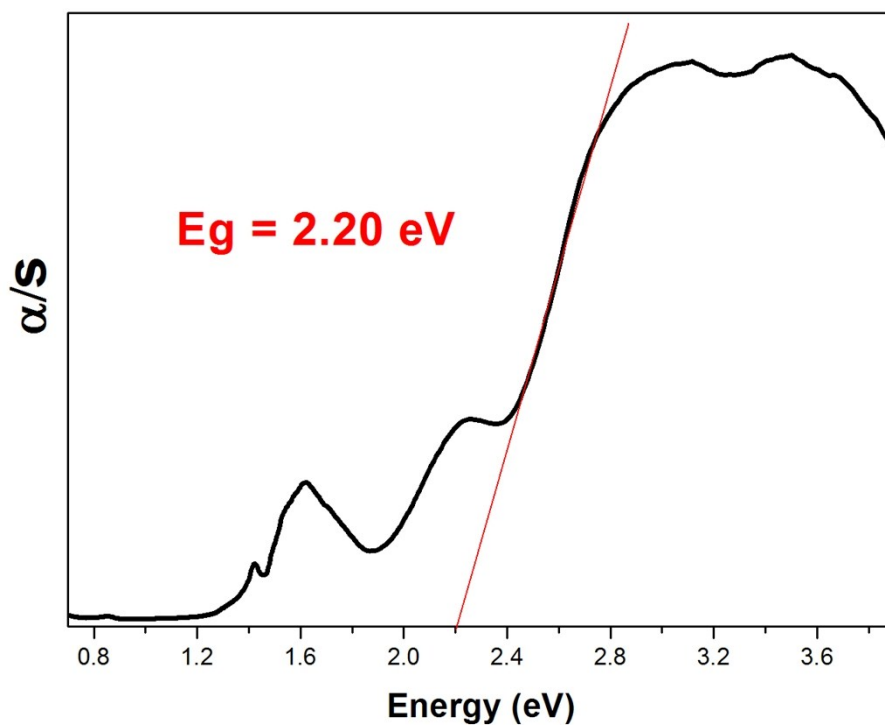


Figure S3. UV diffuse reflectance spectrum of **1** at room temperature. The minor absorptions below 2.20 eV can be ascribed to intraband transition in the valence band or conduction band.

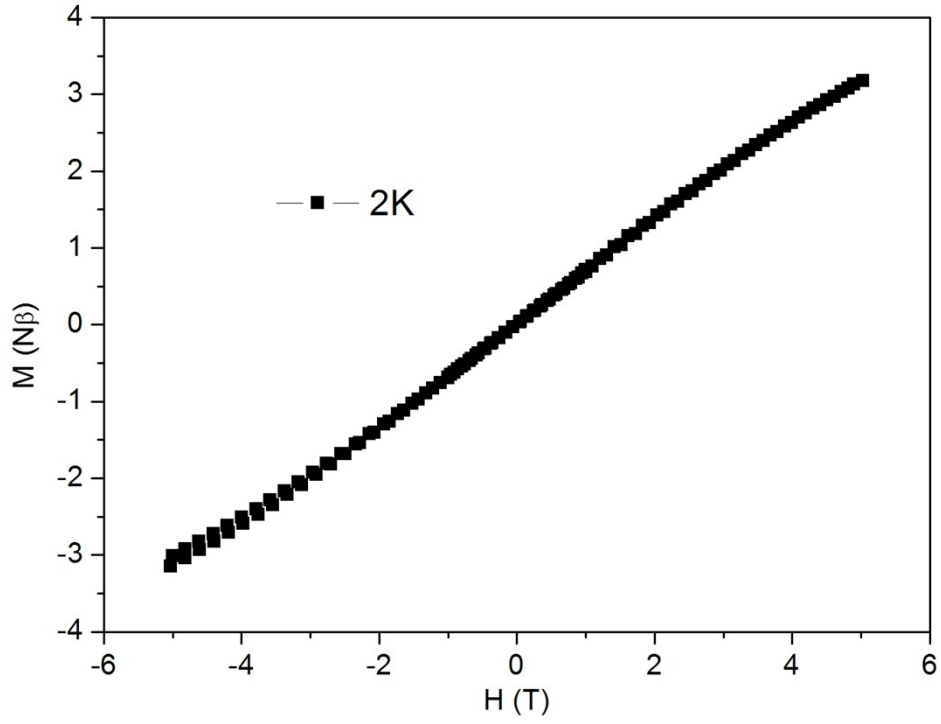


Figure S4. Magnetic loop of 1 at 2K

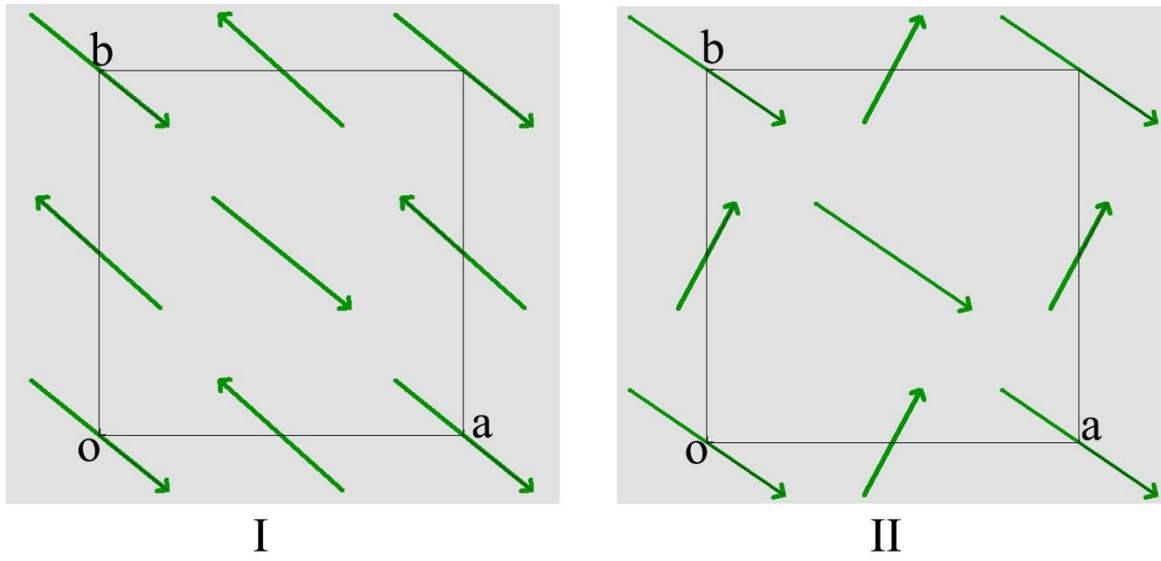


Figure S5. View of spin configurations of phase I and II along the c direction.