Electronic Supplementary Information (ESI)

A New Fe^{III} Substituted Arsenotungstate $[Fe^{III}_2(AsW_6O_{23})_2(As^{III}O_3H)_2]^{12-}$: Synthesis, Structure, Characterization and Magnetic Properties

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Experimental

Materials and methods

All reactions were carried out under aerobic conditions. All other reagents were commercially purchased and were used without further purification. X-Ray powder diffraction pattern was measured at room temperature using a Stoe STADI-P diffractometer with a Cu-Kα radiation at the Institute of Nanotechnology, Karlsruhe Institute of Technology. Fourier transform IR spectrum was measured on a Perkin-Elmer Spectrum One Spectrometer with samples prepared as KBr disks. Elemental compositions were determined by an Inductively Coupled Plasma with Optical Emission Spectroscopy (ICP-OES) at Institute for Applied Materials (IAM-AWP), Karlsruhe Institute of Technology. Thermogravimetric measurement (TGA) was performed using a NETZSCH STA 409C (TA Instruments); 25 mg of the material was

heated up to a temperature of 1000 °C with a heating rate of 10 $Kmin^{-1}$ under nitrogen atmosphere.

Crystallography

Data on a single crystal of **Na-1** was collected at 180 K on a Stoe STADIVARI diffractometer (Ga-Kα, = 1.34143 Å, detector: Dectris Eiger2 R 4M. Absorption corrections were applied using LANA [1].The structure solution was achieved by dual-space direct methods (SHELXT) [2] followed by full-matrix least-squares refinement (SHELXL-2018) [3] within the Olex2 platform (Table 1) [4]. Many of the sodium cations and lattice water molecules were disordered and refined with sets of partial occupancy isotropic atoms, as appropriate. The overall formulation, particularly the number of Na^+ and water molecules, was based on analytical data, and this formula is given in the CIF and the main text. The oxidation numbers of the Fe and As cations were checked using Bond Valence Sum analysis: Fe1: 3.03; As1: 2.99; As2: 3.19 [5,6].

Further details of the crystal structures investigation may be obtained from FIZ Karlsruhe, 76344 Eggenstein-Leopoldshafen, Germany, https://www.ccdc.cam.ac.uk/structures/, on quoting the deposition number CSD-2022893

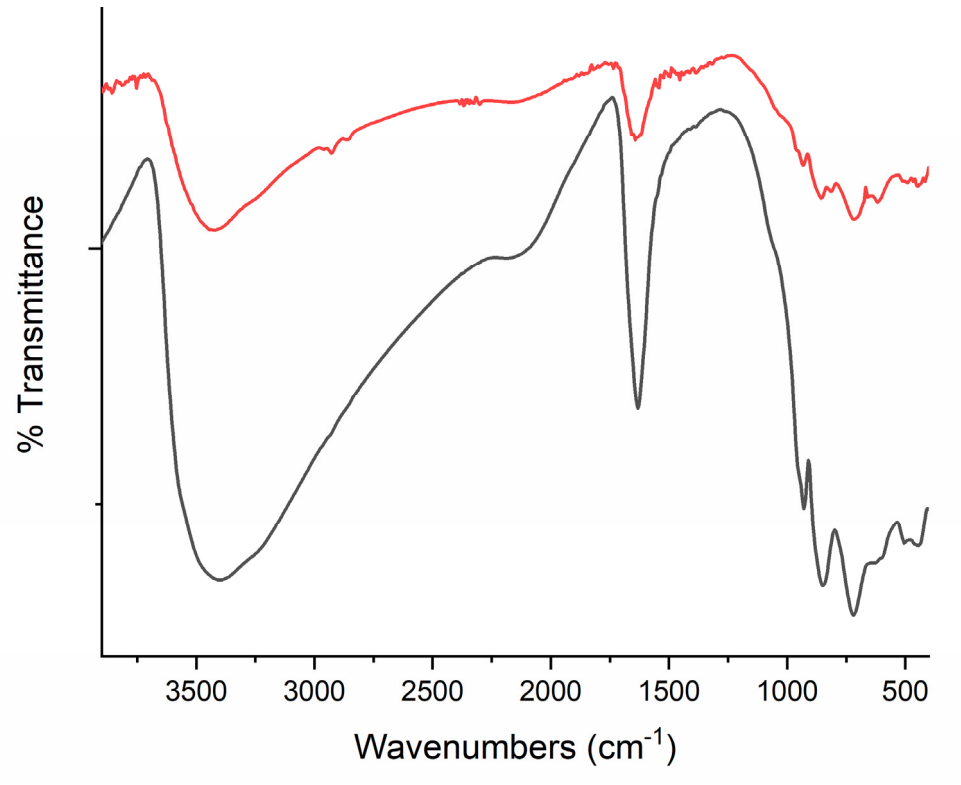

Figure S1. FT-IR spectra of pure **Na-1** (black) and mixture of product obtained in absence of $(Me_2NH_2)^+$ cation (red).

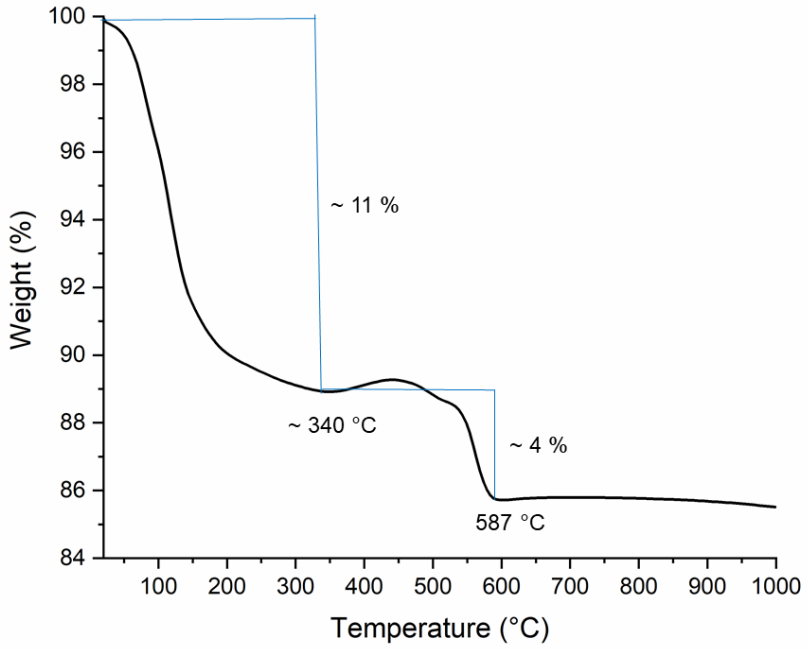

Figure S2. Thermogravimetric analysis (TGA) curve of **Na-1.**

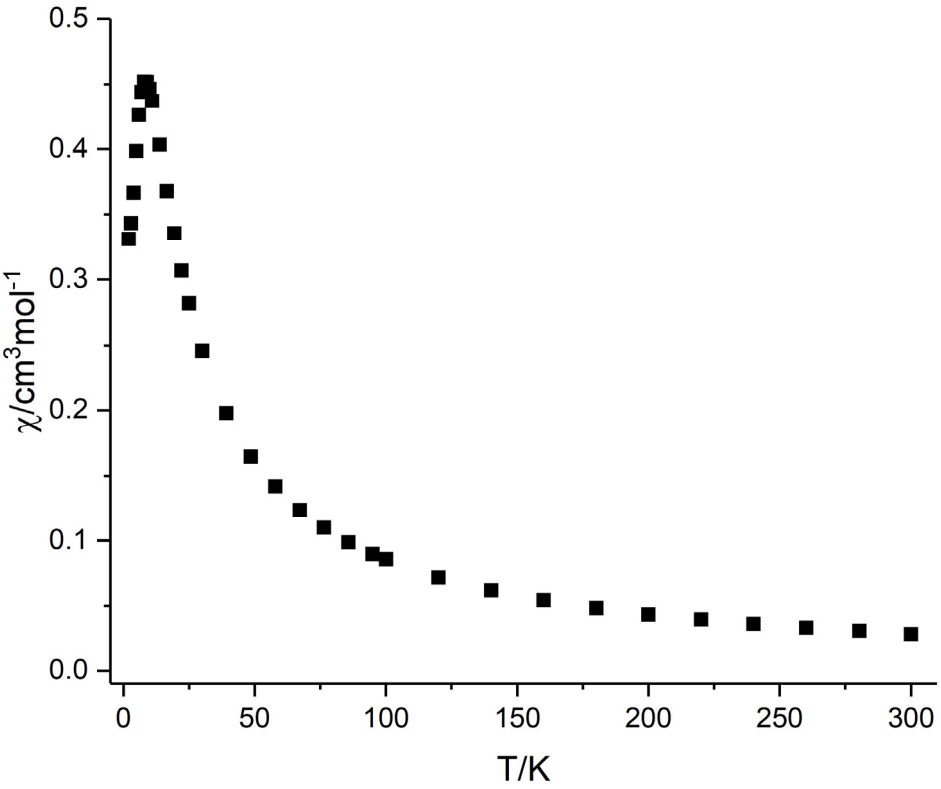

Figure S3. Plot of chiT vs T under 1000 Oe for compound **Na-1.**

References

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