

Supporting Information

A unique dysprosium selenoarsenate(III) exhibiting photocurrent response and slow magnetic relaxation behavior

Jian Zhou,* Hua-Hong Zou,* Rongqing Zhao, Hong Xiao, and Qingran Ding

General Remarks. All analytical grade chemicals were obtained commercially and used without further purification. IR spectra were obtained from a powdered sample pelletized with KBr on an ABB Bomen MB 102 series IR spectrophotometer in the range of 400–4000 cm^{-1} . Energy-dispersive X-ray analysis (EDXA) was taken by using a JEOL JSM-6700F field-emission scanning electron microscope. Room-temperature optical diffuse reflectance spectra of the powdered samples were obtained with a Shimadzu UV-3150 spectrometer. The absorption data were calculated from reflectance spectra by using the Kubelka–Munk function: $a/S = (1-R^2)/2R$, where a is the absorption coefficient, S is the scattering coefficient, and R is the reflectance. PXRD patterns were obtained using a Bruker D8 Advance XRD diffractometer with Cu $K\alpha$ radiation ($\lambda = 1.54056 \text{ \AA}$). The crystals of **1** were grinded and pressed uniformly on the FTO glass. The photocurrent experiment was performed on a CHI650E electrochemistry work station in a three-electrode system, the sample coated ITO glass as the working electrode, a Pt slice as auxiliary electrode and a saturated calomel electrode (SCE) as reference electrode. The supporting electrolyte solution was 0.1 mol·dm⁻³ Na₂SO₄ aqueous solution (100 mL). A 500 W Xe lamp with 420 nm was used as the illumination source. The lamp was kept on continuously, and a manual shutter was used to block exposure of the sample to the light. The sample was typically irradiated at intervals of 60 s.

Crystal Structure Determination

Single-crystal X-ray diffraction data for **1** were recorded on a Rigaku Mercury CCD diffractometer using a ω -scan method with graphite monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) at 173(2) K to a maximum 2θ value (50.20 °). Absorption corrections were applied using multi-scan technique. The structure of **1** was solved by Direct Methods (SHELXS-97) and refined by full-matrix least-squares techniques using the SHELXL-97 program. Non-hydrogen atoms were refined with anisotropic displacement parameters. SIMU restraint prevents the thermal ellipsoids of all adjacent C and N atoms to adopt different orientations. The H atoms bonded to C/N/O atoms were positioned with idealized geometry and refined with fixed isotropic displacement parameters. The As1, As2, Se2 and Se4 atoms were disordered over site occupation factors of 0.85/0.15, 0.88/0.12, 0.85/0.15 and 0.88/0.12, respectively.

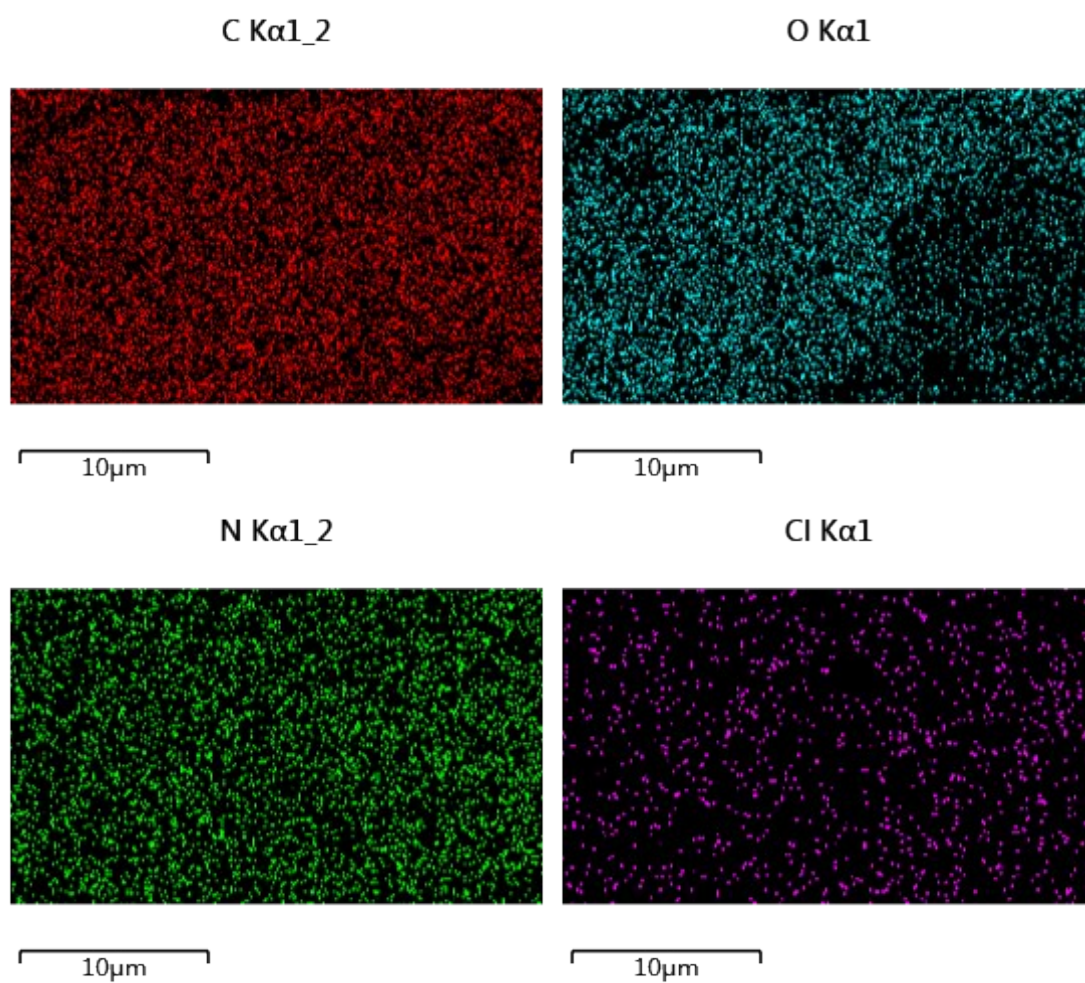


Fig. S1 EDS elemental mappings of C, O, N and Cl for **1**.

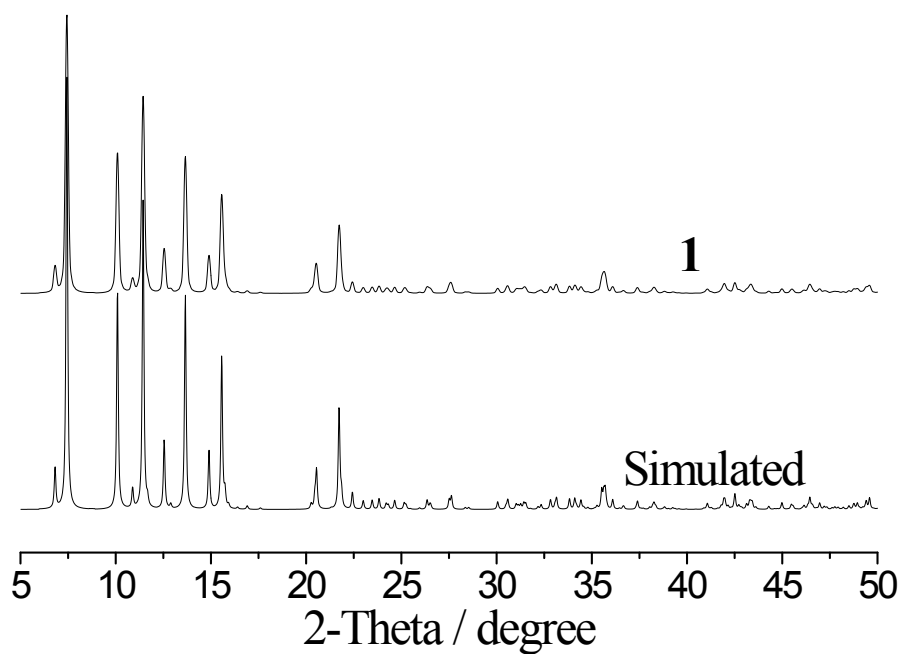


Fig. S2 Simulated and experimental powder XRD patterns of **1**.

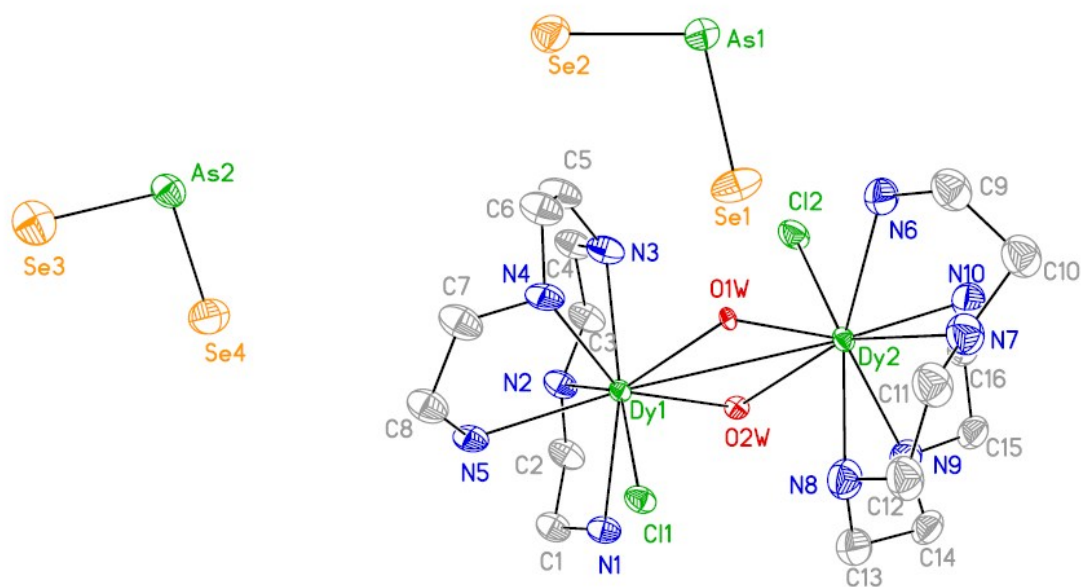


Fig. S3 The asymmetric unit of **1** (H atoms bonded to C and N atoms have been omitted for clarity)

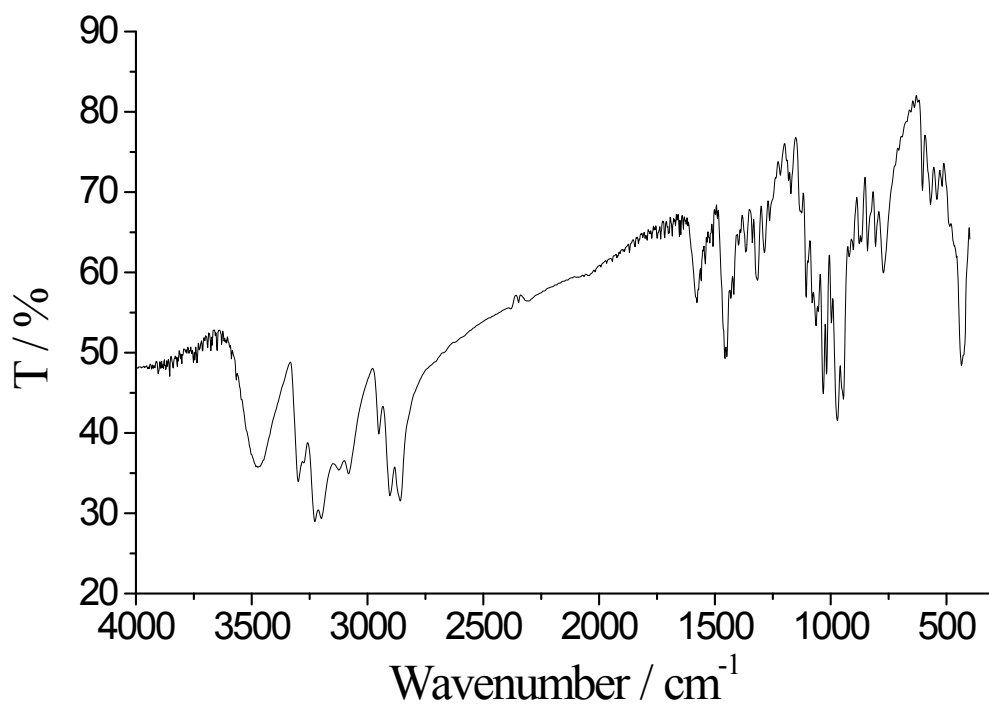


Fig. S4 IR spectrum of 1.

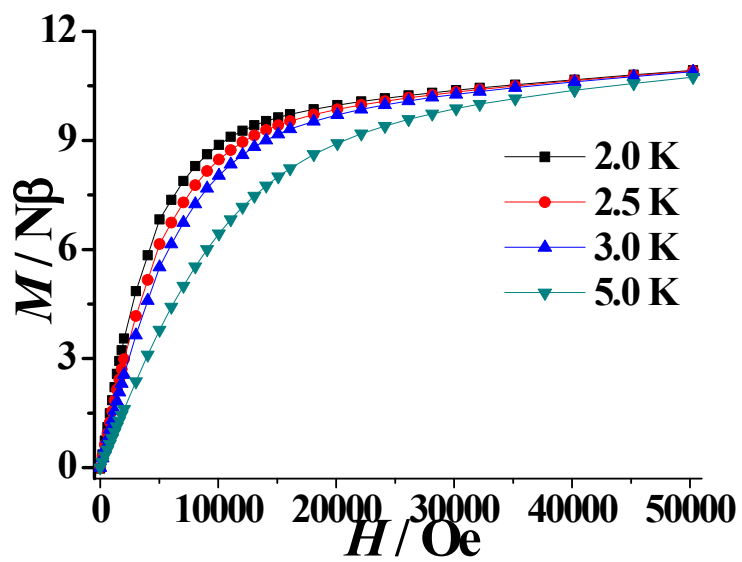


Fig. S5. M vs. H plot at various temperatures for 1.

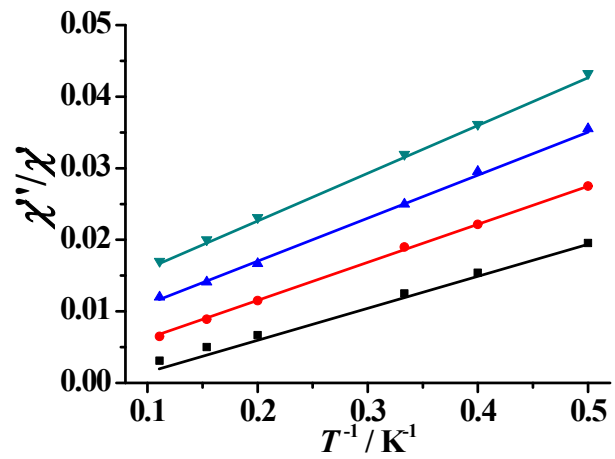


Fig. S6. χ''/χ' vs $1/T$ plot for **1** at four different frequencies (10-1000 Hz range). The solid lines are the best-fit curves.

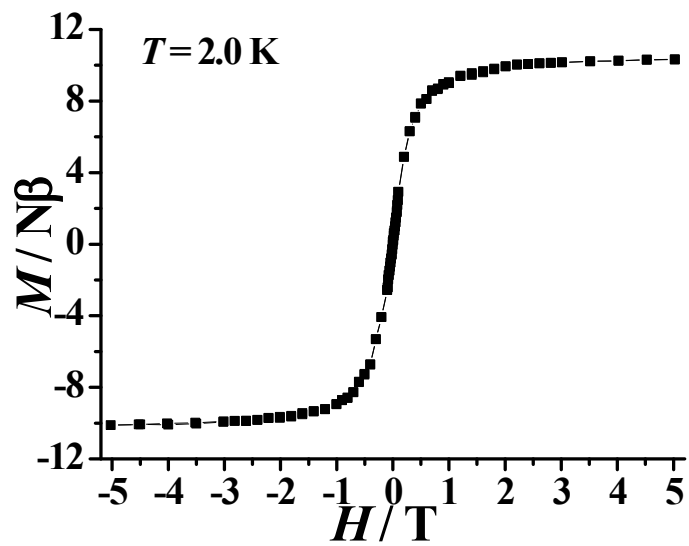


Fig. S7. Magnetic hysteresis loop of **1** recorded at 2 K.