One unprecedented 2-D Mn selenidostannate(IV) incorporating high-nuclear Mn clusters with spin canting behavior

Jian Zhou,* Hong Xiao, Hua-Hong Zou,* Xing Liu and Rongfu Qiu

General Remarks. All analytical grade chemicals were obtained commercially and used without further purification. Elemental analyses (C, N and H) were performed using a PE2400 II elemental analyzer. IR spectra were obtained from a powdered sample pelletized with KBr on an ABB Bomen MB 102 series IR spectrophotometer in the range of 400–4000cm^{-1}. The solide-state UV/Vis spectra were measured at room temperature using a PE Lambda 900 UV/Vis spectrophotometer, and a $BaSO_4$ plate was used as a standard. The absorption data were calculated from reflectance spectra by using the Kubelka-Munk function: $\alpha/S = (1-R^2)/2R$, where α 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 Kα radiation (λ = 1.54056 Å).Variable-temperature magnetic susceptibility measurements were carried out in the temperature range of 2–300 Kwith a Quantum Design MPMS-XL-5 magnetometer.

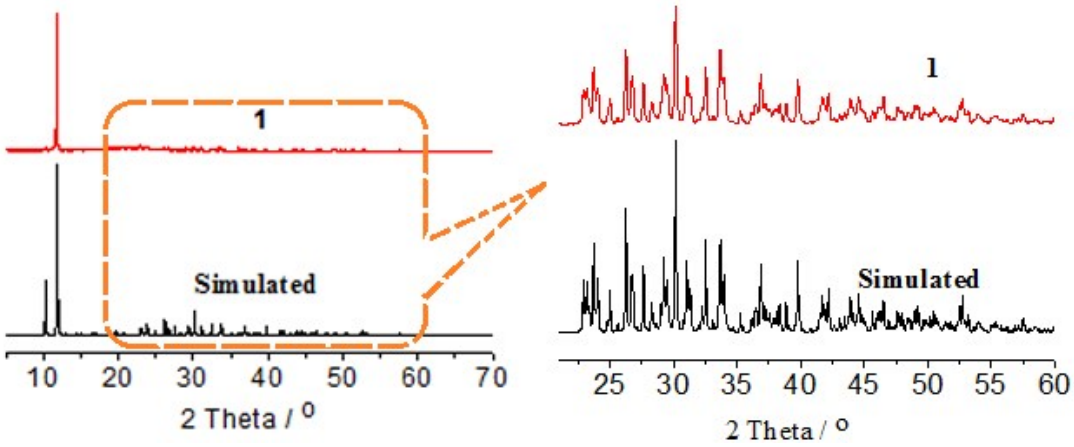


Fig. S1 Simulated, and experimental powder XRD patterns of **1**.

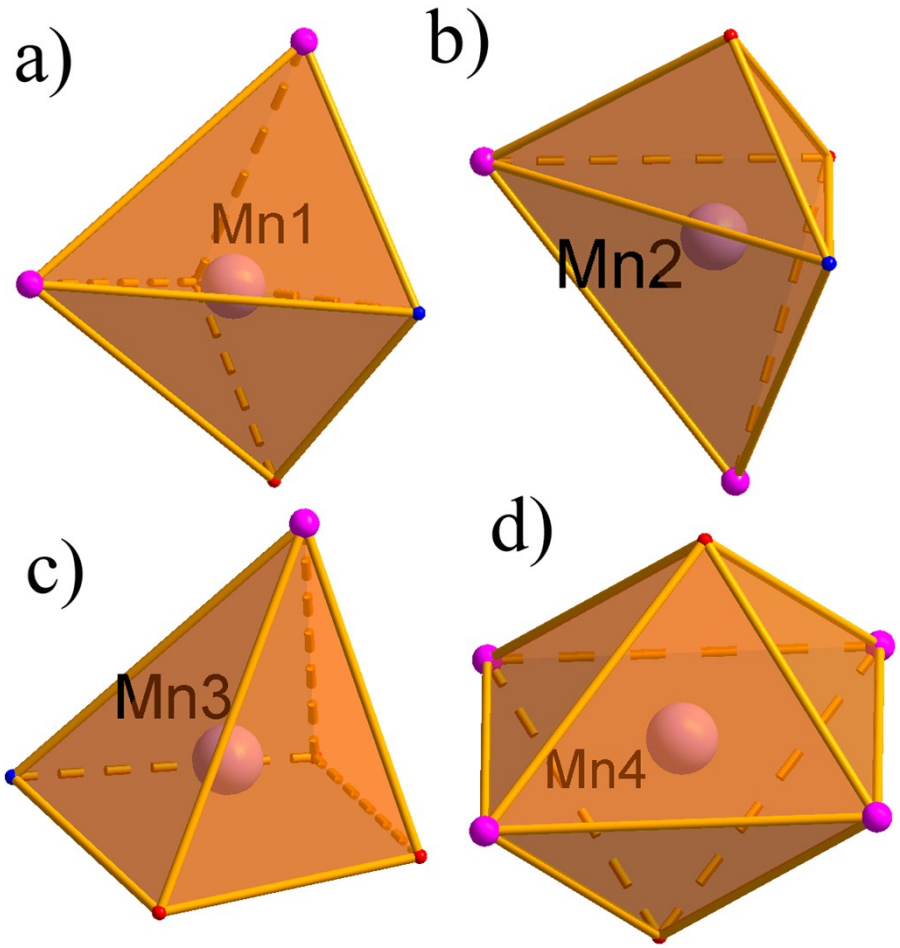


Fig. S2 The coordination environment of $Mn(1)^{2+}$, $Mn(2)^{2+}$, $Mn(3)^{2+}$ and $Mn(4)^{2+}$ ions in **1**.

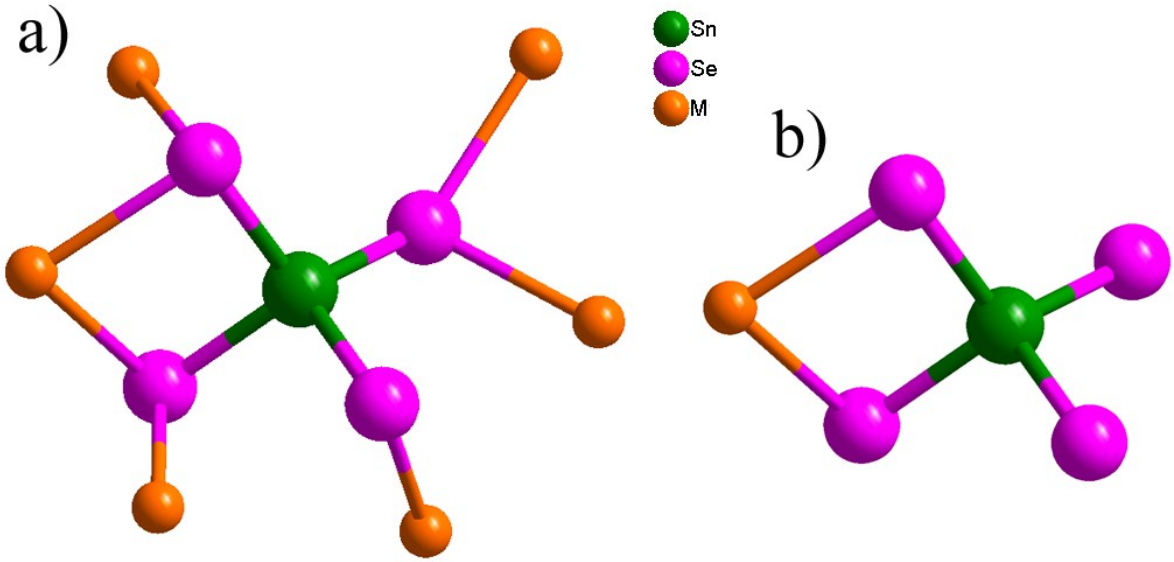


Fig.S3 The link mode of $[SnSe_4]^{4-}$ anion.

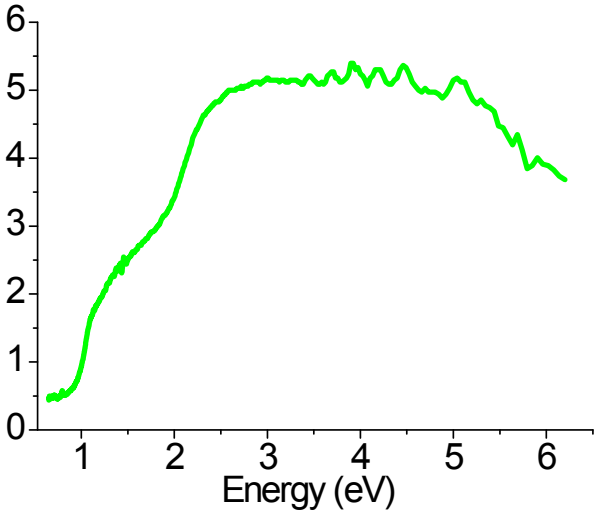
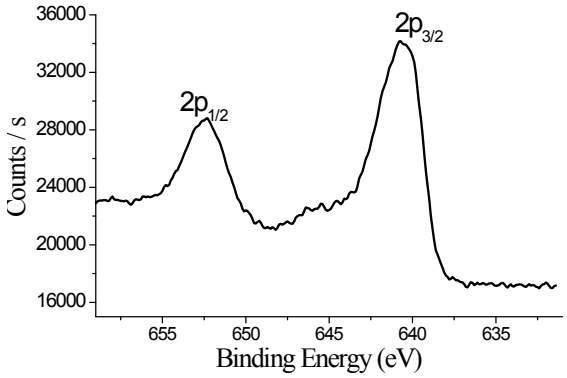
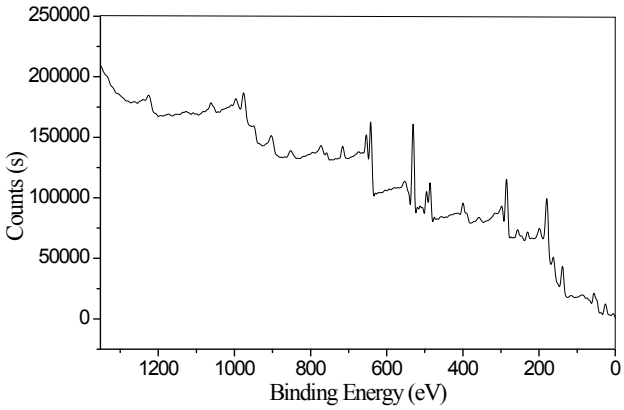


Fig. S4 Solid-state UV-Vis absorption spectrum of **1**.



(a)



(b)

Fig. S5 (a) Mn 2p XPS spectrum of **1**. (b) XPS survey spectrum of **1**.

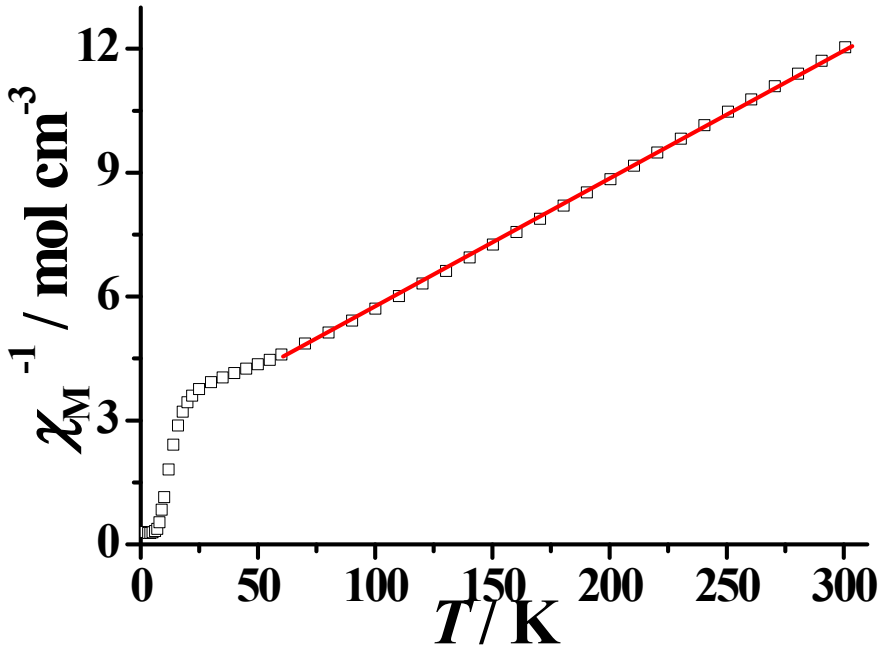


Fig. S6 χ_M^{-1}–T curve of **1.**

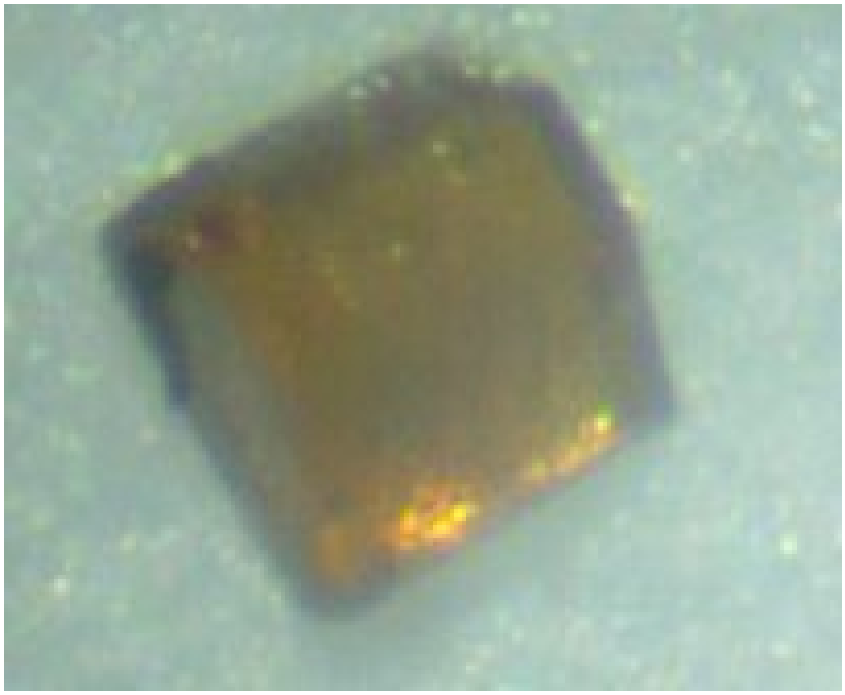


Fig. S7 the photo of single crystal

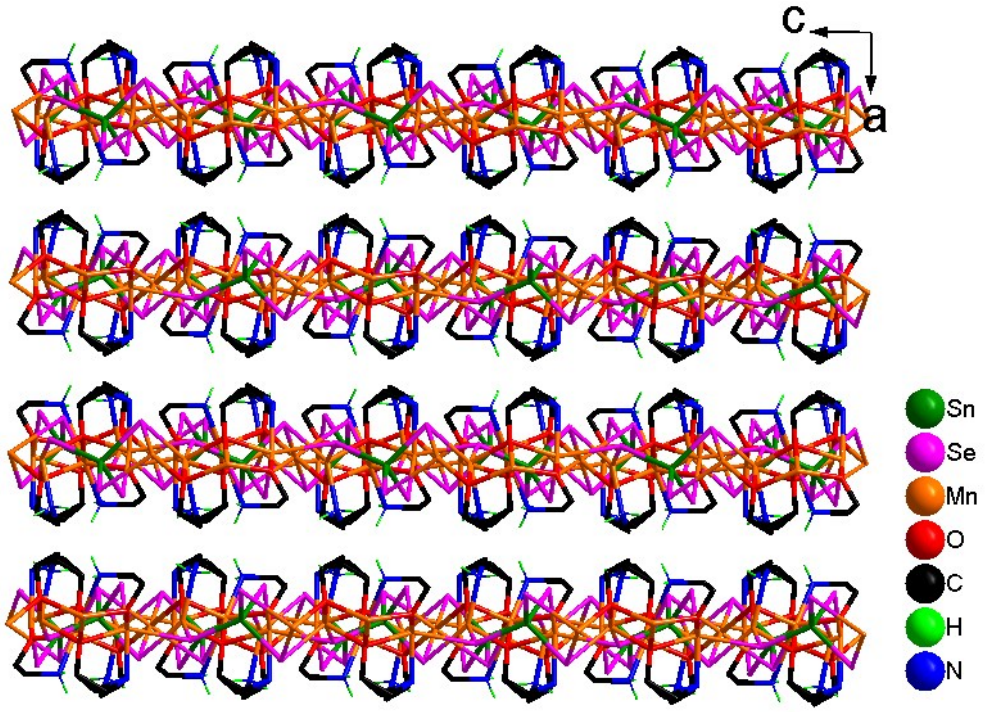


Fig. S8 the crystal packing diagram of **1**. The H atoms on C atoms are omitted for clarity.

Table S1 Selected bond lengths [Å] for **1**.

Sn(1)-Se(4)	2.5017(9)	Sn(1)-Se(2)	2.5241(8)
Sn(1)-Se(1)	2.5180(8)	Sn(1)-Se(3)	2.5471(8)
Mn(1)-O(3)	2.008(5)	Mn(2)-O(1)	2.121(5)
Mn(1)-N(1)	2.202(6)	Mn(2)-N(2)	2.189(6)
Mn(1)-O(1)	2.250(4)	Mn(2)-O(2)	2.312(5)
Mn(1)-Se(4)	2.5611(13)	Mn(2)-Se(3)#2	2.6831(13)
Mn(1)-Se(1)#1	2.8468(13)	Mn(2)-Se(1)	2.7506(13)
Mn(3)-O(3)	2.063(5)	Mn(4)-O(2)#4	2.190(4)
Mn(3)-O(2)	2.121(4)	Mn(4)-O(2)	2.190(4)
Mn(3)-O(1)	2.244(5)	Mn(4)-Se(3)#3	2.8536(7)
Mn(3)-N(3)	2.274(6)	Mn(4)-Se(3)#2	2.8536(7)
Mn(3)-Se(2)#3	2.5765(12)	Mn(4)-Se(2)#3	2.8769(7)
Mn(4)-Se(2)#2	2.8769(7)		

Symmetry transformations used to generate equivalent atoms: #1 x,-y+3/2,z-1/2; #2 x,-y+3/2,z+1/2; #3 -x,y+1/2,-z+1/2; #4 -x,-y+2,-z+1.