# Supporting Information

## Stabilization of $(SnS_4)^{4-}$ Anion by Coordinating to $[TM(\pi\text{-conjugated-ligand})_m]^{n+}$ Complex: A Chain-like Thiostannate(IV) $\{[Mn(phen)]_2(SnS_4)\}_n \cdot nH_2O$ Exhibiting an Unprecedented Link Mode of the $(SnS_4)^{4-}$ Anion

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### 1. Materials and Synthesis

All reagents were purchased commercially and used without further purification. $\{[Mn(phen)]_2(SnS_4)\}_n \cdot nH_2O$ (**1**) was prepared from a mixture of Sn (0.059 g, 0.50 mmol), $MnCl_2 \cdot 4H_2O$ (0.198 g, 1 mmol), S (0.064 g, 2 mmol) and phen (0.090 g, 0.50 mmol) in 4 mL methylamine solution (30% in $H_2O$) which was sealed in a stainless steel reactor with a 25-mL Teflon linear, heated at 170 °C for 5 days and then cooled to room temperature. The product consists of red block crystals of **1** and some indefinite dark-red powder. The crystals of **1** can be selected by hand, washed by ethanol and diethyl ether. The product is stable in air and water. (Yield: 0.025 g, 6.8% based on Sn). Anal. Cala. for $C_{24}H_{18}Mn_2N_4OS_4Sn$ **1**: C, 39.21%; H, 2.47%; N, 7.62%. Found: C, 37.45%; H, 2.51%; N, 7.34%.

### 2. Crystal Structure

The intensity data set was collected on a Rigaku SCXmini CCD diffractometer equipped with graphite-monochromated Mo-$K\alpha$ radiation ($\lambda$ = 0.71073 Å) using $\omega$-scan technique at 293 K. The data set was reduced by CrystalClear program.[1] The structure was solved by

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direct methods using the Siemens SHELXL package of crystallographic software.[2] The difference Fourier maps created on the basis of these atomic positions to yield the other non-hydrogen atoms. The structure was refined using a full-matrix least-squares refinement on $F^2$. All non-hydrogen atoms were refined anisotropically. Crystallographic data and structural refinements are summarized in Table S1. More details on the crystallographic studies as well as atom displacement parameters are given in Table S2.

**Table S1** Crystal and Structure Refinement Data for **1**.

| | **1** |
|---|---|
| Formula | $C_{24}H_{18}Mn_2N_4OS_4Sn$ |
| *M*r (g mol$^{-1}$) | 735.23 |
| Color, habit | Red, Block |
| Cryst size (mm$^3$) | 0.20×0.15×0.15 |
| Cryst syst | Monoclinic |
| Space group | *C*2/*m* |
| $D_{calcd}$ (g cm$^{-3}$) | 1.923 |
| *a* (Å) | 16.146(2) |
| *b* (Å) | 19.262(2) |
| *c* (Å) | 9.938(1) |
| $\alpha$(°) | 90 |
| $\beta$(°) | 124.970(4) |
| $\gamma$(°) | 90 |
| *V* (Å$^3$) | 2532.6(5) |
| *Z* | 4 |
| abs coeff (mm$^{-1}$) | 2.318 |
| *F*(000) | 1448 |
| Reflns collcd/unique ($R_{int}$) | 9625/2436 (0.0300) |
| Data/params/restraints | 2180/173/0 |
| $R_1$[a] [$I>2\sigma(I)$] | 0.0249 |

| | |
|---|---|
| $wR_2$[b] [$I>2\sigma(I)$] | 0.0564 |
| Goodness of fit | 0.995 |
| $\Delta\rho_{max}$ and $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.425, –0.395 |

[a] $R1 = \sum||Fo|-|Fc||/\sum|Fo|$, [b] $wR2 = \{\sum w[(Fo)^2-(Fc)^2]^2/\sum w[(Fo)^2]^2\}^{1/2}$

**Table S2** Selected Bond Lengths (Å) and Angles (°) for **1**.

| Bond | (Å) | Bond | (Å) |
|---|---|---|---|
| Sn(1)-S(1) | 2.411(1) | Mn(2)-N(21)#3 | 2.295(2) |
| Sn(1)-S(1)#1 | 2.411(1) | Mn(1)-S(1) | 2.544(1) |
| Sn(1)-S(2) | 2.343(1) | Mn(1)-S(1)#1 | 2.544(1) |
| Sn(1)-S(3) | 2.405(1) | Mn(1)-S(2)#2 | 2.487(1) |
| Mn(1)-N(11) | 2.290(2) | Mn(2)-S(1)#1 | 2.687(1) |
| Mn(1)-N(11)#1 | 2.290(2) | Mn(2)-S(3) | 2.626(1) |
| Mn(2)-N(21) | 2.295(2) | Mn(2)-S(3)#4 | 2.626(1) |
| | | | |
| Angle | (°) | Angle | (°) |
| S(2)-Sn(1)-S(3) | 115.21(3) | S(2)#2-Mn(1)-S(1)#1 | 113.52(2) |
| S(2)-Sn(1)-S(1) | 119.90(2) | N(11)-Mn(1)-S(1) | 91.24(6) |
| S(3)-Sn(1)-S(1) | 100.30(2) | N(11)#1-Mn(1)-S(1) | 149.54(6) |
| S(2)-Sn(1)-S(1)#1 | 119.90(2) | S(2)#2-Mn(1)-S(1) | 113.52(3) |
| S(3)-Sn(1)-S(1)#1 | 100.30(2) | S(1)#1-Mn(1)-S(1) | 90.83(4) |
| S(1)-Sn(1)-S(1)#1 | 97.42(3) | N(21)-Mn(2)-N(21)#3 | 72.80(11) |
| N(11)-Mn(1)-N(11)#1 | 72.31(11) | N(21)-Mn(2)-S(3)#4 | 168.11(6) |
| N(11)-Mn(1)-S(2)#2 | 93.34(6) | N(21)#3-Mn(2)-S(3)#4 | 95.48(6) |
| N(11)#1-Mn(1)-S(2)#2 | 93.34(6) | N(21)-Mn(2)-S(3) | 95.48(6) |
| N(11)-Mn(1)-S(1)#1 | 149.54(6) | N(21)#3-Mn(2)-S(3) | 168.11(6) |
| N(11)#1-Mn(1)-S(1)#1 | 91.24(6) | S(3)#4-Mn(2)-S(3) | 96.29(3) |

[a] Symmetric codes for **1**: #1 x, –y+1, z; #2 –x+1, –y+1, –z; #3 –x+1, y, –z+1; #4 –x+1, –y+1, –z+1.

**Table S3** Selected Hydrogen Bonds Data for **1**.

| D-H···A | D-H (Å) | H···A (Å) | D···A (Å) | ∠(DHA) (°) |
|---|---|---|---|---|
| O1W-H1WA···S1[a] | 0.82 | 2.44 | 3.245(2) | 172 |
| C12-H12A···O1W | 0.93 | 2.78 | 3.291(4) | 116 |
| C13-H13A···O1W | 0.93 | 2.74 | 3.270(4) | 117 |

Symmetry codes: a 1/2-x, 1/2-y, -z.

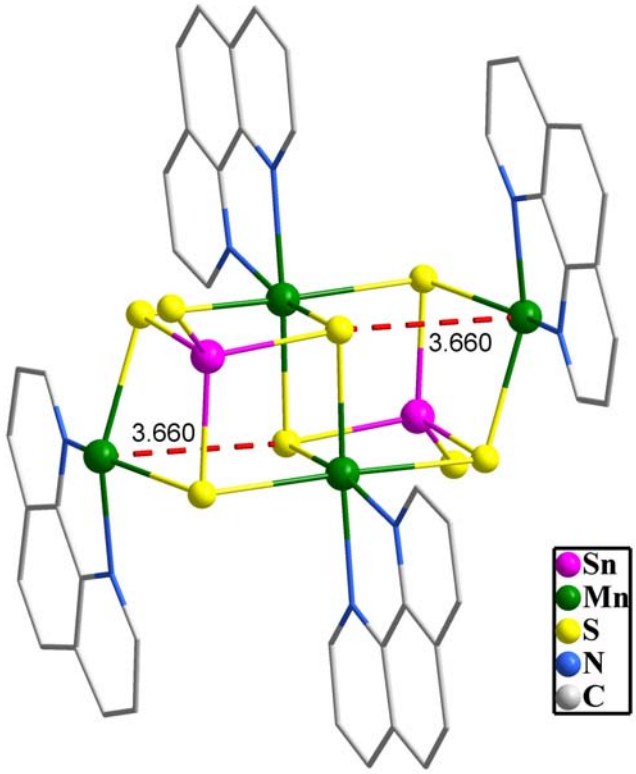


**Fig. S1** The face-shared double-cubane-like unit in **1**. Dash lines show the longer Mn–S separations (Å).

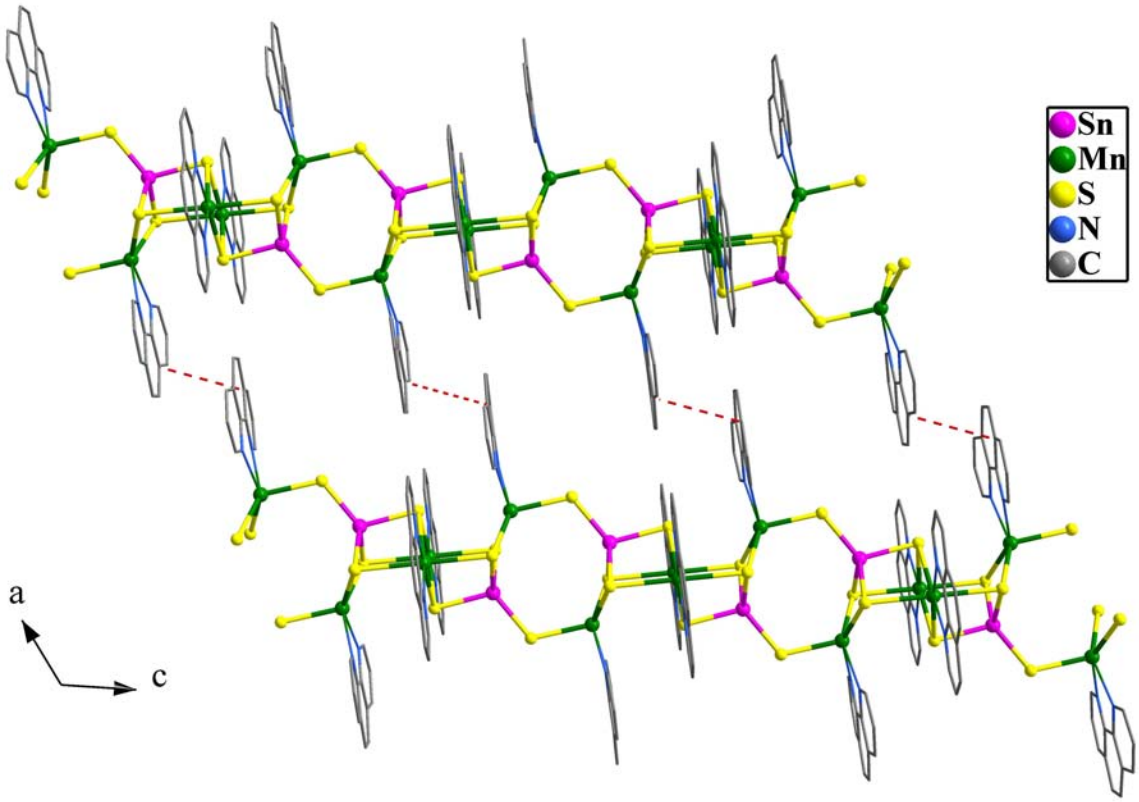


**Fig. S2** 2-D extended layer structure of **1** assembled by the face-to-face $\pi$–$\pi$ stacking interactions (red dashed lines). Hydrogen atoms are omitted for clarity.

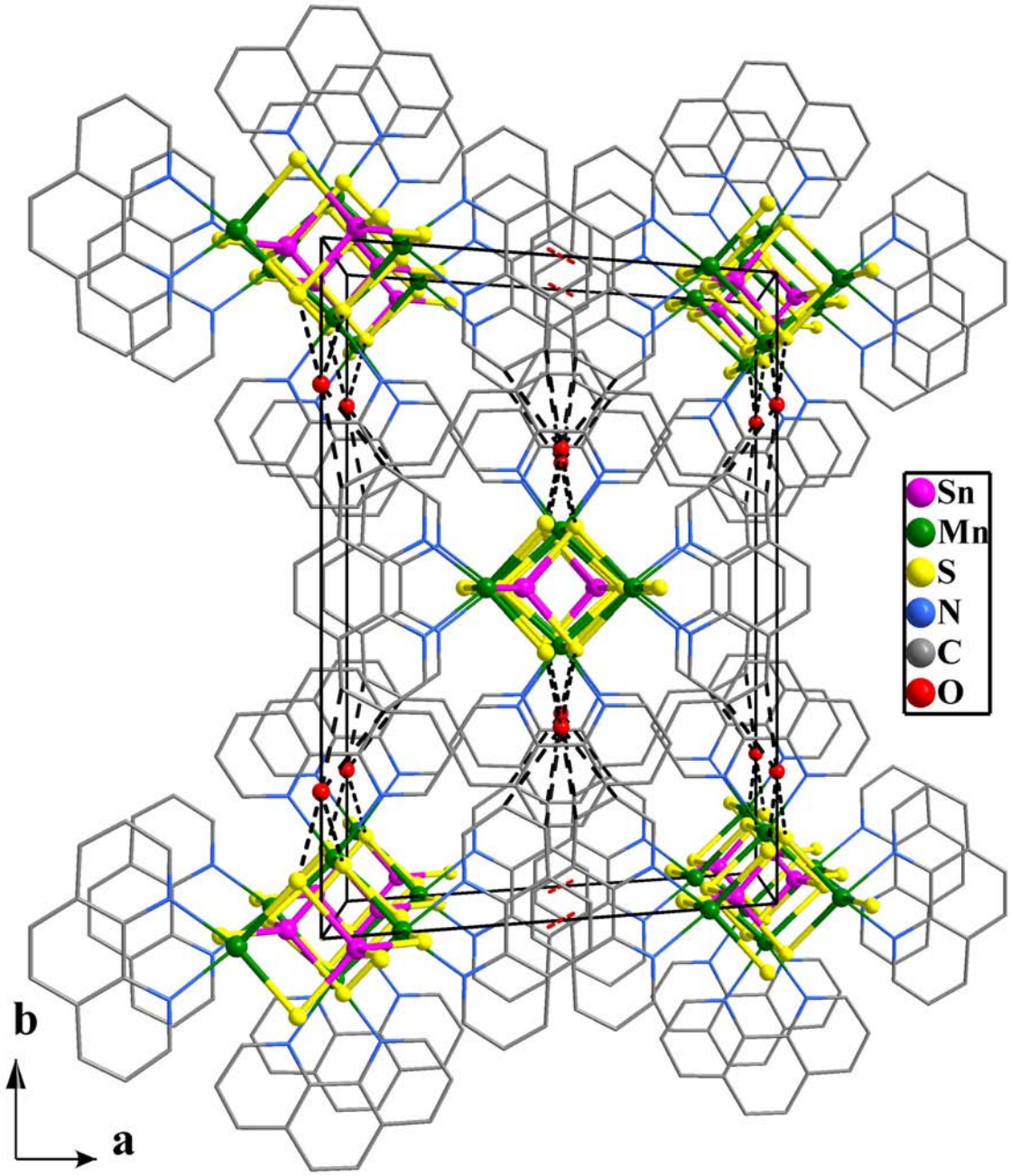


**Fig. S3** The crystal-packing diagram of **1** in a perspective view along the *c* axis showing the face-to-face $\pi$–$\pi$ stacking interactions (red dashed lines) and the intermolecular hydrogen bonds (black dashed lines). Hydrogen atoms are omitted for clarity.

### 3. Physical measurements

Elemental analyses of C, H, and N were performed on an Elementar Vario EL III microanalyzer. A NETZSCH STA 449C thermogravimetric analyzer was used to obtain TG and DTA curves in $N_2$ with a ramp rate of 10 °C·min$^{-1}$ in the temperature range 30–1000 °C.

An empty $Al_2O_3$ crucible was used as the reference. The FT-IR spectrum was obtained on a Perkin-Elmer spectrophotometer using KBr disk in the range 4000–400 $cm^{-1}$. Powder X-ray diffraction (PXRD) pattern was recorded on a PANalytical X'pert PRO diffractometer using Cu-$K\alpha$ radiation. The solid-state fluorescence excitation and emission spectra were performed on an Edinberg EI920 fluorescence spectrophotometer at room temperature with a wavelength increment of 1.0 nm and integration time of 0.2 s. Optical diffuse reflectance spectra was measured at room temperature with a PE Lambda 900 UV-Vis spectrophotometer. The instrument was equipped with an integrating sphere and controlled by a personal computer. The samples were ground into fine powder and pressed onto a thin glass slide holder. The $BaSO_4$ plate was used as a standard (100% reflectance). The absorption spectra was calculated from reflectance spectra using the Kubelka-Munk function: $\alpha/S = (1-R)^2/2R$,[3] where $\alpha$ is the absorption coefficient, $S$ is the scattering coefficient (which is practically wavelength independent when the particle size is larger than 5 $\mu$m), and $R$ is the reflectance. Magnetic susceptibility was measured using a MPMS XL Quantum Design SQUID magnetometer. All data was corrected for diamagnetism estimated from Pascal's constants.

**3.1 IR Spectra**

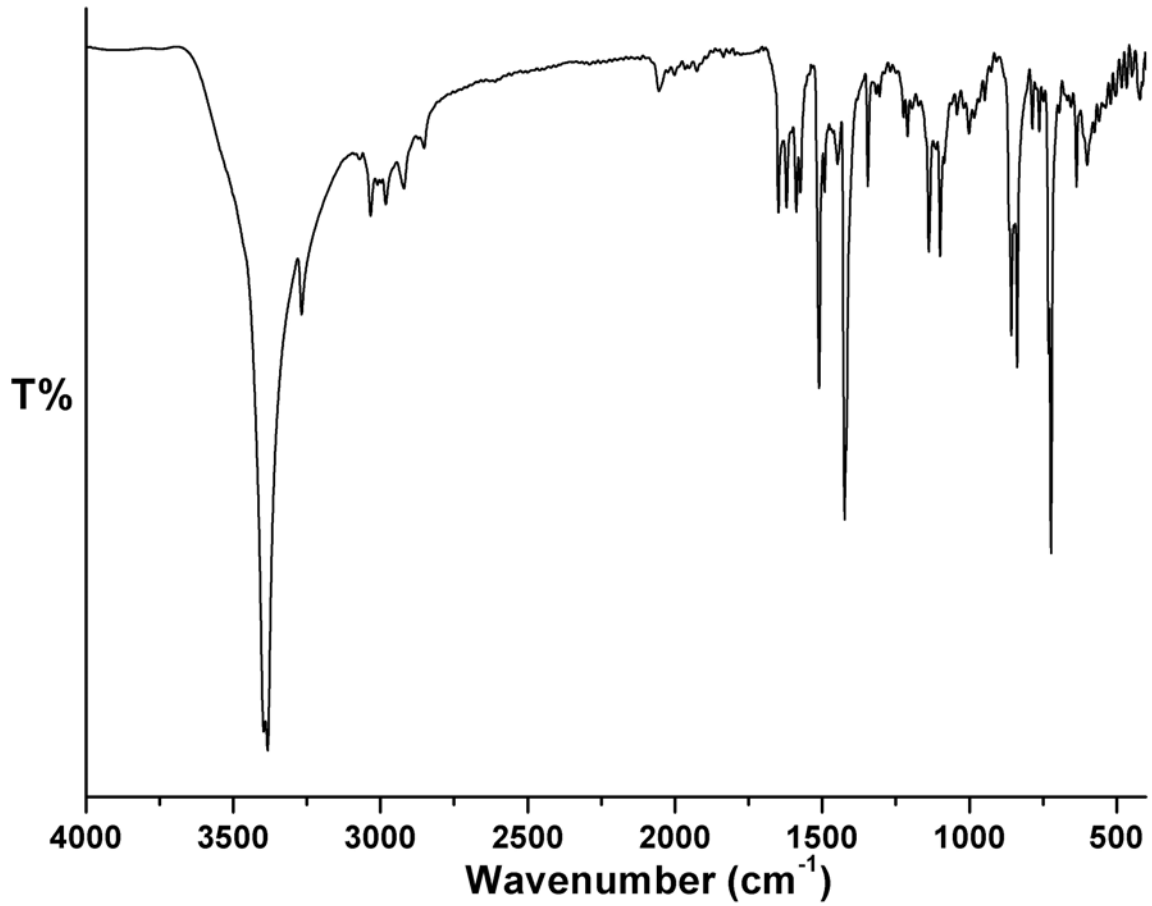


**Fig. S4** IR Spectrum of **1**.

**IR data analysis:**

**Table S4** IR Spectral Data of **1**.

| | |
|---|---|
| Compound **1** | 3383vs, 3267vw, 3033vw, 2984vw, 2919vw, 2848vw, 2054vw, 1648w, 1622w, 1689w, 1511m, 1424s, 1345vw, 1210vw, 1100w, 1002vw, 838m, 723s, 636vw, 575vw |

In the IR Spectrum of **1**, the bands in the region of 3047–2849 $cm^{-1}$ correspond to the C–H vibrations of the aromatic ring hydrogen atoms. The bands in the range 1648–1422 $cm^{-1}$ are attributed to ring vibrations of the phen ligand (C=C and N=N). 3421–3383 $cm^{-1}$ are assigned to the O–H modes of $H_2O$.

**3.2 PXRD**

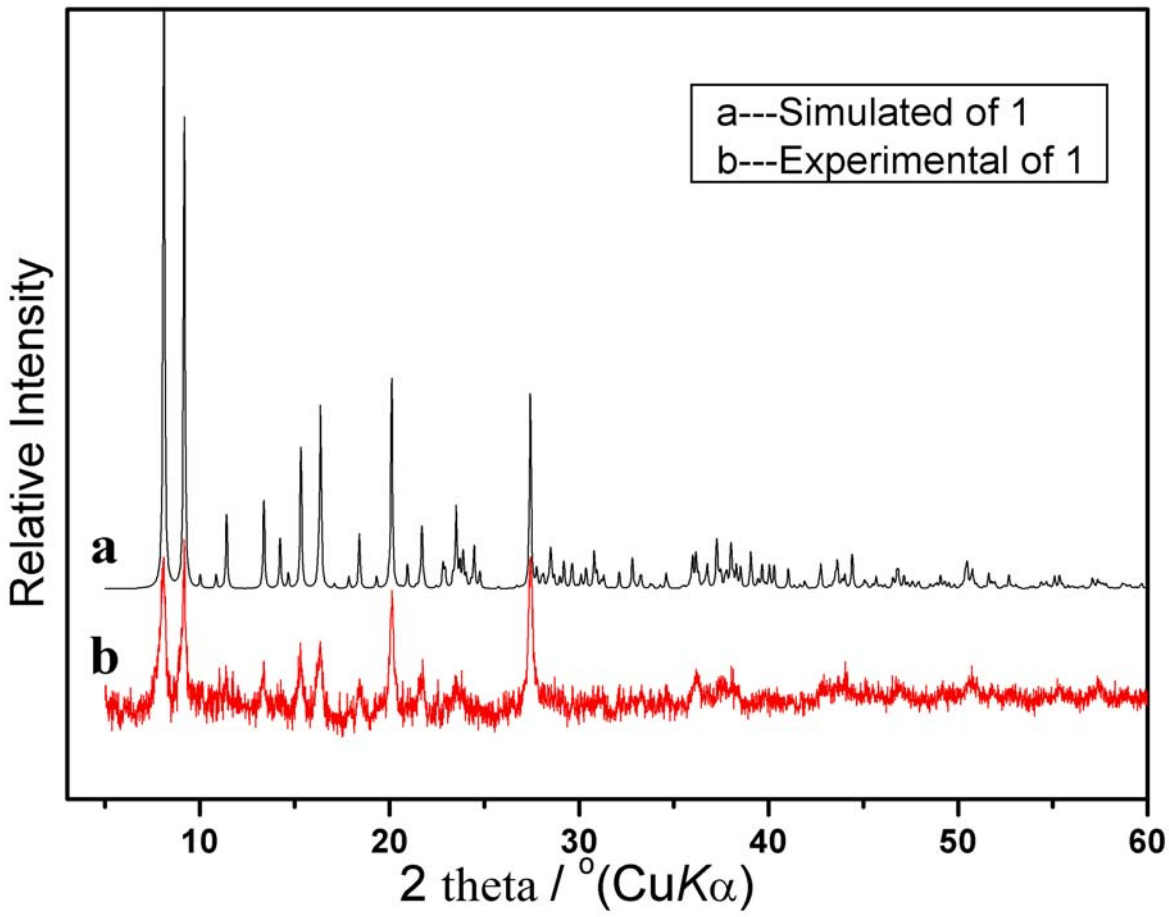


**Fig. S5** The PXRD pattern of **1** (red) is in good agreement with the simulated PXRD pattern calculated from single crystal X-ray data of **1** (black).

### 3.3 TGA

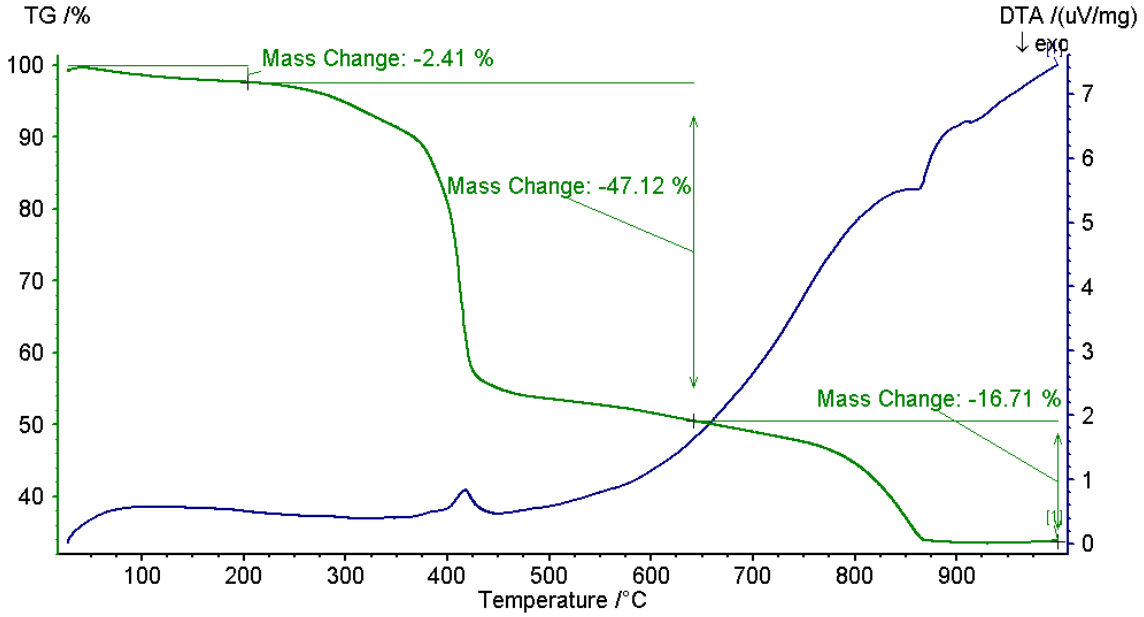


**Fig. S6** TG and DTA curves for **1**.

Thermalgravimetric analyse for **1** revealed a small weight loss of about 2.41% between 30 and 204 °C, which correspond to the removal of one water molecule per formula (calcd 2.45%). A significant weight loss (about 47.12%) was observed between 204 and 614 °C, which is close to the removal of the phen ligands (calcd 49.02%).

### 3.4 Photoluminescence

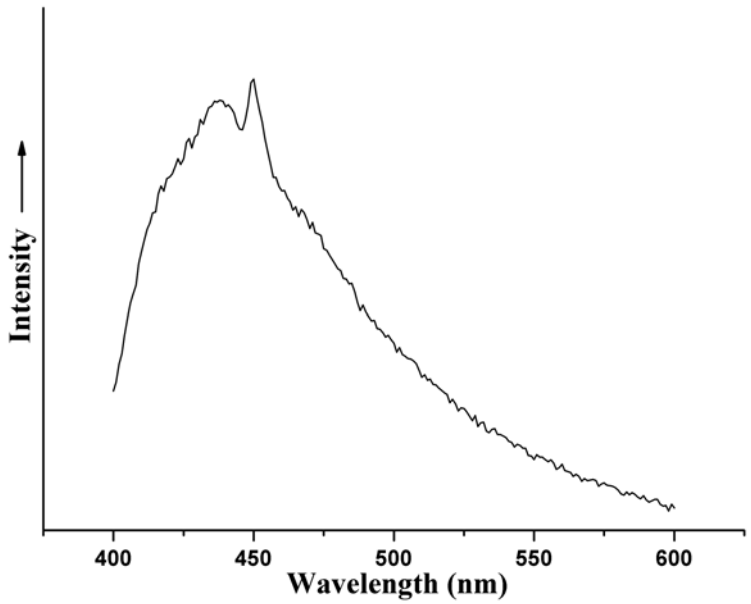


**Fig. S7** Solid-state photoluminescence spectrum of **1** measured at room temperature.

**4. Computational analyses of the roles of TM complex cations (Ligands = phen, 2,2′-bipy, en (ethylenediamine), for example) on the stabilization of $(SnQ_4)^{4-}$ anions**

All selected models were optimized without constraints using 3-21G (S, C, N, H atoms) and LANL2DZ (Sn, Mn atoms) basis sets. A frequencies analysis at the same level was carried out after every geometry optimization to assert the presence of a minimum on the potential energy surface. No imaginary frequencies were found for any of the models studied herein. Single-point calculations and analyses of electron populations with the NBO module in Gaussian 03[4] package on the optimized geometries were carried out at B3LYP levels of theory using the 6-31+G* (S, C, N, H atoms) and LANL2DZ (Sn, Mn atoms) basis set.

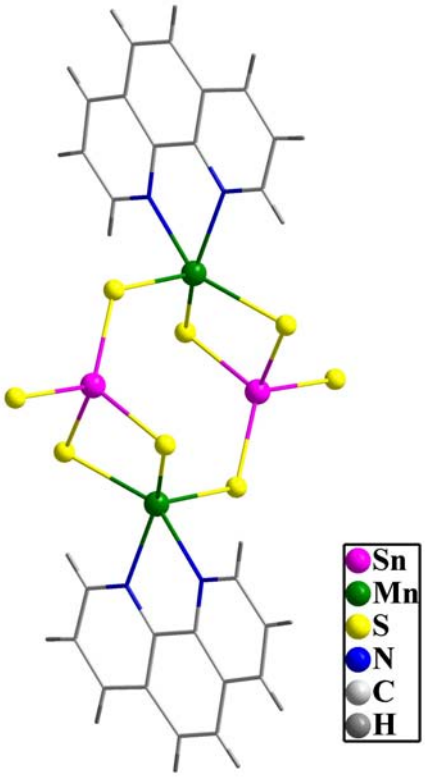


**Fig. S8** The model of $\{[Mn(phen)](SnS_4)\}_2^{4-}$ (**1a**) truncated from the crystal structure of **1** for theoretical calculation.

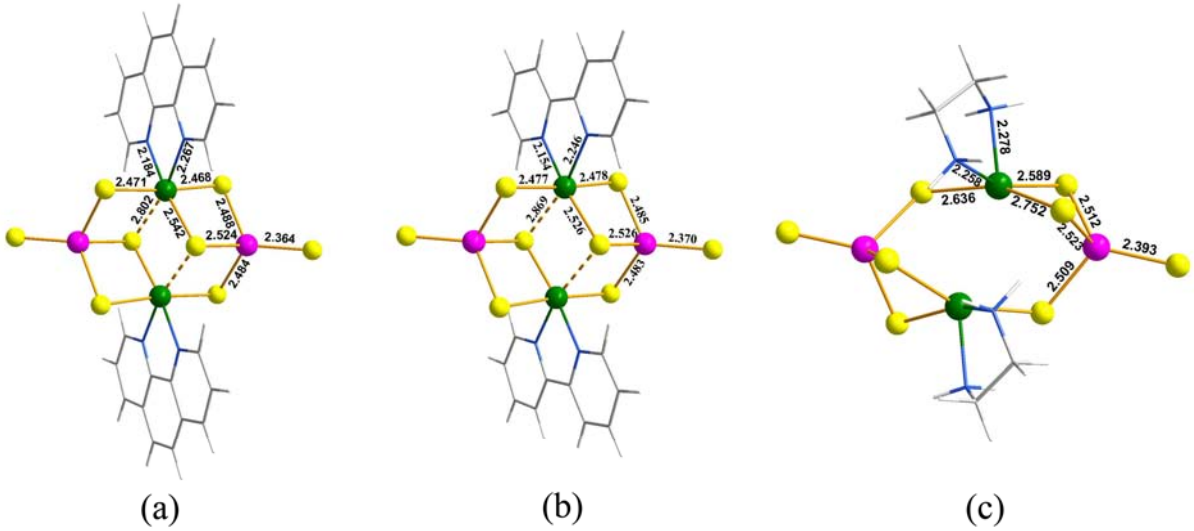


**Fig. S9** Optimized geometrical structures of model **1a'**, **1b'** and **1c'** with selected bond distances (Å). Dotted lines show long Mn–S bonds.

**Table S5** Single-point Calculations and Natural Population Analyses of Model **1a'**, **1b'** and **1c'**.

| | Model **1a'** | Model **1b'** | Model **1c'** |
|---|---|---|---|
| Single-point energies (Hartrees) | –4543.643140 | –4391.167572 | –3781.438926 |
| Average natural charge of per TM complex cation (e) | 0.4867 | 0.5194 | 1.4062 |
| Average natural charge of per $Mn^{2+}$ atom (e) | 1.3417 | 1.3505 | 1.4025 |
| Average natural charge of per $(SnS_4)^{4-}$ species (e) | –2.4867 | –2.5194 | –3.4062 |

**Table S6** Optimized Atomic Coordinates (Å) for Model **1a'**–**1c'**.

| Model of **1a'** | | | |
|---|---|---|---|
| Atom | X | Y | Z |
| Sn | 7.635935 | 10.574215 | 2.833535 |
| Sn | 8.426706 | 8.689923 | -2.846622 |
| S | 5.648815 | 9.258429 | 2.117828 |
| S | 7.878827 | 11.443195 | 0.475976 |

| | | | |
|---|---|---|---|
| S | 9.634568 | 9.109499 | 2.657113 |
| S | 7.439632 | 11.968463 | 4.732814 |
| S | 6.428075 | 10.154645 | -2.670215 |
| S | 8.183816 | 7.820975 | -0.489053 |
| S | 10.413831 | 10.005712 | -2.130935 |
| S | 8.622999 | 7.295652 | -4.745886 |
| Mn | 6.146867 | 9.730501 | -0.252472 |
| Mn | 9.915769 | 9.533688 | 0.239375 |
| N | 4.497507 | 8.372098 | -0.702435 |
| N | 4.306022 | 11.046224 | -0.388577 |
| N | 11.756619 | 8.217961 | 0.375474 |
| N | 11.565133 | 10.892085 | 0.689349 |
| C | 4.655349 | 7.027361 | -0.861891 |
| C | 3.282132 | 8.934787 | -0.839772 |
| C | 4.277320 | 12.392026 | -0.206329 |
| C | 3.176813 | 10.372858 | -0.665281 |
| C | 11.785321 | 6.872161 | 0.193215 |
| C | 12.885829 | 8.891327 | 0.652176 |
| C | 11.407290 | 12.236821 | 0.848822 |
| C | 12.780509 | 10.329396 | 0.826679 |
| C | 3.561418 | 6.215928 | -1.173437 |
| C | 2.099588 | 8.175334 | -1.149289 |
| C | 3.071870 | 13.098294 | -0.304067 |
| C | 1.892480 | 11.011662 | -0.791497 |
| C | 12.990773 | 6.165894 | 0.290938 |
| C | 14.170164 | 8.252523 | 0.778380 |
| C | 10.398922 | 12.608805 | 0.726515 |
| C | 12.501220 | 13.048251 | 1.160376 |
| C | 13.963053 | 11.088847 | 1.136200 |

| | | | |
|---|---|---|---|
| C | 2.292667 | 6.764062 | -1.316956 |
| C | 0.860699 | 8.838385 | -1.268265 |
| C | 1.888307 | 12.432964 | -0.593700 |
| C | 0.757486 | 10.233093 | -1.090252 |
| C | 14.174337 | 6.831223 | 0.580570 |
| C | 15.305158 | 9.031090 | 1.077137 |
| C | 12.341787 | 14.114318 | 1.291429 |
| C | 13.769973 | 12.500117 | 1.303885 |
| C | 15.201943 | 10.425796 | 1.255165 |
| H | 10.833423 | 6.409867 | -0.032076 |
| H | 5.229218 | 12.854320 | 0.018966 |
| H | 3.720850 | 5.149859 | -1.304475 |
| H | 3.076279 | 14.173430 | -0.148252 |
| H | 12.986365 | 5.090760 | 0.135113 |
| H | 5.663716 | 6.655377 | -0.739579 |
| H | 1.436610 | 6.139549 | -1.560182 |
| H | -0.024782 | 8.251996 | -1.504793 |
| H | -0.208311 | 10.725367 | -1.184700 |
| H | 15.114967 | 6.291174 | 0.658973 |
| H | 16.270956 | 8.538817 | 1.171575 |
| H | 14.626030 | 13.124629 | 1.547117 |
| H | 16.087423 | 11.012185 | 1.491699 |
| H | 0.947679 | 12.973014 | -0.672114 |

| Model of **1b'** | | | |
|---|---|---|---|
| Atom | X | Y | Z |
| Sn | 7.75563400 | 10.50684000 | 2.87452500 |
| Sn | 8.41415900 | 8.73975700 | -2.86303100 |
| S | 5.74297700 | 9.21508800 | 2.19875800 |

| | | | |
|---|---|---|---|
| S | 7.90679500 | 11.42922100 | 0.52728300 |
| S | 9.74990300 | 9.05038700 | 2.61885100 |
| S | 7.62526800 | 11.86798300 | 4.81025200 |
| S | 6.41988700 | 10.19620600 | -2.60735400 |
| S | 8.26300000 | 7.81736900 | -0.51579100 |
| S | 10.42681200 | 10.03151300 | -2.18725900 |
| S | 8.54453000 | 7.37861700 | -4.79875800 |
| Mn | 6.16439500 | 9.74519000 | -0.18491500 |
| Mn | 10.00540000 | 9.50139600 | 0.19641100 |
| N | 4.55104900 | 8.38145000 | -0.60761200 |
| N | 4.33102700 | 11.03977800 | -0.28016600 |
| N | 11.83876400 | 8.20680200 | 0.29166100 |
| N | 11.61874900 | 10.86513100 | 0.61911100 |
| C | 4.72734800 | 7.05835000 | -0.75564500 |
| C | 3.27274800 | 8.93798200 | -0.73740400 |
| C | 4.30411700 | 12.36647600 | -0.10261900 |
| C | 3.15488500 | 10.34511500 | -0.56509500 |
| C | 11.86567000 | 6.88010500 | 0.11411100 |
| C | 13.01490700 | 8.90146200 | 0.57659200 |
| C | 11.44245300 | 12.18823000 | 0.76714800 |
| C | 12.89704800 | 10.30859500 | 0.74890500 |
| C | 3.68703900 | 6.17285300 | -1.03775000 |
| C | 2.18104800 | 8.06609400 | -1.03400600 |
| C | 3.13586400 | 13.13039900 | -0.18771000 |
| C | 1.93403300 | 11.08171500 | -0.66493800 |
| C | 13.03392100 | 6.11617800 | 0.19920200 |
| C | 14.23575700 | 8.16485700 | 0.67643500 |
| C | 12.48276400 | 13.07372400 | 1.04925800 |
| C | 13.98875000 | 11.18047800 | 1.04551100 |

| | | | |
|---|---|---|---|
| C | 2.38211000 | 6.71142700 | -1.18046000 |
| C | 1.92660500 | 12.44761600 | -0.47918300 |
| C | 14.24318100 | 6.79895700 | 0.49067700 |
| C | 13.78769200 | 12.53514500 | 1.19196900 |
| H | 5.26907900 | 12.81240500 | 0.11847400 |
| H | 10.90070700 | 6.43417900 | -0.10698400 |
| H | 10.41699300 | 12.52587900 | 0.65548900 |
| H | 3.88625200 | 5.11476700 | -1.15398600 |
| H | 3.16400900 | 14.20199500 | -0.02990200 |
| H | 13.00577200 | 5.04458300 | 0.04139300 |
| H | 12.28355400 | 14.13181000 | 1.16549600 |
| H | 5.75281000 | 6.72070400 | -0.64398600 |
| H | 1.54220700 | 6.05796600 | -1.40879200 |
| H | 15.17776300 | 6.24587000 | 0.56751600 |
| H | 14.62759600 | 13.18860400 | 1.42030500 |
| H | 0.99202200 | 13.00070000 | -0.55602200 |
| H | 14.98263900 | 10.76041600 | 1.15607700 |
| H | 15.15816200 | 8.69019700 | 0.90045600 |
| H | 1.01162900 | 10.55637300 | -0.88895700 |
| H | 1.18715700 | 8.48615300 | -1.14457000 |

Model of **1c'**

| Atom | X | Y | Z |
|---|---|---|---|
| Sn | 7.88580500 | 10.95740500 | 3.35472400 |
| Sn | 8.24611900 | 10.91499000 | -3.39299700 |
| S | 7.29033700 | 8.71886700 | 2.35634000 |
| S | 5.85853300 | 12.10226900 | 2.41269000 |
| S | 9.78135700 | 11.64786600 | 1.86294900 |
| S | 8.29900200 | 11.07481200 | 5.70871100 |

| | | | |
|---|---|---|---|
| S | 6.34138700 | 11.60371600 | -1.91227400 |
| S | 8.86631100 | 8.69678300 | -2.36354800 |
| S | 10.26064500 | 12.09403900 | -2.46584900 |
| S | 7.83370800 | 10.99606100 | -5.74865700 |
| Mn | 6.30635400 | 10.45919300 | 0.46133000 |
| Mn | 9.83344900 | 10.47011200 | -0.49509700 |
| N | 6.05629900 | 8.49011100 | -0.61482100 |
| N | 4.05537200 | 10.37379400 | 0.12431700 |
| N | 10.10317800 | 8.52000500 | 0.61126900 |
| N | 12.08454200 | 10.41479100 | -0.15071200 |
| C | 4.72264600 | 8.43734700 | -1.24214600 |
| C | 3.66885900 | 9.00143500 | -0.25707800 |
| C | 11.43568300 | 8.49176400 | 1.24287100 |
| C | 12.48559000 | 9.05258500 | 0.25193400 |
| H | 9.30034900 | 8.51499000 | 1.28345700 |
| H | 9.95884600 | 7.83187500 | -0.13663000 |
| H | 11.76172100 | 7.48880600 | 1.57839600 |
| H | 11.37290800 | 9.16168100 | 2.10691800 |
| H | 13.48962300 | 8.99642900 | 0.71544300 |
| H | 12.48773800 | 8.43462100 | -0.65437600 |
| H | 12.06196900 | 11.10596600 | 0.60745700 |
| H | 12.41430100 | 10.77281700 | -1.04913900 |
| H | 6.85782700 | 8.48383900 | -1.28845100 |
| H | 6.21008600 | 7.81585900 | 0.14380300 |
| H | 4.06655600 | 11.05475900 | -0.64312100 |
| H | 3.72812900 | 10.74038700 | 1.02030200 |
| H | 2.66447300 | 8.92711500 | -0.71727400 |
| H | 3.67564700 | 8.39703200 | 0.65826200 |
| H | 4.77545200 | 9.09437500 | -2.11662500 |

| | | | |
|---|---|---|---|
| H | 4.40697200 | 7.42573400 | -1.56135600 |

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