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Supporting Information

A series of new manganese thioarsenates(V) based on different unsaturated

[Mn(amine)_x]²⁺ complexes

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Fig. S1 Experimental and simulated powder XRD patterns.(The simulated XRD pattern of **1-4** is slightly different from the measured one. It means that **1-4** are sensitive to the moisture and air)



Fig. S2 The asymmetric unit of **1** (H atoms bonded to C and N atoms have been omitted for clarity).



Fig. S3 The crystal packing of **2**.



Fig. S4 The asymmetric unit of **3** (H atoms bonded to C and N atoms have been omitted for clarity).



Fig. S5 3-D hydrogen bonding network structure.



Fig. S6 The asymmetric unit of **4** (H atoms bonded to C and N atoms have been omitted for clarity).



Fig. S7 Total and partial DOS for 1. The Fermi level is set at 0 eV (dotted line).





Fig. S8 The calculated band structures of 1, 3 and 4. The Fermi level is set at 0 eV (dotted line).