Supporting Information

Modulation of Mn³⁺ Spin State by Guest Molecule Inclusion

Irina A. Kühne¹, Kane Esien², Laurence C. Gavin¹, Helge Müller-Bunz¹, Solveig Felton², and Grace G. Morgan^{1,*}

Contents

Figure S1 . View of asymmetric unit of [MnL ₁]CF ₃ SO ₃ ·0.7H ₂ O at 100 K showing H-bonding connecting complex cation and counterion <i>via</i> a water molecule	.2
Figure S2 . View of asymmetric unit of [MnL ₁]CF ₃ SO ₃ ·0.7H ₂ O at 100 K showing H-bonding connecting complex cation and counterion <i>via</i> a water molecule	.3
Figure S3 . View of asymmetric unit of $[MnL_1]PF_6 \cdot 0.5H_2O$ at 100 K showing H-bonding between phenoxide oxygen and water molecule. A close contact is formed between the water molecule and the disordered PF_6^- counterion.	.4
Figure S4 . View of asymmetric unit of [MnL ₁]PF ₆ ·0.5H ₂ O at 293 K showing H-bonding between phenoxide oxygen and water molecule	. 5
Figure S5 . View of asymmetric unit of $[MnL_1]PF_6 \cdot 0.3H_2O \cdot 0.3sal$ at 100 K illustrating the absence of intermolecular interactions to the complex cation and showing disorder of partial occupancy 4-methoxysalicylaldehyde guest molecule and water.	.6
Figure S6 . Space filling packing arrangement of $[MnL_1]PF_6 \cdot 0.3H_2O \cdot 0.3sal$ at 100 K along the a-axis (left) and along the b-axis (right)	.7
Figure S7 . View of asymmetric unit of [MnL ₁]BPh ₄ at 100 K illustrating the absence of intermolecular interactions.	.8



Figure S1. View of asymmetric unit of $[MnL_1]CF_3SO_3 \cdot 0.7H_2O$ at 100 K showing H-bonding connecting complex cation and counterion *via* a water molecule.



Figure S2. View of asymmetric unit of $[MnL_1]CF_3SO_3 \cdot 0.7H_2O$ at 100 K showing H-bonding connecting complex cation and counterion *via* a water molecule.



Figure S3. View of asymmetric unit of $[MnL_1]PF_6 \cdot 0.5H_2O$ at 100 K showing H-bonding between phenoxide oxygen and water molecule. A close contact is formed between the water molecule and the disordered PF_6^- counterion.



Figure S4. View of asymmetric unit of $[MnL_1]PF_6 \cdot 0.5H_2O$ at 293 K showing H-bonding between phenoxide oxygen and water molecule.



Figure S5. View of asymmetric unit of $[MnL_1]PF_6 \cdot 0.3H_2O \cdot 0.3sal$ at 100 K illustrating the absence of intermolecular interactions to the complex cation and showing disorder of partial occupancy 4-methoxysalicylaldehyde guest molecule and water.



Figure S6. Space filling packing arrangement of $[MnL_1]PF_6 \cdot 0.3H_2O \cdot 0.3sal$ at 100 K along the a-axis (left) and along the b-axis (right) with the $[MnL_1]^+$ in green, PF_6^- in blue, 4-methoxysalicylaldehyde (sal) in red and water molecules in yellow.



Figure S7. View of asymmetric unit of [MnL₁]BPh₄ at 100 K illustrating the absence of intermolecular interactions.