

## Supporting Information for

# Photoinduced electron transfer and remarkable enhancement of magnetic susceptibility in bridging pyrazine complexes

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*Dedicated to Professor Dai-Zheng Liao on the occasion of his 80th birthday*

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## Tables

**Table S1a.** Selected bond lengths (Å) and angles (°) for complex **1**

Bond lengths			
Mn(1)-O(1)	2.1814(11)	Mn(1)-N(1)	2.2840(13)
Mn(1)-Cl(1)	2.5134(3)		
Bond angles			
O(1)-Mn(1)-O(1)#1	180.00(4)	O(1)-Mn(1)-N(1)#1	90.53(4)
O(1)-Mn(1)-N(1)	89.47(4)	O(1)-Mn(1)-Cl(1)	88.36(3)
O(1)-Mn(1)-Cl(1)#1	91.64(3)	N(1)-Mn(1)-N(1)#1	180.00(9)
N(1)-Mn(1)-Cl(1)	89.74(3)	N(1)-Mn(1)-Cl(1)#1	90.26(3)
Cl(1)#1-Mn(1)-Cl(1)	180.0	C(1)-N(1)-Mn(1)	121.52(10)
C(2)-N(1)-Mn(1)	121.64(10)	S(1)-O(1)-Mn(1)	127.22(6)

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

**Table S1b.** Selected bond lengths (Å) and angles (°) for complex **2**

Bond lengths			
Fe(1)-O(1)	2.0957(13)	Fe(1)-N(1)	2.1893(15)
Fe(1)-Cl(1)	2.5023(4)		
Bond angles			
O(1)-Fe(1)-O(1)#1	180.0	O(1)-Fe(1)-N(1)#1	89.55(5)
O(1)-Fe(1)-N(1)	90.45(5)	O(1)-Fe(1)-Cl(1)	92.79(4)
O(1)-Fe(1)-Cl(1)#1	87.21(4)	N(1)-Fe(1)-N(1)#1	180.0
N(1)-Fe(1)-Cl(1)	89.51(4)	N(1)-Fe(1)-Cl(1)#1	90.49(4)
Cl(1)#1-Fe(1)-Cl(1)	180.0	C(1)-N(1)-Fe(1)	121.63(12)
C(2)-N(1)-Fe(1)	121.96(12)	S(1)-O(1)-Fe(1)	126.09(8)

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

**Table S1c.** Selected bond lengths (Å) and angles (°) for complex **3**

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Bond lengths			
Co(1)-O(1)	2.101(4)	Co(1)-N(1)	2.146(5)
Co(1)-Cl(1)	2.4591(19)		

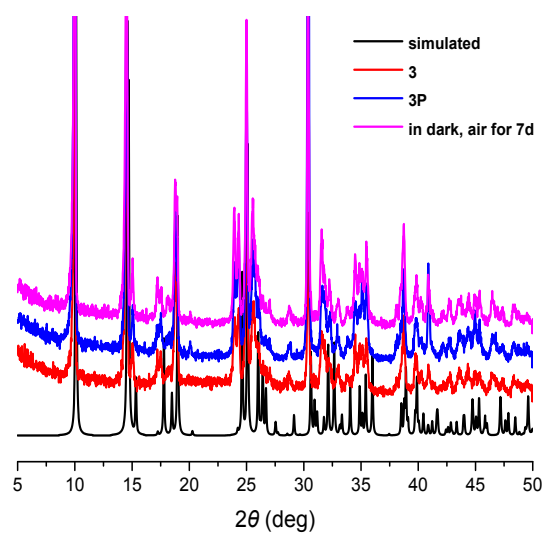
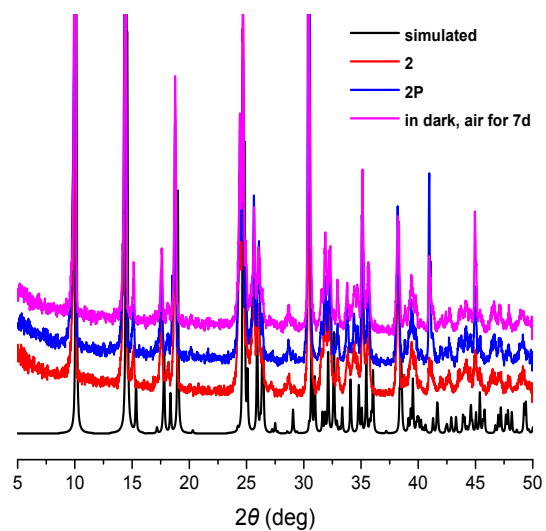
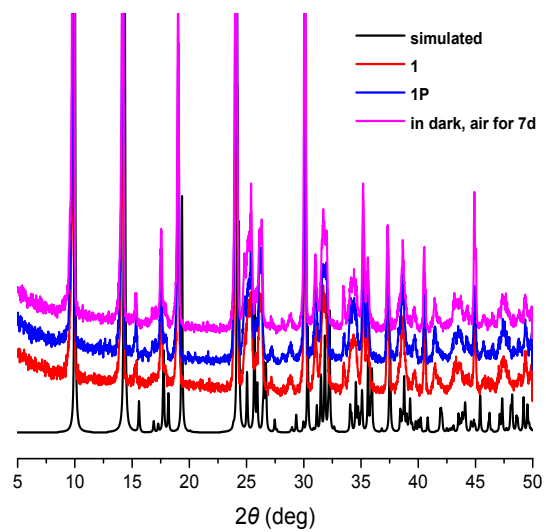
Bond angles			
O(1)-Co(1)-O(1)#1	180.0	O(1)-Co(1)-N(1)#1	90.72(18)
O(1)-Co(1)-N(1)	89.28(18)	O(1)-Co(1)-Cl(1)	87.41(13)
O(1)-Co(1)-Cl(1)#1	92.59(13)	N(1)-Co(1)-N(1)#1	180.0
N(1)-Co(1)-Cl(1)	89.52(14)	N(1)-Co(1)-Cl(1)#1	90.48(14)
Cl(1)#1-Co(1)-Cl(1)	180.0	C(1)-N(1)-Co(1)	122.0(4)
C(2)-N(1)-Co(1)	122.0(4)	S(1)-O(1)-Co(1)	125.9(3)

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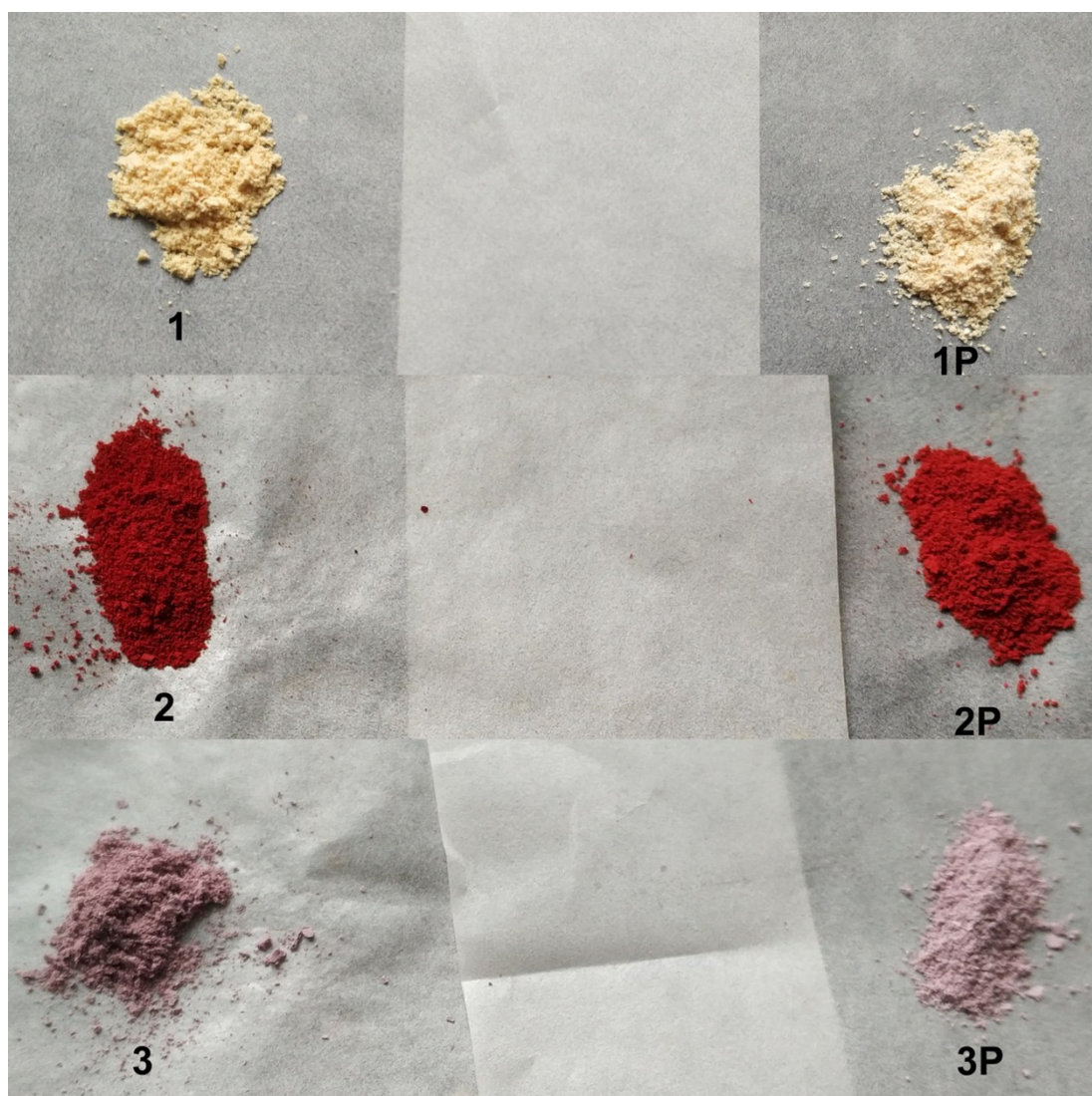
Symmetry transformations used to generate equivalent atoms: #1 -x, -y+2, -z; #2 -x+1, -y+1, -z.

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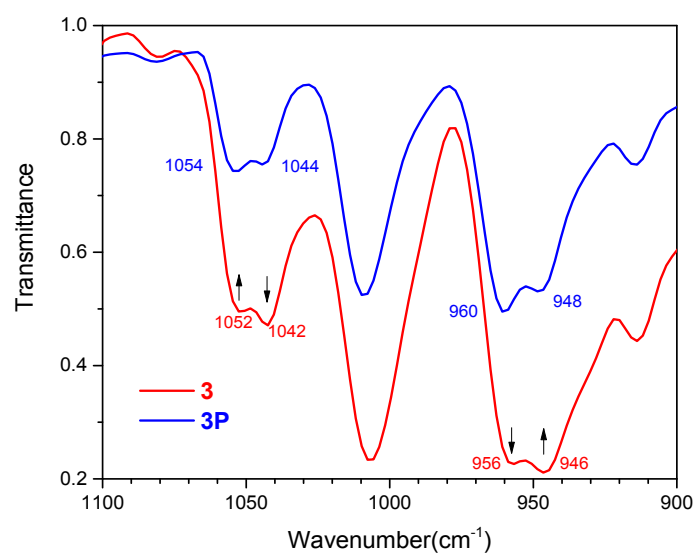
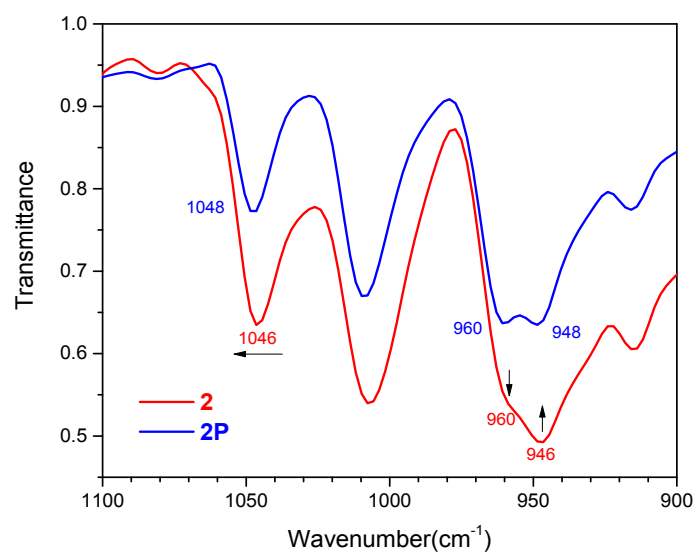
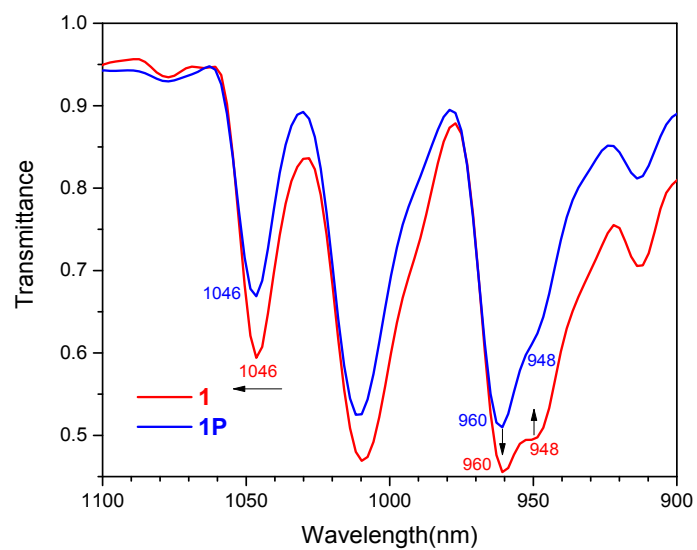
# Graphics



**Fig. S1** PXR D spectra of 1-3.



**Fig. S2** Photochromism of **1-3** after irradiation for an hour.



**Fig. S3** IR spectra and shift of  $\nu(\text{S}=\text{O}-\text{C})$  for **1-3**.

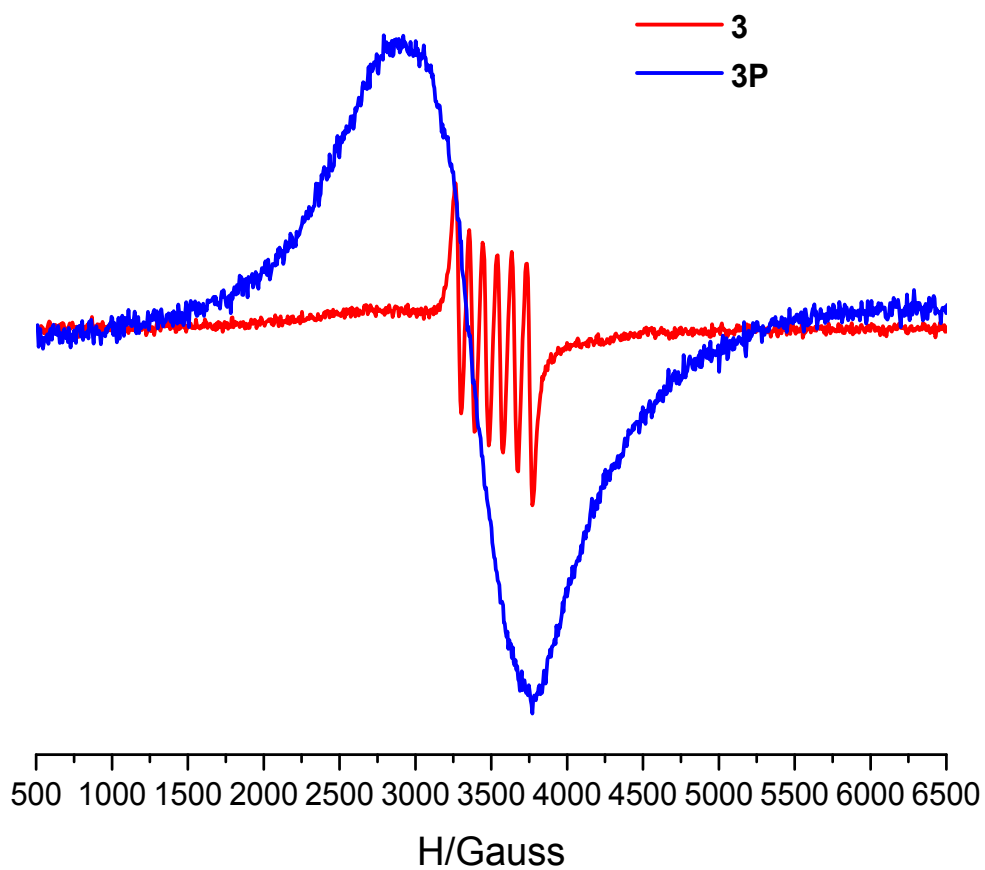
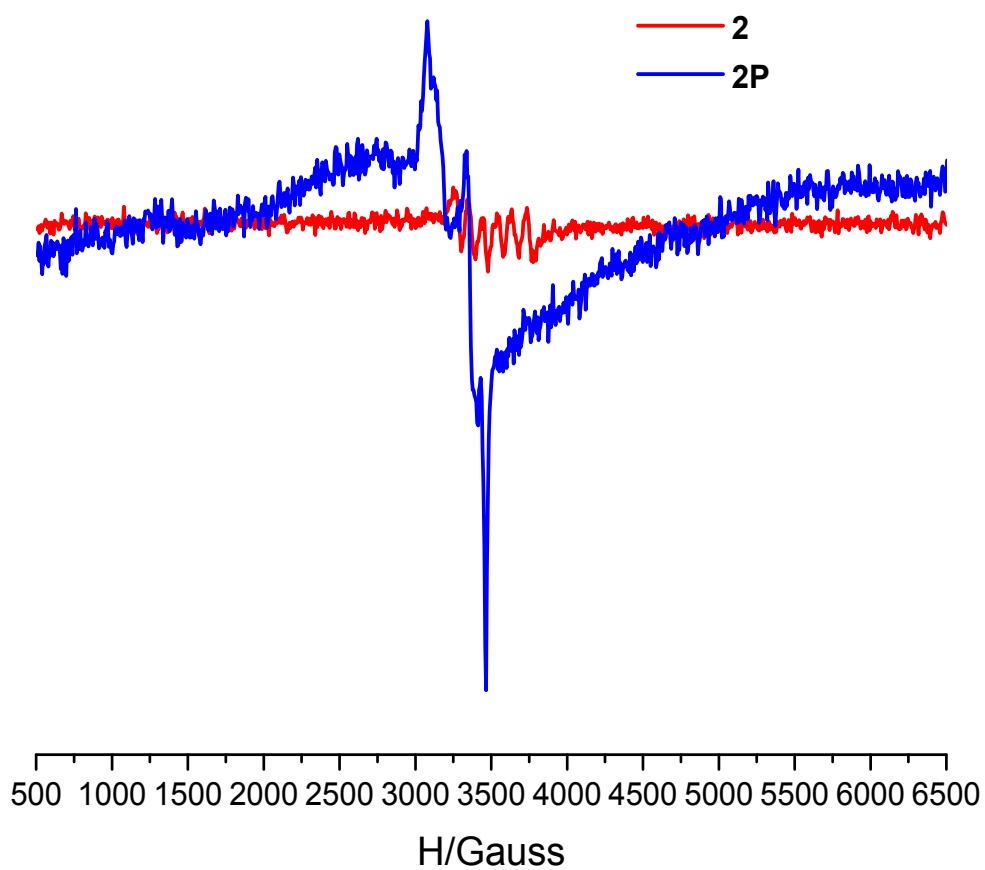
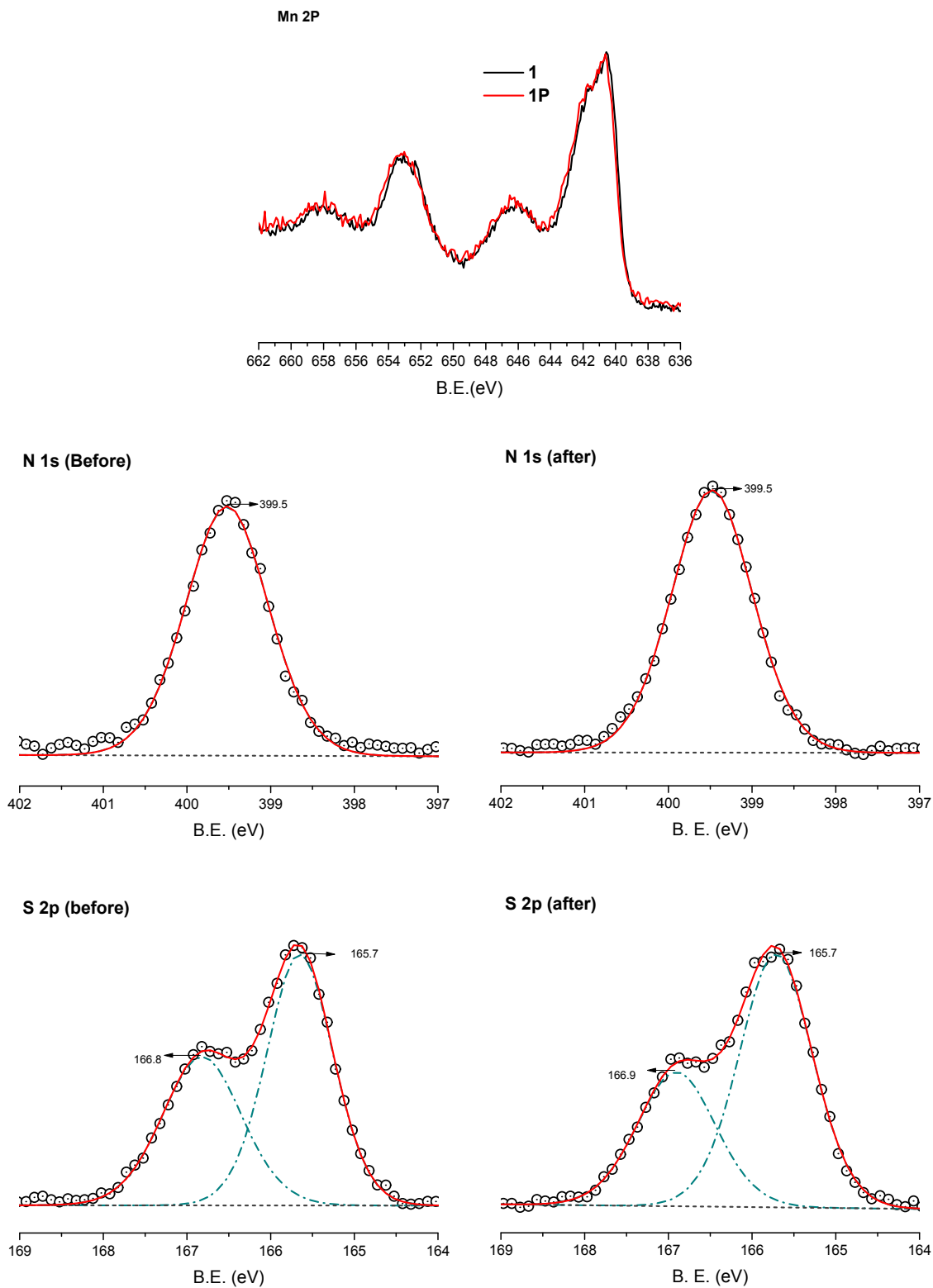


Fig. S4 EPR spectrum of **2** (**2P**) and **3** (**3P**).



**Fig. S5** Mn 2p, N 1s and S 2p XPS (Al-K $\alpha$ ) core-level spectra of **1**(before) and **1P** (after).



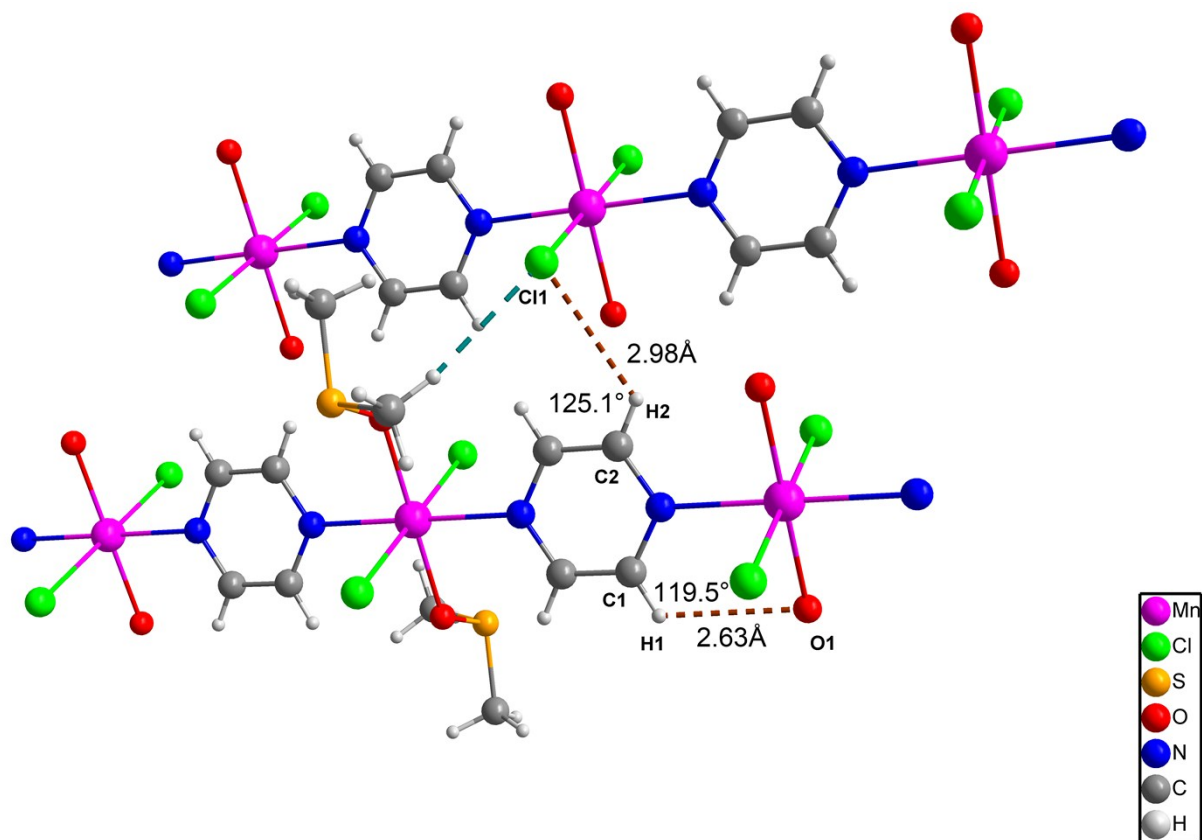


Fig. S6 Potential electron transfer passway (dashed brown lines) in **1**.

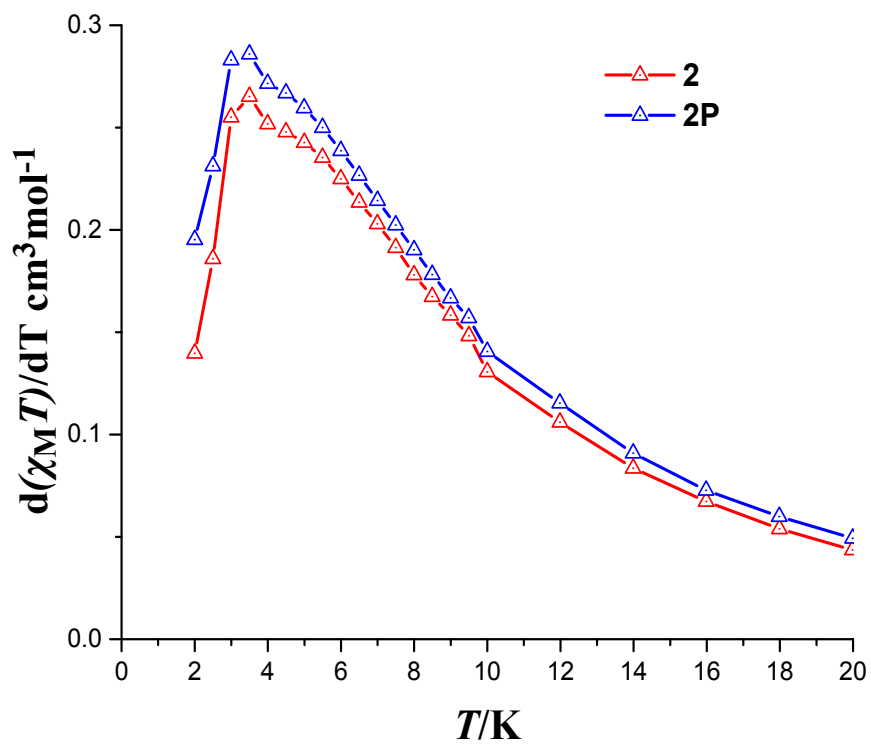
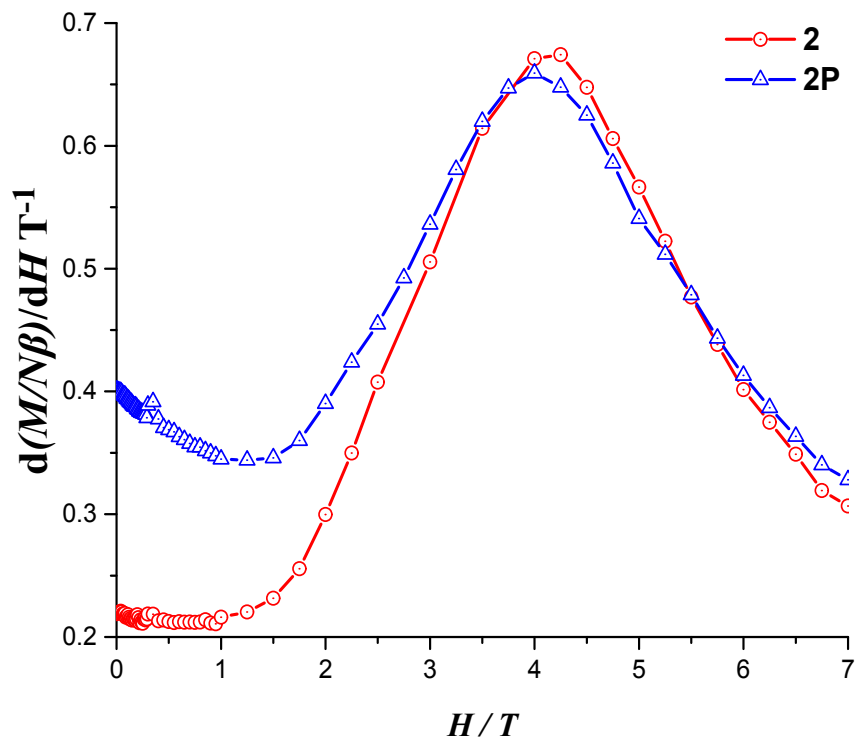


Fig. S7 Plots of temperature dependence of  $d(\chi_M T)/dT$  (top) for **2** and **2P**.



**Fig. S8** Plots of field dependence of  $d(M/N\beta)/dH$  (bottom) for **2** and **2P**.