

## Supplementary Information for:

# A Series of Novel Ion-pair Complexes Based on TCNQ: Syntheses, Crystal Structures and Properties

Guang-Xiang Liu<sup>\*a</sup>, Heng Xu<sup>a</sup>, Xiao-Ming Ren<sup>a</sup> and Wei-Yin Sun<sup>\*b</sup>

<sup>a</sup>*Anhui Key Laboratory of Functional Coordination Compounds, School of Chemistry*

*and Chemical Engineering, Anqing Normal University, Anqing 246003, P. R. China*

<sup>b</sup>*Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry,*

*School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093,*

*P. R. China*

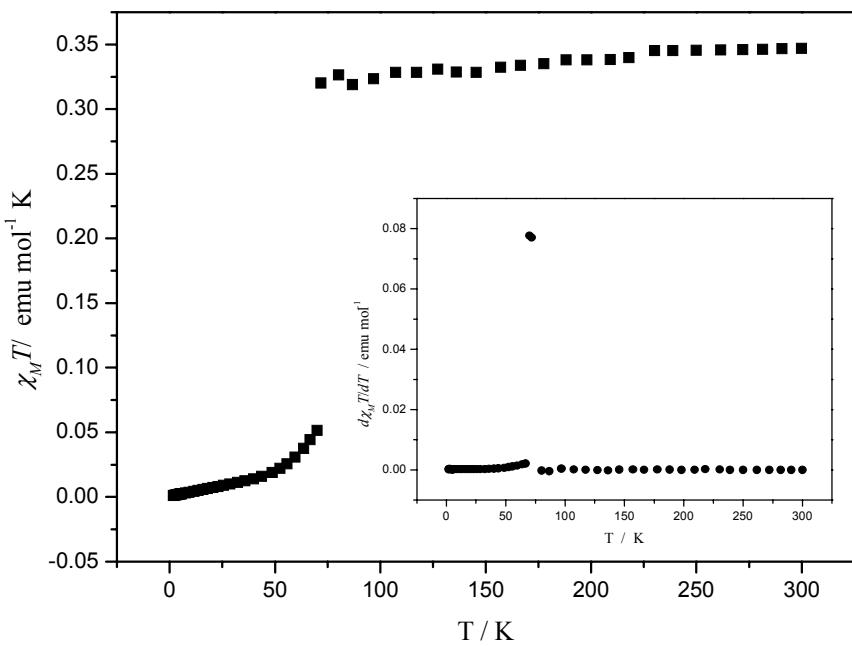
E-mail: [liugx@live.com](mailto:liugx@live.com)

**Table 1S.** Distance [Å] and angles [°] of hydrogen bonding for complexes **1 – 4**

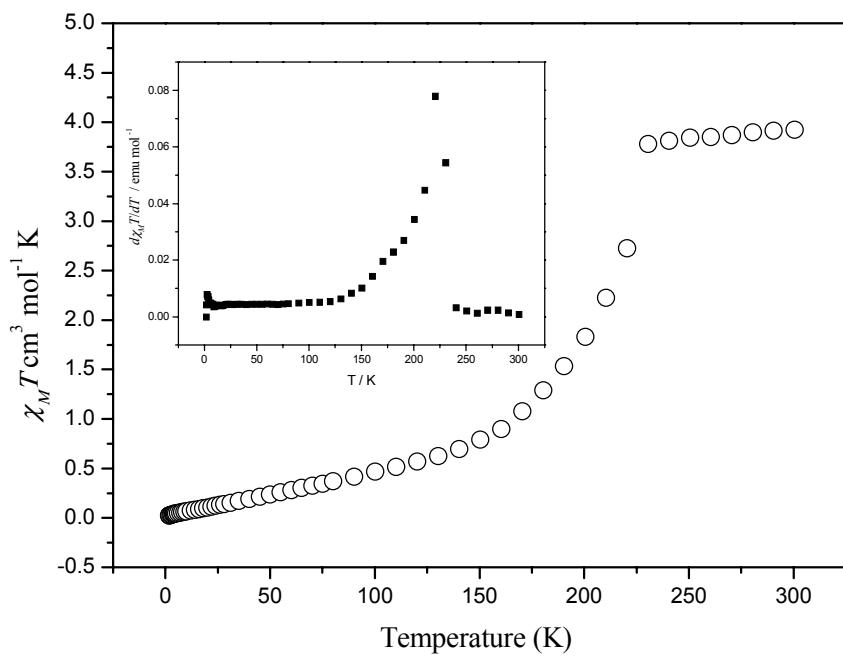
D-H···A	<i>d</i> (D-H)	<i>d</i> (H···A)	<i>d</i> (D···A)	$\angle$ (DHA)
<b>(AP)(TCNQ) (1)</b>				
N2-H2A···N3#1	0.86	2.42	2.991(3)	125
N2-H2B···N5#2	0.86	2.23	3.025(3)	154
C9-H9···N6#3	0.93	2.58	3.215(3)	126
<b>(CP)<sub>2</sub>(TCNQ)<sub>3</sub> (2)</b>				
C12-H12···N6#4	0.93	2.47	3.157(3)	131

C21-H21···N6#5	0.93	2.59	3.367(3)	141
<b>(CMP)(TCNQ) (3)</b>				
C9-H9···N4#6	0.93	2.57	3.331(3)	139
C12-H12···N2	0.93	2.47	3.338(3)	155
C13-H13B···N5#7	0.96	2.59	3.452(4)	150
<b>(BQ)<sub>2</sub>(TCNQ)<sub>2</sub>·CH<sub>3</sub>CN (4)</b>				
C7-H7A···N3#8	0.93	2.57	3.331(3)	139
C8-H8···N3#8	0.93	2.47	3.338(3)	155
C8-H8···N5	0.96	2.59	3.452(4)	150

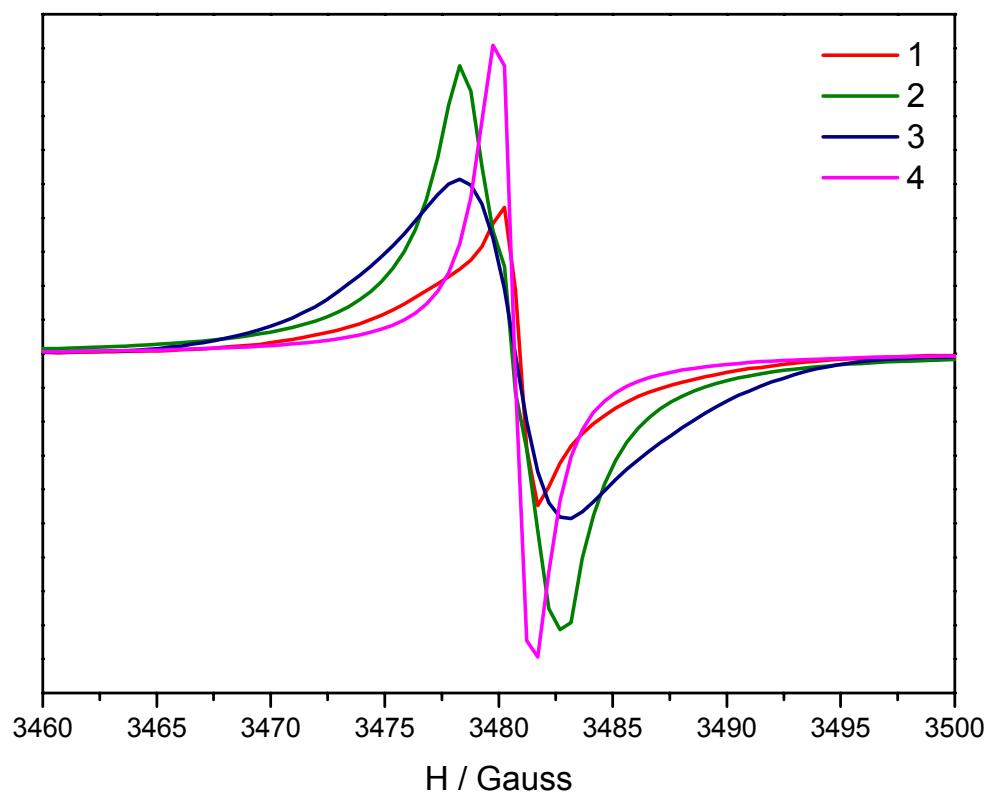
Symmetry codes: #1 x, -1+y, z; #2 -x, 1-y, 2-z; #3 -x, -1/2+y, 3/2-z; #4 2-x, 1-y, 1-z;  
 #5 -1+x, y, z; #6 -x, -1/2+y ; 1/2-z; #7 1-x, -1/2+y, 1/2-z; #8 x, -1+y, z.



**Figure S1.** The plot of  $\chi_M T$  versus  $T$  for complex **3** (inset:  $d(\chi_M T)/dT$  versus  $T$ ).



**Figure S2.** The plot of  $\chi_M T$  versus  $T$  for complex **4** (inset:  $d(\chi_M T)/dT$  versus  $T$ ).



**Figure S3.** EPR spectra of **1** - **4** at room temperature.