

Zhejiang University Avance DMX 500  
QNP 5mm Sample: 07-5-23-8 in DMSO

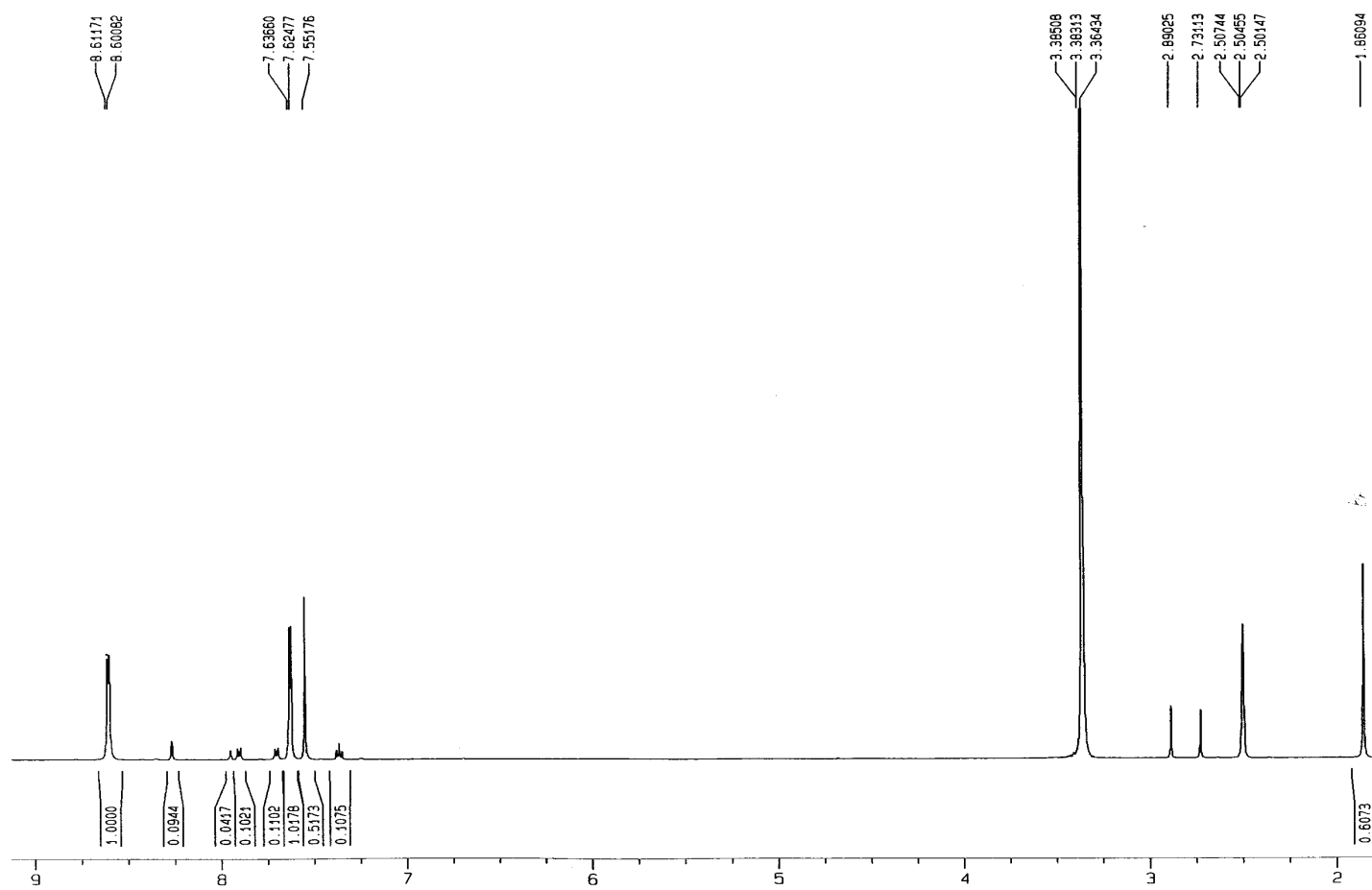


Figure S1. The  $^1\text{H}$  NMR of complex 1.

Zhejiang University Avance DMX 500  
QNP 5mm Sample: 08-10-24-4 in DMSO

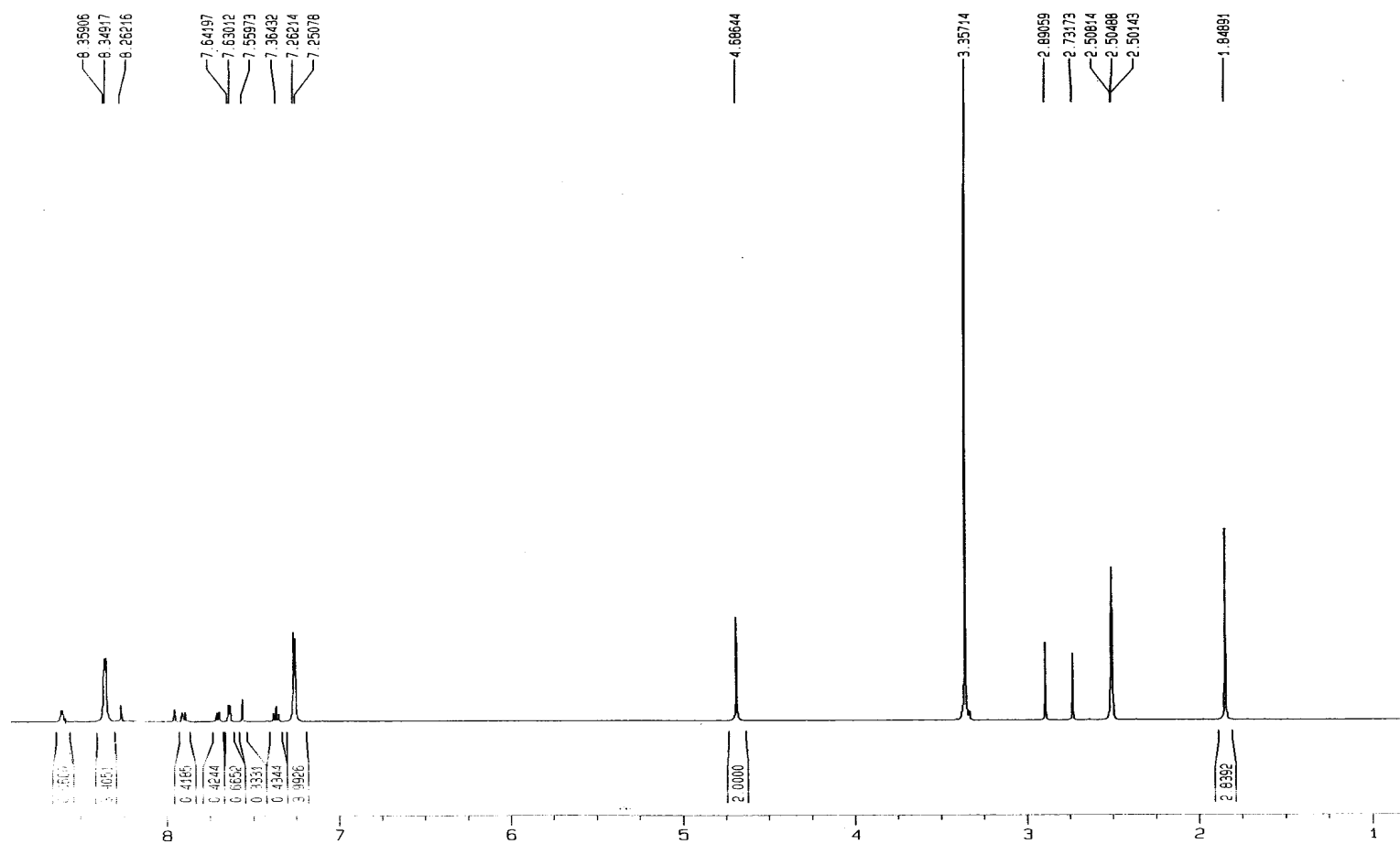
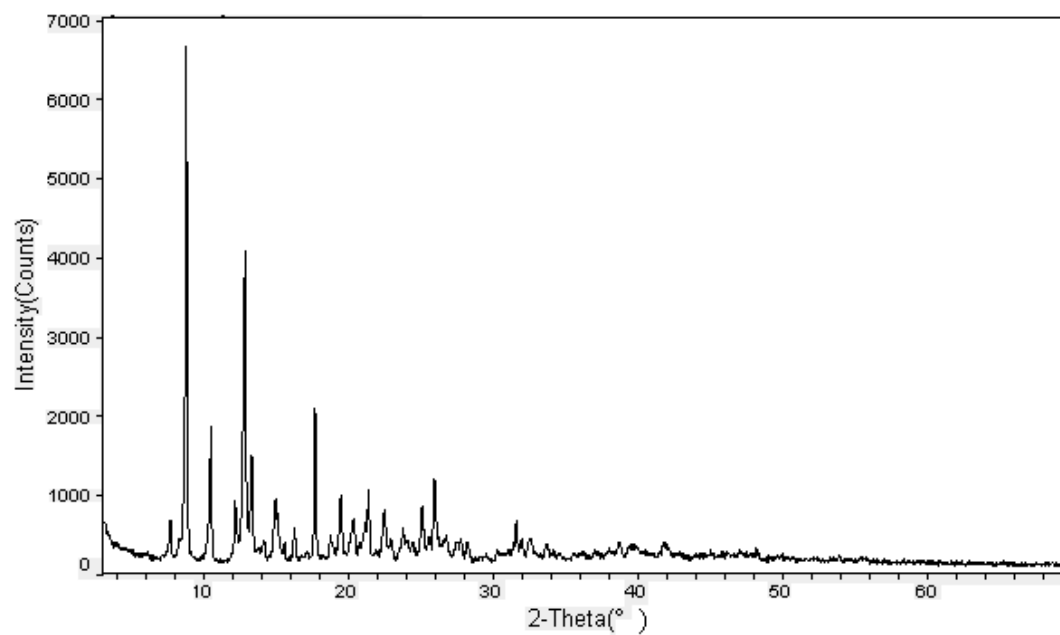
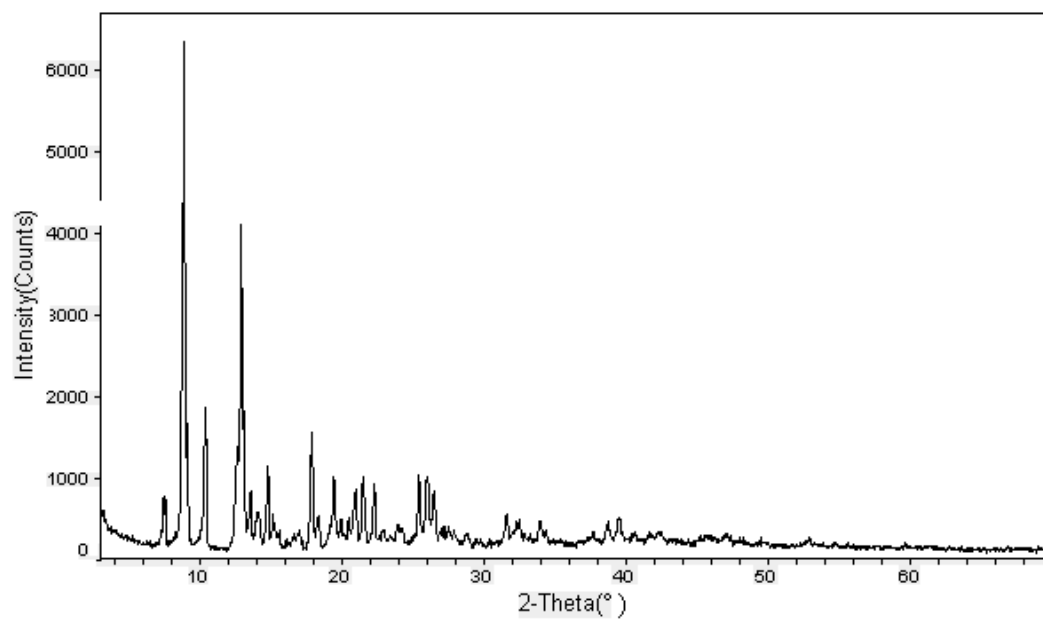


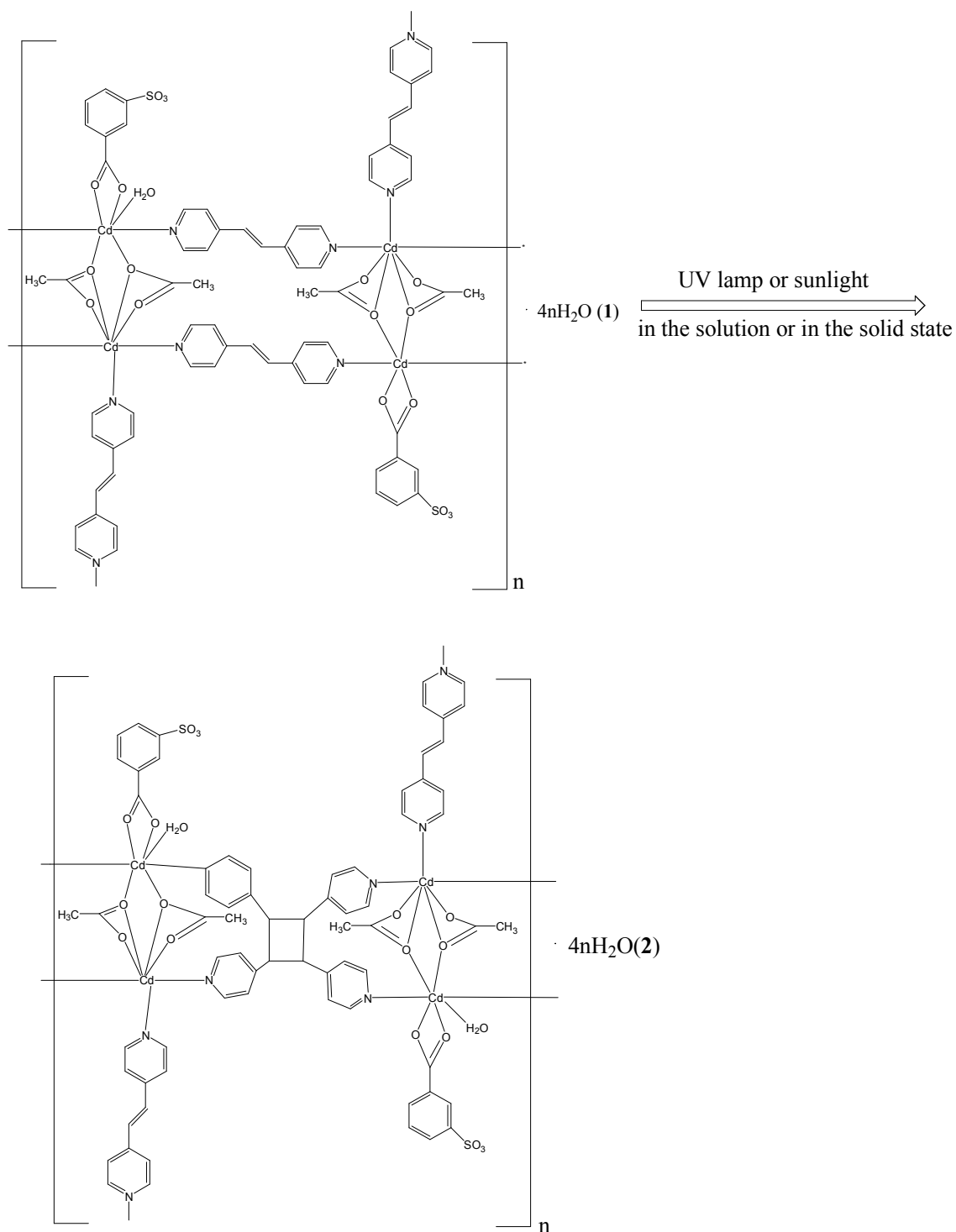
Figure S2. The <sup>1</sup>H NMR of complex 2.



**Figure S3.** Powder X-ray spectrum of complex 1.



**Figure S4.** Powder X-ray spectrum of **2**.



**Scheme S1.** The transformation from **1** to **2** in the solution or in the solid state.

Table S1 Geometrical parameters for O-H...O and C-H...O bonds in complexes **1** and **2**

In complex **1**

Donor --- H....Acceptor	[ ARU ]	D - H	H...A	D...A	D-H...A
O(10) --H(10A) ..O(1W)	[ ]	0.87(3)	2.02(5)	2.651(17)	129(7)
O(10) --H(10B) ..O(3W)	[ ]	0.86(3)	2.05(5)	2.87(2)	158(8)
C(13) --H(13) ..O(1W)	[ 4565.02]	0.93	2.56	3.44(2)	159
C(23) --H(23) ..O(3W)	[ 2755.04]	0.93	2.48	3.13(3)	128
C(25) --H(25) ..O(1)	[ ]	0.93	2.54	3.243(12)	132
C(28) --H(28) ..O(9)	[ 2645.01]	0.93	2.59	3.52(3)	172
C(37) --H(37) ..O(9)	[ ]	0.93	2.58	2.90(2)	101

Translation of ARU-code to Equivalent Position Code

$$[ 2755. ] = 2-x, 1/2+y, 1/2-z$$

$$[ 4565. ] = x, 3/2-y, 1/2+z$$

$$[ 2645. ] = 1-x, -1/2+y, 1/2-z$$

In Complex **2**

Donor --- H....Acceptor	[ ARU ]	D - H	H...A	D...A	D-H...A
O(10) --H(10A) ..O(1W)	[ ]	0.88(8)	1.97(9)	2.735(15)	146(8)
C(6) --H(6) ..O(7)	[ 2756.01]	0.98	2.58	3.489(16)	153
C(22) --H(22) ..O(2)	[ ]	0.93	2.54	3.220(16)	130
C(24) --H(24) ..O(3W)	[ ]	0.93	2.52	3.40(2)	156
C(29) --H(29) ..O(2)	[ ]	0.93	2.56	3.279(13)	135
C(30) --H(30) ..O(9)	[ 2656.01]	0.93	2.55	3.436(15)	158
C(37) --H(37) ..O(8)	[ ]	0.93	2.59	2.936(17)	103

Translation of ARU-code to Equivalent Position Code

$$[ 2656. ] = 1-x, 1/2+y, 3/2-z$$

$$[ 2756. ] = 2-x, 1/2+y, 3/2-z$$