Supporting Information

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1. IR Spectrum of co-crystal

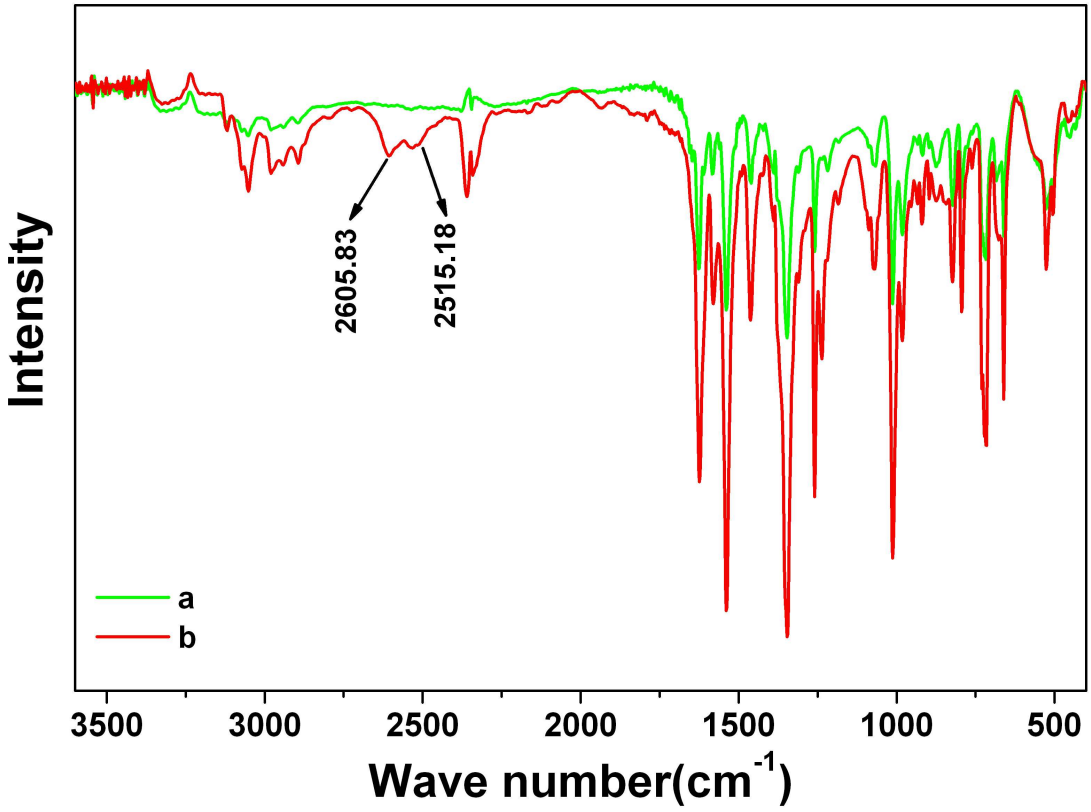
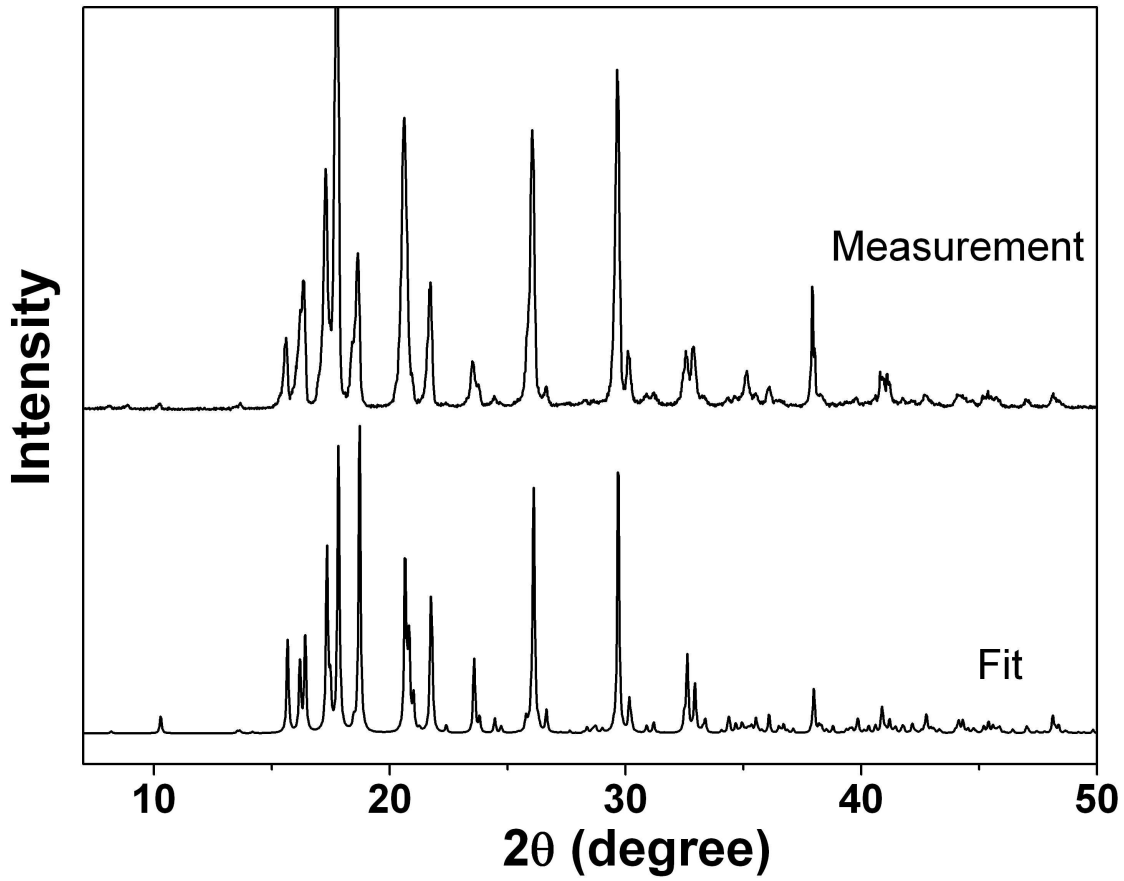


Figure S1 IR spectra of co-crystals **1**(red line, b) and **2** (green line,a).

2. XRD powder pattern of co-crystal **2**:



FigureS2 XRD pattern of co-crystal **2**.

3. XRD powder pattern of co-crystal **1**:

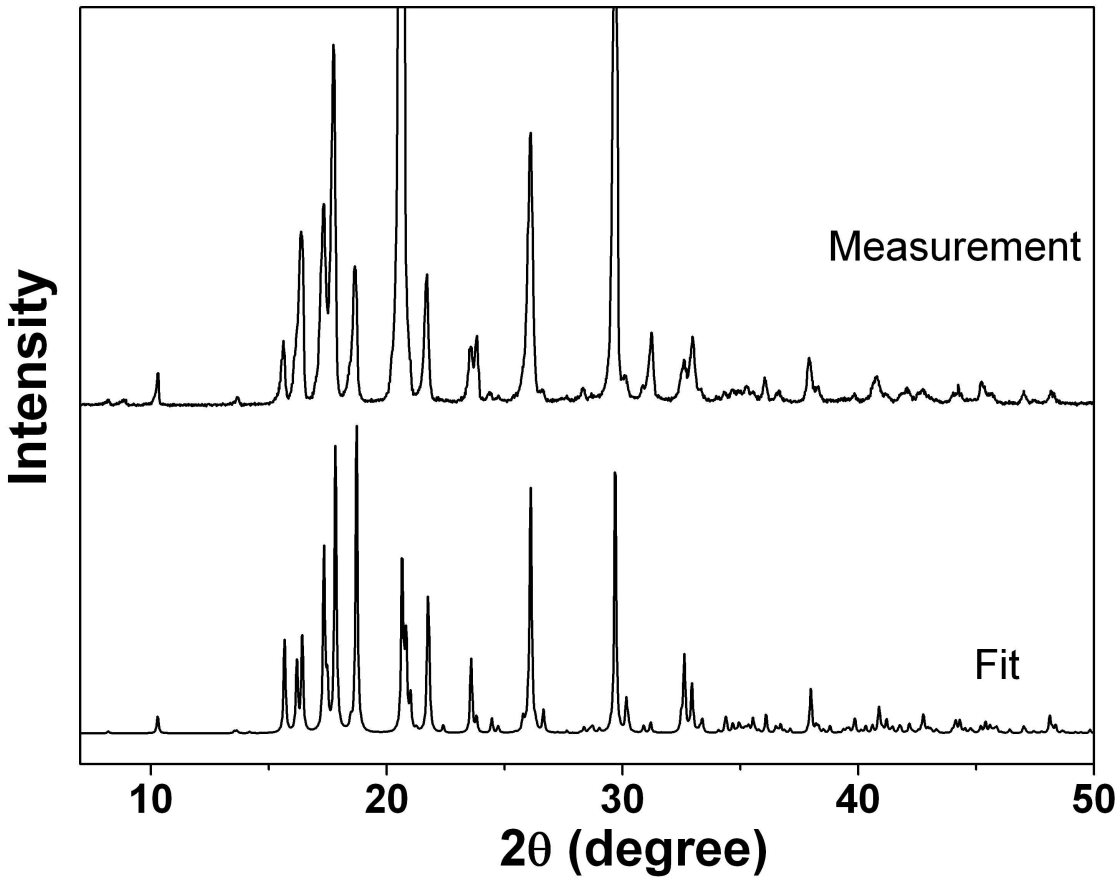


Figure 3S XRD pattern of co-crystal **1**.

Table 1 The D-bondings of co-crystal **1** at 297k (room temperature).

D	H	A	D - H	H...A	D...A	D - H...A
OW	D1	O2	0.91(4)	1.88(4)	2.784(5)	173(4)
OW	D2	O2	0.91(3)	1.94(4)	2.804(5)	159(3)
N3	D3	O1	0.9000	1.8900	2.714(3)	152.00
N3	D3	O2	0.9000	2.4100	3.180(3)	144.00

Table 2 The D-bondings of co-crystal **1** at 163k.

D	H	A	D - H	H...A	D...A	D - H...A
OW	D1	O2	0.90(6)	1.86(6)	2.750(6)	171(6)
OW	D2	O2	0.90(4)	1.86(5)	2.747(6)	169(4)
N3	D3	O1	0.8900	1.8200	2.663(4)	155.00
N3	D3	O2	0.8900	2.5300	3.280(5)	142.00

Table 3 The D-bondings of co-crystal **1** at 123k.

D	H	A	D - H	H...A	D...A	D - H...A
O1W	D1	O11	0.96(3)	1.93(3)	2.818(3)	154(3)
O1W	D2	O4	0.99(3)	1.83(3)	2.799(2)	166(3)
N2	D3	O3	0.97(2)	1.68(2)	2.634(2)	165.8(19)
N2	D3	O4	0.97(2)	2.55(2)	3.275(3)	131.9(17)
N7	D4	O11	0.95(2)	1.80(2)	2.735(3)	171(2)
N7	D4	O12	0.95(2)	2.37(3)	3.010(3)	124.9(19)