Table S1. Selected H-bonded lengths (Å) and angles (º) for **1** and **4**.

D-H…A	d(D..A)	<DHA	Symmetric codes
	Complex **1**		
O1W-H1W...O2	2.617(12)	158.27	
O1W-H2W...O5	2.736(10)	153.69	-x+1/2, -y+1, z
O2W-H3W...O3W	2.497(4)	123.80	
O2W-H4W...O5	2.741(7)	134.43	-x+3/2, -y+1, z
O3W-H3A...O6W	2.646(10)	145.65	
O3W-H3B...O2W	2.497(5)	112.67	
O5W-H5A...O2W	2.653(11)	168.32	
	Complex **4**		
O1W-H1W1...O5	2.816(3)	151.20	1-x,2-y,1-z
O1W-H1W2...O2	2.671(3)	147.31	
O2W-H21...O6	2.817(14)	165.01	

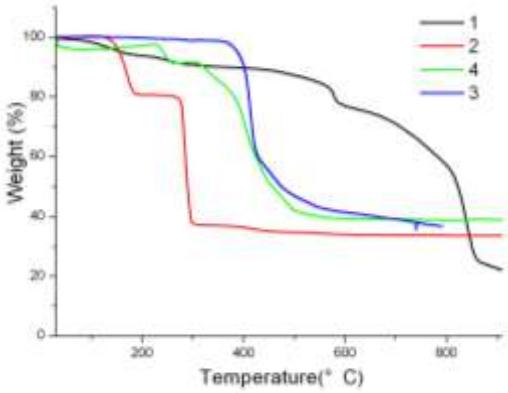

Fig. S1 TG curve of the complexes **1-4**.

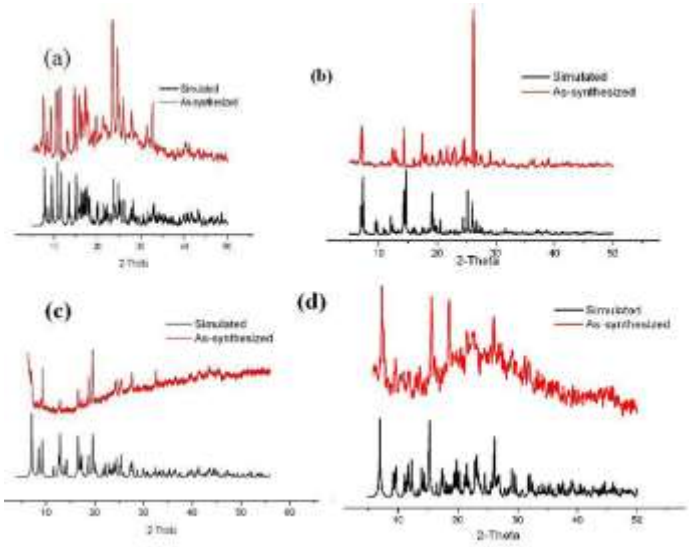

Fig. S2 Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination and the as-synthesized product in compounds **1-4**.