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Supporting information for article:

1. 4, 4'-Bipyridinium acetylenedicarboxylate: a new member of the (H2bipy)[Cu(ox)2] (bipy = 4,4'-bipyridine; ox = oxalate) family

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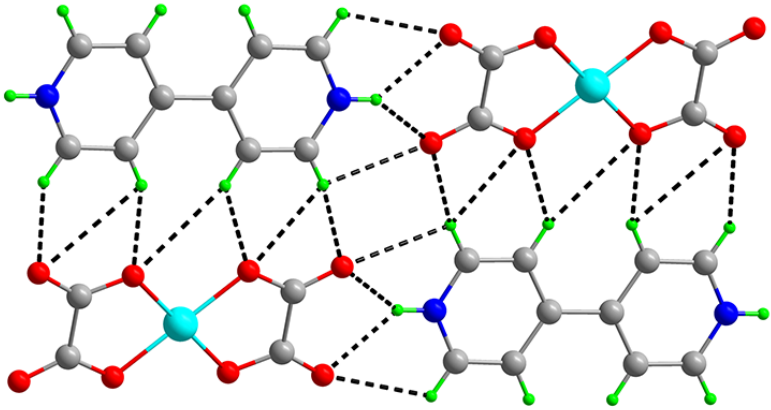
Table S1 The potential hydrogen bonds in compounds (**1**), (**2**), (**3**) and (**4**).

	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	Symmetry
(1)	N1-H1N...O2	0.902(9)	1.659(9)	2.5605(13)	179.1(14)	
	N1-H1N...O1	0.902(9)	2.660(15)	3.239(2)	122.9(10)	
	C1-H1A...O2	0.95	2.39	3.262(2)	151.8	-x, -y+1, -z+1
	C2-H2A...O1	0.95	2.55	3.405(2)	149.9	x, y-1, z
	C4-H4A...O1	0.95	2.39	3.237(2)	148.0	-x+1, -y+1, -z
	C5-H5A...O1	0.95	2.52	3.185(2)	127.3	
(2)	N1-H1N...O3	0.88	2.21	2.888(3)	133.0	
	N1-H1N...O4	0.88	1.98	2.740(3)	144.0	
	C5-H5A...O4	0.95	2.46	3.371(3)	160.8	-x+2, -y+1, -z+1
	C5-H5A...O2	0.95	2.66	3.227(3)	118.5	-x+2, -y+1, -z+1
	C6-H6A...O2	0.95	2.56	3.179(3)	122.8	-x+2, -y+1, -z+1
	C6-H6A...O1	0.95	2.912	3.841(3)	166.0	x-1, y-1, z-1
	C8-H8A...O1	0.95	2.39	3.263(3)	153.4	-x+1, -y+1, -z+2
	C8-H8A...O3	0.95	3.05	3.491(3)	109.7	-x+1, -y+1, -z+2
	C9-H9A...O3	0.95	2.43	3.190(3)	136.4	-x+1, -y+1, -z+2
	C9-H9A...O3	0.95	2.60	3.083(4)	112.2	
(3)	N1-H1A...O3	0.88	1.79	2.595(2)	152.0	
	N1-H1A...O4	0.88	2.36	2.990(2)	128.9	
	C3-H3A...O3	0.95	2.57	3.137(2)	118.7	-x+2, -y+1, -z-1
	C4-H4A...O1	0.95	2.45	3.358(2)	159.2	-x+2, -y+1, -z-1
	C4-H4A...O3	0.95	2.70	3.200(3)	113.6	-x+2, -y+1, -z-1
	C6-H6A...O1	0.95	2.57	3.496(2)	163.5	x, y+1, z
	C7-H7A...O4	0.95	2.58	3.111(2)	115.7	
	C7-H7A...O2	0.95	2.41	3.207(2)	141.6	-x, -y+1, -z
	O4-H4H...O4	0.87(4)	1.60(5)	2.470(2)	171(4)	-x, -y+1, -z
(4)	N1-H1A…O3	0.88	2.47	3.028(3)	122.2	
	N1-H1A…O4	0.88	1.81	2.645(3)	158.6	

	C3-H3A…O3	0.95	2.39	3.003(3)	122.0	
	C3-H3A…O3	0.95	2.72	3.369(4)	126.5	-1-x, -y, 1-z
	C4-H4A…O1	0.95	2.36	3.239(3)	153.2	-1-x, -y, 1-z
	C4-H4A…O3	0.95	2.96	3.490(3)	116.4	-1-x, -y, 1-z
	C6-H6A…O1	0.95	2.62	3.517(3)	156.9	
	C6-H6A…O2	0.95	2.81	3.384(4)	120.0	-x, -y, -z
	C7-H7A…O4	0.95	2.47	3.361(3)	156.5	-x, -y, -z
	C7-H7A…O2	0.95	2.77	3.365(3)	121.6	-x, -y, -z
	O1-H1O…O2	0.94(3)	2.25(3)	2.689(3)	108(2)	
	O1-H1O…O2	0.94(3)	1.77(3)	2.594(3)	145(3)	1-x, 1-y, 1-z



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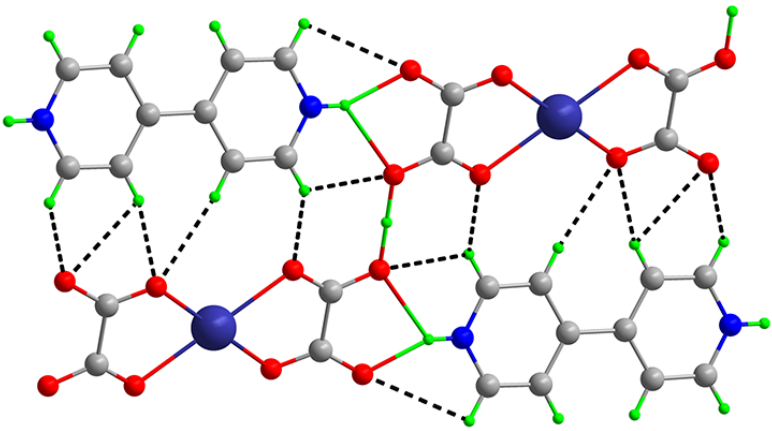

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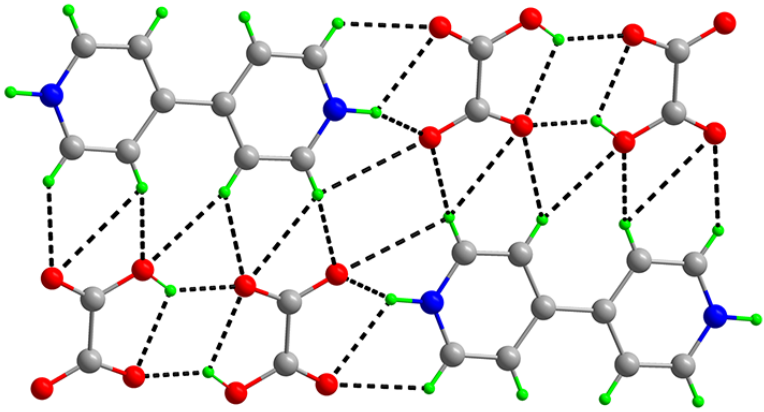

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Fig. S1. The hydrogen-bond networks of (2), (3) and (4). Dashed lines indicate the potential hydrogen bonds.

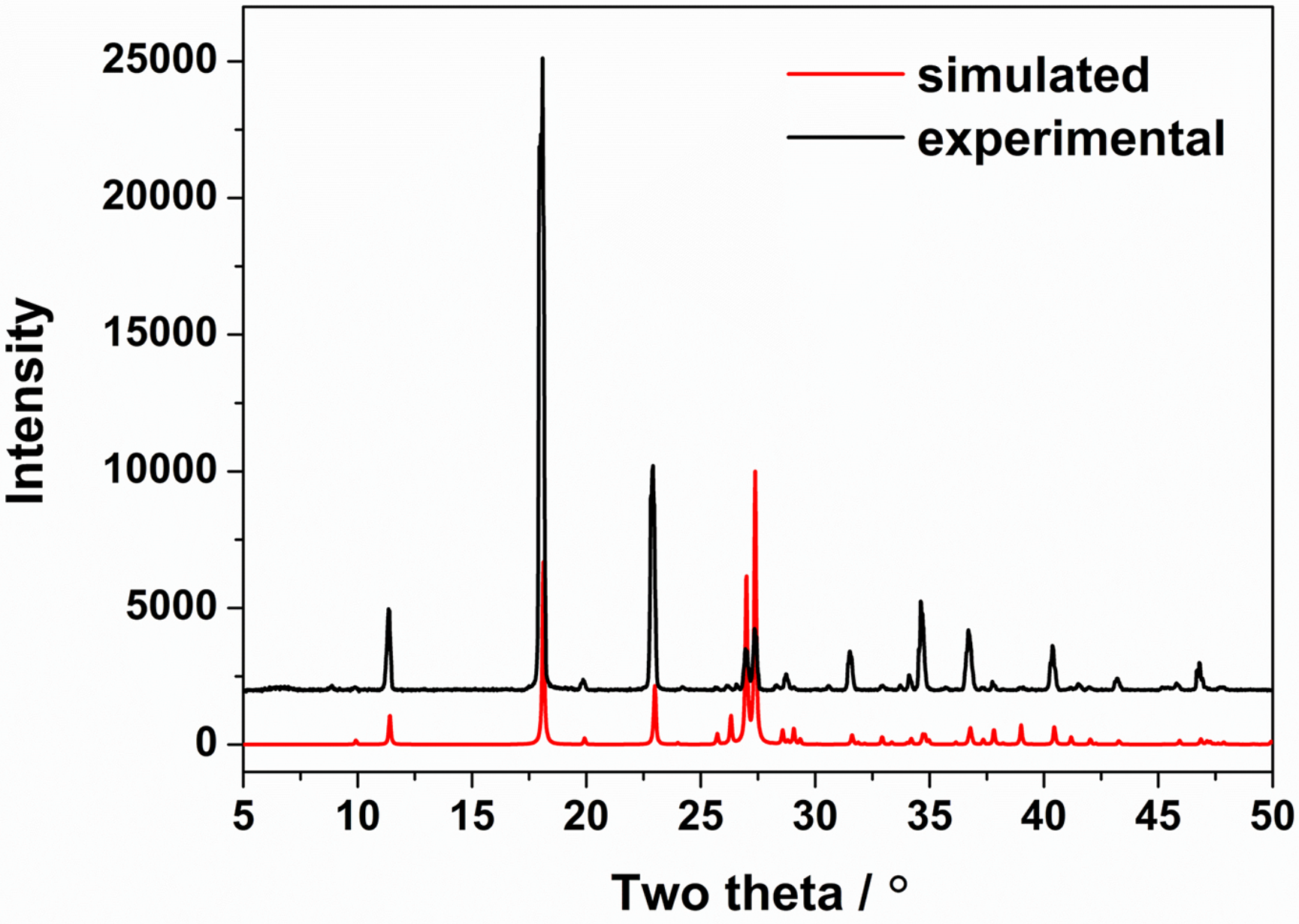

Fig. S2. The examined and simulated powder XRD patterns of compound (1).

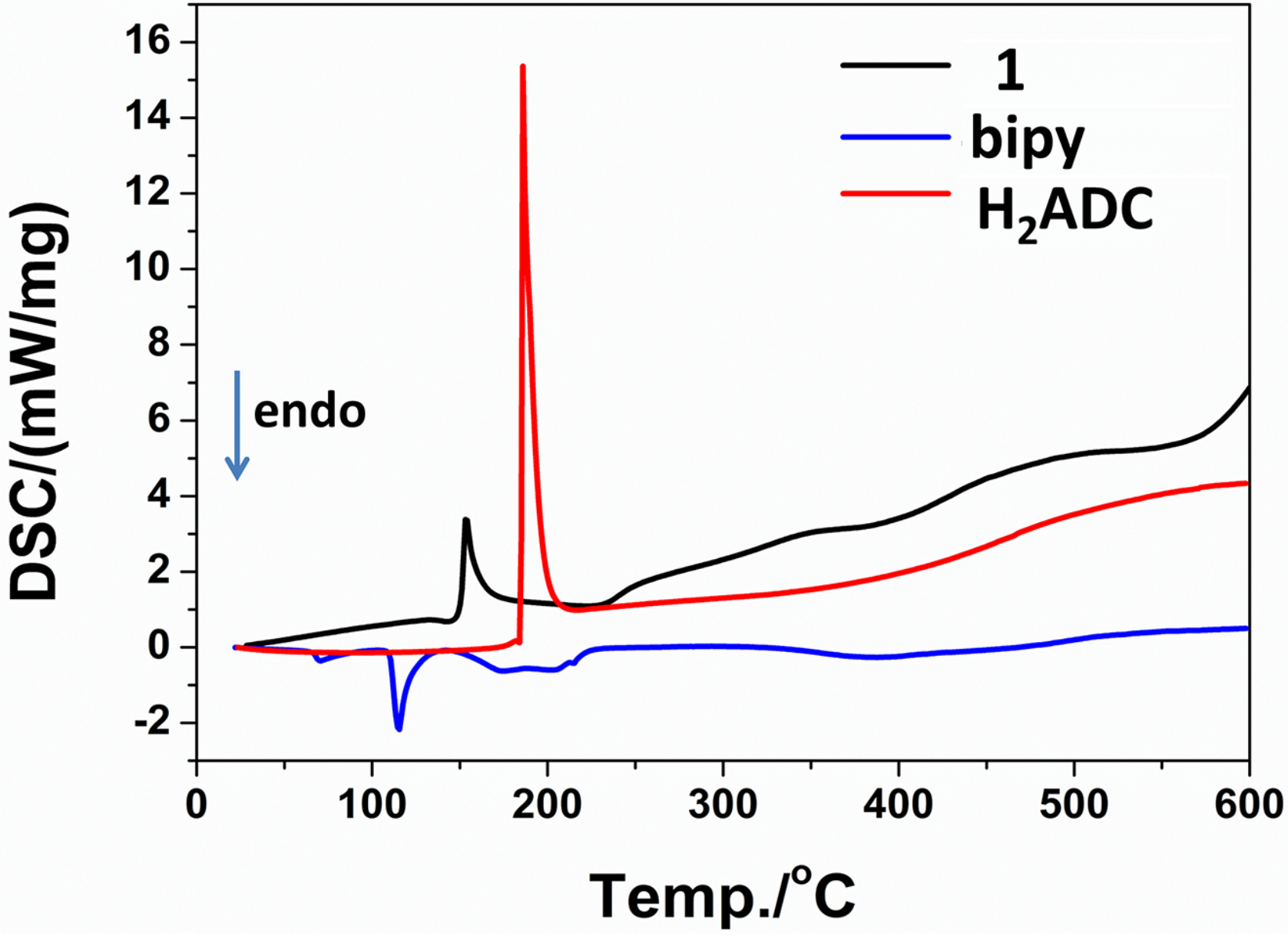

Fig. S3. The DSC diagrams of 4,4’-bipyridine (blue), H2ADC (red) and (1) (black).

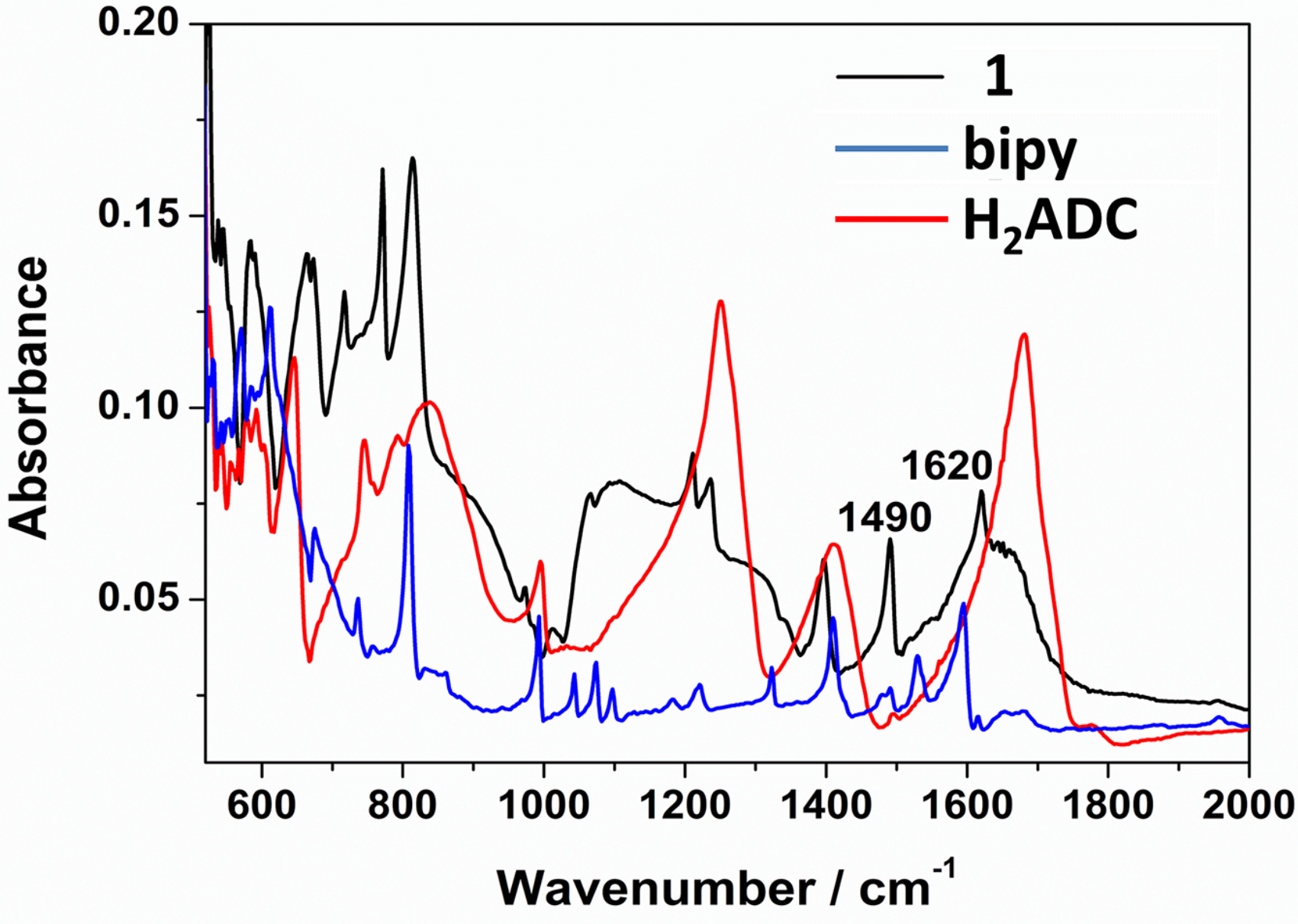

Fig. S4. The FT-IR spectrum of 4,4’-bipyridine (blue), H2ADC (red) and (1) (black).