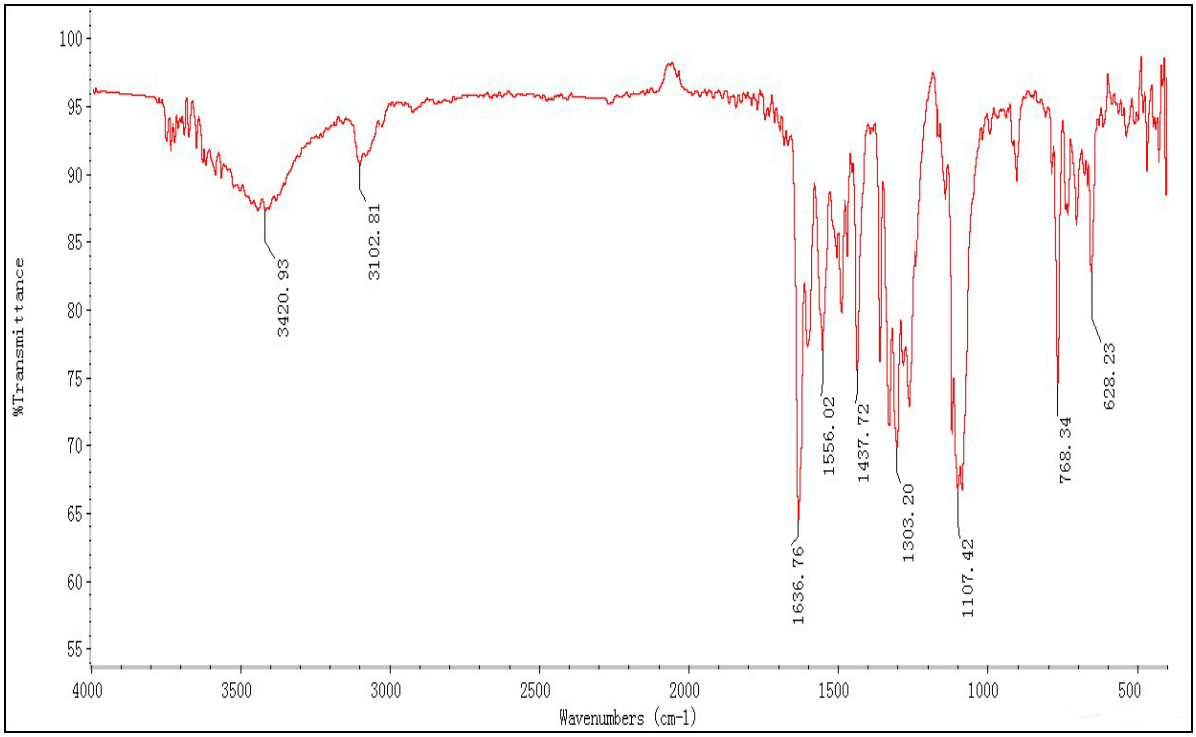

Fig. S1 IR spectrum of complex **1.**

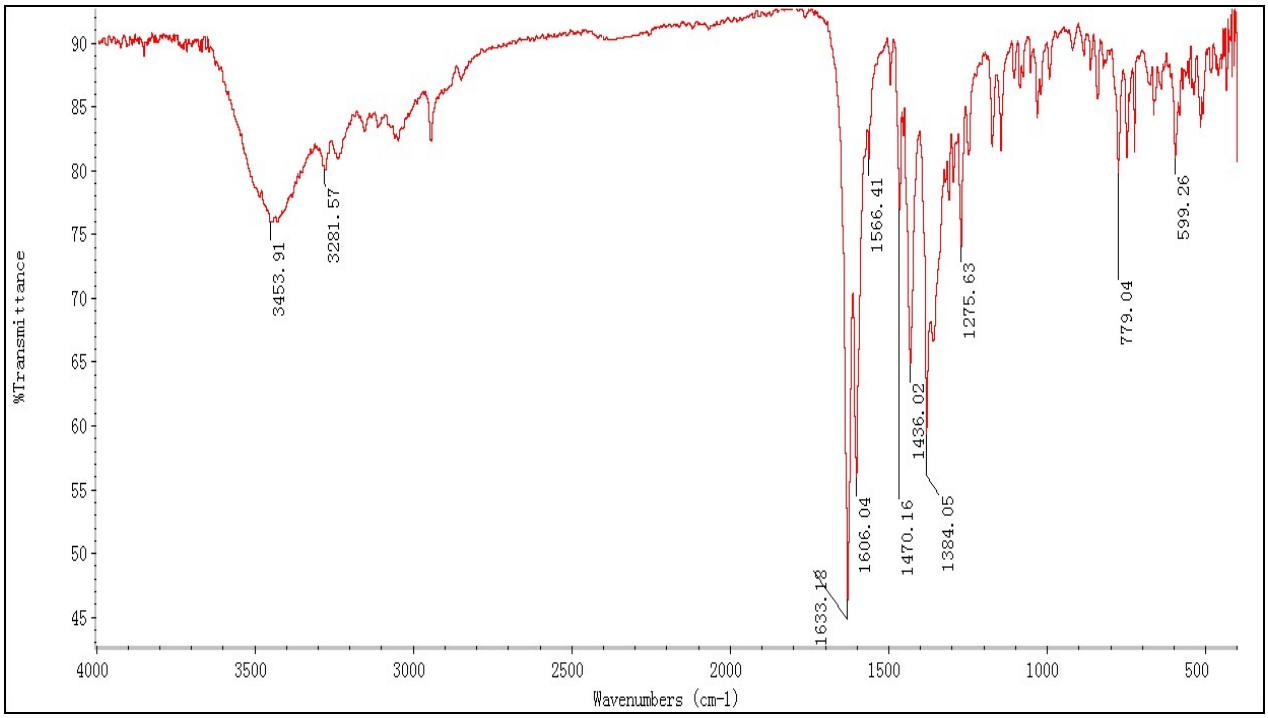

Fig. S2 IR spectrum of complex **2.**

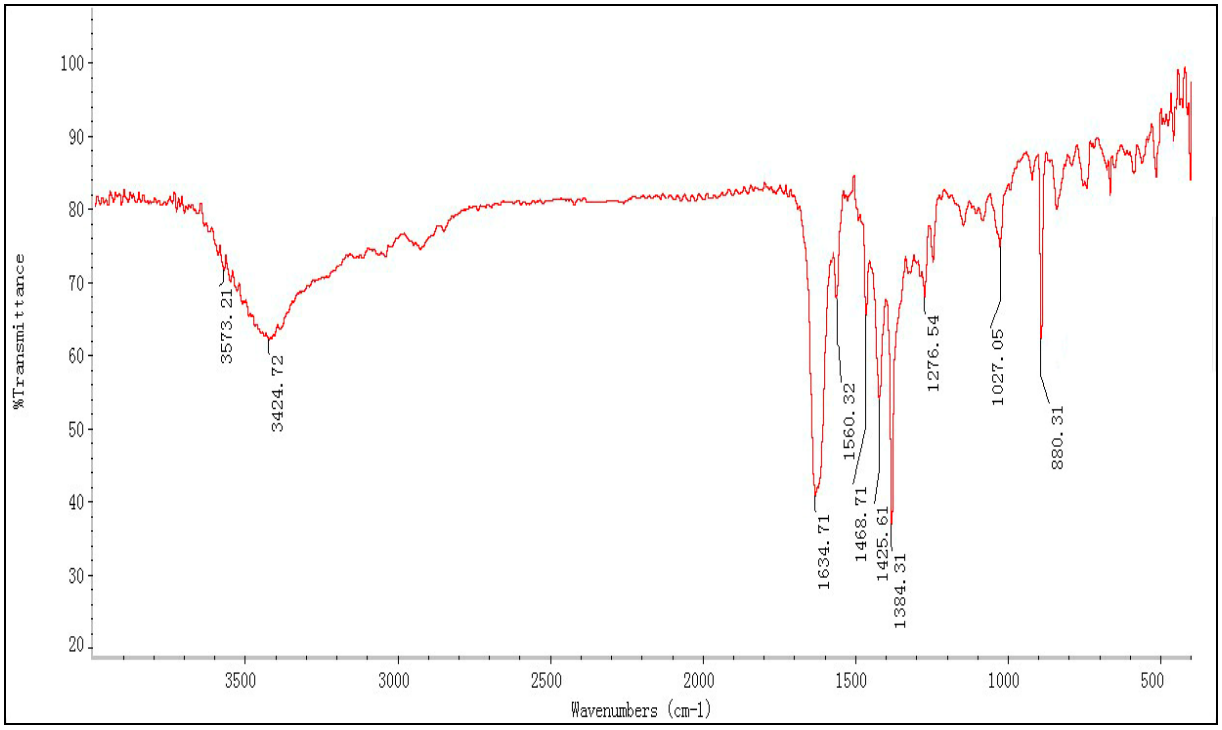

Fig. S3 IR spectrum of complex **3.**

Table S1 Selected bond distances (Å) and bond angles (°) for complexes **1**, **2** and **3**

Bond lengths		Bond angles	
1			
Cu1-O1	1.945(3)	O1-Cu1-N1	83.93(16)
Cu1-N1	1.923(3)	O1-Cu1-N2	164.68(13)
Cu1-N2	1.962(4)	O1-Cu1-N3	96.20(17)
Cu1-N3	1.981(4)	N1-Cu1-N2	83.63(16)
Cu2-O2	1.970(3)	O2-Cu2-O3	85.73(15)
Cu2-O3	1.942(3)	O2-Cu2-O4	93.92(13)
Cu2-O4	2.225(4)	O2-Cu2-N4	97.12(16)
Cu2-N4	2.006(4)	O2-Cu2-N5	169.25(15)
2			
Cu1-O1	1.945(3)	O1-Cu1-N1	83.93(16)
Cu1-N1	1.927(3)	O1-Cu1-N2	164.68(13)
Cu1-N2	1.982(3)	O1-Cu1-N3	96.20(17)
Cu1-N3	1.982(4)	N1-Cu1-N2	83.63(16)
Cu2-O2	1.949(3)	O2-Cu2-O3	85.73(15)
Cu2-O3	1.969(3)	O2-Cu2-O4	93.92(13)
Cu2-O4	2.326(3)	O2-Cu2-N4	169.80(13)
Cu2-N4	1.962(3)	O2-Cu2-N5	92.82(12)
3			
Cu1-O1	1.943(3)	O1-Cu1-N1	83.51(12)
Cu1-N1	1.909(3)	O1-Cu1-N2	167.08(12)
Cu1-N2	1.963(3)	O1-Cu1-N3	95.63(13)
Cu1-N3	1.964(4)	N1-Cu1-N2	83.61(14)
Cu2-O2	1.944(3)	O2-Cu2-O3	85.41(11)
Cu2-O3	1.974(3)	O2-Cu2-O4	87.63(12)
Cu2-O4	2.289(3)	O2-Cu2-N4	92.66(13)
Cu2-N4	1.968(4)	O2-Cu2-N5	169.10(12)

Table S2 Hydrogen-bonding geometries for complex **1** (Å,°)

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(D-H···A)
N3-H3A···O8B^{i}	0.90	2.44	3.334(11)	169
N3-H3B…O9B	0.90	2.28	3.069(11)	145
O4-H4A…O6^{ii}	0.94	1.84	2.761(6)	165
O4-H4B…O5^{iii}	0.90	1.83	2.708(5)	164
O5-H5A…O7	0.91	2.16	3.064(7)	169
O5-H5A…O9B	0.91	2.56	3.261(9)	134
O5-H5B…O1	0.89	2.00	2.884(6)	173
O6-H6A…O8B^{i}	0.88	2.15	2.956(10)	152
O6-H6B…O1	0.86	1.89	2.719(5)	162
C16-H16...O9B^{iv}	0.93	2.56	3.444(10)	158
C17-H17...O4^{v}	0.93	2.45	3.314(9)	155

[Symmetry codes: (i) = 1-x, 1-y, 2-z; (ii) =1-x, -y, 2-z; (iii) = -1+x, y, z;
(iv) = 1-x, -y, 1-z; (v) = -x, -y, 1-z]

Table S3 Hydrogen-bonding geometries for complex **2** (Å,°)

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(D-H···A)
N3-H3A...O7^{iii}	0.90	2.10	2.982(7)	167
N3-H3B...O5^{ii}	0.90	2.22	2.972(7)	141
O4-H4A...O1^{iv}	0.90	1.82	2.709(4)	171
O4-H4B...O8	0.88	1.96	2.821(5)	170
O8-H8A...O7^{v}	0.88	2.22	3.049(6)	157
O8-H8B...O6	0.94	2.17	3.056(8)	156
C18-H18...O4^{i}	0.93	2.40	3.307(5)	164

[Symmetry codes: (i) = 1/2-x,1/2+y, -1/2+z; (ii) = x, -1+y, z; (iii) = 1-x,1-y,1/2+z; (iv) = x, 1+y, z; (v) = 1-x,2-y, 1/2+z]

Table S4 Hydrogen-bonding geometries for complex **3** (Å,°)

D-H···A	d(D-H)	d(H···A)	d(D···A)	∠(D-H···A)
N3-H3A...O6^{iv}	0.90	2.23	2.967(6)	138
N3-H3B...O1^{v}	0.90	2.09	2.983(4)	171
O7-H7A...O1	0.85	1.96	2.759(6)	158
O7-H7B...O5 ^{iv}	0.85	2.40	3.240(6)	173
C18-H18...O7^{vi}	0.93	2.35	3.238(6)	159

[Symmetry codes: (iv) = 1-x, -y, 1-z.; (v) = 1- x, - y, - z; (vi) = 1+x,1+y, 1+z]