Supporting Information

Selective recognition of sulphate in Cu(II) assisted 1D polymer of a simple pentafluorophenyl substituted pyridyl-urea via second sphere coordination

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Figure 1S. Single crystal X-ray structure of **L**[1]

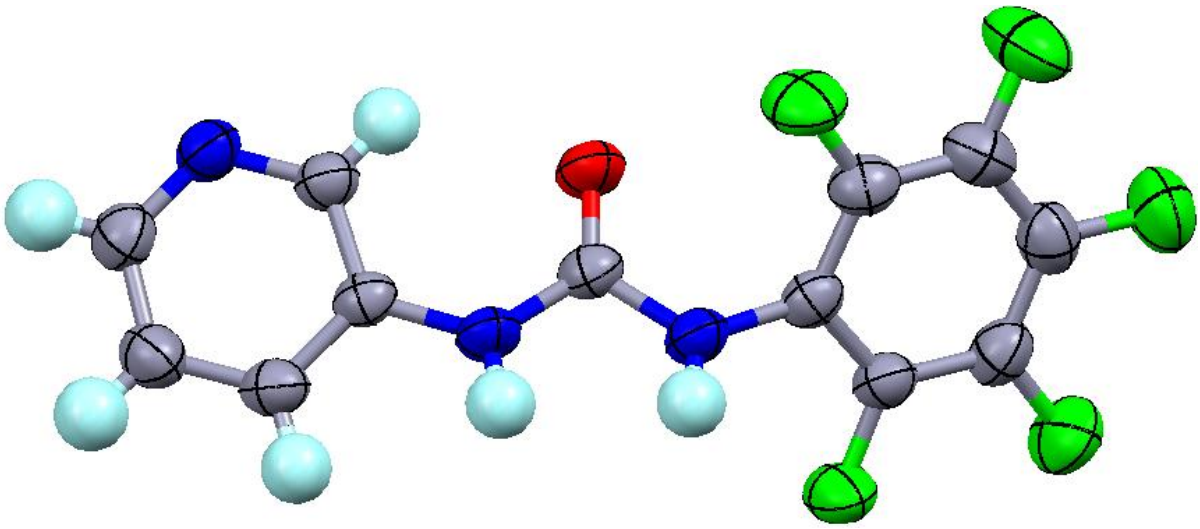


Table 1S. Crystallographic table for $\mathbf{L^1}$

Parameters	$\mathbf{L^1}$
Empirical formula	C12 H6 F5 N3 O
Formula weight	303.20
Crystal system	Orthorhombic
Space group	Pbca
***a* (Å)**	12.7261(15)
***b* (Å)**	10.2498(12)
***c* (Å)**	18.184(2)
α (deg)	90.00
β (deg)	90.00
γ (deg)	90.00
***V* (Å^3)**	2371.9(5)
Z	8
d_{calc} (g/cm^3)	1.765
Crystal size (mm^3)	0.40x0.20x0.06
Diffractometer	Smart CCD
***F*(000)**	1216
μ MoKα (mm^{-1})	0.165
***T* (K)**	150(2)
θ max	27.31
Observed Reflections	2654
Parameters refined	190
R_1; WR_2	0.0407; 0.1558
GOF (F2)	1.038

Table 2S. Crystallographic table for complex **1**

Parameters	**Complex 1**
Empirical formula	C54 H38 Cu F20 N14 O10 S
Formula weight	1518.58
Crystal system	Triclinic
Space group	P-1
***a* (Å)**	11.7823(17)
***b* (Å)**	14.103(2)
***c* (Å)**	23.069(3)
***α* (deg)**	95.942(3)
***β* (deg)**	104.696(3)
γ (deg)	111.866(3)
***V* (Å^3)**	3356.3(8)
Z	2
d_{calc} (g/cm^3)	1.503
Crystal size (mm^3)	1.00x0.08x0.06
Diffractometer	Smart CCD
***F*(000)**	1530
μ MoKα (mm^{-1})	0.476
***T* (K)**	150(2)
***θ* max**	25.66
Observed Reflections	12616
Parameters refined	878
R_1; WR_2	0.0917; 0.2477
GOF (F2)	1.162

Table 3S. Hydrogen bonding table for complex **1**

D-H···A	d(H-A) Å	d(D-A) Å	<DHA (□)
N5-H5···O1	2.11	2.93	157
N6-H6···O3	2.13	2.97	166
N7-H7···O1	2.36	2.97	128
N7-H7···O2	2.49	3.24	146
N8-H8···O2	1.99	2.83	167
N9-H9···O3	2.16	2.87	141
N10-H10···O1	2.04	2.88	168
N11-H11···O4	1.90	2.76	178
N12-H12···O3	2.15	2.93	152
C3-H3···O10	2.37	3.07	132
C27-H27···O8	2.49	3.14	127
C38-H38···F16	2.43	3.20	140
C2-H2···F14	2.54	3.24	133
C45-H45A···F18	2.47	3.29	143

Symmetry codes: 1+x, y, z; x,1+y,z; x,-1+y,z; 2-x,1-y,1-z

Figure 2S. C-F···H-C interactions in complex **1**

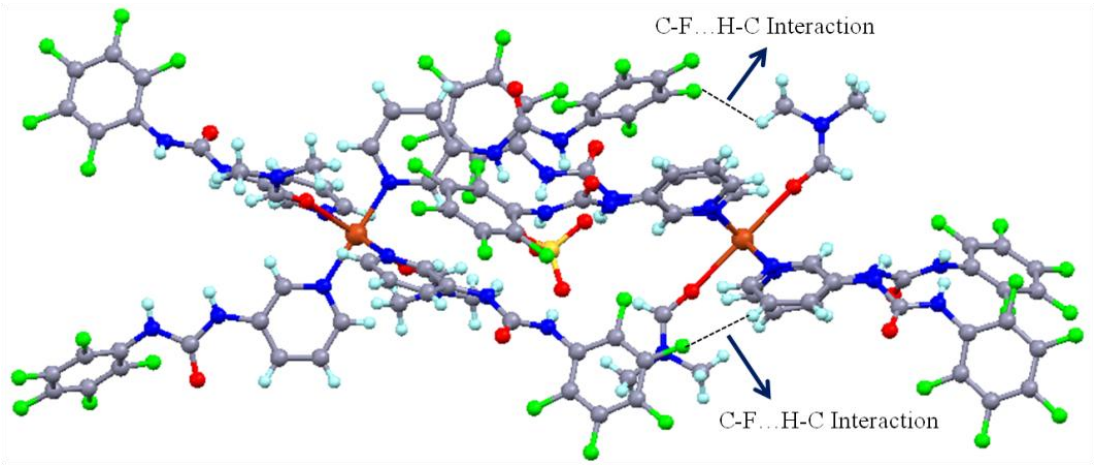


Table 4S. Metal-Ligand bond distances in complex **1**

Atoms	Distance (Å)
Cu1 -O5	2.5027
Cu1 -N1	2.0536
Cu1 -N2	2.0458
Cu2 -N3	2.0538
Cu2 -N4	2.0536
Cu1 -O5a	2.5027
Cu1 -N1a	2.0536
Cu1 -N2a	2.0458
Cu2 -N4b	2.0536
Cu2 -N3b	2.0538

Table 5S. Crystallographic table for complex **2**

Parameters	**Complex 2**
Empirical formula	C48 H32 Cu F20 N14 O14
Formula weight	1472.42
Crystal system	Monoclinic
Space group	C2/c
***a* (Å)**	32.1757(18)
***b* (Å)**	8.1355(5)
***c* (Å)**	25.9525(15)
***α* (deg)**	90.00
***β* (deg)**	119.3470(10)
γ (deg)	90.00
***V* (Å^3)**	5921.6(6)
Z	4
d_{calc} (g/cm^3)	1.652
Crystal size (mm^3)	0.08x0.06x0.04
Diffractometer	Smart CCD
***F*(000)**	2956.0
μ MoKα (mm^{-1})	0.507
***T* (K)**	150
***θ* max**	26.880
Observed Reflections	6334
Parameters refined	447
R_1; WR_2	0.0411; 0.1178
GOF (F2)	1.012

D-H...A	d(H-A) Å	d(D-A) Å	<DHA (□)
N1-H1…O6	2.42	3.020(4)	128
N2-H2…O7	2.10	2.903(3)	156
N5-H5…O5	2.14	2.960(3)	158
N6-H6…O6	2.08	2.923(4)	169
O13-H13…O11	2.06	2.779(3)	149
O14-H14A…O11	2.09	2.824(3)	151
C9-H9…O7	2.54	3.315(3)	141
C14-H14…O5	2.57	3.332(4)	140
C16-H16…F4	2.53	3.109(4)	120

Table 6S. Hydrogen bonding table for complex **2**

Symmetry codes: 1/2-x,-1/2+y,1/2-z; -x,-1+y,1/2-z; -x,2-y,-z

Figure 3S. Scattered plot of complex **2**

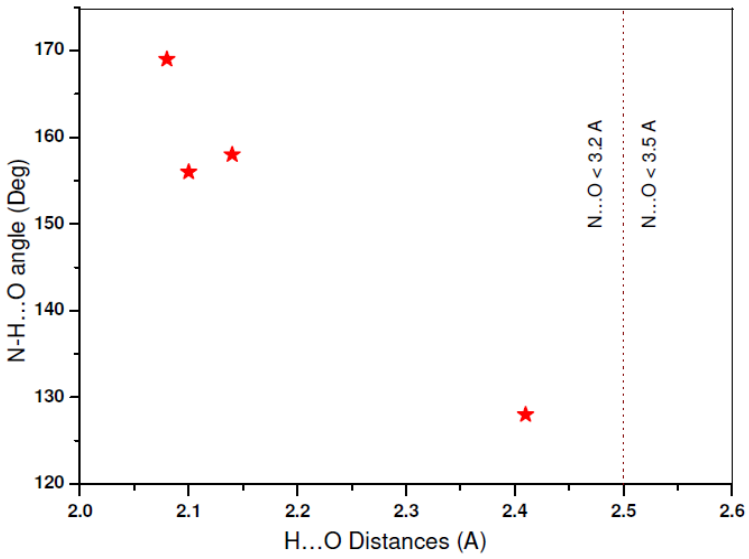


Table 7S. Metal-Ligand bond distances in complex **2**

Atoms	Distance (Å)
Cu1 -O13	2.2809(1)
Cu1 -O14	2.4167(1)
Cu1 -N3	2.0554
Cu1 -N4	2.0499
Cu1 -N3a	2.0554
Cu1 -N4a	2.0499

Table 8S. Crystallographic table for complex **3**

Parameters	**Complex 3**
Empirical formula	C48 H48 Co F15 N13 O12 S
Formula weight	1374.98
crystal system	Monoclinic
Space group	P2(1)/c
***a* (Å)**	17.833(2)
***b* (Å)**	12.8082(17)
***c* (Å)**	26.372(3)
α (deg)	90.00
β (deg)	105.751(3)
γ (deg)	90.00
***V* (Å^3)**	5797.4(13)
Z	4
d_{calc} (g/cm^3)	1.575
Crystal size (mm^3)	1.00x0.08x0.06
Diffractometer	Smart CCD
***F*(000)**	2804
μ MoKα (mm^{-1})	0.451
***T* (K)**	150(2)
θ max	25.00
Observed Reflections	10204
Parameters refined	827
R_1; WR_2	0.0349; 0.0927
GOF (F2)	0.985

Table 9S. Hydrogen bonding table for complex **3**

D-H…A	d(H-A) Å	d(D-A) Å	<DHA (□)
N7-H7…O8	2.04	2.840(2)	155
N8-H8…O9	1.99	2.807(2)	158
N9-H9…O7	2.18	2.897(2)	141
N10-H10…O7	2.17	2.946(2)	150
N10-H10…O9	2.36	3.110(2)	146
N11-H11…O7	1.98	2.811(2)	163
N12-H12…O11	2.03	2.826(2)	153
C1-H1…F9	2.48	3.384(2)	164
C2-H2...O8	2.49	3.236(3)	138
C14-H14...F5	2.53	3.184(3)	127
C33-H33…O6	2.57	3.316(2)	137
C38-H38C…O11	2.57	3.473(3)	158
C44-H44C...O3	2.59	3.489(3)	156

Symmetry codes: x,-1+y,z; 1-x,1-y,-z; -x,1-y,-z; -x,2-y,-z; x,1+y,z; -1+x,y,z; 1-x,-1/2+y,1/2-z

Table 10S. Crystallographic table for complex **4**

Parameters	**Complex 4**
Empirical formula	C48 H48 F15 N13 Ni O12 S
Formula weight	1374.76
crystal system	Monoclinic
Space group	P2(1)/c
***a* (Å)**	17.8094(11)
***b* (Å)**	12.7781(8)
***c* (Å)**	26.5467(17)
α (deg)	90.00
β (deg)	105.688(2)
γ (deg)	90.00
***V* (Å^3)**	5816.2(6)
Z	4
d_{calc} (g/cm^3)	1.570
Crystal size (mm^3)	0.06x0.04x0.02
Diffractometer	Smart CCD
***F*(000)**	2808
μ MoKα (mm^{-1})	0.488
***T* (K)**	150(2)
θ max	22.41
Observed Reflections	7513
Parameters refined	809
R_1; WR_2	0.0522; 0.1518
GOF (F2)	1.045

Table 11S. Hydrogen bonding table for complex **4**

D-H...A	d(H-A) Å	d(D-A) Å	<DHA (□)
N(4) --H(4) ..O(4)	2.06	2.8657	155
N(5) --H(5A) ..O(2)	1.99	2.8104	160
N(6) --H(6) ..O(3)	1.97	2.8089	164
N(7) --H(7) ..O(11)	2.05	2.8514	155
N(8) --H(8) ..O(3)	2.21	2.9403	143
N(9) --H(9) ..O(2)	2.33	3.0875	147
N(9) --H(9) ..O(3)	2.22	2.9930	149
C(3) --H(3) ..O(4)	2.53	3.2764	138
C(26) --H(26) ..F(10)	2.52	3.1771	128

Symmetry codes: 1-x,-y,-z; -x,-y,-z; -1+x,y,z; -x,1-y,-z; x,1+y,z

Table 12S .Crystallographic table for complex **5**

Parameters	**Complex 5**
Empirical formula	C27 H31 Cu N7 O9 S
Formula weight	693.19
crystal system	Monoclinic
Space group	C2/c
***a* (Å)**	32.699(5)
***b* (Å)**	10.4948(17)
***c* (Å)**	23.118(4)
***α* (deg)**	90.00
***β* (deg)**	129.583(2)
γ (deg)	90.00
***V* (Å^3)**	6114.2(16)
Z	8
d_{calc} (g/cm^3)	1.506
Crystal size (mm^3)	1.00x0.08x0.06
Diffractometer	Smart CCD
***F*(000)**	2872
μ MoKα (mm^{-1})	0.847
***T* (K)**	150(2)
***θ* max**	25.00
Observed Reflections	5388
Parameters refined	410
R_1; WR_2	0.0403; 0.1075
GOF (F2)	S = 1.041

Table 13S. Hydrogen bonding table for complex **5**

D-H...A	d(H-A) Å	d(D-A) Å	<DHA (□)
N3-H3...O5	2.07	2.771(5)	139
N4-H4...O5	2.20	2.922(4)	141
N5-H5...O4	2.08	2.931(3)	171
N6-H6...O7	2.13	2.966(4)	165
O8-H8A...O2	1.97	2.736(3)	155
C3-H3A...O1	2.42	3.251(5)	148
C4-H4A...O7	2.49	3.276(4)	142

Symmetry codes: -x,y,1/2-z; 1/2-x,3/2-y,1-z; x,-1+y,z

Figure 4S. Comparison of PXRD pattern of complex **3**: (Blue) simulated and (Red) experimental

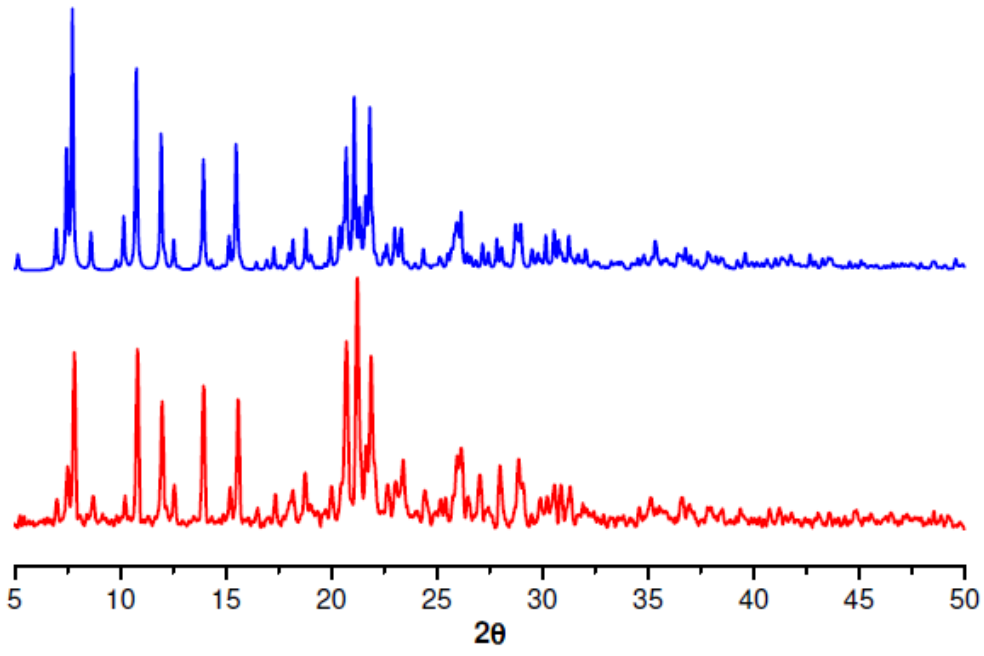


Figure 5S. Comparison of PXRD pattern of complex **4**: (Blue) simulated and (Red) experimental

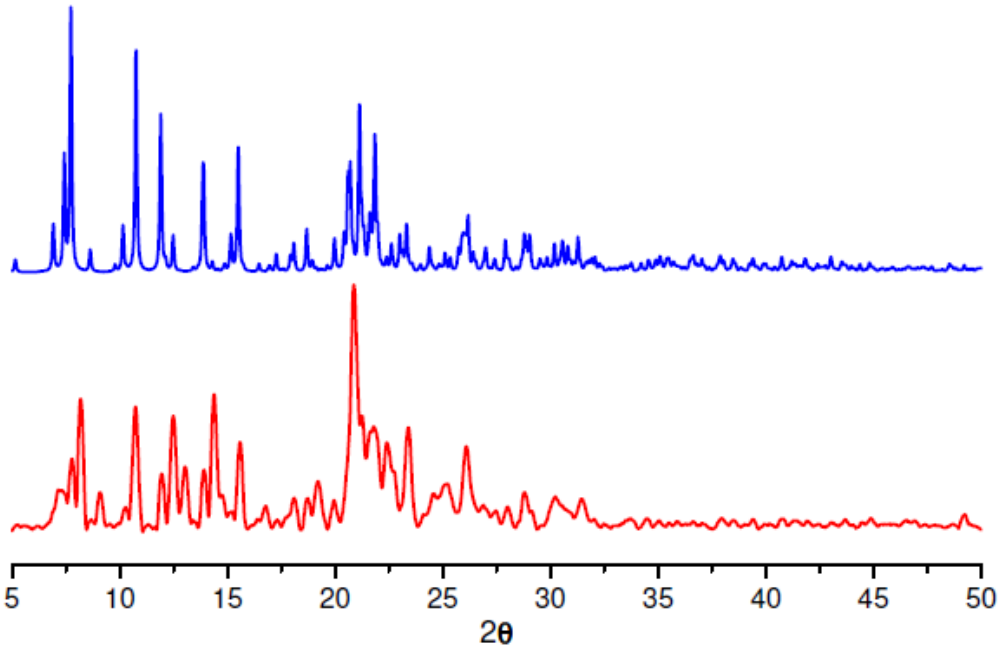


Figure 6S. Comparison of PXRD pattern of complex **5**: (Blue) simulated and (Red) experimental

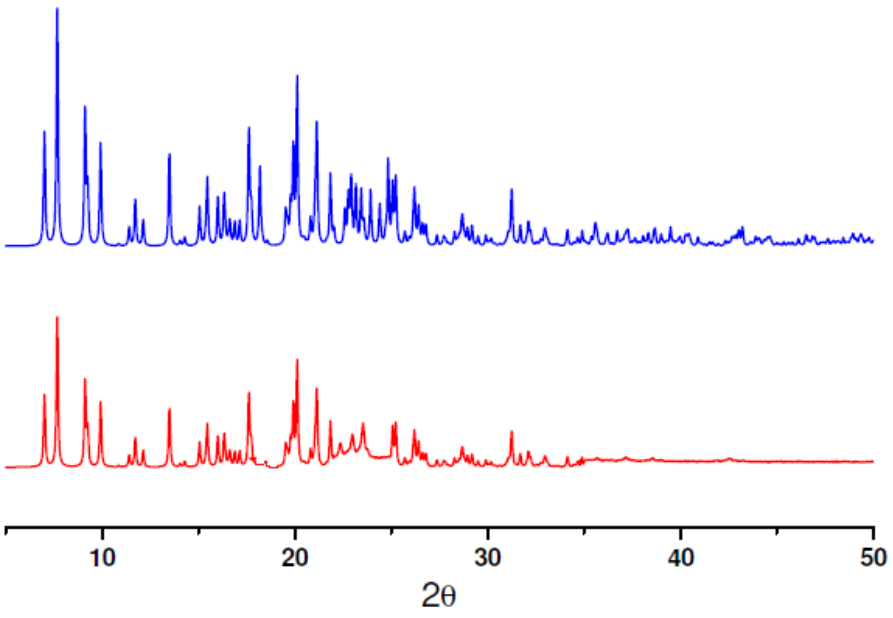


Figure 7S. PXRD pattern of $CuCl_2$ complex of **L**[1]

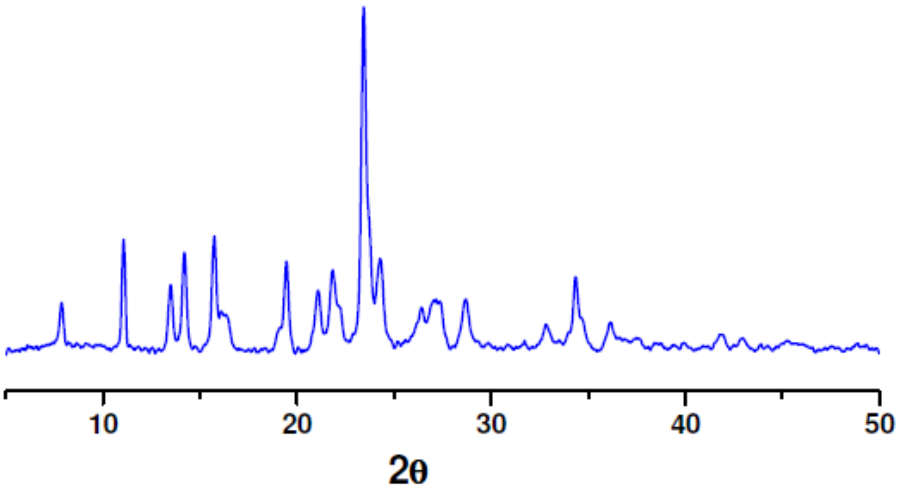


Figure 8S. PXRD pattern of $CuBr_2$ complex of **L**[1]

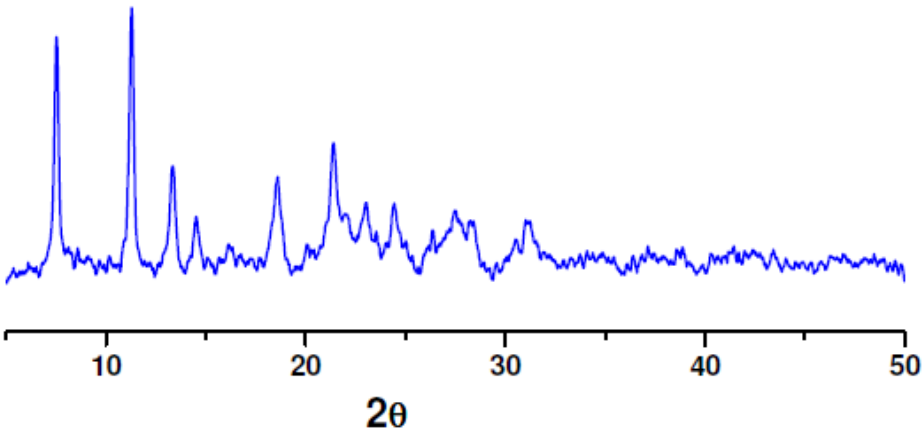


Figure 9S. ESI-MS spectrum of $\mathbf{L}^{1}$

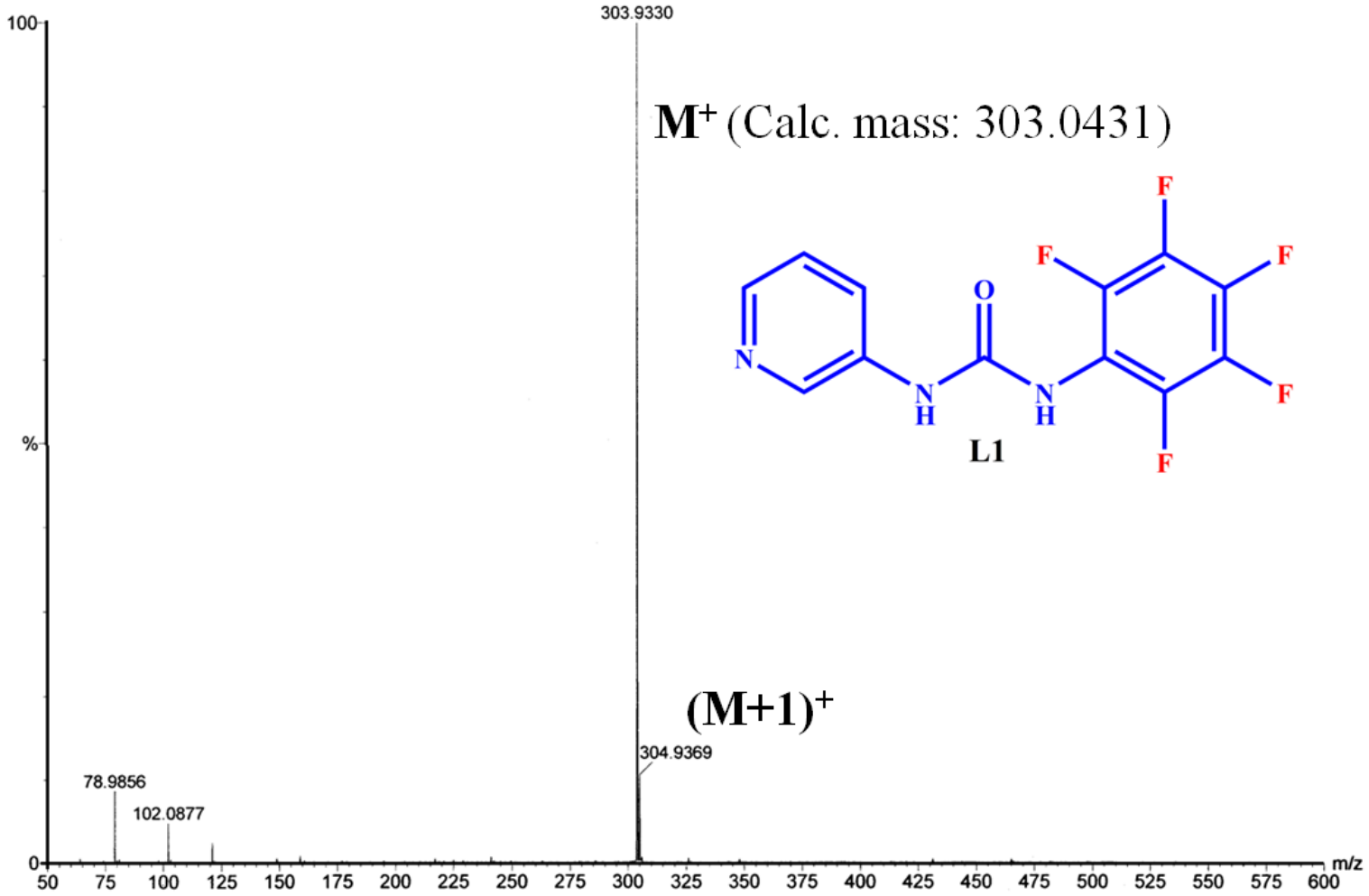


Figure 10S. ^{1}H-NMR spectrum of **L^{1}**

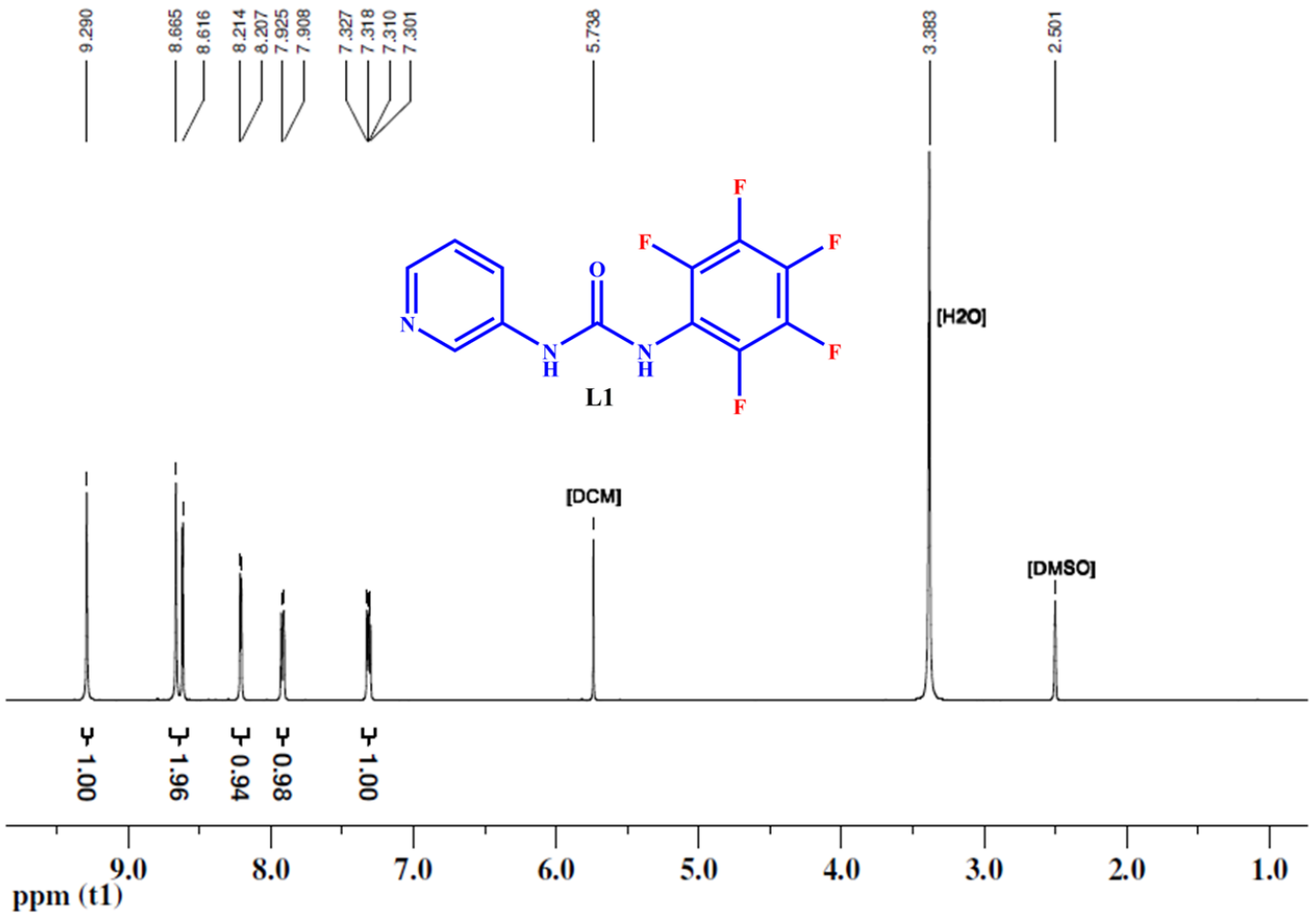


Figure 11S. ^{13}C-NMR spectrum of **L^1**

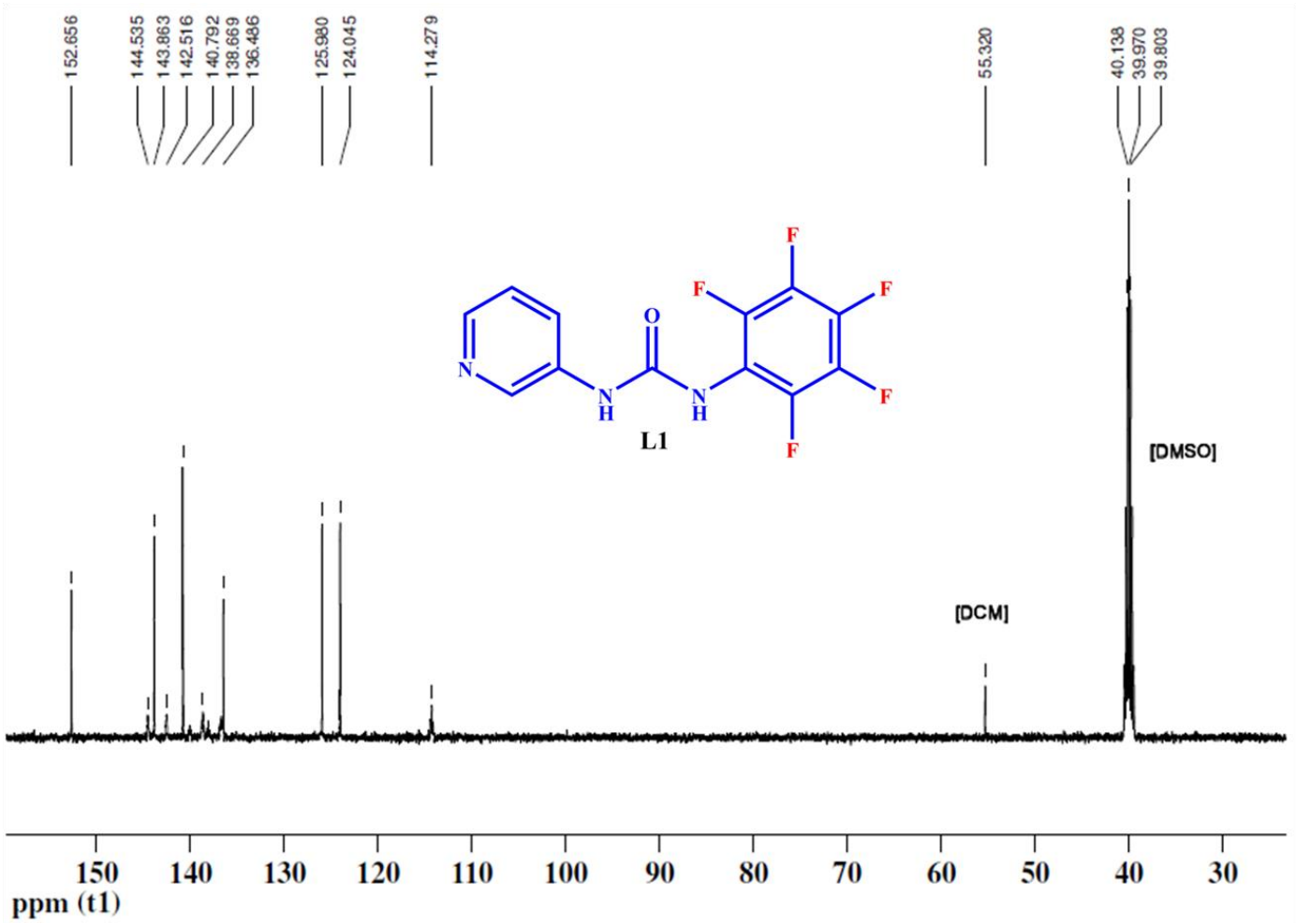


Figure 12S. ESI-MS spectrum of $\mathbf{L^2}$

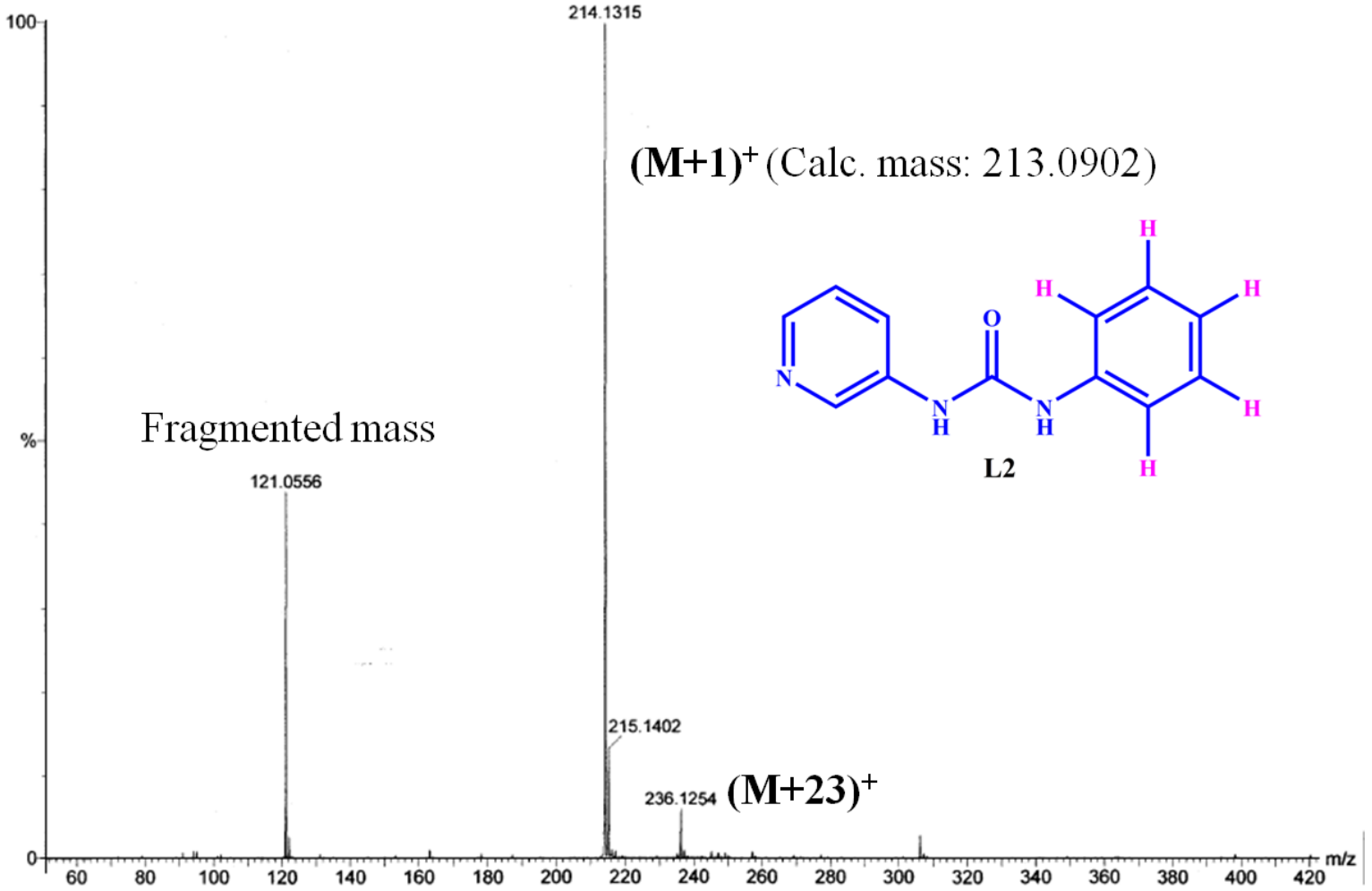


Figure 13S. ^{1}H-NMR spectrum of **L**^{2}

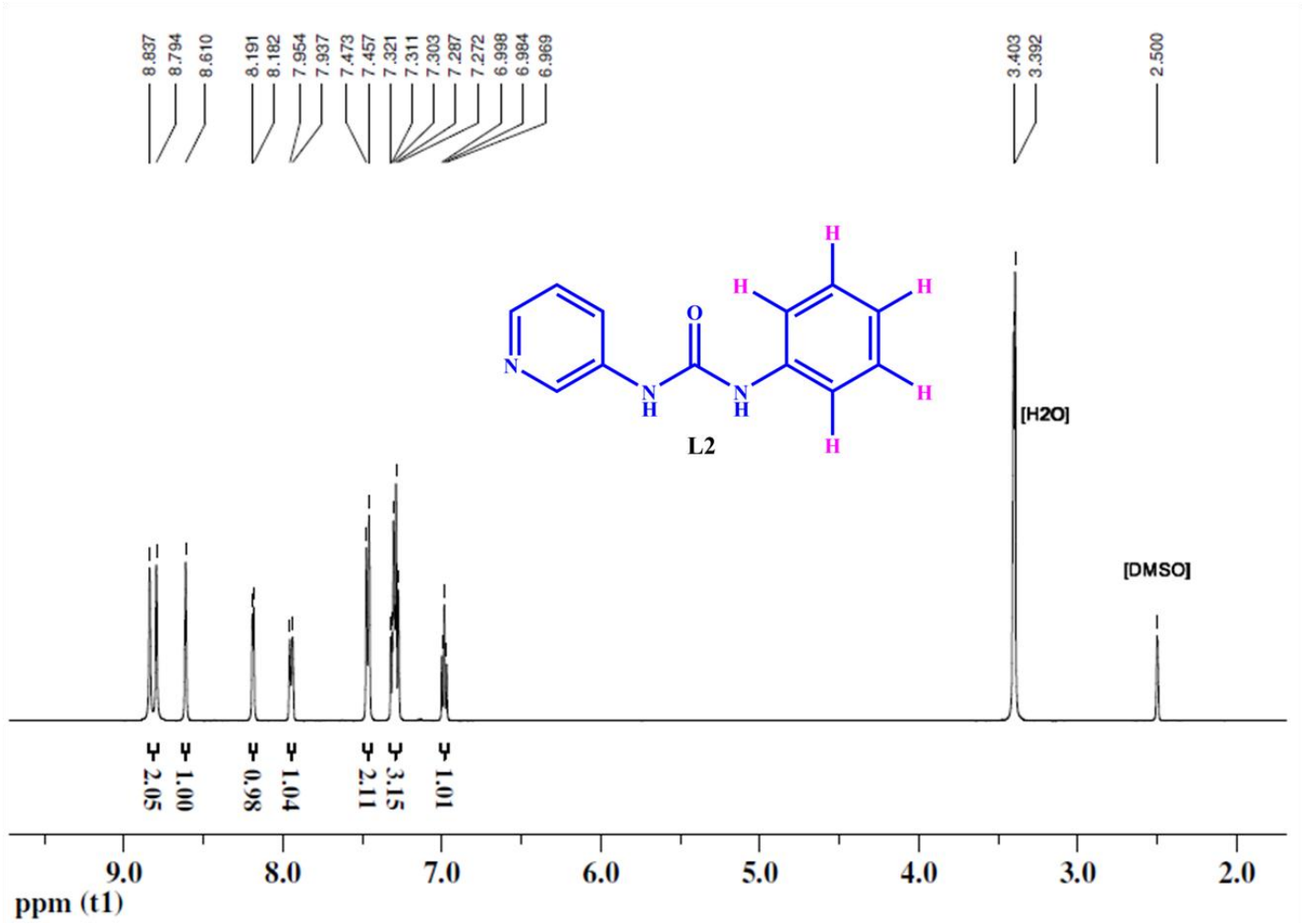


Figure 14S. ^{13}C-NMR spectrum of **L^2**

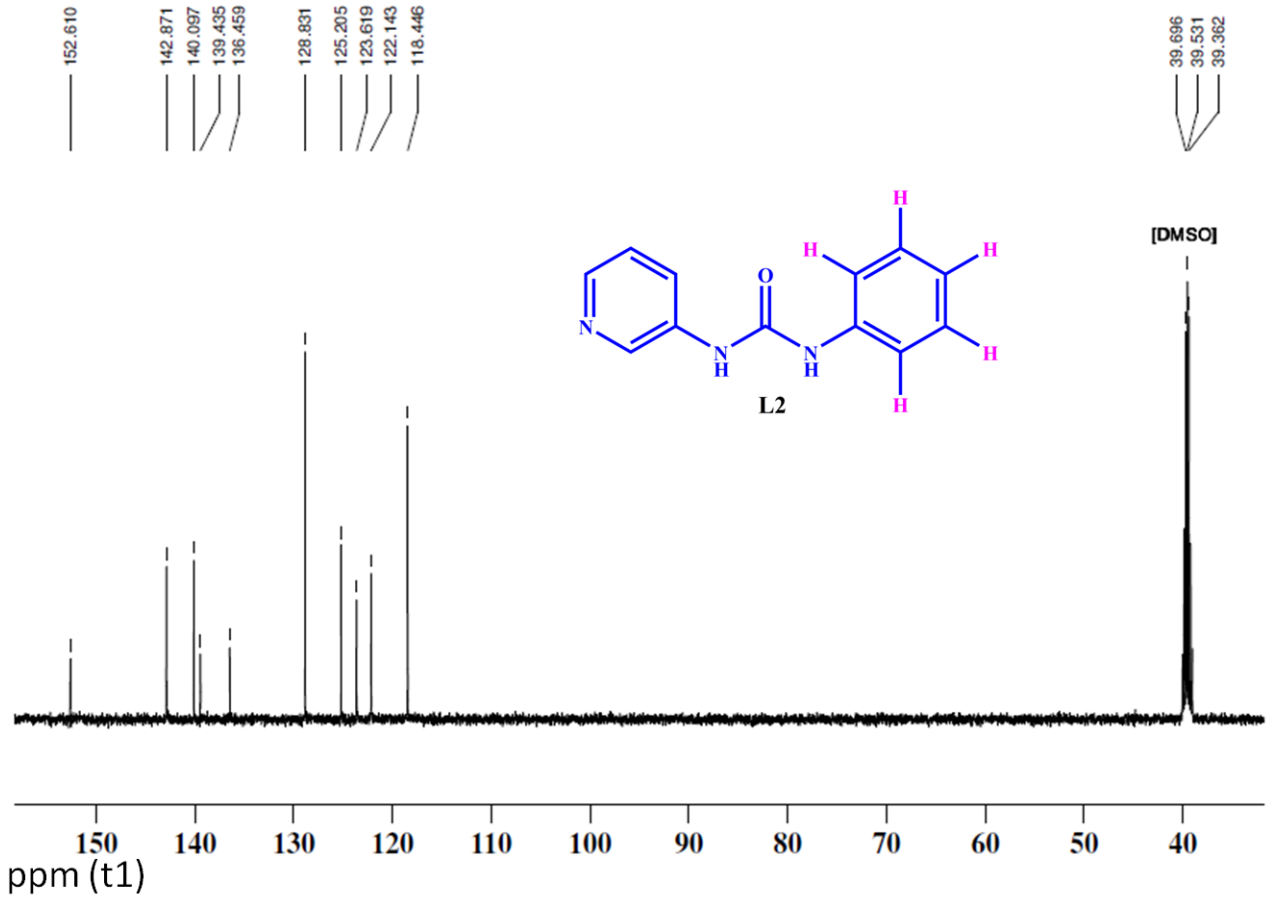
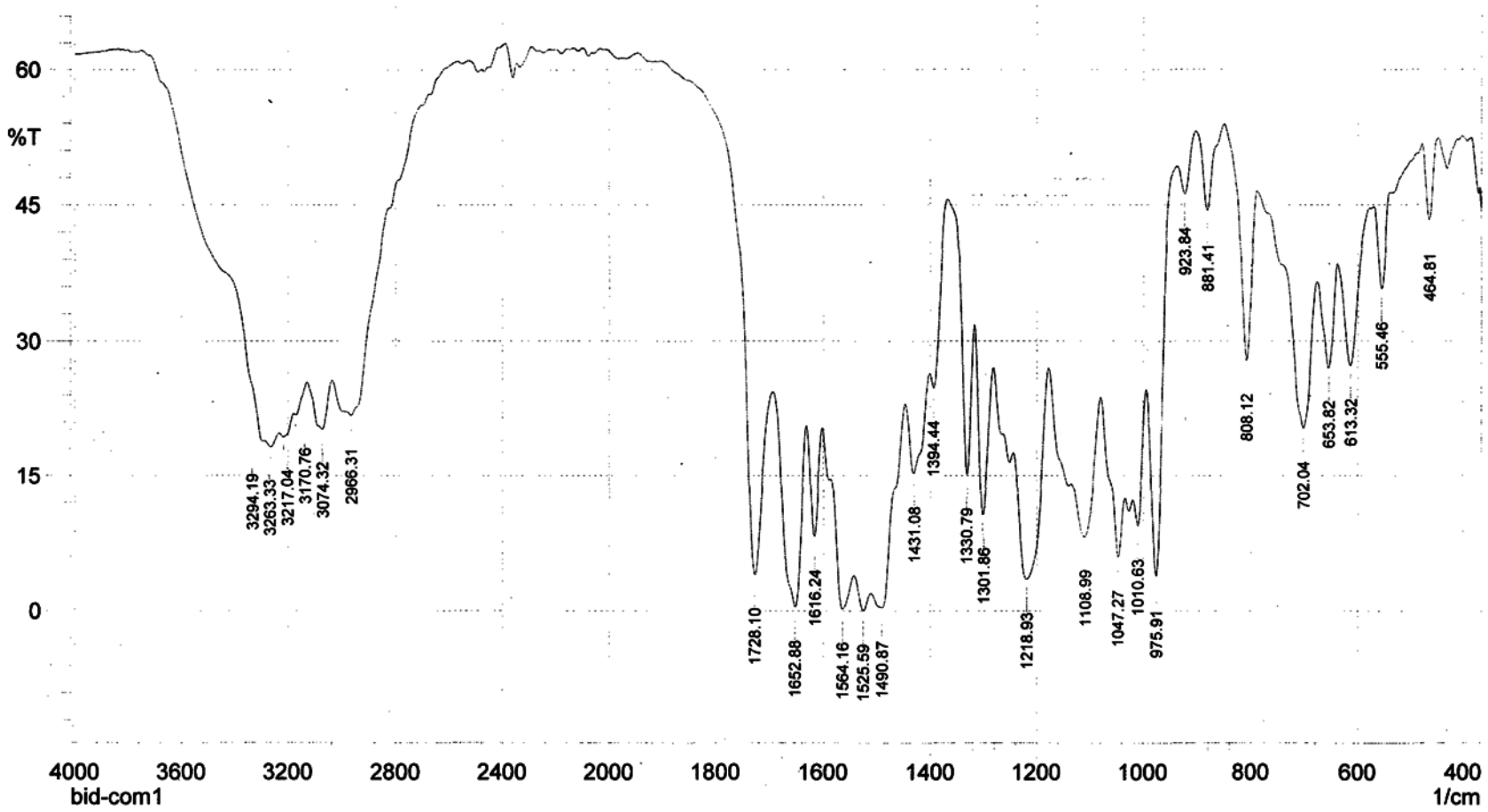


Figure 15S. FT-IR spectrum of complex **1**



Peak at 1109 cm^{-1} (symmetric stretching frequency of SO_4^{2-}) indicate the presence of SO_4^{2-}.

Figure 16S. FT-IR spectrum of complex **2**

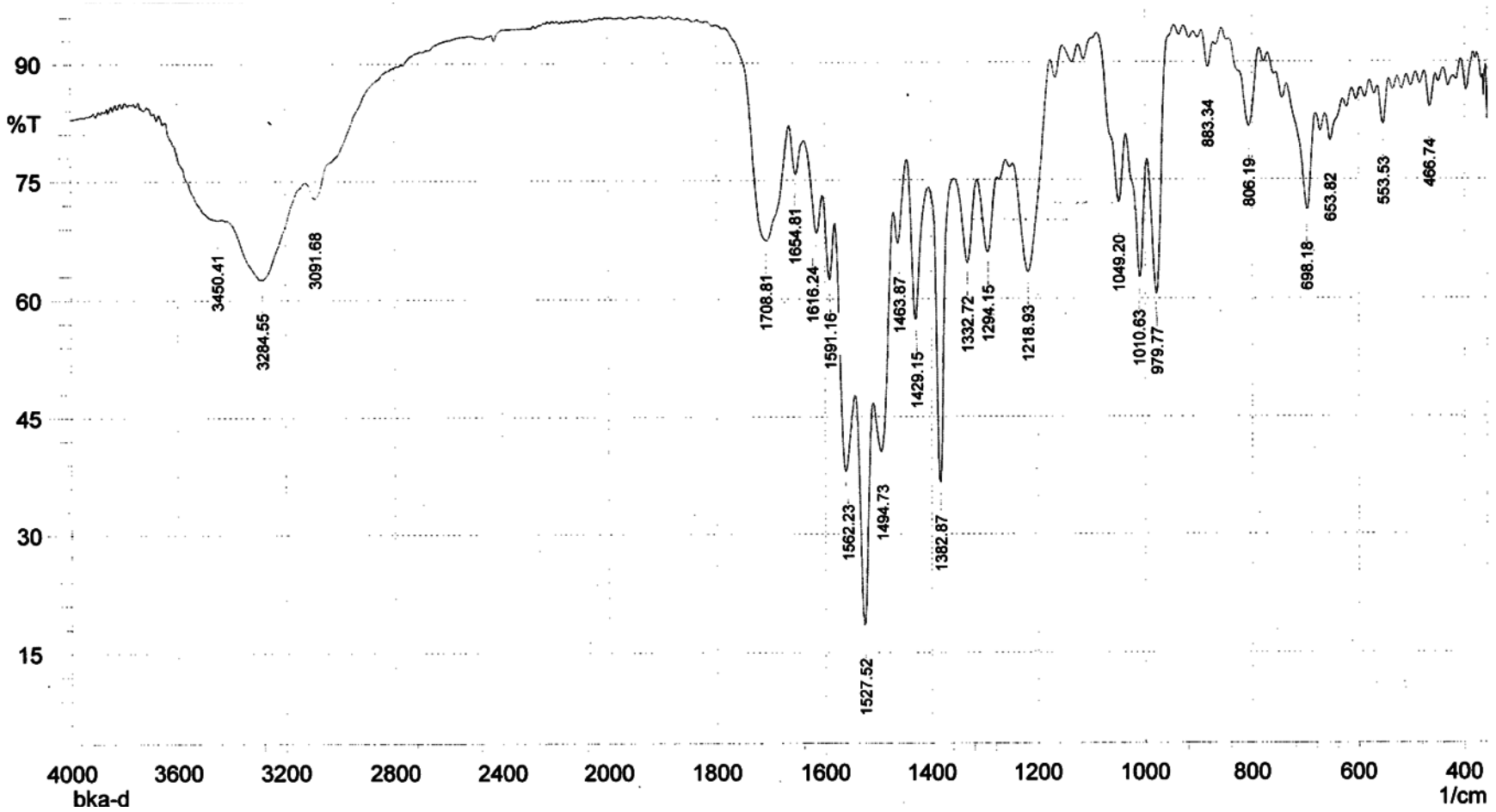
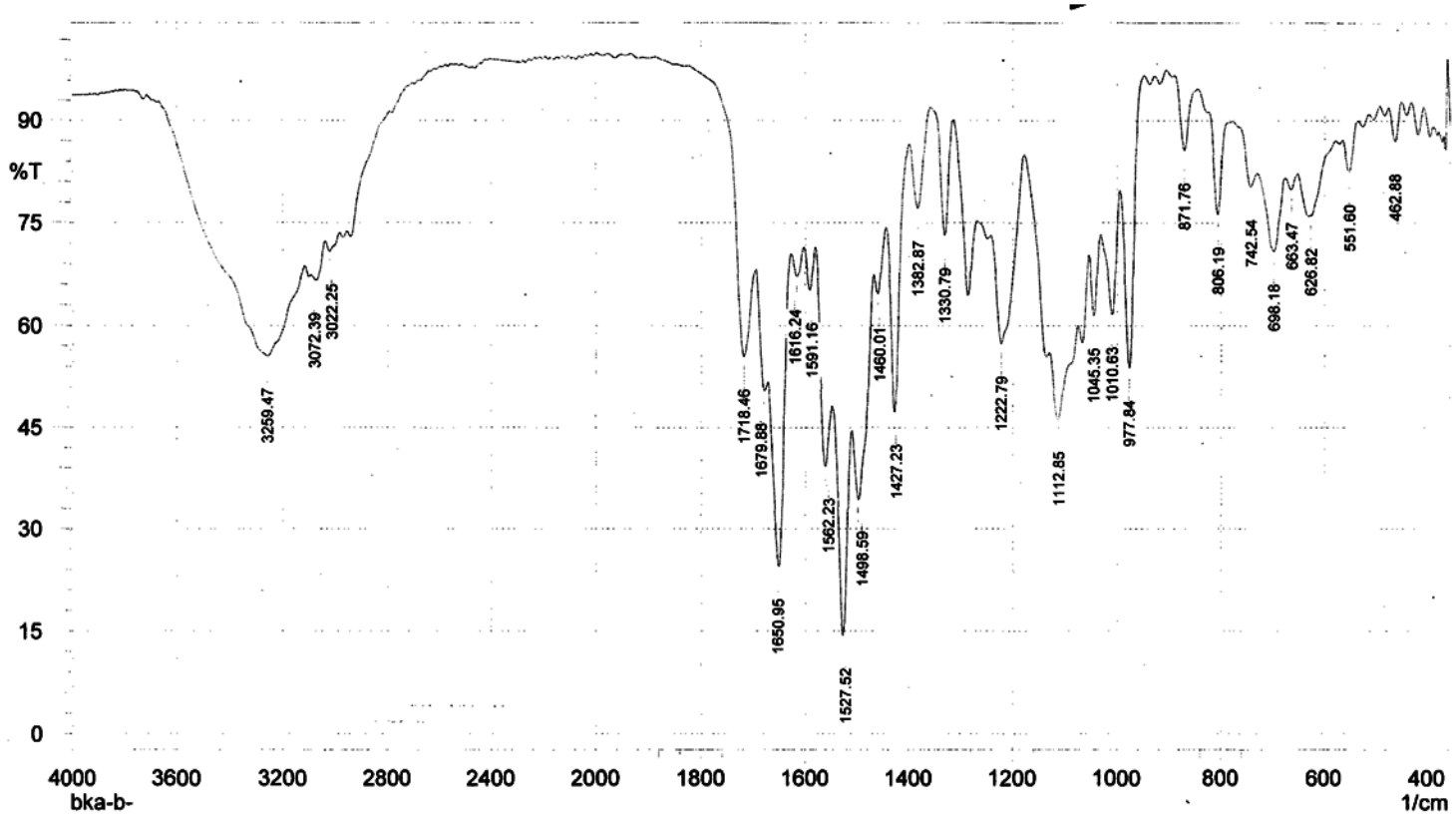
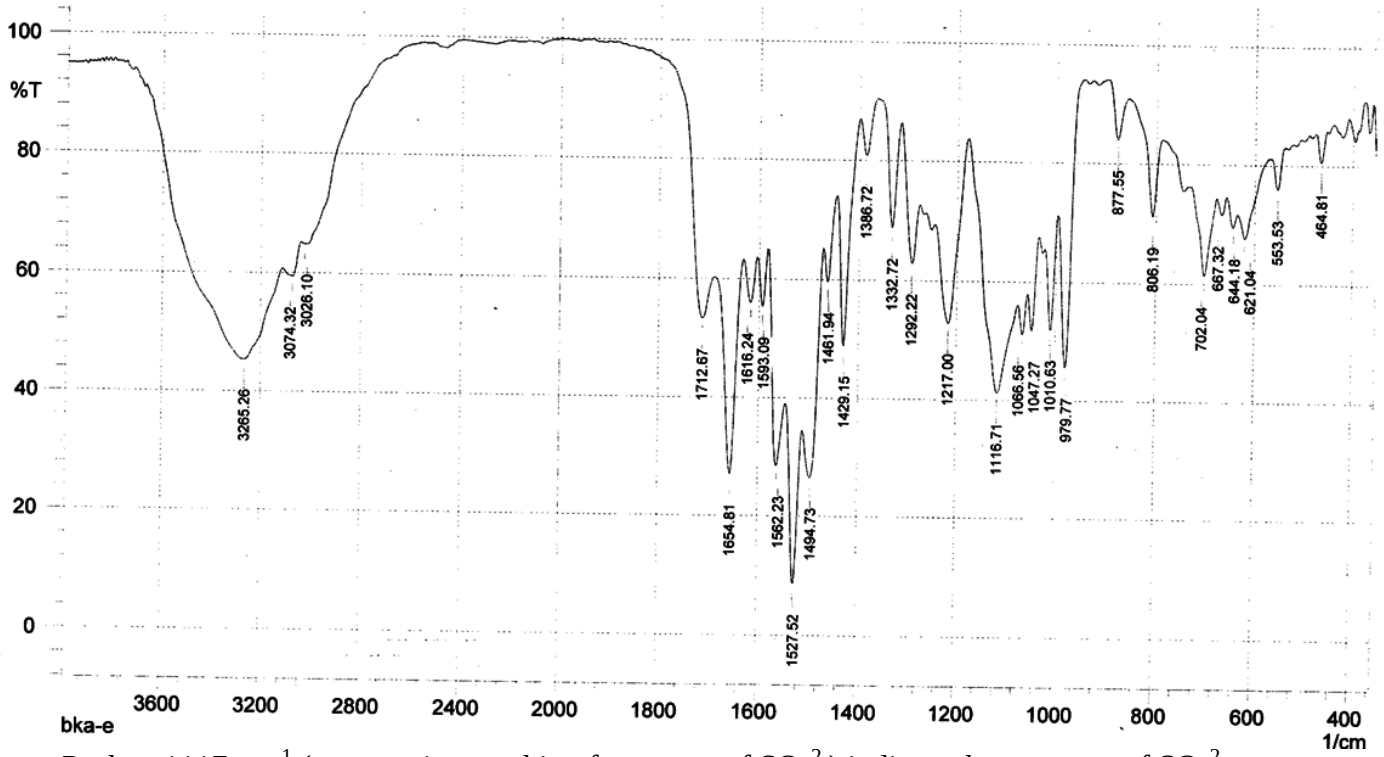


Figure 17S. FT-IR spectrum of complex **3**



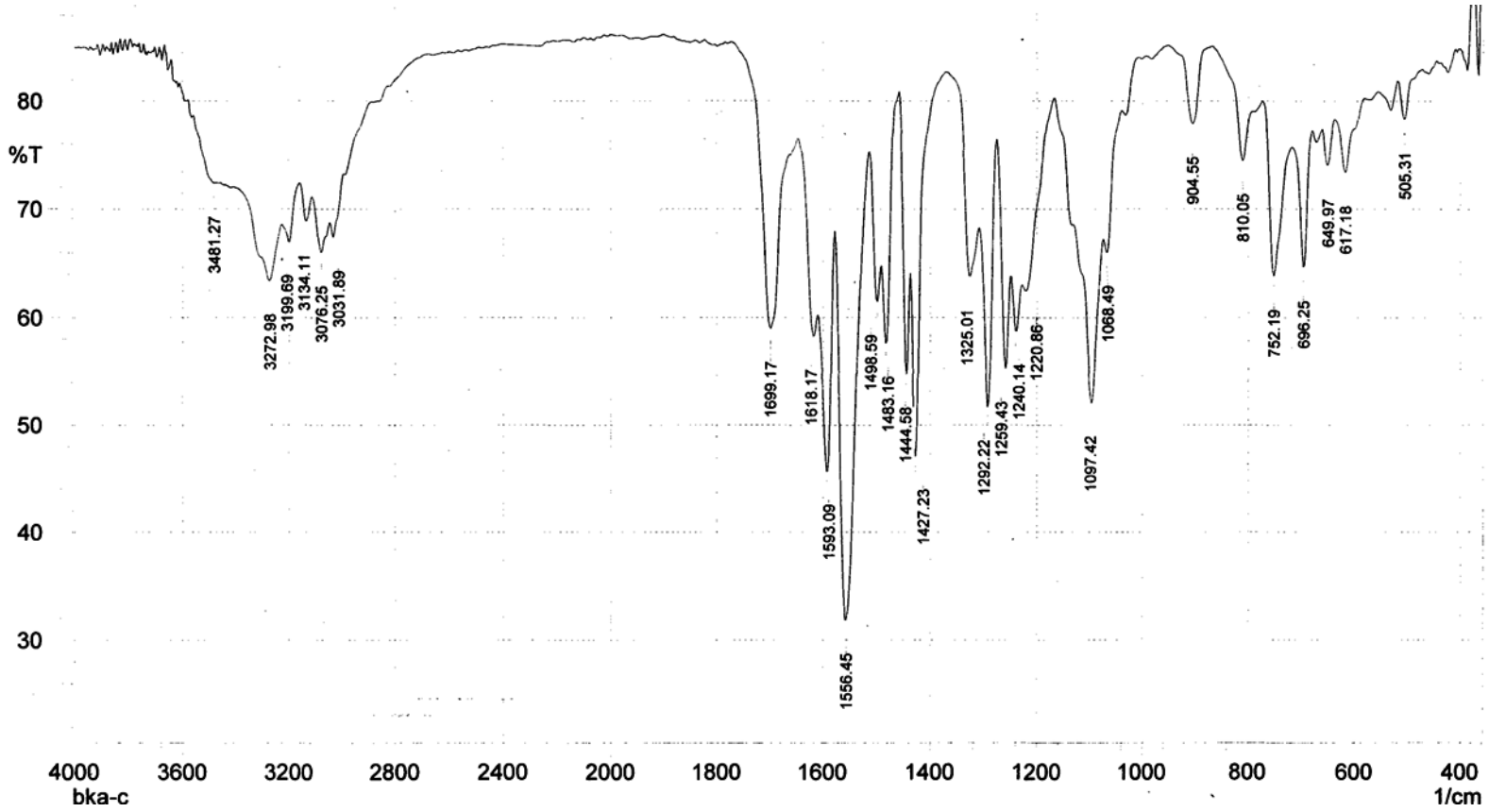
Peak at 1113 cm^{-1} (symmetric stretching frequency of SO_4^{2-}) indicate the presence of SO_4^{2-}.

Figure 18S. FT-IR spectrum of complex **4**



Peak at 1117 cm^{-1} (symmetric stretching frequency of SO_4^{2-}) indicate the presence of SO_4^{2-}.

Figure 19S. FT-IR spectrum of complex **5**



Star sign at 1097 cm^{-1} (symmetric stretching frequency of SO_4^{2-}) indicate the presence of SO_4^{2-}.

Figure 20S. FT-IR spectrum of $CuBr_2$ complex of $\mathbf{L^1}$

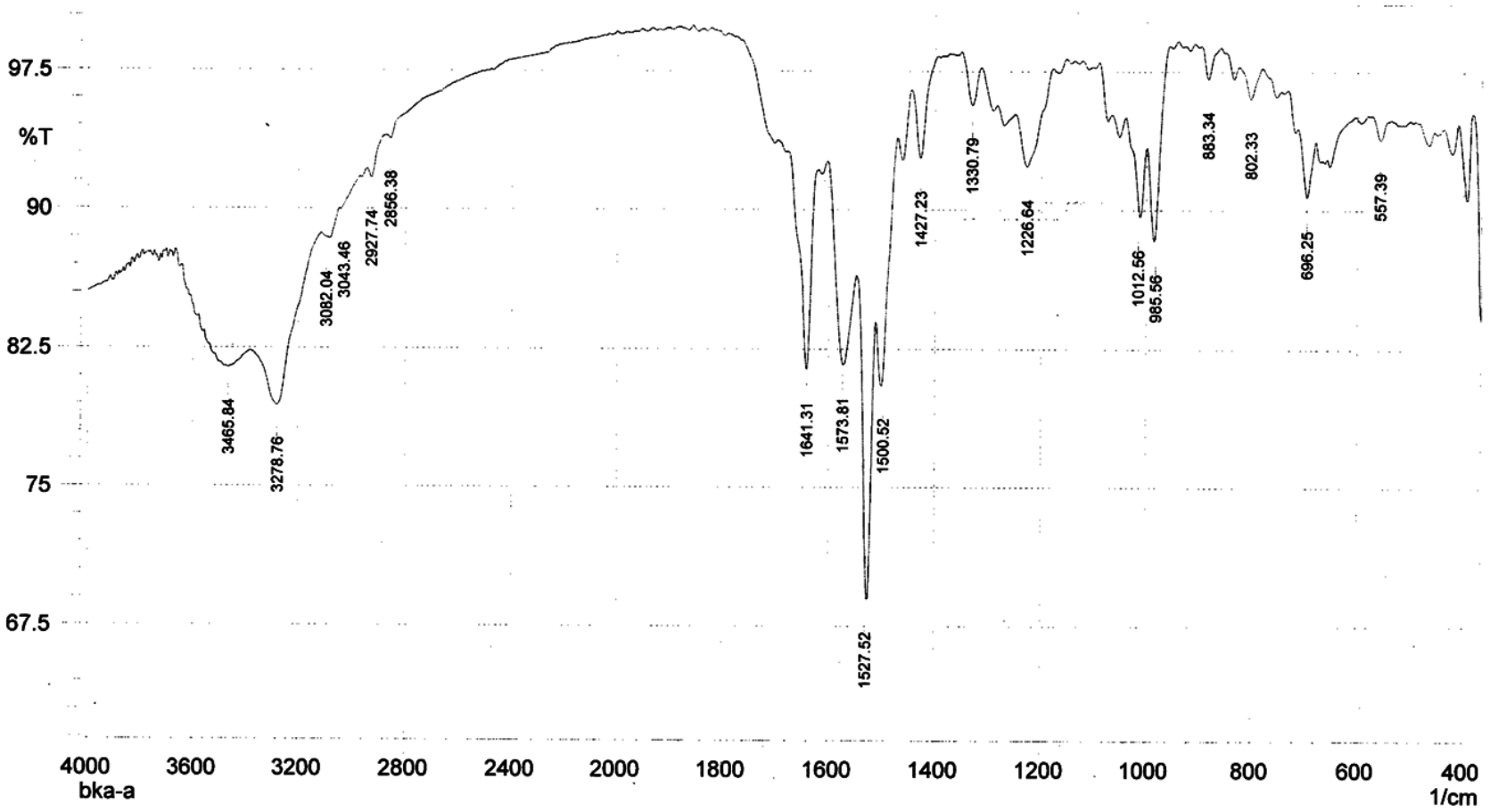


Figure 21S. FT-IR spectrum of $CuCl_2$ complex of $\mathbf{L^1}$