

Supporting information

Self-organization to Double Columnar Arrays of K⁺-Crown Ether Derivatives into Double-Columnar Arrays Controlled by Supramolecular Isomers of Hydrogen-Bonded Anionic Biimidazolate Ni Complexes

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Table 1S. Crystal data of 1 ~ 5

Table 2S. Selected bond lengths and angles for Crystals 1~5

Figure 1S. ORTEP view of crystal 1 with the numbering scheme

Figure 2S. ORTEP view of crystal 2 with the numbering scheme

Figure 3S. ORTEP view of crystal 3 with the numbering scheme

Figure 4-1S. ORTEP view of crystal 4 with the numbering scheme

Figure 4-2S. ORTEP view of crystal 4 with the numbering scheme

Figure 5S. ORTEP view of crystal 5 with the numbering scheme

Table 1S.

Crystal data of 1 ~ 5

	1	2	3	4	5
Formula	C ₄₁ H ₆₇ N ₁₂ O ₁₁ NiK	C ₃₄ H ₅₁ N ₁₂ O ₈ NiK	C ₃₅ H ₄₃ N ₁₂ O ₇ NiK	C ₇₄ H ₁₁₀ N ₅₆ O ₁₄ Ni ₂ K ₂	C ₃₈ H ₅₉ N ₁₄ O ₁₆ NiK
<i>M</i> _w	1001.85	853.65	841.60	1811.46	937.77
Crystal system	<i>monoclinic</i>	<i>monoclinic</i>	<i>monoclinic</i>	<i>triclinic</i>	<i>monoclinic</i>
Space Group	<i>C2/m</i> (#14)	<i>P2₁/n</i> (#14)	<i>P2₁/n</i> (#14)	<i>P</i> -1 (#2)	<i>C2/c</i> (#15)
<i>T</i> [K]	296	296	296	296	296
<i>a</i> [Å]	19.077(3)	8.7797(11)	9.294(2)	13.962(1)	18.966(2)
<i>b</i> [Å]	29.074(3)	17.039(3)	25.183(5)	25.636(3)	19.058(2)
<i>c</i> [Å]	9.769(3)	28.3270(18)	17.099(2)	12.937(1)	25.469(2)
α [°]				100.034(8)	
β [°]	110.39(2)	91.496(1)	95.64(1)	93.221(8)	103.201(8)
γ [°]				101.778(7)	
<i>V</i> [Å ³]	5078(1)	4236.3(9)	3982(1)	4443.4(7)	8962.9(14)
<i>Z</i>	4	4	4	2	8
<i>D</i> _{calc} /g cm ⁻³	1.310	1.338	1.403	1.354	1.390
<i>F</i> (000)	2128.00	1800.00	1760.00	1912.00	3968.00
μ (CuK α) [cm ⁻¹]	18.38	20.567	21.65	19.89	20.076
Total Reflections	4004	6774	5702	12450	6233
Unique reflections	3797	6113	4243	11840	5820
No. variables	322	562	544	1165	587
Goodness of fit	0.996	1.113	1.829	1.513	1.189
<i>R</i> ₁ (<i>I</i> > 3.00 σ (<i>I</i>))	0.0665	0.0751	0.0659	0.0938	0.0742
<i>wR</i> ₂ (<i>I</i> > 3.00 σ (<i>I</i>))	0.1435	0.1736	0.1791	0.2128	0.1635
Residual max. (min.) peak [eÅ ⁻³]	0.36 (-0.23)	0.49 (-0.86)	0.22 (-0.22)	0.98 (-1.14)	1.03 (-0.59)

Table 2S. Selected bond lengths [Å] and angles [°] for Crystals 1~5

Crystal 1			
Ni(1)-N(1)	2.13(1)	Ni(1)-N(5)	2.13(9)
Ni(1)-N(3)	1.975(8)		1
			13(9)
N(3)-Ni(1)-N(1)	77.8(4)	Ni(1)-N(3)-C(3)	143.2(9)
N(5)-Ni(1)-N(1)	163.5(3)	Ni(1)-N(3)-C(6)	120.0(7)
N(5)-Ni(1)-N(3)	90.8(3)	Ni(1)-N(5)-C(7)	141.6(7)
Ni(1)-N(1)-C(1)	139.4(8)	Ni(1)-N(5)-C(9)	112.3(7)
Ni(1)-N(1)-C(5)	111.7(7)		
Crystal 2			
Ni(1)-N(1)	2.142(5)	Ni(1)-N(7)	2.083(6)
Ni(1)-N(3)	2.079(5)	Ni(1)-N(9)	2.136(6)
Ni(1)-N(5)	2.091(6)	Ni(1)-N(11)	2.078(5)
N(3)-Ni(1)-N(1)	78.5(2)	N(11)-Ni(1)-N(9)	78.5(2)
N(5)-Ni(1)-N(1)	92.8(2)	Ni(1)-N(1)-C(1)	142.8(5)
N(7)-Ni(1)-N(1)	165.7(2)	Ni(1)-N(1)-C(5)	112.0(4)
N(9)-Ni(1)-N(1)	93.4(2)	Ni(1)-N(3)-C(3)	140.4(5)
N(11)-Ni(1)-N(1)	97.4(2)	Ni(1)-N(3)-C(6)	114.6(4)
N(5)-Ni(1)-N(3)	99.7(2)	Ni(1)-N(5)-C(7)	143.5(5)
N(7)-Ni(1)-N(3)	91.4(2)	Ni(1)-N(5)-C(11)	112.9(4)
N(9)-Ni(1)-N(3)	165.4(2)	Ni(1)-N(7)-C(9)	141.0(5)
N(11)-Ni(1)-N(3)	90.4(2)	Ni(1)-N(7)-C(12)	114.1(4)
N(7)-Ni(1)-N(5)	79.0(2)	Ni(1)-N(9)-C(13)	142.8(5)
N(9)-Ni(1)-N(5)	92.7(2)	Ni(1)-N(9)-C(17)	111.5(5)
N(11)-Ni(1)-N(5)	166.9(2)	Ni(1)-N(11)-C(15)	141.0(5)
N(9)-Ni(1)-N(7)	98.6(2)	Ni(1)-N(11)-C(18)	114.6(4)
N(11)-Ni(1)-N(7)	92.6(2)		
Crystal 3			
Ni(1)-N(1)	2.147(4)	Ni(1)-N(7)	2.109(4)
Ni(1)-N(3)	2.078(4)	Ni(1)-N(9)	2.112(4)
Ni(1)-N(5)	2.079(4)	Ni(1)-N(11)	2.073(4)
N(3)-Ni(1)-N(1)	79.0(1)	N(9)-Ni(1)-N(5)	101.0(2)
N(5)-Ni(1)-N(1)	92.1(1)	N(11)-Ni(1)-N(5)	92.9(2)
N(7)-Ni(1)-N(1)	96.5(1)	Ni(1)-N(5)-C(7)	142.3(3)
N(9)-Ni(1)-N(1)	162.1(1)	Ni(1)-N(5)-C(11)	113.8(3)
N(11)-Ni(1)-N(1)	88.1(1)	N(9)-Ni(1)-N(7)	97.8(1)
Ni(1)-N(1)-C(1)	141.8(3)	N(11)-Ni(1)-N(7)	170.9(2)
Ni(1)-N(1)-C(5)	110.8(3)	Ni(1)-N(7)-C(9)	142.7(3)
N(5)-Ni(1)-N(3)	167.5(1)	Ni(1)-N(7)-C(12)	112.8(3)
N(7)-Ni(1)-N(3)	93.1(1)	N(11)-Ni(1)-N(9)	79.2(1)
N(9)-Ni(1)-N(3)	89.6(1)	Ni(1)-N(9)-C(13)	141.4(3)
N(11)-Ni(1)-N(3)	95.6(1)	Ni(1)-N(9)-C(17)	112.4(3)
Ni(1)-N(3)-C(3)	141.7(3)	Ni(1)-N(11)-C(15)	143.2(3)
Ni(1)-N(3)-C(6)	114.2(3)	Ni(1)-N(11)-C(18)	112.7(3)
N(7)-Ni(1)-N(5)	79.1(2)		
Crystal 4			
Ni(1)-N(1)	2.10(1)	Ni(2)-N(13)	2.08(1)
Ni(1)-N(3)	2.10(1)	Ni(2)-N(15)	2.122(9)

Ni(1)-N(5)	2.06(1)	Ni(2)-N(17)	2.11(1)
Ni(1)-N(7)	2.13(1)	Ni(2)-N(19)	2.07(1)
Ni(1)-N(9)	2.18(1)	Ni(2)-N(21)	2.15(1)
Ni(1)-N(11)	2.02(1)	Ni(2)-N(23)	2.08(1)
N(3)-Ni(1)-N(1)	78.7(4)	N(15)-Ni(2)-N(13)	78.7(4)
N(5)-Ni(1)-N(1)	92.0(4)	N(17)-Ni(2)-N(13)	89.6(4)
N(7)-Ni(1)-N(1)	165.5(4)	N(19)-Ni(2)-N(13)	96.3(4)
N(9)-Ni(1)-N(1)	88.0(4)	N(21)-Ni(2)-N(13)	162.4(4)
N(11)-Ni(1)-N(1)	98.3(4)	N(23)-Ni(2)-N(13)	95.0(4)
Ni(1)-N(1)-C(1)	141.1(9)	Ni(2)-N(13)-C(19)	141.2(8)
Ni(1)-N(1)-C(5)	113.4(9)	Ni(2)-N(13)-C(23)	114(1)
N(5)-Ni(1)-N(3)	97.7(4)	N(17)-Ni(2)-N(15)	162.7(4)
N(7)-Ni(1)-N(3)	91.3(4)	N(19)-Ni(2)-N(15)	89.6(4)
N(9)-Ni(1)-N(3)	162.1(4)	N(21)-Ni(2)-N(15)	86.1(4)
N(11)-Ni(1)-N(3)	91.1(5)	N(23)-Ni(2)-N(15)	99.8(4)
Ni(1)-N(3)-C(3)	142.3(8)	Ni(2)-N(15)-C(21)	144.5(9)
Ni(1)-N(3)-C(6)	113(1)	Ni(2)-N(15)-C(24)	114.0(8)
N(7)-Ni(1)-N(5)	78.8(5)	N(19)-Ni(2)-N(17)	78.8(4)
N(9)-Ni(1)-N(5)	94.6(4)	N(21)-Ni(2)-N(17)	107.1(4)
N(11)-Ni(1)-N(5)	167.5(4)	N(23)-Ni(2)-N(17)	94.0(4)
Ni(1)-N(5)-C(7)	144(1)	Ni(2)-N(17)-C(25)	140(1)
Ni(1)-N(5)-C(11)	113.2(8)	Ni(2)-N(17)-C(29)	111.3(9)
N(9)-Ni(1)-N(7)	103.8(4)	N(21)-Ni(2)-N(19)	92.6(5)
N(11)-Ni(1)-N(7)	92.2(4)	N(23)-Ni(2)-N(19)	166.5(4)
Ni(1)-N(7)-C(9)	140(1)	Ni(2)-N(19)-C(27)	143.7(9)
Ni(1)-N(7)-C(12)	110.4(9)	Ni(2)-N(19)-C(30)	114.2(9)
N(11)-Ni(1)-N(9)	78.9(4)	N(23)-Ni(2)-N(21)	78.6(5)
Ni(1)-N(9)-C(13)	138.3(8)	Ni(2)-N(21)-C(31)	136.5(9)
Ni(1)-N(9)-C(17)	107.6(9)	Ni(2)-N(21)-C(35)	109.4(9)
Ni(1)-N(11)-C(15)	144(1)	Ni(2)-N(23)-C(33)	144(1)
Ni(1)-N(11)-C(18)	117(1)	Ni(2)-N(23)-C(36)	115.1(9)
Crystal 5			
Ni(1)-N(1)	2.151(6)	Ni(1)-N(7)	2.089(6)
Ni(1)-N(3)	2.092(6)	Ni(1)-N(9)	2.088(6)
Ni(1)-N(5)	2.140(6)	Ni(1)-N(11)	2.139(5)
N(3)-Ni(1)-N(1)	79.4(2)	N(9)-Ni(1)-N(5)	90.6(2)
N(5)-Ni(1)-N(1)	105.9(2)	N(11)-Ni(1)-N(5)	165.0(2)
N(7)-Ni(1)-N(1)	93.5(2)	Ni(1)-N(5)-C(7)	140.3(5)
N(9)-Ni(1)-N(1)	162.9(2)	Ni(1)-N(5)-C(11)	110.5(5)
N(11)-Ni(1)-N(1)	86.2(2)	N(9)-Ni(1)-N(7)	94.2(2)
Ni(1)-N(1)-C(1)	139.5(5)	N(11)-Ni(1)-N(7)	91.7(2)
Ni(1)-N(1)-C(5)	108.5(5)	Ni(1)-N(7)-C(9)	142.0(5)
N(5)-Ni(1)-N(3)	90.4(2)	Ni(1)-N(7)-C(12)	113.1(5)
N(7)-Ni(1)-N(3)	165.2(2)	N(11)-Ni(1)-N(9)	78.4(2)
N(9)-Ni(1)-N(3)	96.1(2)	Ni(1)-N(9)-C(13)	141.8(5)
N(11)-Ni(1)-N(3)	100.8(2)	Ni(1)-N(9)-C(17)	114.0(5)
Ni(1)-N(3)-C(3)	141.5(5)	Ni(1)-N(11)-C(15)	140.8(5)
Ni(1)-N(3)-C(6)	112.1(5)	Ni(1)-N(11)-C(18)	111.8(5)
N(7)-Ni(1)-N(5)	78.9(2)		

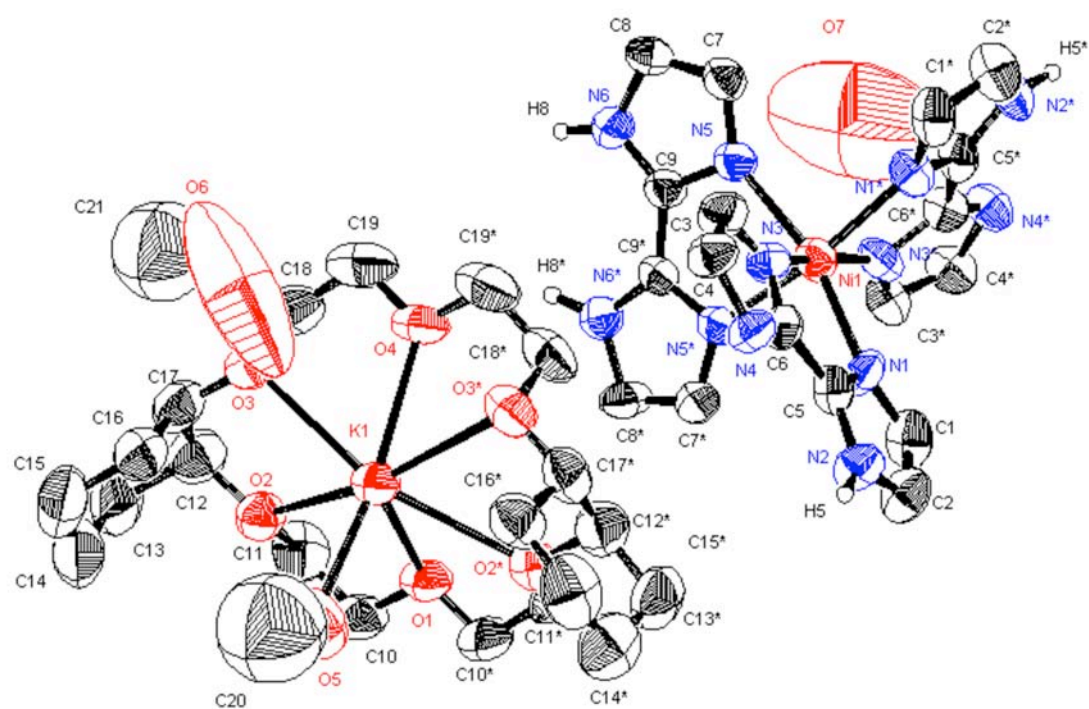


Figure 1S. ORTEP view of crystal 1

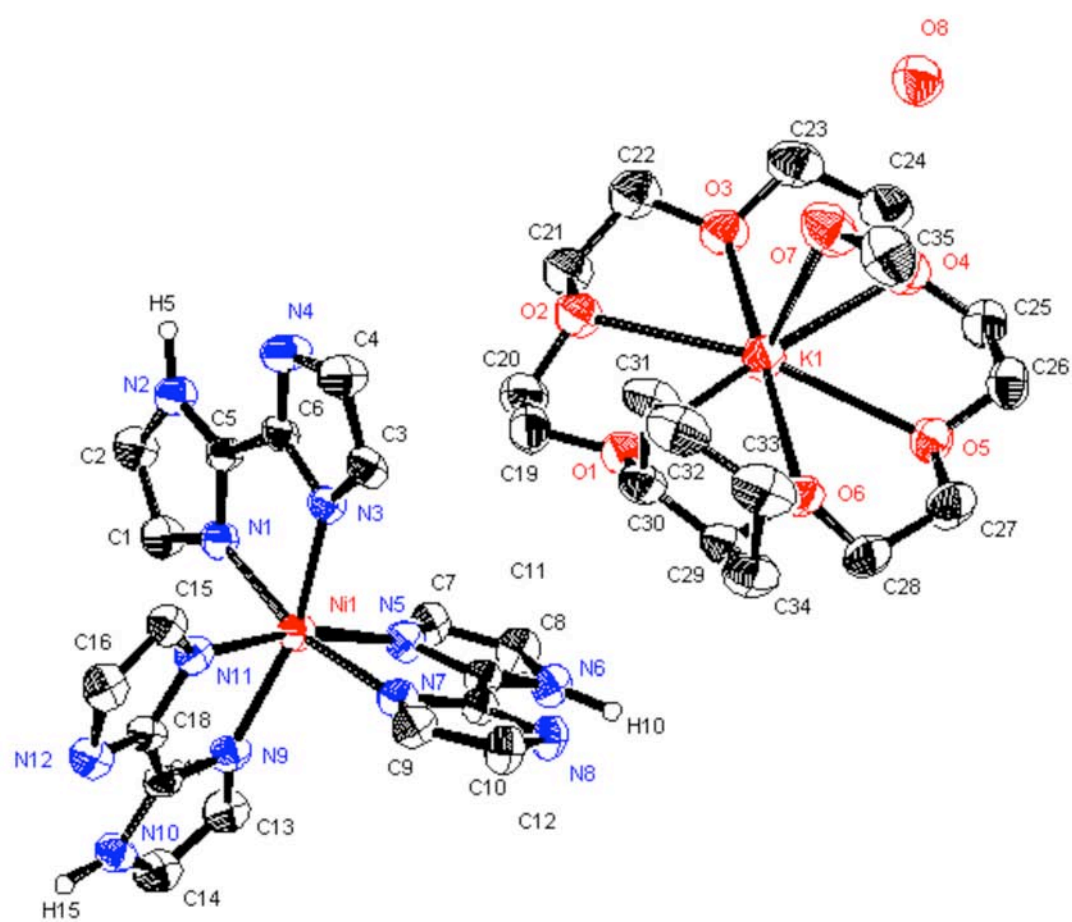


Figure 2S. ORTEP view of crystal 2

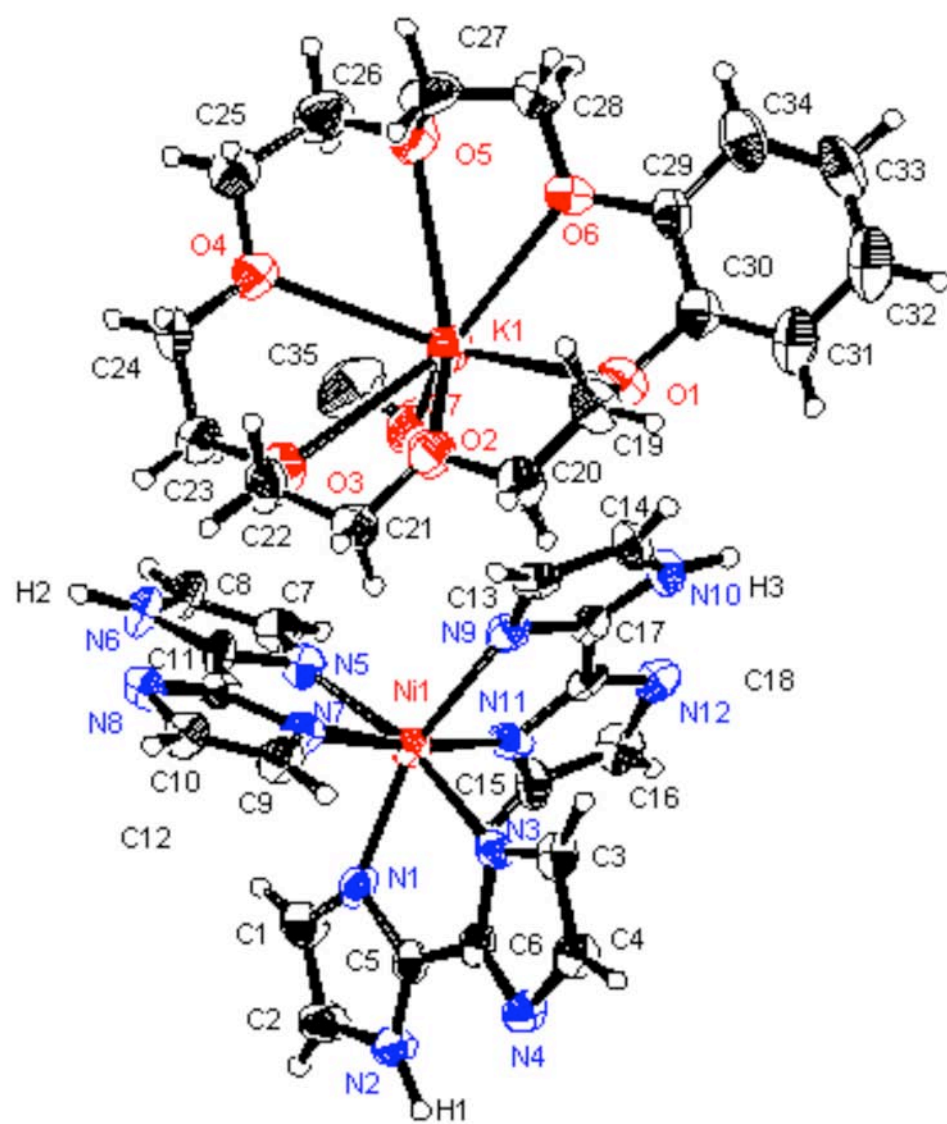


Figure 3S. ORTEP view of crystal 3

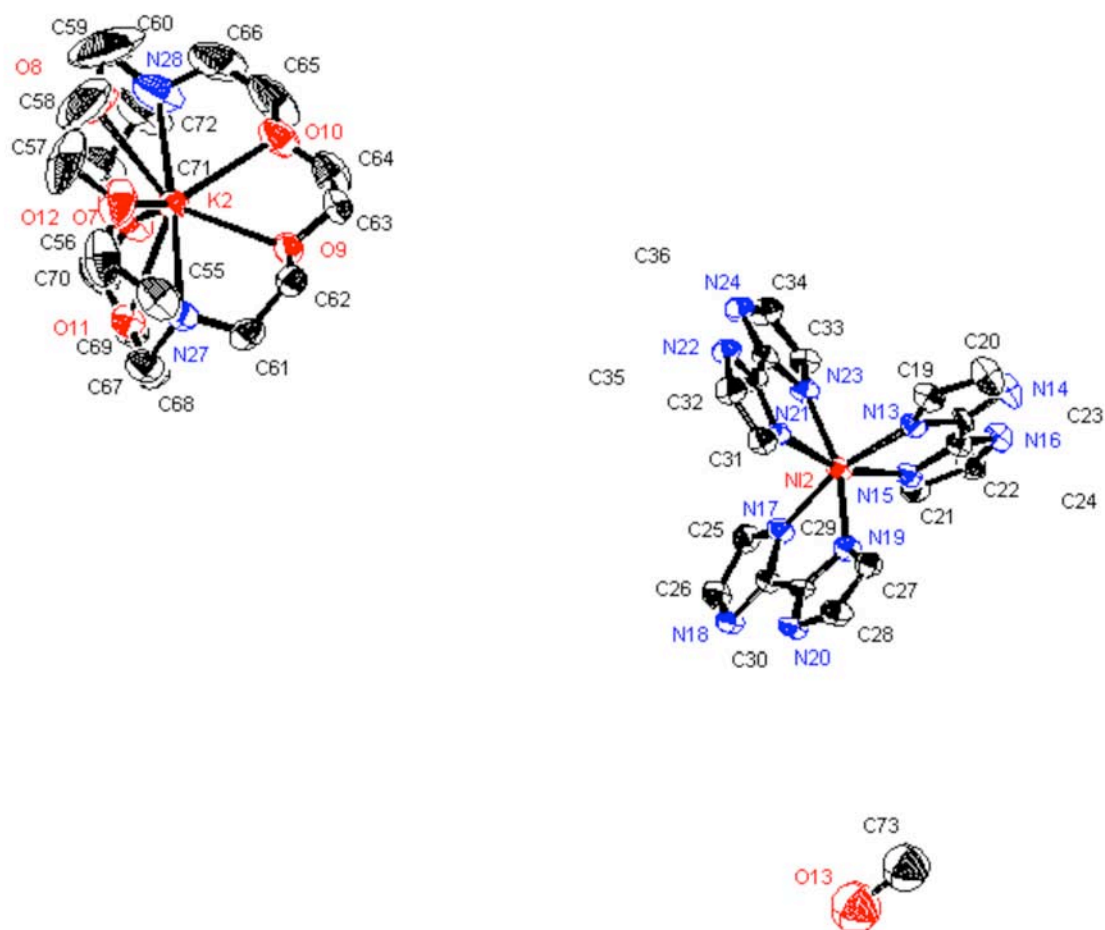


Figure 4S-1. ORTEP view of crystal 4

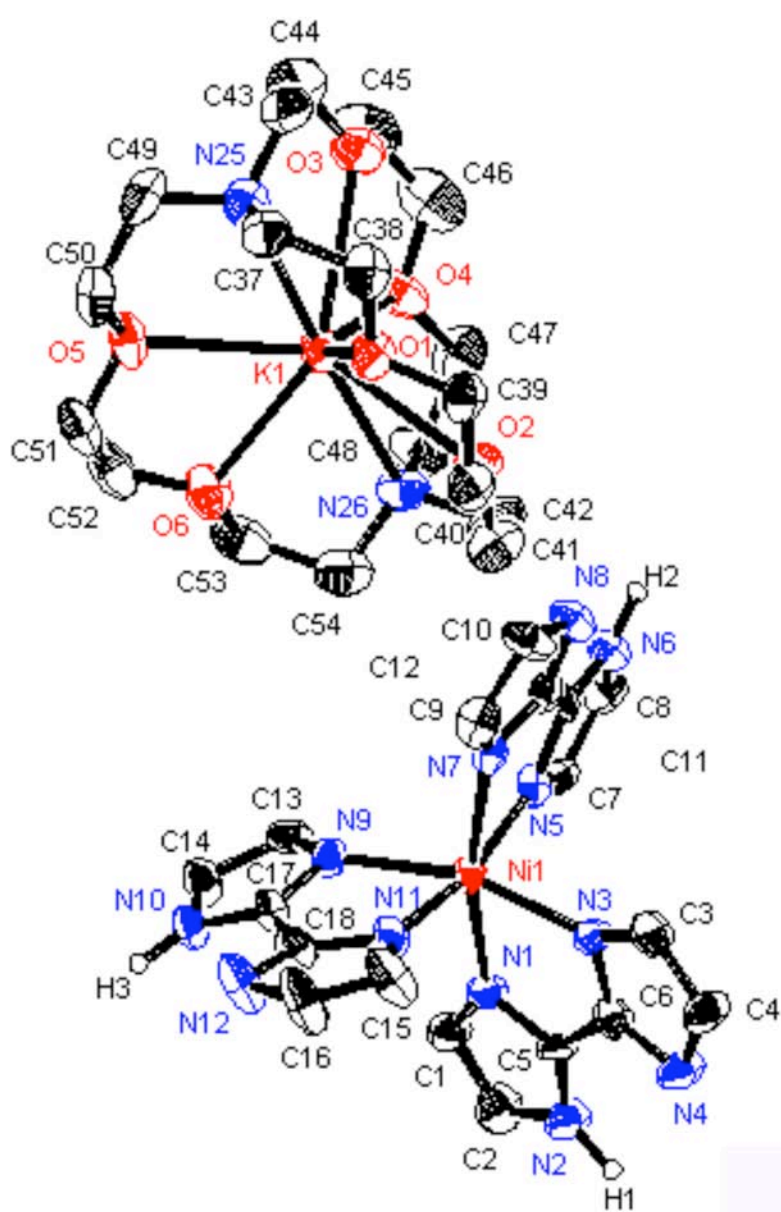


Figure 4S-2. ORTEP view of crystal 4

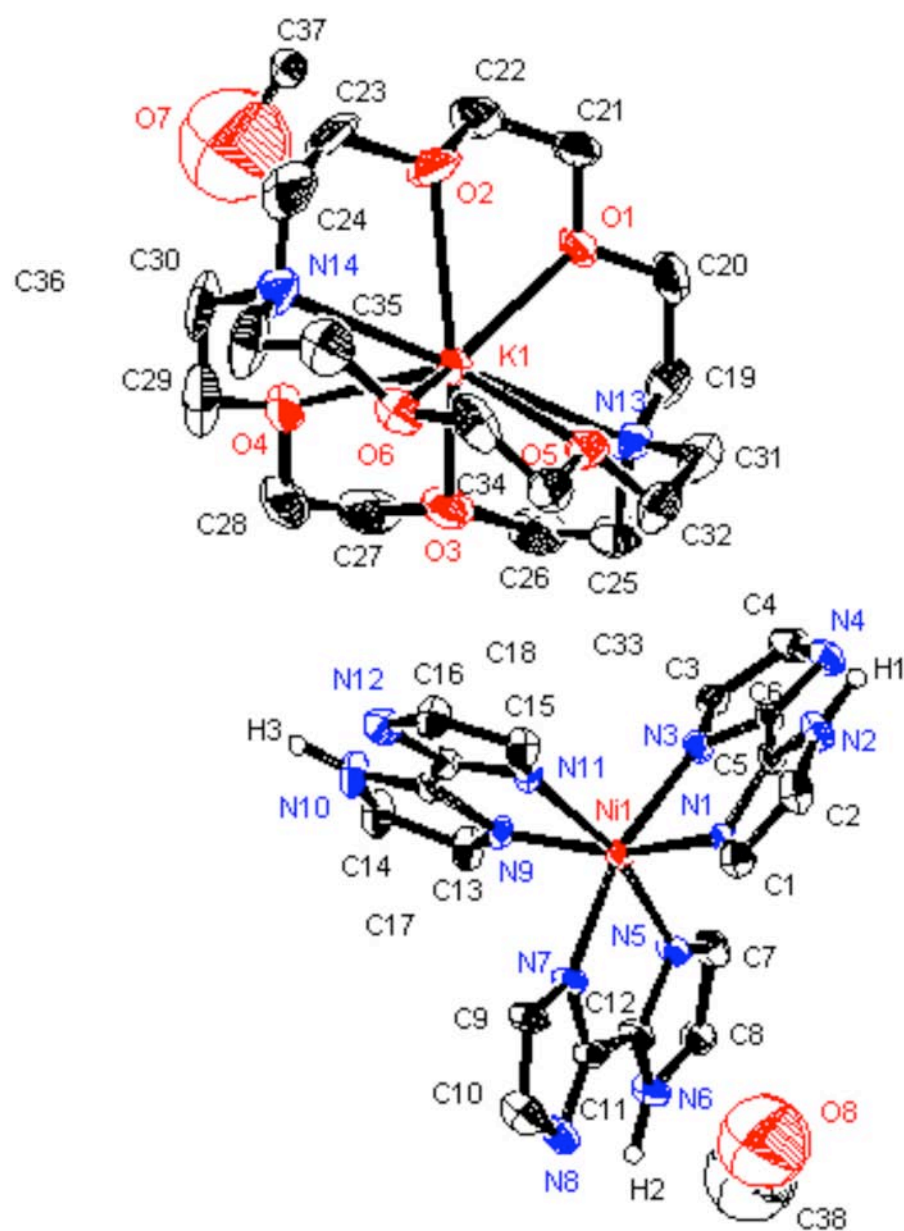


Figure 5S. ORTEP view of crystal 5

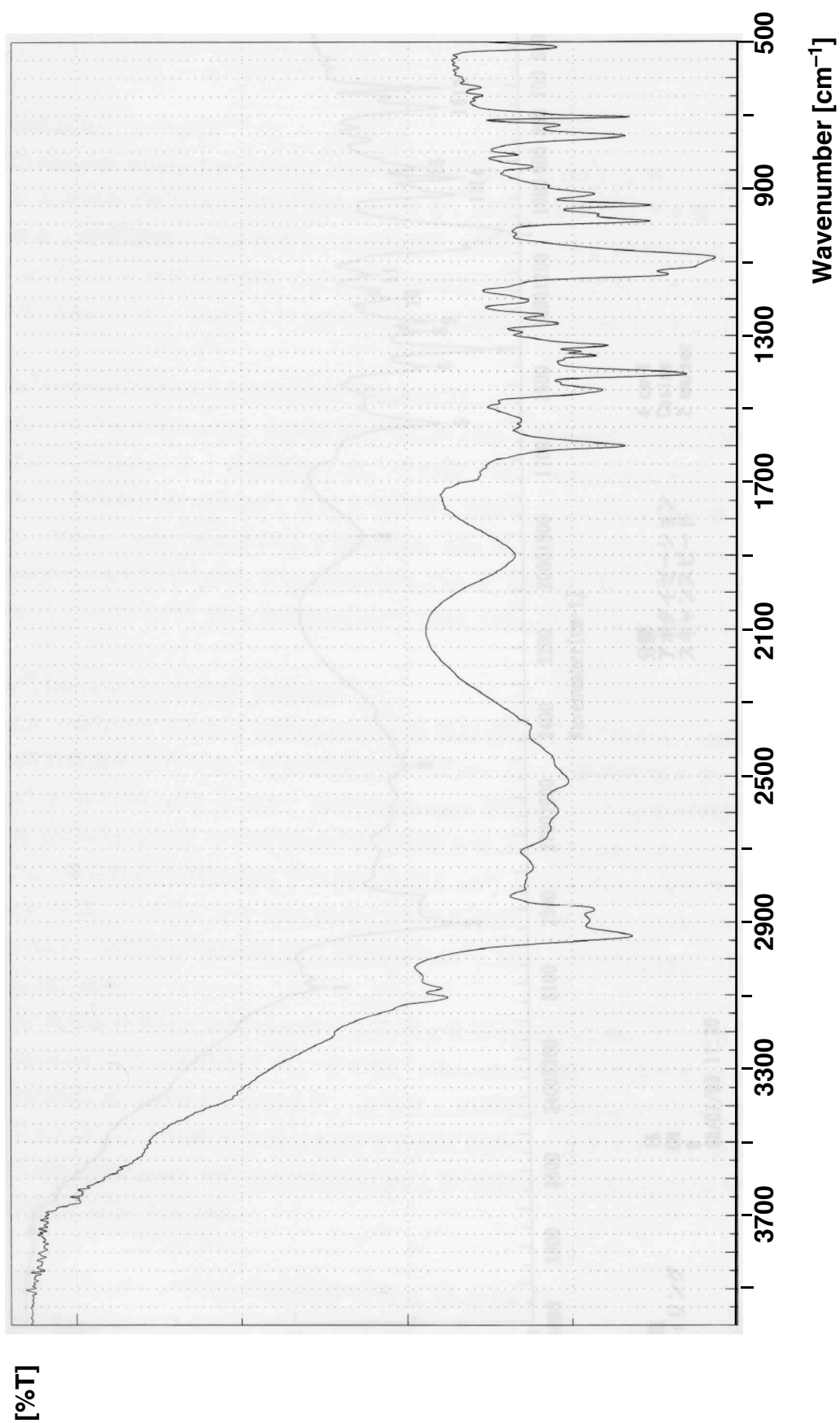


Figure 6S.

IR spectrum of the crystal 1 ($[\text{Ni}^{\text{II}}(\text{Hbim})_3][\text{K-DHC}(18\text{-crown-}6)]_n$)