Supporting information

Syntheses, Structures and Magnetic Properties of Tetranuclear Cubane-type and Heptanuclear Wheel-type Nickel(II) Complexes with 3-Methoxysalicylic Acid Derivatives

Fumiya Kobayashi, Ryo Ohtani, Saki Teraoka, Wataru Kosaka, Hitoshi Miyasaka, Yingjie Zhang, Leonard F. Lindoy, Shinya Hayami*, Masaaki Nakamura*

Table S1. Selected bond length (Å) and angles (°) for **1**.

Bond lengths			
Ni1-O2	1.988(2)	O4-C8	1.346(4)
Ni1-O3	2.032(2)	O4-C9	1.445(4)
Ni1-O17	2.093(2)	O5-C16	1.432(4)
Ni1-O18	2.037(2)	O5-C18	1.364(4)
Ni1-O19	2.045(2)	O6-C17	1.294(4)
Ni1-O20	2.074(2)	O7-C23	1.226(4)
Ni2-O6	1.993(2)	O8-C23	1.356(4)
Ni2-O7	2.035(2)	O8-C24	1.447(4)
Ni2-O19	2.032(2)	O9-C31	1.434(4)
Ni2-O20	2.048(2)	O9-C33	1.374(4)
Ni2-O21	2.071(2)	O10-C32	1.299(4)
Ni2-O24	2.108(2)	O11-C38	1.229(4)
Ni3-O10	1.993(2)	O12-C38	1.353(4)
Ni3-O11	2.055(2)	O12-C39	1.444(4)
Ni3-O18	2.065(2)	O13-C46	1.431(4)
Ni3-O20	2.040(2)	O13-C48	1.374(4)
Ni3-O21	2.051(2)	O14-C47	1.301(4)
Ni3-O22	2.091(2)	O15-C53	1.228(4)
Ni4-O14	2.003(2)	O16-C53	1.353(4)
Ni4-O15	2.034(2)	O16-C54	1.445(4)
Ni4-O18	2.048(2)	O17-C61	1.420(4)
Ni4-O19	2.069(2)	O18-C62	1.425(4)
Ni4-O21	2.033(2)	O19-C63	1.423(3)

Ni4-O23	2.104(2)	O20-C64	1.411(4)
O1-C1	1.426(4)	O21-C65	1.416(4)
O1-C3	1.379(4)	O22-C66	1.382(4)
O2-C2	1.286(4)	O23-C67	1.427(4)
O3-C8	1.231(4)	O24-C68	1.427(4)

Angles

O2-Ni1-O3	88.21(9)	O3-Ni1-O18	94.86(9)
O18-Ni1-O17	91.65(9)	O18-Ni1-O19	84.60(9)
O18-Ni1-O20	81.09(9)	O19-Ni1-O17	87.81(9)
O19-Ni1-O20	83.53(8)	O19-Ni2-O7	93.33(9)
O6-Ni2-O7	88.26(9)	O19-Ni2-O21	80.43(9)
O19-Ni2-O20	84.50(8)	O20-Ni2-O21	83.14(8)
O19-Ni2-O24	91.69(9)	O20-Ni3-O18	81.22(9)
O20-Ni2-O24	87.35(9)	O20-Ni3-O22	87.87(10)
O10-Ni3-O11	88.35(9)	O21-Ni3-O18	82.57(8)
O20-Ni3-O11	96.14(9)	O14-Ni4-O15	88.84(9)
O20-Ni3-O21	83.86(9)	O18-Ni4-O23	87.14(9)
O21-Ni3-O22	90.98(9)	O21-Ni4-O15	92.85(9)
O18-Ni4-O19	83.74(8)	O21-Ni4-O19	80.49(9)
O21-Ni4-O18	83.43(8)	O21-Ni4-O23	91.99(9)
Ni1-O18-Ni3	98.97(9)	Ni1-O18-Ni4	95.45(9)
Ni4-O18-Ni3	95.86(9)	Ni1-O19-Ni4	94.57(9)
Ni2-O19-Ni1	96.00(9)	Ni2-O19-Ni4	99.53(9)
Ni2-O19-Ni1	94.63(9)	Ni3-O20-Ni1	98.59(9)
Ni3-O20-Ni2	96.24(9)	Ni3-O21-Ni2	95.21(9)
Ni4-O21-Ni2	99.41(9)	Ni4-O21-Ni3	96.78(9)

Table S2. Selected bond length (Å) and angles (°) for **2**.

bond lengths			
Ni(1)-O(2)	2.207(3)	Ni(1)-O(2)	1.976(3)
Ni(1)-O(2)	1.949(3)	Ni(1)-O(3)	2.017(3)
Ni(1)-O(4)	2.084(3)	Ni(2)-O(4)	2.081(3)
O(2)-C(2)	1.312(5)	O(3)-C(8)	1.249(5)
N(1)-C(8)	1.329(6)	N(2)-C(11)	1.276(7)
Angles			
O2-Ni1-O1	74.79(11)	O2-Ni1-O1	99.71(12)
O2-Ni1-O3	85.84(12)	O2-Ni1-O3	97.15(12)
O2-Ni1-O4	97.24(12)	O2-Ni1-O4	79.82(12)
O2-Ni1-O4	79.82(11)	O3-Ni1-O4	87.00(13)
O3-Ni1-O4	99.11(13)	O4-Ni1-O1	95.65(13)
O4-Ni2-O4	95.98(11)	O4-Ni2-O4	84.02(11)
Ni1-O2-Ni1	103.56(13)	Ni1-O4-Ni2	96.13(12)
Ni1-O4-Ni1	95.98(13)	Ni1-O4-Ni1	95.15(13)

Table S3. Selected bond length (Å) and angles (°) for **3**.

Bond lengths			
Ni(1)-O(1)	1.814(16)	Ni(1)-N(1)	1.837(19)
Ni(1)-N(2)	1.831(19)	Ni(1)-N(3)	1.906(19)
C(1)-O(1)	1.320(3)	C(7)-O(2)	1.277(3)
C(7)-N(1)	1.331(3)	C(10)-N(2)	1.281(3)
Angles			
O(1)-Ni(1)-N(1)	97.59(8)	O(1)-Ni(1)-N(2)	175.78(8)
O(1)-Ni(1)-N(3)	92.82(7)	N(1)-Ni(1)-N(2)	86.49(9)
N(1)-Ni(1)-N(3)	168.98(9)	N(2)-Ni(1)-N(3)	83.18(8)

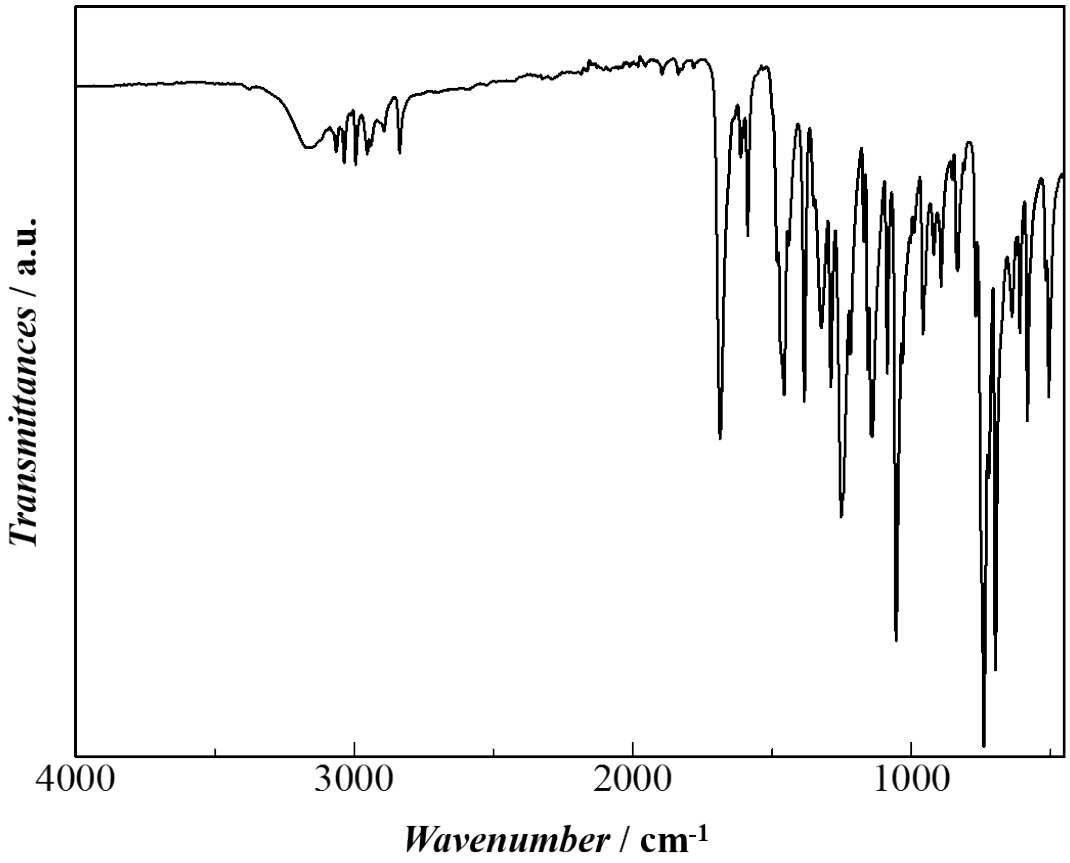

Figure S1. FT–IR spectra for Benzyl 2-hydroxy-3-methoxybenzoate (HL^1).

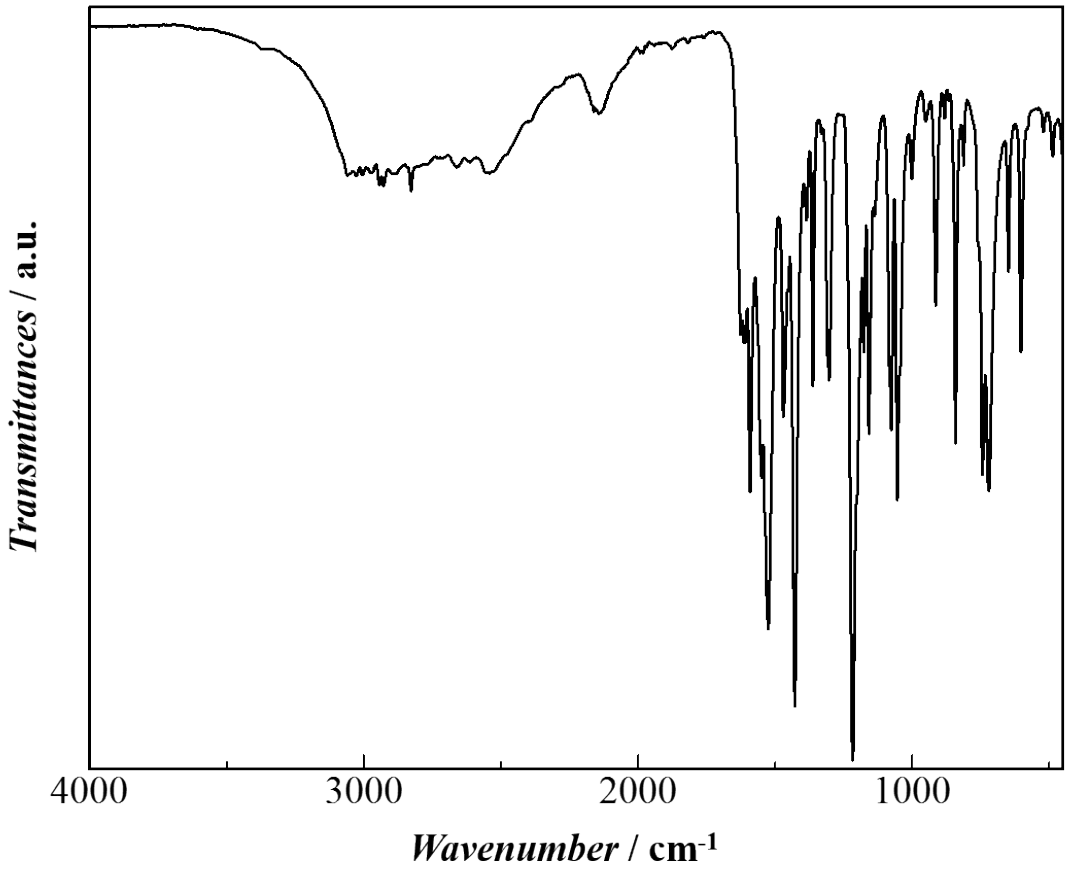

Figure S2. FT–IR spectra for 1-(2-hydroxy-3-methoxybenzamido)-2-aminoethane.

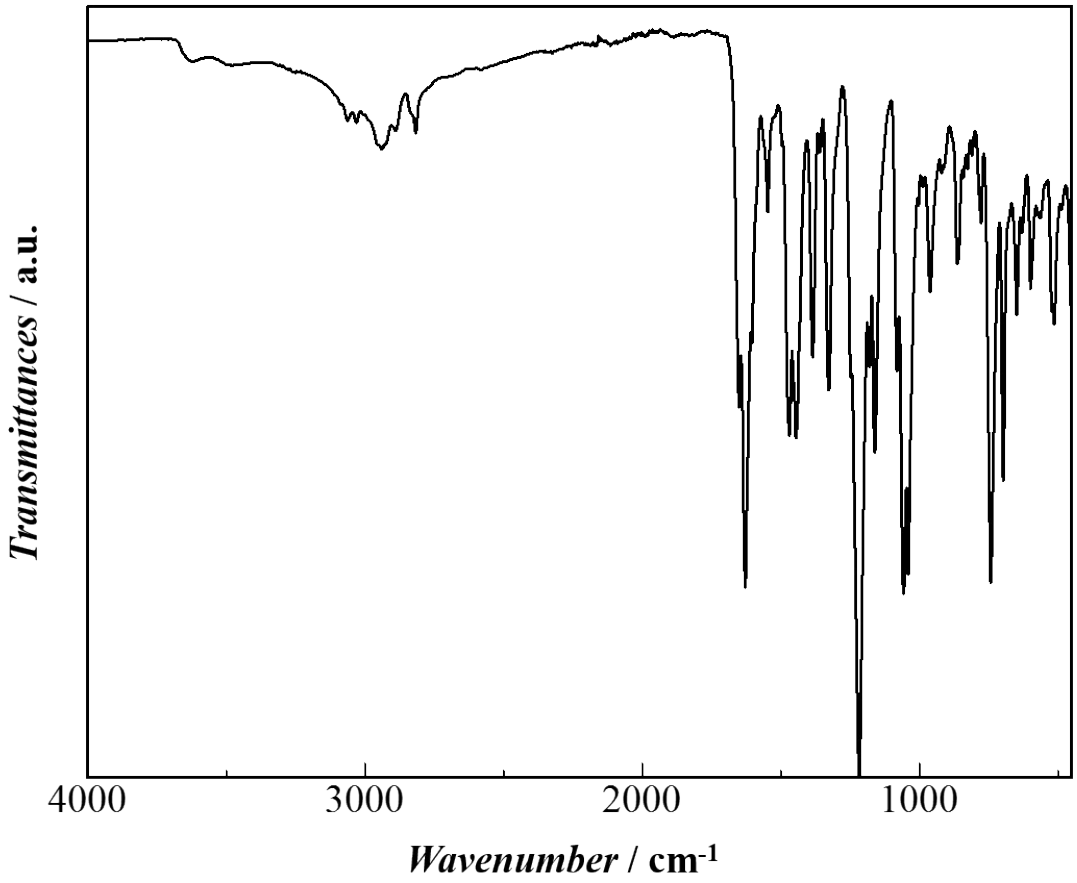

Figure S3. FT–IR spectra for $[Ni_4L^1{}_4(\mu_3\text{-OMe})_4(CH_3OH)_4]$ (**1**).

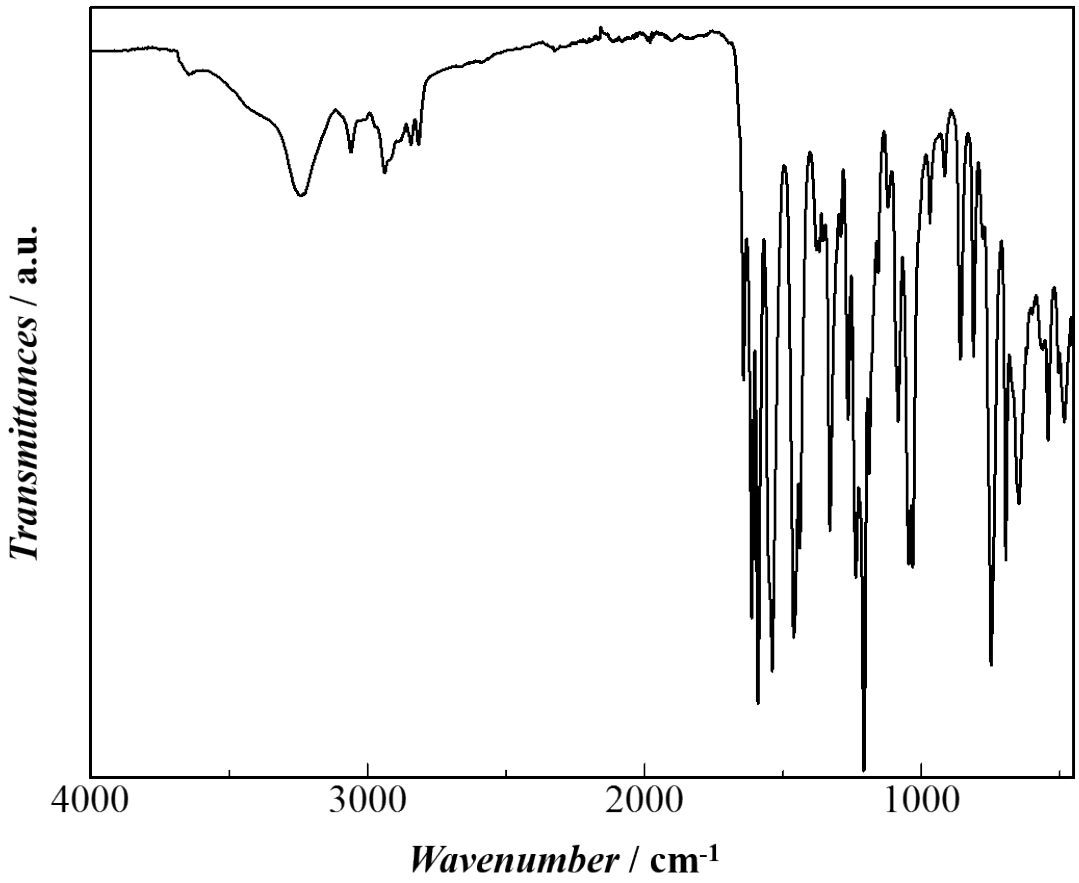

Figure S4. FT–IR spectra for $[Ni_7(HL^2)_6(\mu_3\text{-}OMe)_6]Cl_2$ (**2**).

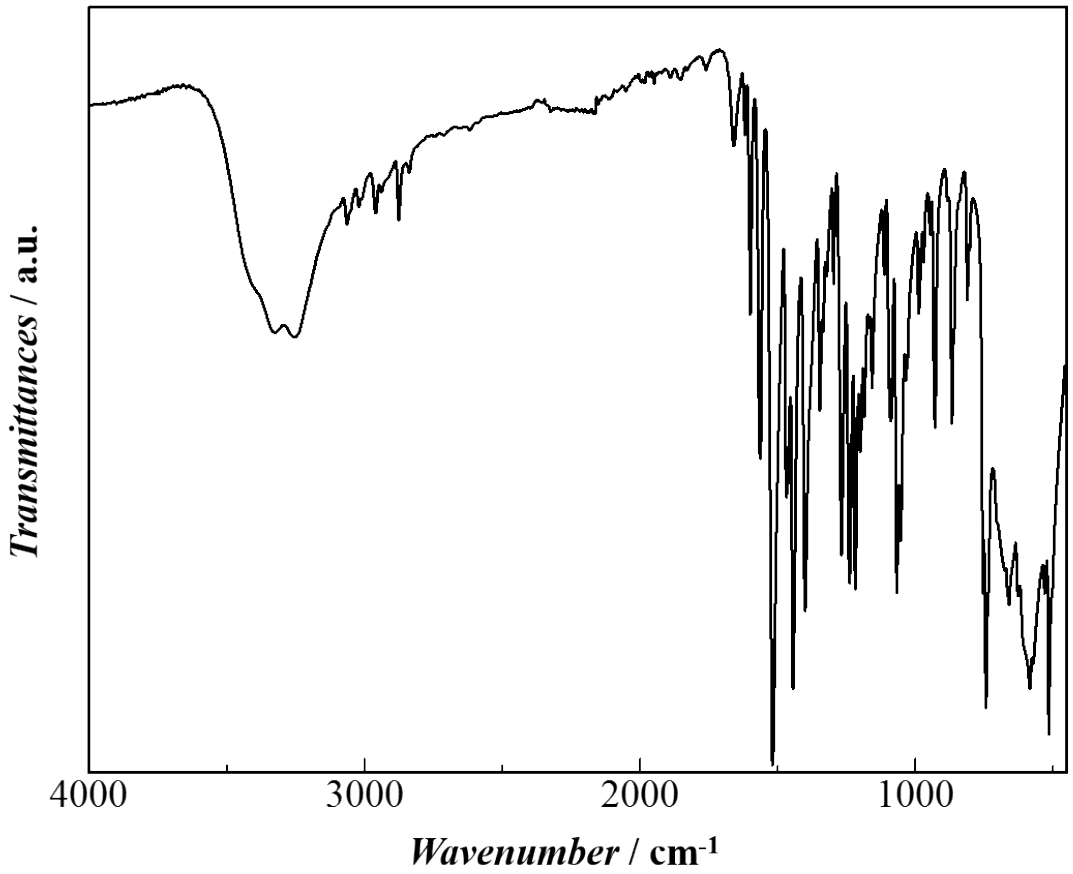

Figure S5. FT−IR spectra for $NiL^3 \cdot 2H_2O$ (**3**).