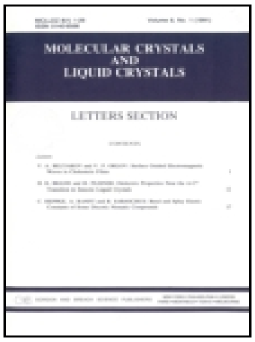

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Microwave Assisted Synthesis, and Structure of a Co-Crystal Nickel Complex with 2-ethoxy-6-methyliminomethyl-phenol

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A new co-crystal complex $[Ni_7(emmp)_6(OH)_6][Ni(emmp)_2]\cdot(CH_3CN)_2\cdot(ClO_4)_2$ *(**1**, Hemmp is 2-ethoxy-6-methyliminom-ethyl-phenol) has been synthesized by microwave-assist solvothermal method. Complex **1** was characterized by IR spectroscopy, elemental analysis, and X-ray single-crystal diffraction. The **1** was consist of a nano-bowl-like heptanuclear cation cluster* $[Ni_7(emmp)_6(OH)_6]^{2+}$*, two counterion* ClO_4^-*, one neutral mononuclear complex* $[Ni(emmp)_2]$ *and two acetonitrile molecules. The five part of **1** constructed a whole through M···H interaction, O–H···N hydrogen bonds and C–H···O hydrogen bonds.*

Keywords Co-crystal complex; hydrogen bonds, microwave chemistry; N,O ligands

1. Introduction

In the past decade, much attention has been given to the design and synthesis of the polymetallic cluster since the discovery of “single-molecule magnets” (SMMs) [1, 2]. The search for *key ligands* to suit respective needs is one of most important process to advance this research. Recently, Schiff base, as old ever green ligands, is widely used in the synthesis of magnetic clusters [3–10]. Previous investigations implied that the Schiff base of 2-hydroxy-benzaldehyde ramification ligand derivatives metal-cluster structure probably favors ferromagnetic coupling through μ_3-O-bridges [4, 11–15]. On the other hand, relatively small modifications in the bridging ligand may lead to significant changes in the overall structures of the assemblies [7, 16–18]. In order to study the steric hindrances resulting from the nature of the substituted groups, we chose an analogous ligand 2-ethoxy-6-methylimino- methyl-phenol to serve as a chelating/bridging ligand to bring metal ions into new type of multinuclear clusters.

As well known, the “conventional” techniques—mixed metal ion and ligands in a common solvent at temperatures limited by the boiling point of that solvent at atmospheric pressure have been superbly successful in producing the vast majority of paramagnetic compounds. With the development of new preparative routes for the synthesis

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of molecular cluster under nonambient conditions, a few groups have explored higher temperature routes–solvothermal methods to clusters, including very high spin ground state example [19–21]. Furthermore, in recently, microwave heating has been introduced into to solvothermal methods, as a new and extremely attractive method for synthesizing polymetallic clusters, and provide a clean, cheap, and convenient method of heating that can result not only in higher yields and shorter reaction times but also in the formation of completely new products [4,7,12,13,22–26]. An interesting aspect for synthetic inorganic chemists is the exploring and widening of new preparative routes under nonambient conditions in different reaction systems. Herein, we constructed a co-crystal compound complex $[Ni_7(emmp)_6(OH)_6][Ni(emmp)_2]\cdot(CH_3CN)_2\cdot (ClO_4)_2$ (**1**) which is consist of a nano-two-double-like heptanuclear unit $[Ni_7(emmp)_6(OH)_6]\cdot(ClO_4)_2$, mononuclear complex $[Ni(emmp)_2]$ and two acetonitrile molecules using nickel(II) ions and a new Schiff base Hemmp as the reactants.

2. Experimental

2.1 Material and Physical Measurements

All chemicals were commercially available and used as received without further purification. Microwave syntheses are carried out using a XH-800C microwave digestion system. The C, H, N microanalyses were carried out with a PE 2400 series II elemental analyzer. The FT-IR spectra were recorded from KBr pellets in the range 4000–400 cm^{-1} on a Bio-Rad FTS-7 spectrophotometer. The crystal structure was determined by single-crystal X-ray diffraction and using SHELXS-97, SHELXL-97 software for structure solution and refinement, respectively.

2.2 Microwave Synthesis

$Ni(ClO_4)_2\cdot 6H_2O$ (0.360 g, 1 mmol), 3-ethoxy-2-hydroxy-benzaldehyde (Hehb, 0.166 g, 1 mmol), methylamine [0.5 mL (50%)], and acetonitrile (15 mL), water (15 mL) were placed in a 60-mL Teflon-lined autoclave, which was then inserted into the cavity of a microwave reactor. The reaction mixture was maintained at $T = 140°C$, power = 300 W, and pressure = 2.8 atm for a total of 29 min. After cooling (*ca.* 120 min), and **1** as green crystals were collected by filtration, washed with water, and dried in air. The phase pure **1** was obtained by manual separation (yield: 135 mg, *ca.* 47.41% based on Ni). *Anal. Calcd.* (%): $C_{84}H_{108}Cl_2N_{10}Ni_8O_{30}$: C, 44.28; H, 4.78; N, 6.15; Found C, 44.21; H, 4.86; N, 6.24%. IR data for **1** (KBr, cm^{-1}): 3628(m), 3439(s), 2925(w), 1631(s), 1475(s), 1462(m), 1305(s), 1234(m), 1216(s), 1121(s), 1089(s), 1052(m), 966(w), 793(m), 636(w), 623(w), 490(w).

Caution: Perchlorate salts with organic ligands are potentially explosive.

2.3 Crystal Structure Determination

A diffraction data were collected on a Bruker Smart Apex CCD diffractometer with graphite monochromated Mo -Kα radiation ($\lambda = 0.71073$ Å) at 298 K. Using the ω-θ scan mode in the range $2.31 \le \theta \le 25.10°$. Raw frame data were integrated with the SAINT program [27]. The structure was solved by direct methods using SHELXS-97 and refined by full-matrix least-squares on F^2 using SHELXS-97 [27]. An empirical absorption correction was applied with the program SADABS [27]. All non-hydrogen atoms were refined anisotropically. H

Table 1. Crystal data and structure refinement for **1**

Compound	**1**
Mol. form.	$C_{84}H_{108}Cl_2N_{10}Ni_8O_{30}$
Form. weight	2278.22
T / K	298(2)
Color and form	Green, block
Crystal system	Triclinic
Space group	$P\bar{1}$ (no. 2)
a / Å	10.932(3)
b / Å	14.816(4)
c / Å	16.869(5)
α / °	111.397(3)
β / °	101.865(3)
γ / °	90.626(3)
V / Å^3	2478.4(12)
Z	1
F(000)	1180
$D_{calcd.}$/ g cm^{-3}	1.526
μ/ mm^{-1}	1.619
θ range / °	2.31 to 25.10
Ref. coll./unique	17,928 / 8712
R_{int}	0.0451
Completeness	98.8%
Parameters	165
GOF	1.038
R_1 $[I \geq 2\sigma(I)]^{a,b)}$	0.0573
wR_2 (all data)$^{a,b)}$	0.1739
Residues / e Å^{-3}	1.305 and –0.800

$^{(a)}$ $R_1 = \sum||F_o|–|F_c||/\sum|F_o|$, $^{(b)}$ $wR_2 = [\sum w(F_o{}^2–F_c{}^2)^2/\sum w(F_o{}^2)^2]^{1/2}$.

atoms of the hydroxide radicals were located in difference Fourier maps. The O -H distances were normalized to 0.7507 $\sim$ 0.8501 Å for **1**. And the H-atoms were then allowed to ride on their parent O atoms, with Uiso(H) $= 1.5U$iso(O). All calculations and graphics were performed with SHELXTL. The highest peak in the residual electron density of **1** are located 1.00 Å from atom Ni_4. The crystallographic details are provided in Table 1, while the selected bond distances and angles are listed in Table 2. Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Center. CCDC reference numbers for **1** is 986275.

3. Results and Discussion

The molecular structure of the co-crystal compound **1** contains a double-bowl-like heptanuclear nickel cation cluster unit, $[Ni_7(emmp)_6(OH)_6]^{2+}$ as in the reference [4,11–15], a mononuclear unit, $[Ni(emmp)_2]$, two counterions $ClO_4{}^-$ and two acetonitrile molecules (Fig. 1). The coordination properties of the [Ni7] unit in **1** share a great similarity with in the references [4, 11–15], but μ_3-O bridges are different. In **1**, μ_3-O bridges are composed with six μ_3-OH bridges while in the reference, six μ_3-O bridges are all μ_3-OMe bridges

Table 2. Selected bonds lengths (Å) and angles (°) for **1**

Ni1–O7	2.070(3)	Ni1–O8	2.072(3)
Ni1–O9	2.078(3)	Ni2–O3	1.991(3)
Ni2–O5	2.029(4)	Ni2–O6	2.270(4)
Ni2–O7	2.040(4)	Ni2–O8	2.113(3)
Ni2–N2	2.064(5)	Ni3–O1	2.019(4)
Ni3–O2	2.265(3)	Ni3–O5	1.990(4)
Ni3–O7	2.114(4)	Ni3–O9	2.045(3)
Ni3–N3	2.069(5)	Ni4–O1	1.998(3)
Ni4–O9	2.112(3)	Ni4–N1	2.061(5)
Ni4–O3a	2.023(3)	Ni4–O4a	2.249(4)
Ni4–O8a	2.049(4)	Ni5–O10	1.823(4)
Ni5–N4	1.919(5)	O7–Ni1–O8	82.2(1)
O7–Ni1–O9	82.6(1)	O7–Ni1–O7a	180.0
O7–Ni1–O8a	97.8(1)	O7–Ni1–O9a	97.4(1)
O8–Ni1–O9	98.1(1)	O7a–Ni1–O8	97.8(1)
O8–Ni1–O8a	180.0	O8–Ni1–O9a	81.9(1)
O7a–Ni1–O9	97.4(1)	O8a–Ni1–O9	81.9(1)
O9–Ni1–O9a	180.0	O7a–Ni1–O8a	82.2(1)
O7a–Ni1–O9a	82.6(1)	O8a–Ni1–O9a	98.1(1)
O3–Ni2–O5	162.6(2)	O3–Ni2–O6	92.6(2)
O3–Ni2–O7	113.5(2)	O3–Ni2–O8	78.6(1)
O3–Ni2–N2	87.9(2)	O5–Ni2–O6	73.9(2)
O5–Ni2–O7	79.3(2)	O5–Ni2–O8	92.2(1)
O5–Ni2–N2	103.1(2)	O6–Ni2–O7	153.2(2)
O6–Ni2–O8	98.4(2)	O6–Ni2–N2	91.2(2)
O7–Ni2–O8	81.9(1)	O7–Ni2–N2	95.4(2)
O8–Ni2–N2	163.8(2)	O1–Ni3–O2	73.9(1)
O1–Ni3–O7	92.7(2)	O9–Ni4–N1	164.5(2)
O1–Ni3–N3	102.7(2)	O4a–Ni4–O9	98.8(2)
O2–Ni3–O7	97.4(1)	O3a–Ni4–N1	102.4(2)
O2–Ni3–N3	91.3(2)	O8a–Ni4–N1	96.3(2)
O5–Ni3–O9	113.5(2)	O3a–Ni4–O8a	79.4(1)
O7–Ni3–O9	82.3(1)	O1–Ni3–O5	162.9(2)
O9–Ni3–N3	96.0(2)	O1–Ni3–O9	79.2(1)
O5–Ni3–O7	78.4(2)	O2–Ni3–O5	92.7(2)
O5–Ni3–N3	87.8(2)	O2–Ni3–O9	153.0(2)
O7–Ni3–N3	163.9(2)	O1–Ni4–O4a	93.2(1)
O1–Ni4–O9	78.1(1)	O1–Ni4–N1	88.7(2)
O1–Ni4–O3a	163.0(2)	O8a–Ni4–O9	81.6(1)
O1–Ni4–O8a	112.5(1)	O4a–Ni4–N1	90.0(2)
O3a–Ni4–O9	92.4(1)	O3a–Ni4–O4a	74.2(1)
O4a–Ni4–O8a	153.7(1)	O10–Ni5–N4	93.3(2)
O10–Ni5–N4b	86.7(2)	N4–Ni5–N4b	180.0
O10–Ni5–O10b	180.0	Ni3–O1–Ni4	103.1(2)
Ni2–O3–Ni4a	103.1(2)	Ni2–O5–Ni3	103.1(2)
Ni1–O7–Ni3	95.7(1)	Ni2–O7–Ni3	98.5(1)

(Continued on next page)

Table 2. Selected bonds lengths (Å) and angles (°) for **1** *(Continued)*

Ni1–O7–Ni2	98.2(1)	Ni1–O8–Ni4a	98.5(1)
Ni1–O8–Ni2	95.9(1)	Ni2–O8–Ni4a	98.0(1)
Ni3–O9–Ni4	98.6(1)	Ni1–O9–Ni4	96.4(1)
Ni1–O9–Ni3	97.7(1)	Ni1···Ni3	3.103(1)
Ni1···Ni2	3.108(1)	Ni2···Ni3	3.147(1)
Ni1···Ni4	3.122(1)	Ni2···Ni4a	3.142(1)
Ni3···Ni4	3.151(1)		

Symmetry codes for **1**: (a) 1 – *x*, 1 – *y*, 1 – *z*; (b): 1 – *x*, 2 – *y*, –*z*.

[4, 11–15]. In the $[Ni_7(emmp)_6(OH)_6]^{2+}$ core, the coordination bond lengths involving the μ_3-O atom are in the range of 2.070(3)–2.078(3) Å. The angles of the Ni–O–Ni bridged by μ_3-O are in the range of 95.7(1)–98.6(1)°, while the angles of the Ni–O–Ni bridged by μ_2-O are 103.1(2)° (Table 2). In the double-bowl-like heptanuclear unit, the emmp anionic ligands (single deprotonated at the phenolate site) bridge the peripheral Ni^{II} centers adopting a μ_4:η^1:η^2:η^1 coordinated motif (Scheme 1a), lying alternately above and below the double-bowl basal plane. Close inspection of the double-bowel conformation shows approximate bowel dimensions of 2.77 × 6.25 × 10.27 × 11.89 Å (base thick × base diameter × depth × rim diameter) which is a nano-double-bowl, while two acetonitrile molecules lie on the double-bowl (Fig. 1). The acetonitrile molecule on the double-bowl were linked the double-bowl through bottom O–H···N hydrogen bonds (O8–H8D···N5,

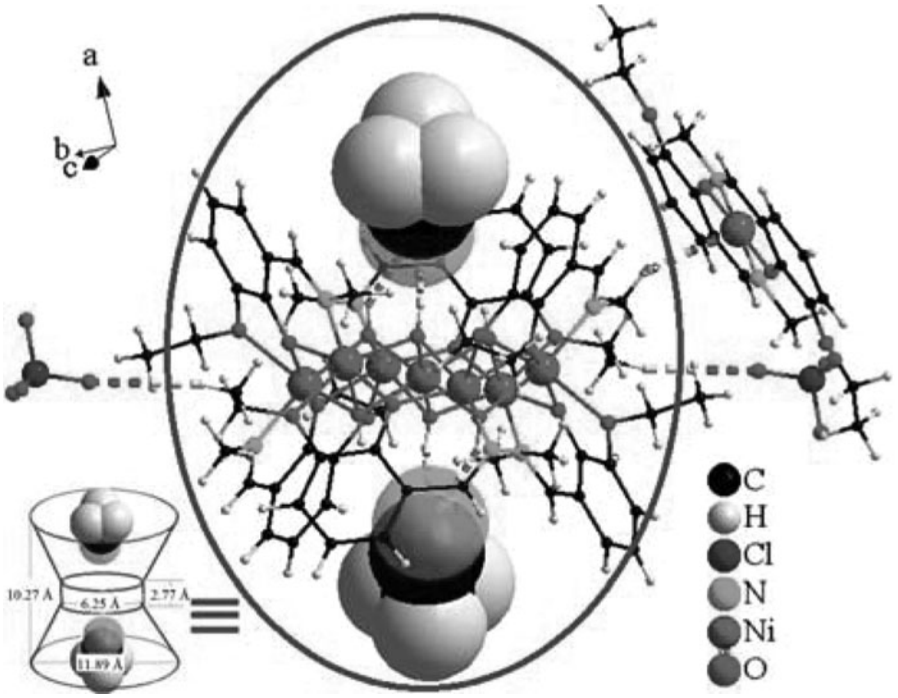
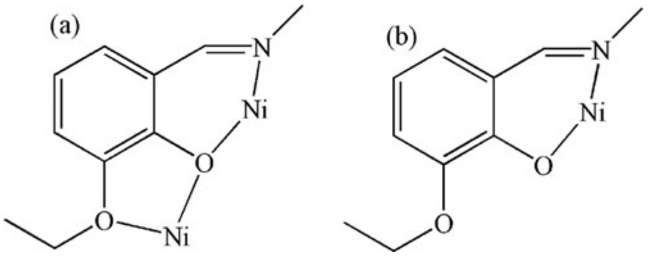


Figure 1. Structure of 1.



Scheme 1. Coordination mode of the emmp ligand.

3.243(2); O9–H9D···N5, 3.204(2) Å, Table 3). Another important part comes from the mononuclear unit [Ni(emmp)$_2$]; the Ni5 ion has a N2O2 square planar coordination geometry, in which one phenolato oxygen atom and one imino nitrogen atom belonging to one deprotonated emmp$^-$ ligand, (Ni5–O11, 1.823(4) Å and Ni5–N4, 1.919(5) Å), and the resulting mononuclear unit is thus neutral. In the mononuclear unit, the emmp$^-$ ligand displays an another coordination mode which is μ_2:η^1:η^1 coordinated mode (Scheme 1b). The T-shaped C–H···π stacking interactions were observed between the [Ni$_7$(emmp)$_6$(OH)$_6$]$^{2+}$ and mononuclear units (Fig. 2), which were characterized by a C–H···ring centroid contact (C3–H3···Q, Q is the centroid one of the aryl rings of the emmp$^-$ ligand in the mononuclear unit) with a H···Q distance of 2.830 Å [28, 29]. Another weak inter-unit interaction in **1** was evidenced by the short contact between Ni5 and H18C with a Ni5···H18C [C18–H18C···Ni5$^{\mathrm{I}}$, symmetry code: (i) x, y – 1, z] bond length of 2.649(1) Å and a Ni5 ···C18 bond length of 3.528(1) Å, while the C18–H18C···Ni5$^{\mathrm{I}}$ angle bond was 152.3(1)°. Ni5 can be considered as a Lewis acid, where in the mononuclear unit the Ni$^{\mathrm{II}}$ in a square planar configuration is a 16e species with an empty orbital on the metal atom that can adapt to receive the electrons in the C–H bond. However, the contact distances of Ni5···H18C (2.649(1) Å) and Ni5···C18 (3.528(1) Å) were not comparable, and the angle of C18–H18C···Ni5$^{\mathrm{I}}$ was greater than 100°. Thus according to G. R. Desiraju et al., [30,31] the weak interaction should probably be classified as a four-electron-three-center C–H···M hydrogen bond compared to those considered as agostic interactions [24, 32]. The mononuclear compound [Ni(emmp)$_2$] is "locked" at the edge of the double-bowl-like [Ni7] unit by C–H···π together with C–H···M hydrogen-bond interactions thus forming a 1-D chain (Fig. 2).

To compare the references [4, 11–15], we found that the bulk of the Hemmp ligand plays a vital important role with construction structure. Herein, we give an example that relatively small modifications in the bridging ligand may lead to significant changes in the overall structures of the assemblies.

Table 3. Hydrogen bond lengths (Å) and bond angles (°)

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA
O8—H8D···N5	0.85	2.50	3.243(2)	147.0
O9—H9D···N5	0.85	2.40	3.204(2)	159.1

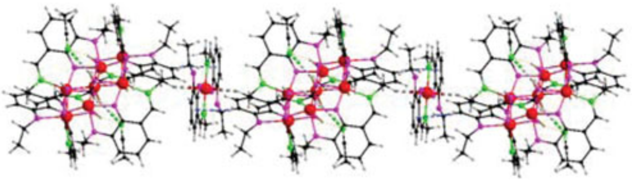


Figure 2. The 1-D chain through C–H···π hydrogen bonds and C–H···Ni5 interaction.

Conclusions

Using microwave assisted, we synthesized a co-crystal complex $[Ni_7(emmp)_6(OH)_6][Ni(emmp)_2]\cdot(CH_3CN)_2\cdot(ClO_4)_2$. The heptanuclear cation unit is a nano-double-bowl, while the acetonitrile molecules stay at the bowl. The structure indicates that that the bulk of the ligand plays a very important role with construction structure.

Supplemental Data

Crystallographic data (excluding structure factors) for the structure in this paper has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication CCDC 986275. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: 44 1223 336033, e-mail: deposit@ccdc.cam.ac.uk).

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