



# Novel heteroligand Ni(II) complexes with benzylmalonate dianions: synthesis, structure, and thermal behavior

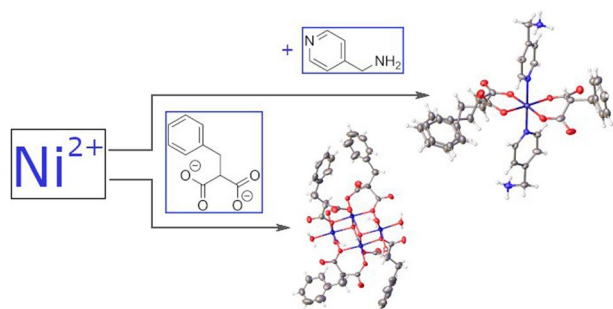
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## Abstract

The two heteroligand Ni(II) complexes were synthesized: tetranuclear ionic complex  $(\text{NBu}_4)_4[\text{Ni}_4(\text{OH})_2(\text{Bzmal})_4(\text{H}_2\text{O})_6](\text{OAc})_2 \cdot 8\text{H}_2\text{O}$  and mononuclear neutral complex  $[\text{Ni}(\text{Bzmal})_2(4\text{-ampyH})_2] \cdot 2\text{H}_2\text{O} \cdot 2\text{DMF}$  (where  $\text{NBu}_4^+$  is the tetrabutylammonium cation,  $\text{Bzmal}^{2-}$  are benzylmalonate dianions, and  $4\text{-ampyH}^+$  is the 4-(ammoniummethyl)pyridine). The structure of the complexes was determined by single-crystal X-ray diffraction analysis. The simultaneous thermal analysis of  $[\text{Ni}(\text{Bzmal})_2(4\text{-ampyH})_2] \cdot 2\text{H}_2\text{O} \cdot 2\text{DMF}$  was performed.

## Graphical abstract



**Keywords** Nickel(II) · Dicarboxylic acid · Substituted malonates · Crystal structure · Thermal decomposition · Coordination chemistry

## Introduction

Malonic acid and its derivatives belong to a class of organic ligands capable of performing a chelate-bridging function in the formation of coordination compounds with metal ions, especially transition metals. Varying the substituents in the substituted malonic acid anions, initial metal salt and the use of additional ligands enable to affect the structure of

the resulting compounds, thus affecting the properties of complexes [1–6]. The 3d-metal malonates and substituted malonates are of interest from the point of view of magnetic properties or as precursors for mixed oxide materials [7–14].

Malonate homometallic complexes of nickel(II) comprising only water molecules as additional ligands are represented by molecular mononuclear compounds [15] and polymers [16–18]. The malonate fragments in molecular nickel(II) compounds can be an anionic, for example, a bichelate moiety is widespread in such systems [19–22]. Another nickel(II) malonate moiety comprising hydroxo groups along with coordinated water molecules is a 36-nuclear anion known for dimethylmalonic and cyclobutane-1,1-dicarboxylic acids [23–25]. However, the nickel(II)

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benzylmalonates have not been reported in literature before, homometallic benzylmalonates with other 3d metals are known [4, 8, 26–29]. Coordination of N-donor ligands results in mono- [30–35] or binuclear [36, 37] molecular compounds and polymers [38–42], depending on the structure of the N-containing ligand.

Here, we present the synthesis and the structure of novel nickel(II) coordination compounds with benzylmalonic acid anions ( $\text{H}_2\text{Bzmal}$ ) along with additional coordinated water molecules and hydroxo groups ( $\text{NBu}_4$ ) $[\text{Ni}_4(\text{OH})_2(\text{Bzmal})_4(\text{H}_2\text{O})_6](\text{OAc})_2 \cdot 8\text{H}_2\text{O}$  (**1**,  $\text{NBu}_4^+$  is the tetrabutylammonium cation) or 4-(ammoniummethyl)pyridine cations  $[\text{Ni}(\text{Bzmal})_2(4\text{-ampyH})_2] \cdot 2\text{H}_2\text{O} \cdot 2\text{DMF}$  (**2**,  $4\text{-ampyH}^+ = 4\text{-(ammoniummethyl)pyridine}$ ). Thermal behavior of **2** was investigated by TGA and DTA methods in argon (simultaneous thermal analysis).

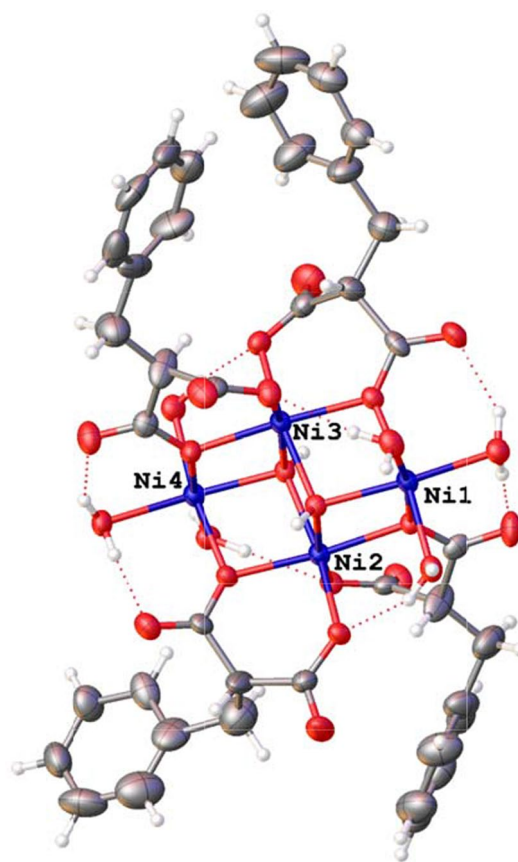
## Results and discussion

The reaction of nickel(II) acetate, benzylmalonic acid, and tetrabutylammonium hydroxide produced a tetranuclear heteroligand nickel(II) complex ( $\text{NBu}_4$ ) $[\text{Ni}_4(\text{OH})_2(\text{Bzmal})_4(\text{H}_2\text{O})_6](\text{OAc})_2 \cdot 8\text{H}_2\text{O}$  (**1**). With the initial salt being nickel(II) perchlorate and 4-(aminomethyl)pyridine (4-picolyamine) being an additional ligand, the neutral  $[\text{Ni}(\text{Bzmal})_2(4\text{-ampyH})_2] \cdot 2\text{H}_2\text{O} \cdot 2\text{DMF}$  (**2**) complex is formed. The IR spectra of **1** and **2** contain asymmetric  $\nu_{\text{as}}(\text{COO}^-)$  ( $1598$  and  $1593$ ,  $1577$   $\text{cm}^{-1}$ ) and symmetric  $\nu_{\text{s}}(\text{COO}^-)$  ( $1401$  and  $1409$ ,  $1389$   $\text{cm}^{-1}$ ) stretching vibrations of the carboxylic groups, respectively.

The asymmetric unit of **1** contains six cations of tetrabutylammonium, one and a half complex anion, three acetate anions, and twelve water molecules (Fig. 1).

Six *n*-butyl groups and two phenyl groups in **1** are equally disordered over two sites. The best available single crystal is found to have poor quality that affected the convergence factors and did not allow us to locate hydrogen atoms. Thus, an additional analysis was performed to clarify the chemical composition. First, the C–O bond lengths are the intermediates between those of single and double bonds, thus, no  $\text{HBzmal}^-$  monoanions or acetic acid molecules are present in the crystal. Nickel atoms are undoubtedly in the 2+ oxidation state, as follows from a crystal-chemical analysis according to <https://crystalpredictor.com> for complexes containing nickel in an oxygen environment [43]. Thus, though the  $\mu_3$ -bridge oxygen atom does not participate in any hydrogen bonds, it corresponds to the hydroxo rather than oxo group, and the overall chemical formula of this solid is ( $\text{NBu}_4$ ) $[\text{Ni}_4(\text{OH})_2(\text{Bzmal})_4(\text{H}_2\text{O})_6](\text{OAc})_2 \cdot 8\text{H}_2\text{O}$ .

The nickel(II) atoms in the tetranuclear anions of **1** form octahedral  $\text{NiO}_6$  coordination polyhedra, however, they are formed by a different environment. Three of the metal

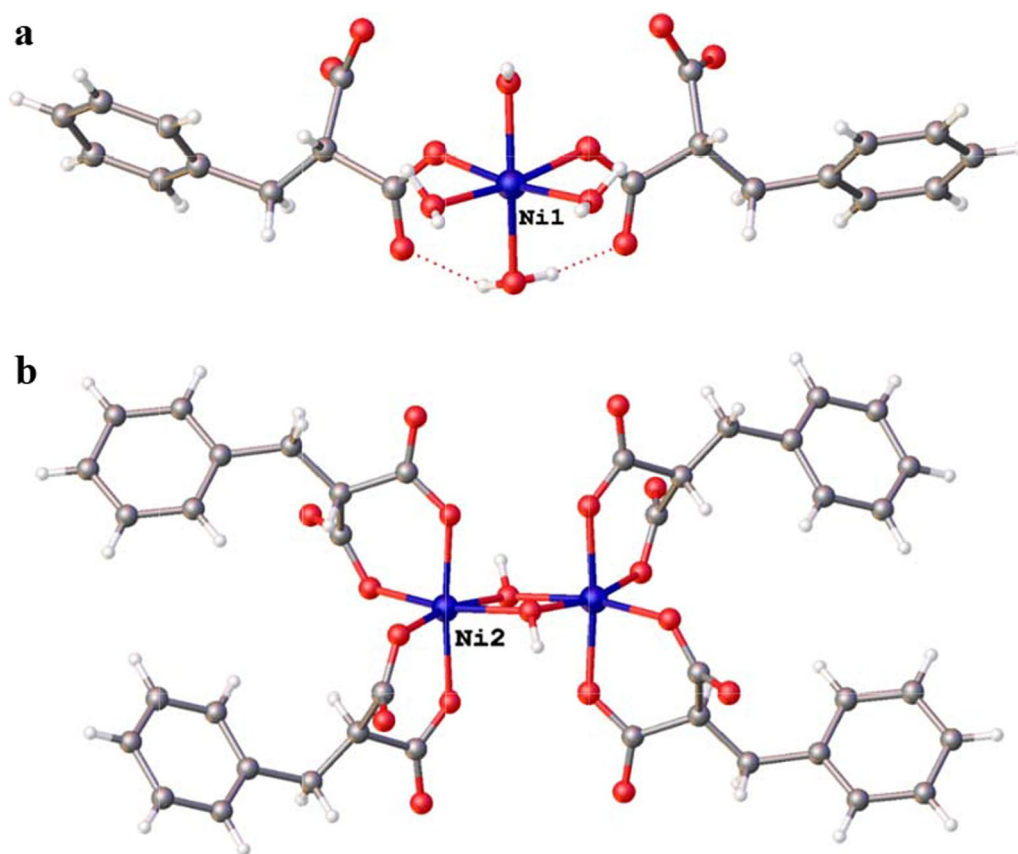


**Fig. 1** Complex anions  $[\text{Ni}_4(\text{OH})_2(\text{Bzmal})_4(\text{H}_2\text{O})_6]^{2-}$  in representation of atoms with thermal ellipsoids ( $p=50\%$ )

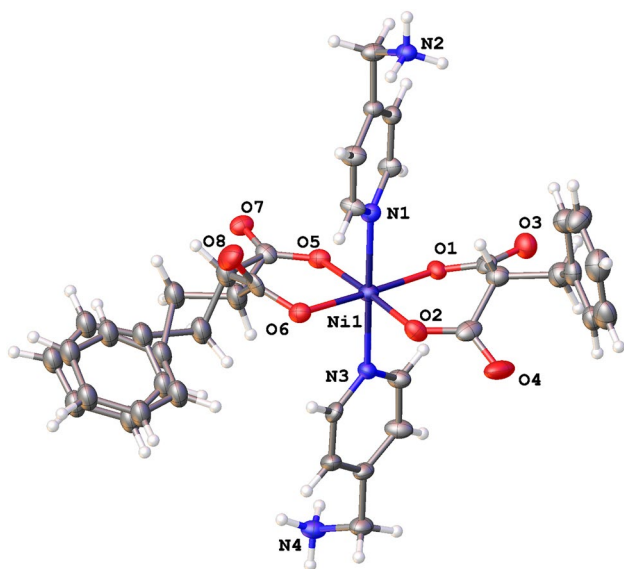
atoms (Ni1, Ni4, and Ni5) are coordinated with three water molecules, one hydroxide anion and two  $\text{Bzmal}^{2-}$  anions, while the others (Ni2, Ni3, and Ni6) are coordinated with oxygen atoms of the two chelate anions and two hydroxides (Fig. 2a, b).

The asymmetric unit of **2** contains a Ni(II) atom, two chelate benzylmalonate dianions, two 4-(ammoniummethyl)pyridine cations coordinated by the metal atom through the nitrogen atom of the heterocycle, and two water and DMF molecules (Fig. 3). Previously, the only two complexes were described, where a metal atom is coordinated with this cation. Aside from this compound,  $[\text{Co}(4\text{-ampyH})_2(\text{H}_2\text{O})_4](\text{SO}_4)_2 \cdot 3\text{H}_2\text{O}$  [44] and  $[\text{Ag}(4\text{-ampyH})_2](\text{ClO}_4)_3 \cdot 2\text{H}_2\text{O}$  [45] contain the 4-(ammoniummethyl)pyridine bound with metals. In contrast to known compounds, complex **2** contains two acid dianions, which completely compensate for the charge of the metal cation and two protonated amino groups of the ligands, forming a complex zwitterion, similar to the betaines.

The bond lengths of all the coordination bonds are listed in Table 1. In general, these bond lengths increase from (Ni–O(OH)) to (Ni–O( $\text{H}_2\text{O}$ )) and to (Ni–O $_{\text{An}}$ ). The chelate



**Fig. 2** Environment of Ni1/Ni4/Ni5 **a** and Ni2/Ni3/Ni6 **b** atoms in the  $[\text{Ni}_4(\text{OH})_2(\text{Bzmal})_4(\text{H}_2\text{O})_6]^{2-}$  complex anion



**Fig. 3** Complex  $[\text{Ni}(4\text{-ampyH})_2(\text{Bzmal})_2]$  in representation of atoms with thermal ellipsoids ( $p = 50\%$ )

(Ni–O<sub>An</sub>) bonds are shorter than the additional bridging Ni–O<sub>An</sub> bond. All Bzmal<sup>2-</sup> dianions bridge two metal atoms

through both of its oxygen atoms. To put it simply, Bzmal<sup>2-</sup>, OH<sup>-</sup> and H<sub>2</sub>O implement the B<sup>11</sup>, M<sup>3</sup>, and M<sup>1</sup> coordination modes in terms of the notation described in Ref. [46]. The overall crystal-chemical formula of the tetranuclear  $[\text{Ni}_4(\text{OH})_2(\text{Bzmal})_4(\text{H}_2\text{O})_6]^{2-}$  anions is A<sub>4</sub>M<sub>3</sub>B<sup>11</sup><sub>4</sub>M<sup>1</sup><sub>6</sub>, where A = metal atom. It is worth noting that no similar tetranuclear heteroligand complexes have previously been obtained before among hydroxo-carboxylates.

The stability of the tetranuclear complex in **1** is additionally enhanced by intramolecular hydrogen bonds (Fig. 1). All coordinated water molecules take part in at least one intramolecular hydrogen bond. Besides, two neighboring water molecules form two hydrogen bonds with acetate anions (O(30)–H...O(2S) and O(31)–H...O(1S) with one anion, and O(34)–H...O(3S) and O(35)–H...O(4S) with another one). The parameters of H-bonds are listed in Table S1. It stands to mention that in addition to coordinated water molecules, the asymmetric unit of **1** also contains twelve water molecules that are involved in H-bonding. Although the positions of hydrogen atoms could not be located and were assumed based on the most likely hydrogen-bonding, one can suggest that water molecules, three anions and acetate anions in solid **1** form isolated H-bonded associates (Fig. 4). The cations are located between the H-bonded associates,

**Table 1** Coordination bond lengths/Å in complexes **1** and **2**

Central atom	Bond		
	Ni–O (OH)	Ni–O (H <sub>2</sub> O)	Ni–O/Bzmal <sup>2-</sup>
<b>1</b>			
Ni (1)	2.019 (4)	2.051 (5)–2.079 (5)	2.076 (5)–2.081 (4)
Ni (2)	2.033 (5)–2.060 (4)		2.023 (5)–2.055 (5)
Ni (3)	2.045 (5)–2.046 (4)		2.023 (5)–2.056 (5)
Ni (4)	2.018 (4)	2.046 (5)–2.082 (5)	2.063 (5)–2.108 (5)
Ni (5)	2.025 (4)	2.048 (5)–2.063 (5)	2.078 (5)–2.086 (5)
Ni (6)	2.051 (5)–2.053 (4)		2.028 (4)–2.059 (5)
		Ni–O/Bzmal <sup>2-</sup>	Ni–N
<b>2</b>			
Ni (1)		2.011 (3)–2.046 (3)	2.142 (3)–2.142 (4)

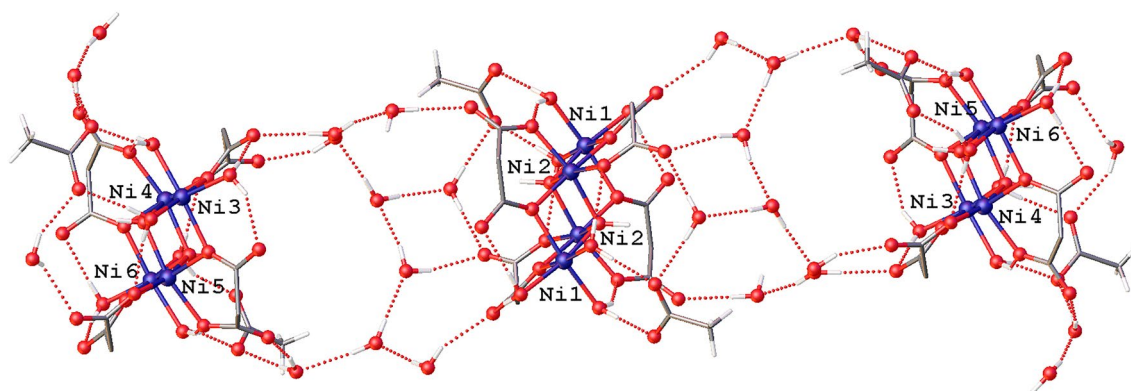
and due to the absence of strong intermolecular bonding, prominent thermal motion occurs even at 120(2) K.

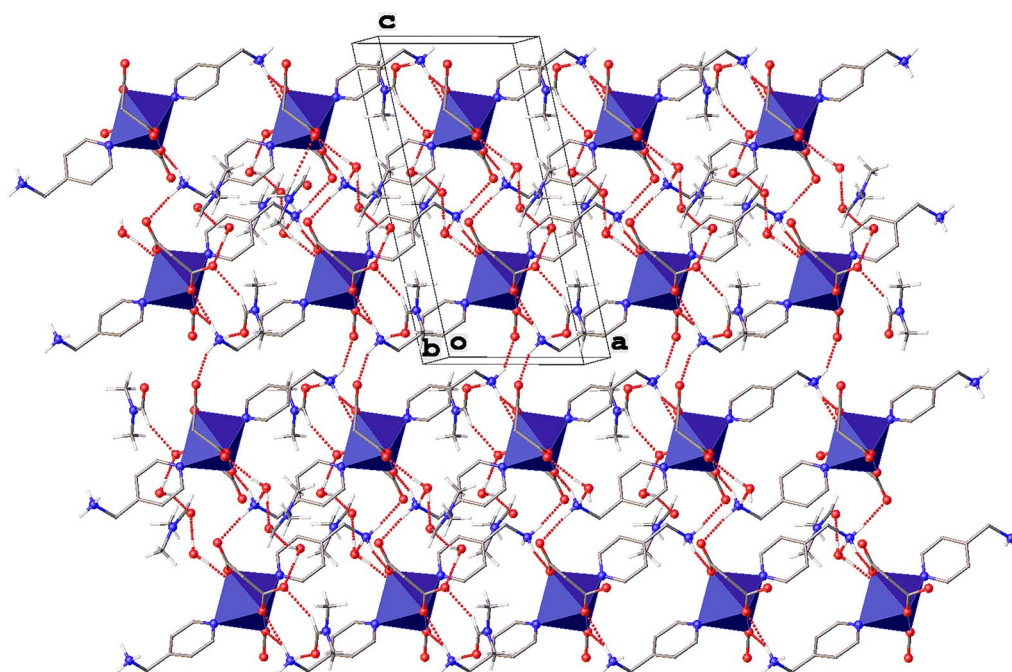
As a result of the presence of ammonium groups and solvent molecules in solid **2**, the dimensionality of H-bonded associates is higher. In this solid, H-bonded parallel to the (1 0 1) plane layers are observed (Fig. 5). The layers are formed by water molecules, dimethylformamide, and the neutral complex. The amino group and water molecules are donors in H-bonding, with water molecules, along with oxygen atoms of DMF and benzylmalonate anions being acceptors (Table S1).

Thermal decomposition of complex **2** was studied using simultaneous thermal analysis, a combination TGA and DTA, in Ar flow (Fig. 6a, b). Thermal decomposition starts at 37 °C from dehydration process (37–102 °C,  $\Delta m = 3.88\%$ ,  $m_{\text{calc}} = 4.26\%$ ), followed by DMF removal ( $t = 101\text{--}155$  °C,  $\Delta m = 17.70\%$ ,  $m_{\text{calc}} = 17.30\%$ ).

These two thermolysis stages are accompanied by two endothermic peaks on DTA curve with maxima at 65 and 128 °C. At 150 °C the melting process with maximum

at 155 °C takes place. This process is overlapped with start of the 4-(aminomethyl)pyridine ligand degradation (b.p. = 230 °C) in the temperature range of 156–201 °C with mass loss 11.16% and followed at 202–254 °C by benzylmalonic acid partial decarboxylation with  $\Delta m = 9.98\%$  (DTA curve shows an exothermic and endothermic effect with maxima at 201 and 206 °C, respectively). Apparently, 4-(aminomethyl)pyridine continues to remove at 254 °C, which combines with the further benzylmalonic fragments destructive elimination in the range 254–410 °C. Final mass loss is  $\Delta m = 85.74\%$ . For more complete oxidation of the end thermolysis product air atmosphere annealing of **2** at 550 °C for 2 h was performed (heating rate was 10 °C/min). PXRD data shows that the major phase in the final product of thermolysis is a cubic NiO (Fig. S1, S2) [47].

**Fig. 4** H-bonded associate observed in **1** (H-bonds are dashed; benzyl fragments and cations are omitted for clarity)



**Fig. 5** H-bonded layers observed in **2** (view along the crystallographic axis *b*;  $\text{PhCH}_2$  moieties are omitted;  $\text{NiN}_2\text{O}_4$  coordination polyhedra are depicted as octahedra; H-bonds are dashed)

## Conclusion

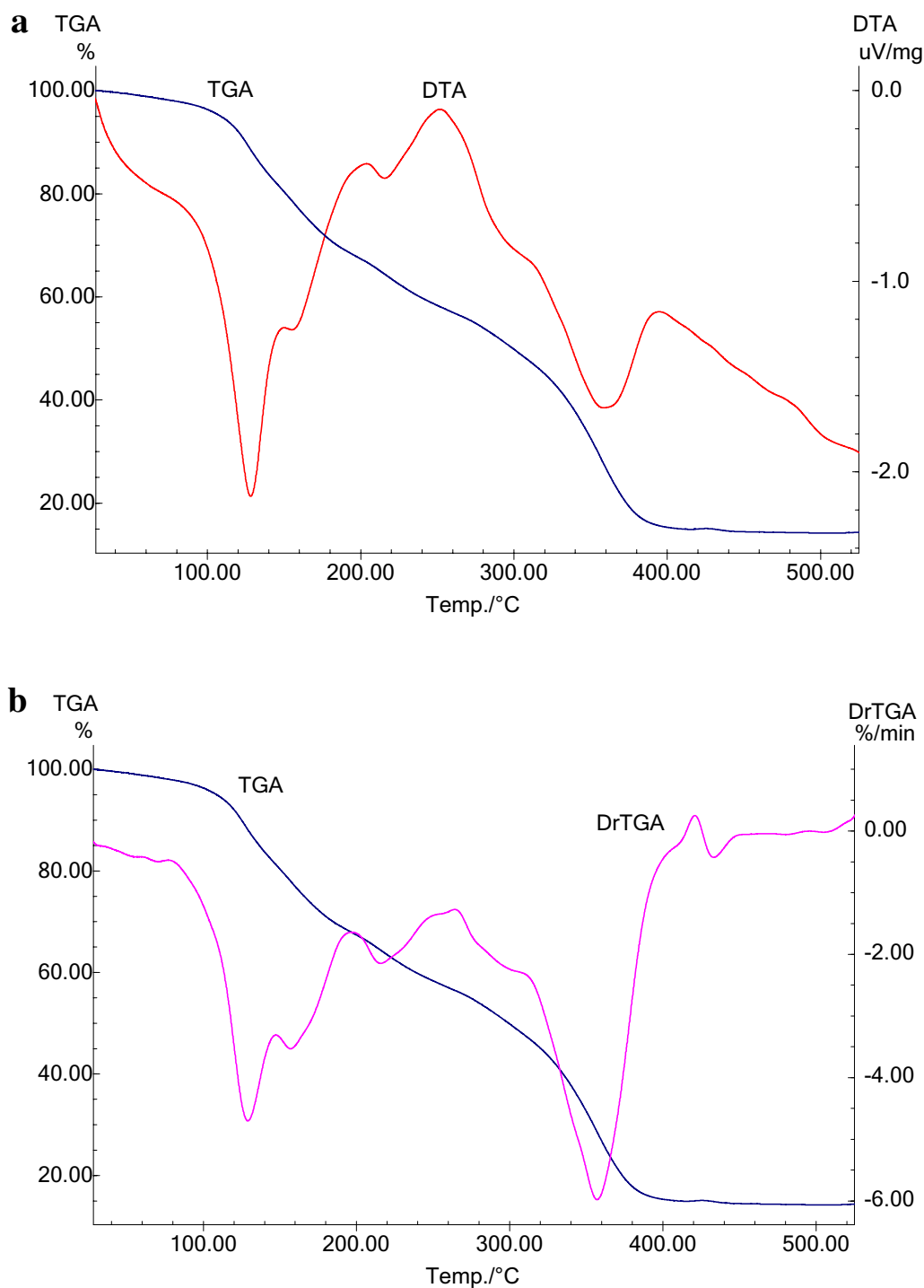
To sum up, two novel heteroligand complexes of nickel(II) with benzylmalonic acid anions and additionally coordinated water and hydroxide groups for **1**, or 4-(ammoniummethyl)pyridine cations for **2** were obtained in this work. A tetranuclear hydroxomalonate was obtained in the absence of N-donor ligands from nickel(II) acetate, whereas a mononuclear complex was synthesized in the presence of 4-(aminomethyl)pyridine from nickel(II) perchlorate. It should be noted that the latter complex is the third example where the 4-(ammoniummethyl)pyridine is coordinated by a metal atom; on the other hand, it is a unique complex that can be considered as a zwitterion. The thermal destruction of complex **2** in an Ar atmosphere shows its lability: it begins at 37 °C from stepwise elimination of water and DMF molecules, the degradation of the organic part of the molecule almost completely ending at 410 °C. Annealing sample **2** in air at 550 °C has been shown to make it possible to obtain a cubic NiO phase as a major product.

## Experimental

The synthesis of all compounds was carried out in air using distilled water and commercially available reagents: ethanol, methanol, nickel(II) acetate tetrahydrate (Reakhim, “pure” grade), nickel(II) perchlorate hexahydrate (Sigma Aldrich,

“chem. pure” grade), tetrabutylammonium hydroxide (Sigma Aldrich, 40% in water), benzylmalonic acid (Sigma Aldrich, 99%), and 4-(aminomethyl)pyridine (Alfa Aesar, 97 + %). The IR spectrum of **1** were recorded on a Perkin Elmer Spectrum FT-IR 65 spectrometer by the ATR method in the range of 4000–400  $\text{cm}^{-1}$ . IR spectrum of **2** was recorded using JASCO FT/IR-4700 spectrometer by ATR method in the range of 4500–550  $\text{cm}^{-1}$ .

The monocrystal X-ray diffraction study was conducted using Bruker APEX II and Bruker D8 Venture ( $\lambda(\text{MoK}\alpha) = 0.71073 \text{ \AA}$ ) diffractometers (Bruker AXS, Madison, WI, USA) at 120.0(2) K. Absorption was corrected by semiempirical methods in accordance with R. Blessing’s methodology [48] using the SADABS program [49]. Crystal structures were solved and refined with the OLEX<sup>2</sup> package. The ShelXT program was applied to solve [50], and the ShelXL program was used to refine structures against  $F^2(\text{hkl})$  [51]. Positions and thermal parameters of non-hydrogen atoms were refined first in isotropic and then in anisotropic approximation for all ordered fragments. Carbon atoms of two  $\text{Bzmal}^{2-}$  anions and four butyl groups in the structure of **1** are equally disordered over two sites. They were refined isotropically with fixed C–C bond distances. The positions of hydrogen atoms were calculated and refined in isotropic approximation as ‘riding’ atoms with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{X})$  for methyl groups and water molecules, and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{X})$  for the other atoms. The crystal and experimental parameters, as well as the convergence factors



**Fig. 6** TGA (blue), DTA (red;  $\uparrow$ exo) **a** and derivative of TGA (DrTGA, purple) **b** curves of **2** (colour figure online)

are listed in Table 2. All crystallographic information can be obtained from the Cambridge Crystallographic Data Centre at <http://www.ccdc.cam.ac.uk/structures> (CCDC No. 2243916 (**1**), 2243915 (**2**)).

Simultaneous Thermal Analysis (STA), which combines Thermogravimetric Analysis (TGA) with Differential

Thermal Analysis (DTA) for **2**, was carried out on simultaneous thermal analyzer DTG-60 (Shimadzu) under argon flow ( $50\text{ cm}^3/\text{min}$ ) at a heating rate of  $10\text{ }^{\circ}\text{C}/\text{min}$ . The study was performed in Al crucibles under a lid with a hole. The sample mass was in the range 4.97–5.05 mg.

**Table 2** Crystallographic details, experimental parameters, and convergence factors for complexes **1** and **2**

Parameter	Value	
	<b>1</b>	<b>2</b>
Formula	C <sub>108</sub> H <sub>212</sub> N <sub>4</sub> Ni <sub>4</sub> O <sub>36</sub>	C <sub>38</sub> H <sub>52</sub> N <sub>6</sub> NiO <sub>12</sub>
<i>F</i> <sub>w</sub> /g mol <sup>-1</sup>	2377.64	843.56
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> $\bar{1}$
<i>a</i> /Å	17.577(2)	8.3952(8)
<i>b</i> /Å	16.870(2)	14.9092(14)
<i>c</i> /Å	68.454(9)	17.2804(16)
$\alpha$ /°	90	98.553(3)
$\beta$ /°	109.189(2)	102.966(3)
$\gamma$ /°	90	91.670(3)
<i>V</i> /Å <sup>3</sup>	19171(4)	2079.9(3)
<i>D</i> <sub>calc</sub> /g cm <sup>-3</sup>	1.236	1.347
$\mu$ /mm <sup>-1</sup>	0.654	0.533
$\theta$ range/°	1.36–26.00	1.99–26.43
No. of collected reffs	169908	28088
No. of independent reffs	33389	8492
<i>R</i> <sub>int</sub>	0.068	0.092
GooF	1.133	1.068
<i>R</i> <sub>1</sub> ( <i>I</i> > 2 $\sigma$ ( <i>I</i> ))	0.1065	0.0749
<i>wR</i> <sub>2</sub> (all data)	0.2426	0.1501
Residual electron density (min/max)/e Å <sup>-3</sup>	–1.175/2.022	–0.872/1.215

The powder patterns of compound **2** and thermolysis product were measured on Bruker D8 Advance ( $\lambda(\text{CuK}\alpha) = 1.54060 \text{ \AA}$ ) diffractometer (Bruker AXS, Madison, WI, USA) using LynxEye detector in Bragg–Brentano geometry, with the sample dispersed thinly on zero-background Si sample holder ( $\theta/\theta$  scan with variable slits (beam length 20 mm) from 3° to 50°  $2\theta$  (**2**) and 3° to 80°  $2\theta$  (thermolysis product), stepsize of 0.020°). The experimental diffraction patterns were processed using the TOPAS software (Version 4.2. Karlsruhe: Bruker AXS, 2009), using single-crystal structures.

[(Hexa(aqua- $\kappa\text{O}$ )bis( $\mu_3$ -hydroxo)-tetra( $\mu$ -benzylmalonato- $\kappa^2\text{O},\text{O}'$ )tetrnickel(II))-tetrakis(tetrabutylammonium)diacetate octahydrate ((NBu<sub>4</sub>)<sub>4</sub>[Ni<sub>4</sub>( $\mu_3$ -OH)<sub>2</sub>( $\mu$ -Bzmal- $\kappa^2\text{O},\text{O}'$ )<sub>4</sub>(H<sub>2</sub>O- $\kappa\text{O}$ )<sub>6</sub>(OAc)<sub>2</sub>·8H<sub>2</sub>O, C<sub>108</sub>H<sub>212</sub>N<sub>4</sub>Ni<sub>4</sub>O<sub>36</sub>, **1**) Benzylmalonic acid (0.312 g, 1.608 mmol) was dissolved in ethanol (30 cm<sup>3</sup>), and 40% aqueous solution of tetrabutylammonium hydroxide was added (2.082 g of solution, 3.216 mmol). Then nickel(II) acetate (0.200 g, 0.803 mmol) was added to the reaction mixture. As a result, a pale green suspension was formed, which was stirred with heating (70 °C) for 30 min. The suspension was cooled to room temperature and filtered, with the filtrate placed in a Schlenk flask and concentrated to one-third. A week later, another half of the

solvent evaporated. One week later, crystallization of green crystals suitable for X-ray diffraction analysis was observed. The crystals were isolated and dried in air at room temperature, with the yield being 0.011 g (23% based on nickel(II) acetate). IR (ATR):  $\nu = 3679 \text{ w}, 2961 \text{ m}, 2940 \text{ m}, 2875 \text{ m}, 1598 \text{ s}, 1488 \text{ m}, 1468 \text{ m}, 1454 \text{ m}, 1401 \text{ s}, 1349 \text{ m}, 1310 \text{ m}, 1268 \text{ w}, 1200 \text{ w}, 1175 \text{ w}, 1107 \text{ w}, 1068 \text{ w}, 1031 \text{ w}, 1009 \text{ w}, 977 \text{ w}, 930 \text{ w}, 895 \text{ m}, 855 \text{ m}, 839 \text{ m}, 742 \text{ m}, 725 \text{ m}, 699 \text{ m}, 641 \text{ m}, 624 \text{ m}, 598 \text{ m}, 550 \text{ m}, 484 \text{ w}, 440 \text{ w}, 415 \text{ w}, 405 \text{ w} \text{ cm}^{-1}$  (w = weak, m = medium, s = strong).

[Bis(benzylmalonato- $\kappa^2\text{O},\text{O}'$ )bis((4-(ammoniummethyl)pyridine)- $\kappa\text{O}$ )] nickel(II) dihydrate *N,N'*-dimethylformamide disolvate ([Ni(Bzmal- $\kappa^2\text{O},\text{O}'$ )<sub>2</sub>(4-ampyH- $\kappa\text{O}$ )<sub>2</sub>·2H<sub>2</sub>O·2DMF, C<sub>38</sub>H<sub>52</sub>N<sub>6</sub>NiO<sub>12</sub>, **2**) A solution of nickel(II) perchlorate (0.030 g, 0.082 mmol) and benzylmalonic acid (0.064 g, 0.328 mmol) in 5 cm<sup>3</sup> of water was placed at the bottom of a test tube. Then a layer of a MeOH–H<sub>2</sub>O mixture (1:1, 3 cm<sup>3</sup>) was slowly added on top. A solution of 4-(aminomethyl)pyridine (4-ampy) (0.032 cm<sup>3</sup>, 0.328 mmol) in 5 cm<sup>3</sup> of MeOH was slowly added as a third layer and the test tube was closed. Two months later, crystallization of blue crystals suitable for X-ray diffraction analysis was observed. The crystals were isolated and dried in air at room temperature, with the yield being 0.045 g (65% based on nickel(II) perchlorate). IR (ATR):  $\nu = 3618 \text{ w}, 3056 \text{ w}, 3029 \text{ w}, 2932 \text{ w}, 2758 \text{ w}, 2646 \text{ w}, 2160 \text{ w}, 1989 \text{ w}, 1672 \text{ m}, 1651 \text{ m}, 1633 \text{ m}, 1593 \text{ s}, 1577 \text{ s}, 1497 \text{ m}, 1455 \text{ m}, 1409 \text{ s}, 1389 \text{ s}, 1341 \text{ m}, 1316 \text{ m}, 1267 \text{ m}, 1227 \text{ m}, 1213 \text{ m}, 1171 \text{ m}, 1103 \text{ m}, 1070 \text{ m}, 1021 \text{ m}, 1000 \text{ m}, 956 \text{ m}, 911 \text{ m}, 863 \text{ m}, 840 \text{ m}, 801 \text{ m}, 758 \text{ m}, 727 \text{ m}, 702 \text{ s}, 665 \text{ s}, 625 \text{ m}, 594 \text{ s} \text{ cm}^{-1}$  (w = weak, m = medium, s = strong).

**Supplementary Information** The online version contains supplementary material available at <https://doi.org/10.1007/s00706-023-03114-y>.

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