Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

(ESI)

An octanuclear Schiff-base complex with the Na_2Ni_6 core: structure, magnetism and DFT calculations

Marek Machata, Ivan Nemec, Radovan Herchel, Zdeněk Trávníček*

Department of Inorganic Chemistry, Regional Centre of Advanced Technologies and Materials, Faculty of Science, Palacký University, 17. listopadu 12, CZ-771 46 Olomouc, Czech Republic.

Table S1 Crystal data and structure refinement parameters for compound **1.**

Formula	$C_{110}H_{107}N_5Na_2Ni_6O_{24}$
M (g·mol^{-1})	2281.19
Crystal system	Monoclinic
Space group	$P2_1/c$
λ (Å)	0.71073
a (Å)	17.9459(5)
b (Å)	27.5058(6)
c (Å)	26.7230(7)
α (°)	90.000
β (°)	126.788(12)
γ (°)	90.000
V (Å^3)	10564.0(14)
Z	4
T (K)	150(2)
ρ_{calcd} (g·cm^{-3})	1.434
μ (mm^{-1})	1.131
Data/restraints/ parameters	18415/9/1297
$R_1{}^a$ [I > 2σ(I)]/R_1 (all)	0.0622/0.1244
$wR_2{}^b$ [I > 2σ(I)]/wR_2 (all)	0.1629/0.1802
Goodness-of-fit	0.938
largest peak and hole (e Å^{-3})	1.324 and -0.687
CCDC number	1530435

Table S2 The metal-ligand bond distances (in Å), the Ni–O–Ni bridging angles (in °) and values of angular distortion parameters Σ^i (in °) for Ni^{II} atoms in **1**.

Ni1–O1	2.075(4)	Ni4–O2	2.026(4)	Na1–O1	2.303(4)	Ni2–O5–Ni3	90.70(13)
Ni1–O2	1.993(4)	Ni4–O4	2.050(4)	Na1–O3	3.040(4)	Ni2–O8–Ni3	91.18(13)
Ni1–O3	2.035(4)	Ni4–O7	2.086(4)	Na1–O10	3.004(4)	Ni2–O8–Ni5	102.22(15)
Ni1–O5	2.071(3)	Ni4–O9	1.983(4)	Na1–O16	2.334(5)	Ni2–O10–Ni5	104.97(15)
Ni1–O9	2.059(3)	Ni4–O11	2.167(4)	Na1–O22	2.256(5)	Ni2–O6–Ni6	98.98(15)
Ni1–N1	1.996(4)	Ni4–O12	2.107(4)	Na1–O23	2.260(5)	Ni2–O10–Ni6	101.84(15)
Ni2–O1	2.080(4)	Ni5–O8	2.091(3)	Na2–O9	2.987(4)	Ni3–O7–Ni4	100.52(17)
Ni2–O5	2.193(3)	Ni5–O10	2.038(3)	Na2–O12	2.369(4)	Ni3–O9–Ni4	102.06(16)
Ni2–O6	2.028(4)	Ni5–O13	2.064(4)	Na2–O13	2.308(4)	Ni3–O8–Ni5	90.91(13)
Ni2–O8	2.074(4)	Ni5–O14	2.006(4)	Na2–O18	2.777(4)	Ni3–O13–Ni5	94.92(15)
Ni2–O10	2.050(3)	Ni5–O18	2.046(4)	Na2–O20	2.319(5)	Ni5–O10–Ni6	93.85(14)
Ni2–N2	2.010(5)	Ni5–N4	2.002(5)	Na2–O21	2.279(4)	Ni5–O14-Ni6	93.53(14)
Ni3–O5	2.076(3)	Ni6–O6	2.093(4)	Ni1–O1–Ni2	94.43(15)	Σ(Ni1)	63.84
Ni3–O7	2.026(4)	Ni6–O10	1.986(3)	Ni1–O5–Ni2	91.29(13)	Σ(Ni2)	119.43
Ni3–O8	2.178(4)	Ni6–O14	2.029(4)	Ni1–O5–Ni3	102.40(15)	Σ(Ni3)	119.55
Ni3–O9	2.083(4)	Ni6–O15	2.092(4)	Ni1–O9–Ni3	102.56(15)	Σ(Ni4)	110.10
Ni3–O13	2.067(3)	Ni6–O16	2.133(4)	Ni1–O2–Ni4	93.91(15)	Σ(Ni5)	78.35
Ni3–N3	2.026(5)	Ni6–O17	2.063(4)	Ni1–O9–Ni4	93.18(14)	Σ(Ni6)	96.98

[i] The octahedral distortion calculated from 12 *cis* angles found in the coordination polyhedron.

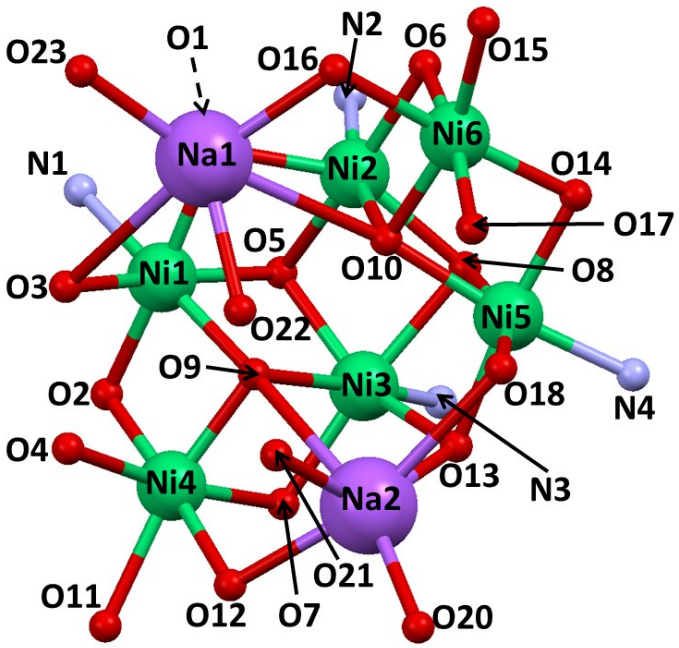

Fig. S1 The figure of the Na_2Ni_6 core showing all the donor atoms in **1**. The remaining atoms are omitted for clarity.

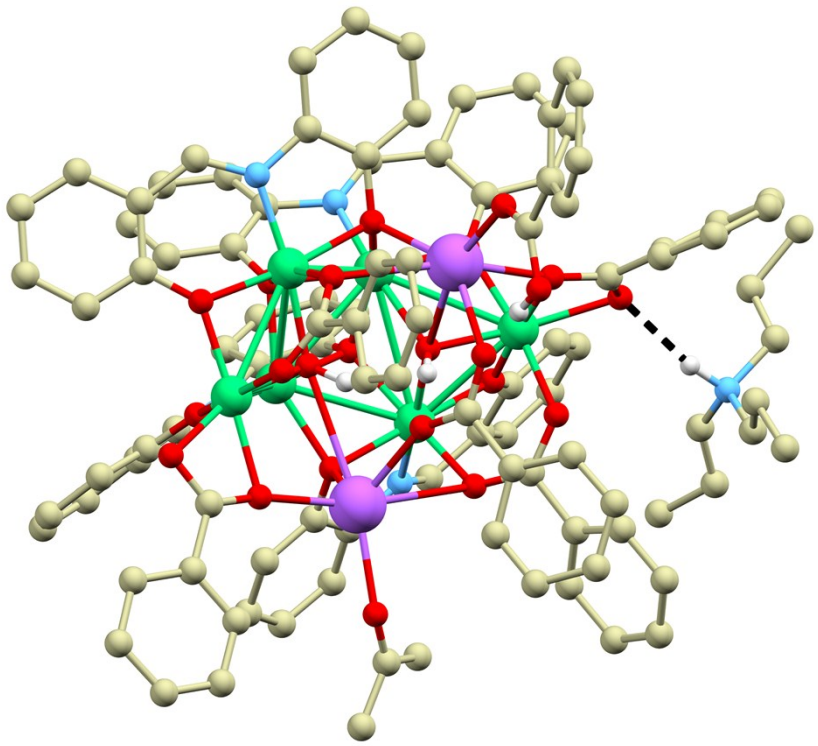

Fig. S2 Picture showing the N-H···O hydrogen bond (black dashed line) between the tripropylamonium cation and complex anion in **1**. The hydrogen atoms not involved into non-covalent interactions are omitted for clarity.