Journal of Molecular Structure 1127 (2017) 266–274

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: http://www.elsevier.com/locate/molstruc

Crystal structure, vibrational and magnetic properties of the monohydrated cobalt (II) complex with 1-(4-Nitrophenyl)-1H-imidazolium cation, $(C_9H_8N_3O_2)_2CoCl_4 \cdot H_2O$

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ARTICLE INFO

Article history:
Received 11 May 2016
Received in revised form
27 July 2016
Accepted 28 July 2016
Available online 30 July 2016

Keywords:
X-ray diffraction
Crystal structure
Cobalt (II) complex
Vibrational studies
Thermal analysis
Magnetic properties

ABSTRACT

Single crystals of organic-inorganic hybrid compound Bis(1-(4-Nitrophenyl)-1H-imidazolium) tetrachlorocobaltate monohydrate, was obtained by slow evaporation of an aqueous solution at room temperature and characterized by a single-crystal X-ray diffraction, an elemental and thermal analysis, UV−Vis spectra, FT-IR and FT-Raman spectroscopies as well as magnetic measurements. The entitled compound crystallizes into triclinic system of P-1 space group. The Co(II) ion of the $[CoCl_4]^{2-}$ anion shows a tetrahedral coordinating geometry. The atomic arrangement can be described as an alternation of organic and inorganic layers along the c-axis. The different components are connected by N–H···Cl, O–H···Cl and O–H···O hydrogen bonds. The differential scanning calorimetry (DSC) of the title compound revealed an endothermic peak at 52 °C related with a phase transformation caused by a slight deformation of the inorganic group. The room temperature IR and Raman spectra were recorded and analyzed on the basis of literary data to gain more information about the entitled compound. The magnetic susceptibility measurements in the temperature range 2–100 K shows that the complex displays a weak antiferromagnetic exchange interaction at very low temperatures.

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1. Introduction

A great deal of interest has arisen in the synthesis of hybrid materials as a result of their special functional properties such as ferroelectric transitions, conductivity, optical, catalytic and magnetic properties [1–5]. Quite recently, have been many research papers reporting the growth, their properties and the structural studies of novel compounds with various divalent metals such as Cd, Mn, Zn, Cu and Co in order to allow a rational application of such materials, a good characterization and an understanding of the supramolecular desired [6–10]. Furthermore, the various families of inorganic–organic hybrid are of considerable interest due to their catching characteristics and their potential applications as insulators in the electronics industry. When deposited in thin film form, this class of materials enables the fabrication of a wide variety of low-cost electronic and optoelectronic devices [11–16]. These include light emitting diodes, solar cells, photodetectors, field-effect transistors as well as chemical and biological sensors [17–19]. The structural topology of the hybrid compounds can be tuned by careful selection of the anions and the organic cation, and some weak interactions such as directional hydrogen bonds, D-H···X (X = Cl, Br, I; and D = N, O etc.) and C–H···π or π···π interactions. These interactions also often play an important role in the construction of these molecular materials. The structures of organic cation play an important role in determining the final structures and topologies [20]. Taking the above into consideration, we are interested in understanding the role played by the organic groups because they not only control distance between the layers, but are actively involved in the hydrogen bonding, whose importance is ambiguous [21–23]. In this paper the 1-(4-Nitrophenyl)-1H-imidazole cation are used in view of these following characteristics: (1) they possess extended aromatic system, which provide supramolecular interactions such as π–π interactions between the aryl rings to construct intriguing structures; (2) they possess rigidity of coordination to metal atoms; (3) they have strong coordination with two nitrogen atoms.

Considering the attractive properties and the attributes of the

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http://dx.doi.org/10.1016/j.molstruc.2016.07.111
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Cobalt (II) complex and the new promising opportunities they may open with regard to the development of the useful organic–inorganic hybrid materials, the present study reports on the synthesis and structural characterization of the $(C_9H_8N_3O_2)_2CoCl_4\cdot H_2O$ compound by X-ray diffraction, UV–vis spectra, thermal analysis (TGA/DSC). In addition, a vibrational study and magnetic properties of the entitled compound was investigated and discussed.

2. Experimental

2.1. Materials and physical measurements

Differential scanning calorimetry (DSC) runs were recorded using a DSC 822P METTLER TOLEDO in the temperature range 25–200 °C at a heating rate of 10 °C min^{-1}. Thermogravimetric analysis (TGA) was carried out with an ATG PYRIS 6 instrument at the temperature range from 30 to 250 °C. The UV–vis absorption (DMF solution) was measured at room temperature with a PerkinElmer Lambda 900 UV-VIS-NIR spectrometer in the range of 200–500 nm. As for the Raman spectra, they were recorded on a HORIBA JOBIN–YVON (T64000) spectrometer in the region 50–3500 cm^{-1}. The Raman Measurements on heating from 30 to 60 °C have been carried out under a microscope in a furnace. The heating rate is 10 °C/min, waiting time after stabilization of temperature is 1 min and the collecting time for each spectrum is 320 s (The temperatures in the 30–60 °C intervals were monitored by a Linkam TP 94 hot stage controller). The spectra slit widths were set to maintain a resolution of approximately 2 cm^{-1}. The excitation light was 514 nm line of He–Ne (20 mV) ion laser. The IR spectrum (KBr pellets) was obtained with a Nicolet Impact 410 spectrometer in the 400–4000 cm^{-1} range. Magnetic measurements were

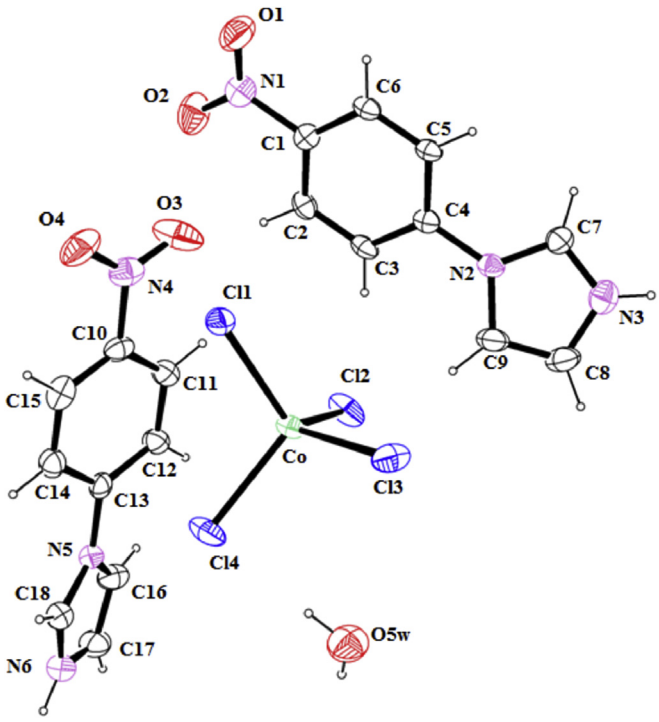

Fig. 1. ORTEP drawing of the asymmetric unit of $(C_9H_8N_3O_2)_2CoCl_4\cdot H_2O$.

Table 1
Crystal data and summary of intensity data collection and structure refinement.

Crystal data	
Empirical formula	$C_{18}H_{18}N_6O_5CoCl_4$
Formula weight (g/mol)	599.11
Crystal system,	Triclinic
Space group	P-1
a (Å)	7.9630(10)
b (Å)	10.5000(9)
c (Å)	14.9510(6)
α	91.609(5)
β	102.997(6)
γ	90.809(10)
v (Å^3)	1217.30(19)
Z	2
D_{calc} (g.cm^{-3})	1.635
Absorption coefficient (mm^{-1})	0.615
F(000)	606
Crystal size (mm) Crystal habit	0.3 × 0.18 × 0.12
Data collection	
Diffractometer	Bruker Apex II Kappa CCD diffractometer
Monochromator	Graphite
Radiation type, λ (Å)	Ag-*Kα*, 0.5608 Å
T (K)	293(2)
Θ Range (°)	2.602–25.00
Indexes range	$-9 \le h \le 9$
	$-12 \le k \le 12$
	$-16 \le l \le 17$
Measured reflections	7947
Independent reflections	3905
Observed refl. ($I > 2\sigma(I)$)	2634
Rint	0.053
Refinement	
Refinement on	F^2
Data/rastraints/parameters	3905/3/313
$R(F0^2) > 2\sigma(F0^2)]$	R1 = 0,059
	wR = 0.12
GooF = *S*	1.06
Δρmax/Δρmin (e Å^{-3})	0.845/−0.372
CCDC	1,450,995

Table 2
Atomic coordinates and Ueq for $(C_9H_8N_3O_2)_2CoCl_4\cdot H_2O$.

	x	y	z	Ueq
Co	−0.13,479 (9)	0.25,659 (7)	0.77,237 (5)	0.0474 (2)
Cl1	−0.19,776 (19)	0.04854 (13)	0.78,413 (10)	0.0611 (4)
Cl2	0.08286 (19)	0.29,522 (18)	0.70,174 (10)	0.0770 (5)
Cl3	−0.37,205 (19)	0.35,679 (15)	0.69,241 (12)	0.0749 (5)
Cl4	−0.0578 (2)	0.34,604 (17)	0.91,753 (11)	0.0825 (5)
C1	0.3207 (6)	−0.1394 (5)	0.5711 (4)	0.0510 (13)
C2	0.1992 (6)	−0.1364 (5)	0.4909 (3)	0.0506 (13)
C3	0.1603 (6)	−0.0223 (5)	0.4499 (3)	0.0468 (13)
C4	0.2449 (6)	0.0874 (5)	0.4921 (3)	0.0474 (13)
C5	0.3698 (6)	0.0816 (6)	0.5733 (4)	0.0550 (14)
C6	0.4074 (6)	−0.0329 (6)	0.6138 (4)	0.0557 (14)
C7	0.1486 (7)	0.2229 (6)	0.3594 (4)	0.0629 (15)
C8	0.1796 (10)	0.4105 (6)	0.4284 (6)	0.084 (2)
C9	0.2248 (9)	0.3247 (6)	0.4929 (5)	0.079 (2)
C10	0.2762 (7)	0.0303 (5)	0.9074 (4)	0.0595 (15)
C11	0.3822 (7)	0.1103 (5)	0.8732 (4)	0.0621 (15)
C12	0.4599 (7)	0.2116 (5)	0.9270 (4)	0.0594 (15)
C13	0.4291 (6)	0.2308 (5)	1.0133 (4)	0.0502 (13)
C14	0.3263 (7)	0.1495 (6)	1.0478 (4)	0.0640 (16)
C15	0.2479 (7)	0.0480 (6)	0.9945 (5)	0.0688 (17)
C16	0.6619 (8)	0.4017 (6)	1.0644 (5)	0.0712 (17)
C17	0.6948 (10)	0.4936 (7)	1.1276 (5)	0.085 (2)
C18	0.4538 (10)	0.3962 (7)	1.1375 (5)	0.080 (2)
N1	0.3620 (7)	−0.2638 (6)	0.6154 (4)	0.0746 (15)
N2	0.2061 (5)	0.2077 (4)	0.4496 (3)	0.0521 (11)
N3	0.1319 (7)	0.3460 (6)	0.3463 (4)	0.0822 (16)
N4	0.1944 (7)	−0.0818 (5)	0.8520 (5)	0.0763 (15)
N5	0.5124 (6)	0.3382 (4)	1.0699 (3)	0.0584 (12)
N6	0.5626 (11)	0.4876 (6)	1.1729 (4)	0.106 (2)
O1	0.2666 (8)	−0.3545 (5)	0.5862 (4)	0.1119 (19)
O2	0.4877 (7)	−0.2675 (5)	0.6790 (4)	0.1111 (19)
O3	0.2165 (7)	−0.0953 (6)	0.7749 (5)	0.126 (2)
O4	0.1107 (7)	−0.1553 (5)	0.8858 (4)	0.1106 (19)
O5	−0.0861 (7)	0.6163 (5)	0.8388 (4)	0.1086 (17)

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