Available online at http://www.journalcra.com

International Journal of Current Research
Vol. 9, Issue, 09, pp.57931-57934, September, 2017

INTERNATIONAL JOURNAL OF CURRENT RESEARCH

ISSN: 0975-833X

RESEARCH ARTICLE

SYNTHESIS AND STRUCTURAL ANALYSIS OF THE CYSTAL TRANS-DIAQUATETRAKIS (IMIDAZOLE) NICKEL (II) DIBROMIDE

[1]Sivaranjani, T., [*,1]Sakthimurugesan, K., [2]Thirumurugan, S., [2]Anbalagan, K. and [3]Ganesh Raja, A.S.

[1]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India,
[2]Department of Chemistry, Pondicherry University, Pondicherry 605 014, India,
[3]Mossbauer Effect Data Center, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

ARTICLE INFO

Article History:
Received 20th June, 2017
Received in revised form
14th July, 2017
Accepted 22nd August, 2017
Published online 30th September, 2017

Key words:

Structure analysis,
Imidazole,
Hydrogen bonding,
Ortep,
Packing diagram.

ABSTRACT

The crystal structure of the title compound, (C_{12} H_{16} N_8 Ni O_2, 2(Br) is shown below. The cation Ni(II) ion sits on an inversion centre and is octahedrally coordinated by four imidazole rings. The compound contains a six-coordinate Ni(II) ion lying on an Inversion center, which is bonded to four imidazole N atoms and two O atoms. Intermolecular hydrogen-bonding interactions are present, linking the nickel complex cations and bromide anions in the crystal structure. A two-dimensional perpendicular network is formed via N2-Br1, N4-Br1 intermolecular hydrogen bonds. The imidazole ring systems are inclined to one another with dihedral angles varying between 81.2 (4) and 170.9 (4). In the crystal, molecules are linked via N-H-Br hydrogen bonds involving one Ni(II)cation and the Oxygen atom in the equatorial plane, forming an inversiondimer-like arrangement.

Citation: Sivaranjani, T., Sakthimurugesan, K., Thirumurugan, S., Anbalagan, K. and Ganesh Raja, A.S., 2017. "Synthesis and structural analysis of the cystal trans-diaquatetrakis (Imidazole) Nickel(ii) dibromide", *International Journal of Current Research*, 9, (09), 57931-57934

INTRODUCTION

Synthesis of imidazole derivatives has attracted great interest in recent years due to their broad spectrum of biological activities (Gaonkar *et al.*, 2009). In addition, imidazole-containing compounds exhibit a wide spectrum of pharmaceutical properties such as pesticides, fungicides, antibacterial, anti-inflammatory, anti-tubercular, anti-diabetic, antimalarial and antitumour (Roman *et al.*, 2007; Nanterment *et al.*, 2004; Congiu *et al.*, 2008; Venkatesan*et al.*, 2008; Bhatnagar*et al.*, 2011; Puratchikody & Doble 2007). The chemistry of imidazole occupies an extremely important position within the family of five-membered heterocyclic compounds. This paper describes the synthesis and crystal structure of the nickel(II) complex of the imidazole ligand Diaquatetrakis-1H-imidazole.

Corresponding author: **Tufail Ahmad,**
Registrar, Department of Anaesthesiology and Critical care, GMC Srinagar Kashmir, India

MATERIALS AND METHODS

MATERIALS

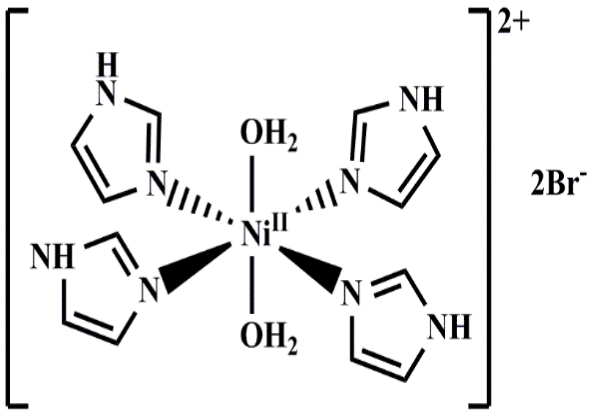
$NiBr_2.3H_2O$, ethanol, imidazole

METHOD (EXPERIMENTAL)

$NiBr_2.3H_2O$ (2.0 g) was dissolved in ethanol (10 ml). The solution was kept in ice and added slowly the solution of imidazole (2.0 g in 10 ml EtOH) with stirring. The reaction mixture was stirred 3 hours and filtered the solution.

Then initiate the crystallization, the cold ethanol(5 ml) was added to the above solution. To obtain blue crystalline solid crystals, the solution was washed with 10 ml of ethanol under suitable refrigeration condition and dried over in air for one hour.

Structure of the crystal



Data Collection

Bruker SMART APEXII CCD diffractometer, Radiation source: fine-focus sealed tube, Graphite monochromatorω and φ scans, Absorption correction: multi-scan (*SADABS*; Bruker, 2008), *T*min = 0.964, *T*max = 0.979

Computer Programs

APEX2, SAINT and XPREP (Bruker, 2004), SHELXS97 and SHELXL97 (Sheldrick, 2008), ORTEP-3 for Windows (Farrugia, 1997) and PLATON
(Spek, 2009).

RESULTS

ORTEP

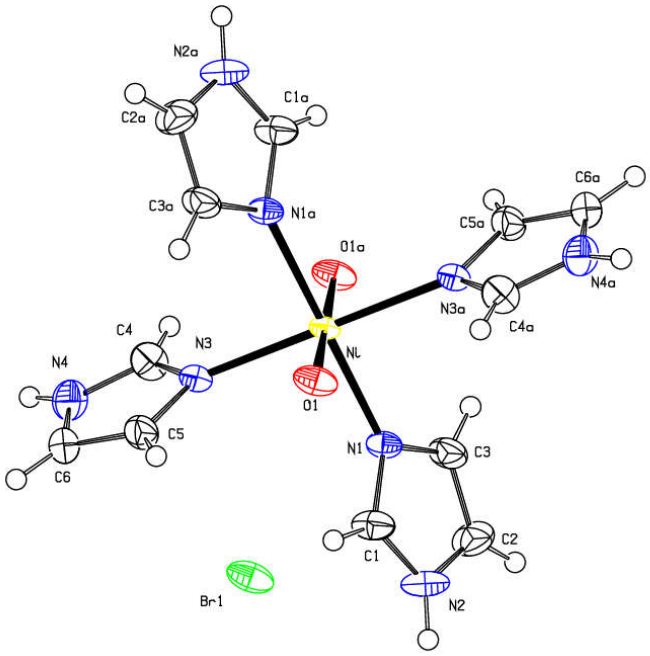


Figure 1. (ORTEP)

The molecular structure of the title compound, with the atomic numbering scheme and displacement ellipsoids drawn at 30% probability level.

Packing 1:

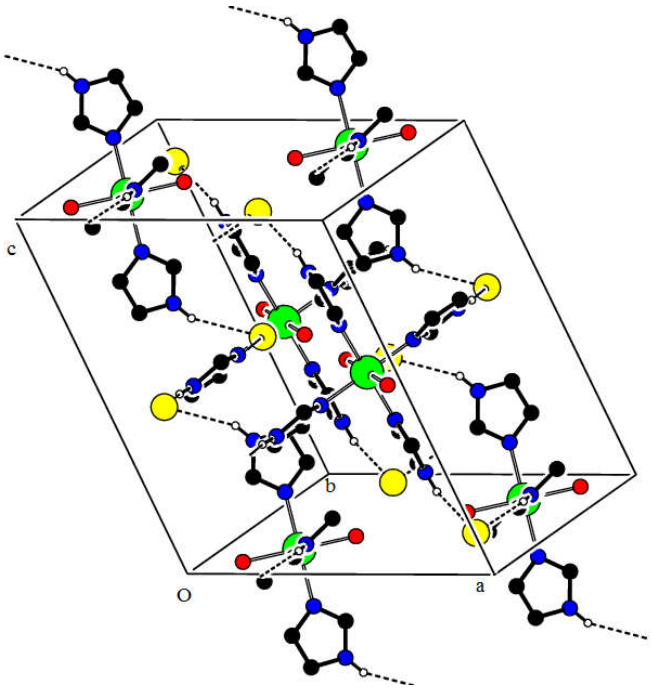


Figure 2.

A partial view of the crystal packing of the title compound is viewed like a chain along the(001)(see Table 2).

Packing 2:

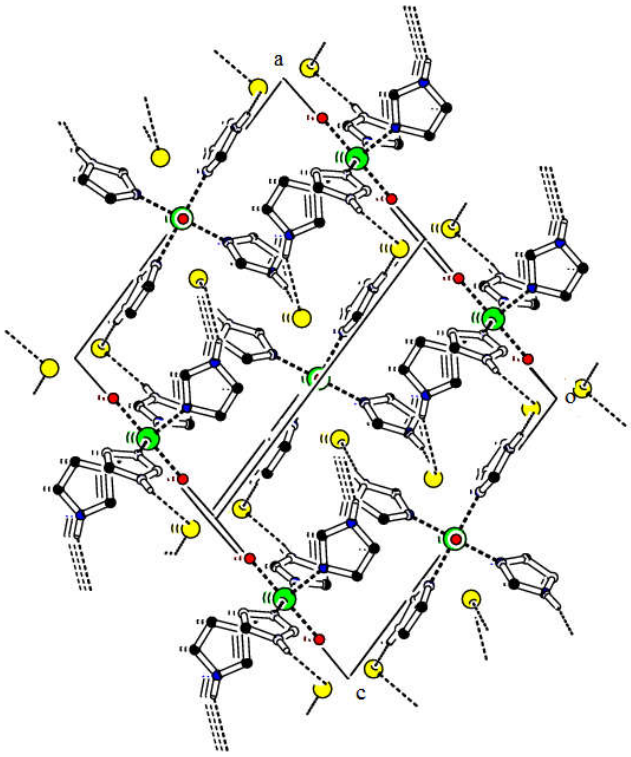


Figure 3.

A partial view of the crystal packing of the title compound is viewed in an expanded form along the(010), showing intramolecular N4—H…Br1 hydrogen bonds.

Table 1. Experimental details

Crystal data Chemical formula	C_{12} H_{16} N_8 Ni O_2, 2(Br)
Mr	522.86
Crystal system, space group	Monoclinic, c2/c
Temperature(K)	295(2)
a, b, c, (Å)	12.6295(15), 11.2390(11), 14.3124(18)
β(°)	109.324(13)
V(Å^3)	1917.1(4)
Z	4
Radiation type	Mo Kα
μ(mm^{-1})	0.11
Crystal size (mm)	0.70 x 0.65 x 0.50
Data collection Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (SADABS; Bruker, 2008)
Tmin, Tmax	0.1216, 0.1806
No. of measured, independent and observed [I > 2σ(I)] reflections	4600
Rint	0.0420
(sin θ/λ)max (A° $^{-1}$)	0.0472
Refinement R[F^2> 2σ(F^2)], wR(F^2), S	0.0354, 0.0872, 1.044
No. of reflections	1674
No. of parameters	116
No. of restraints	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρmax, Δρmin (e A ° $^{-3}$)	16, -0.16

Table :2
Hydrogen-bonding geometry (Å ,º) D-Donor, H-Hydrogen, A-Acceptor

D-H-A	D-H	H-A	D-A
N4-H4-Br1	0.86	2.68	3.400
N2-H2-Br1	0.86	2.61	3.485

Table 3:
Selected geometric parameters(Å,º)

Ni---O1	2.137
Ni---N1	2.078
Ni---N3	2.133
N1---Ni---O1A	89.67
N1A---Ni---O1	89.67
N3---Ni---O1	90.42
N3A---Ni---O1A	89.58

Packing 3:

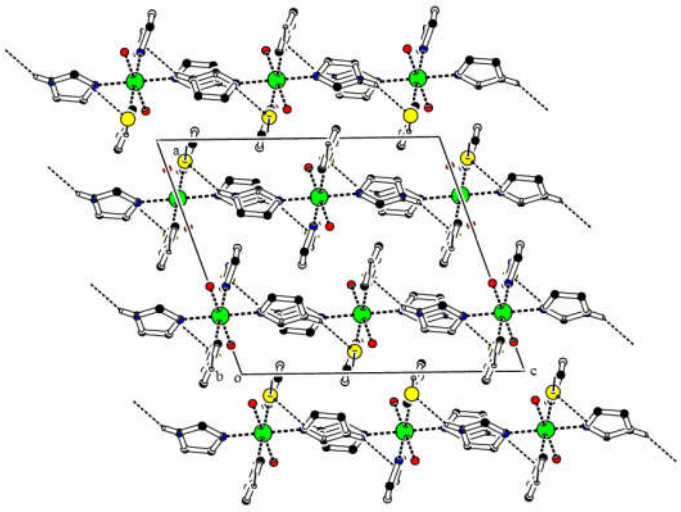


Figure 4.

The packing diagram shows the 2D-network structure on plane form of the Crystal packing. (011)

Packing 5:

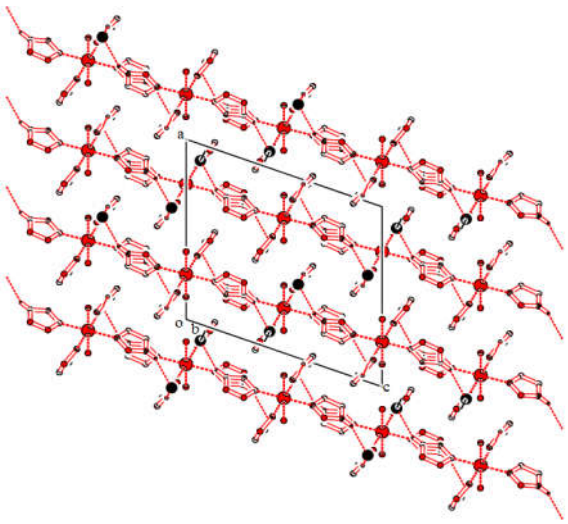


Figure 6.

The above figure shows the packing of intermolecular interactions along (011) In a plane with attractive colour.

DISCUSSION

The molecular structure of the title compound is illustrated in Fig. 1. From the structure the nickel (II) ion has a distorted tetrahedral coordination environment. It is surrounded by four N and two O atoms; an N1 and N1A atom are in the perpendicular positions, and the other (N2, N2A) are also in the perpendicular position. The oxygen atom (C1/N1/Ni–O1) makes dihedral angles of 29.9 (4)°, and 33.3 (4)° with the other oxygen atom (C1/N1/Ni–O1A). In the crystal, molecules are linked via N—H・・・Br hydrogen bonds, involving one Br- anion and the oxygen molecule (O2) in the equatorial plane, to form an inversion dimer-like arrangement. The Nitrogen in the axial position hydrogen-bonded to Br- anions. There are a number of N—H・・・Br interactions present forming a three dimensional structure. The atom Ni (II) lies on an inversion center and is octahedrally coordinated by four imidazole N atoms (N1, N3, N1A and N3A) and two O atoms in trans positions (O1 and O1A) (Fig. 1). For the mirror symmetry the Ni-N bond lengths, having similar values. This is apparently caused by many intermolecular interactions between H atoms of the coordinated imidazole and oxygen atoms with the bromide ions. The hydrogen-bonding interactions are weak (Steed& Atwood, 2000), based on H--A distances of 2.61±2.68 Å, D--A distances of 3.400 (3)±3.485 (4) Å. In the packing diagram two various Imidazole rings are linked via Br atom with the Nitrogen atoms. The packing diagram (Fig. 2) gives two molecules center linked chain like structure.

REFERENCES

Bhatnagar, A., Sharma, P. K. and Kumar, N. 2011. Int. J. Pharm. Tech. Res. 3, 268-282.

Bruker, 2004. APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.

Gaonkar, S. L., Rai, K. M. L. and Shetty, N. S. 2009. Med. Chem. Res. 18, 221– 230.

Kannan, P. S., Ganeshraja, A. S., Rajkumar, K., Anbalagan, K. and Subbiah Pandi, A. 2013. *ActaCryst*. E69, m498–m499.

Nanterment, P. G., Barrow, J. C., Lindsley, S. R., Young, M., Mao, S., Carroll, S., Bailey, C., Bosserman, M., Colussi, D., McMasters, D.R., Vacca, J. P. and Selnick, H. G. 2004. Bioorg. Med. Chem. Lett. 14, 2141–2145.

Puratchikody, A. and Doble, M. 2007. Bioorg. Med. Chem. Lett. 15, 1083–1090.

Roman, G., Riley, J. G., Vlahakis, J. Z., Kinobe, R. T., Brien, J. F., Nakatsu, K. and Szarek, W. A. 2007. Bioorg. Med. Chem. 15, 3225–3234.

Sheldrick, G. M. 2008. ActaCryst. A64, 112–122.

Shiu, K-B., Yen, C-H., Liao, F-L., Wang, S-L. 2003. *Acta Cryst*. E59, m1189 - m1191

Spek, A. L. 2009. ActaCryst. D65, 148–155.

Venkatesan, A. M., Agarwal, A., Abe, T., Ushirogochi, H. O., Santos, D., Li, Z., Francisco, G., Lin, Y. I., Peterson, P. J., Yang, Y.,Weiss,W. J., Shales, D. M. and Mansour, T. S. (2008). *Bioorg. Med. Chem.* 16, 1890–1902.

****