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Crystal structure analysis of dichloridobis(2-Isopropylimidazole)Zinc(II)

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Abstract: The Crystal structure of dichloridobis(2-Isopropylimidazole)Zinc(II)[Zn(2-Isopropylimdazole)$_2$Cl$_2$]. The structure of title compound, [$C_{12}H_{20}Cl_2N4Zn$], Consists of centrosymmetric monomeric units, in which the Zn^{II} atom has a tetragonallydistorded coordination involving two imidazole N atoms and two Cl atoms in the square plane [Zn-N = 1.998(1)Å and Zn-Cl = 2.2541(7)Å. The angles Cl-Zn-Cl and N-Zn-N are 110.34(4)° and 116.07(12)°, respectively. In the crystal there are no classical hydrogen bonds present.Crystal data were collected using CrysAlis CCD Oxford DiffractionX-ray diffractometer. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares procedures to the final R_1 of 0.0370usingSHELXL programs.

Key Words: Imidazole, Zinc(II) and crystal structure.

Introduction

Recently, we are interested in the synthesis, structures and thermal properties of coordination polymers based on zinc(II) halides and N-donor ligands[1], we have started systematic investigation of their thermal behavior becausewe have demonstrated that new ligand-deficient coordination polymers can be conveniently prepared by thermal decomposition of suitable ligand-rich precursur compounds[2,3]. We have found for example that most of the ligand rich compounds can be transformed into ligand deficient compounds on heating. Starting from these findings we have initiated systematic investigations on this topic. In these investigations we have reacted zinc(II) chloride with bis(2-Isopropylimidazole).

Experimental

X-ray Structure Determination

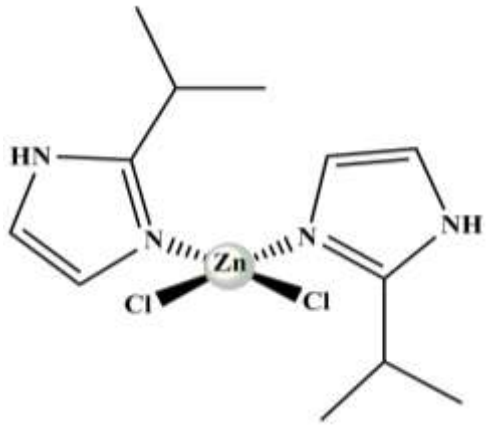
Single crystal of the compound suitable for x-ray diffraction was obtained by slow evaporationmethod. Three dimensional intensity data were collected on a CrysAlis CCD[4]Oxford diffraction Xcaliburdiffractometer with Eos detector using graphite monochromatized Mo-Kα radiation (λ= 0.71073 Å) at Department of chemistry, Department of Chemistry, Pondicherry University, Pondicherry 605 014, India. The structure was solved by direct methods and refined on F^2 by full-matrix least-squares procedures using the SHELXL programs[5]. All the non-hydrogen atoms were refined using isotropic and later anisotropic thermal parameters. The hydrogen atoms were included in the structure factor calculation at idealized positions by using a riding model, but not refined. Images were created with ORTEP-3[6].The crystallographic data for the compound are listed in Table 1.

Table 1: Crystal data and structure refinement of the titled compound

Compound	**Parameters**
Empirical formula	C12 H20 Cl2 N4 Zn
Formula weight	475.45
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic,Pbcn
Unit cell dimensions	a = 11.1856(3)Å alpha = 90°
	b = 11.3266(4)Å beta = 90°
Empirical formula	c = 13.0627(6)Å gamma = 90°
Volume	1654.98(11) A^3
Z, Calculated density	3, 1.431 Mg/m^3
Absorption coefficient	1.799 mm^[1]
F(000)	736
Crystal size	0.20 x 0.24 x 0.28 mm
Theta range for data collection	3.92 to 29.33°
Limiting indices	-14<=h<=14, -15<=k<=15, -16<=l<=16
Reflections collected / unique	10733 / 2056 [R(int) = 0.0372]
Completeness to theta = 29.33	90.80%
Max. and min. transmission	0.9655 and 0.9488
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2056 / 0 / 89
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	**R1 = 0.0349**, wR2 = 0.0897
R indices (all data)	R1 = 0.0658, wR2 = 0.1017
Extinction coefficient	0.0023(4)
Largest diff. peak and hole	0.544 and -0.316 $e.A^{-3}$

Synthesis of the compound

Zinc(II) complexes with organic ligands show typical electronic properties that potentially give great advantages in the field of catalysis. The interest is also increasing, owing to the relevance of these compounds in basic and applied research in various fields to chemistry, material science, life science, and so forth. Furthermore, from the materialsviewpoint, the metallic complexes can exhibit a full spectrum ofnew magnetic, optical, and redox properties. To an ethanol solution (30 mL) of 2-isopropyl imidazole (2 M) was added to an ethanol solution (10 mL) of $ZnCl_2$ (1 M) and the mixture was stirred for 5 hours at room temperature. The reactionmixture was stirred under a blanket of argon during which time a microcrystallinewhite solid precipitated from the solution.After repeated recrystallization the white solid was intensified into X-ray quality colorless crystals. The crystals were filtered, washed with cold ethanol, and dried in desiccators over $CaCl_2$. The scheme diagram is given below.



Results and Discussion

The symmetric unit of the title compound is shown in Fig. 1. The dihedral angle between the mean planes of the two imidazole five-membered rings is 47.7(18)°. For the ring comprising atoms N1/C1/C2/N2/C3, the out-of-plane distance are 0.201Å for Zn1, 2.298Å for Cl1 and 0.005Å for Cl2, with two Cl atoms on the same side of the mean plane. The two imidazole rings connected at Zn with the torsion angle C1-N1-Zn1-N1a of -137.24(17)° indicating a -Anti-clinalconformation for this group. Atoms C5 and C6 deviate from the imidazole ring which it is attached by -1.035Å and 1.412Å, respectively. In the crystal, molecule are linked by N---H…Cl hydrogen bonds, forming Zigzag and chains along c axis (Fig. 2). There are a number of π—π interactions present linking the ribbons andforming a three dimensional structure. The selected bond lengths and angles are listed in table 3 and 4, respectively.

Table 2: Hydrogen-bond geometry [Å]

Distance (Å)				Angle (º)
D—H…A	D—H	H…A	D…A	D—H…A
N2-H2A…Cl1	0.86	2.52	3.358(2)	166

Symmetry code: i) 1/2-x,-1/2+y,z

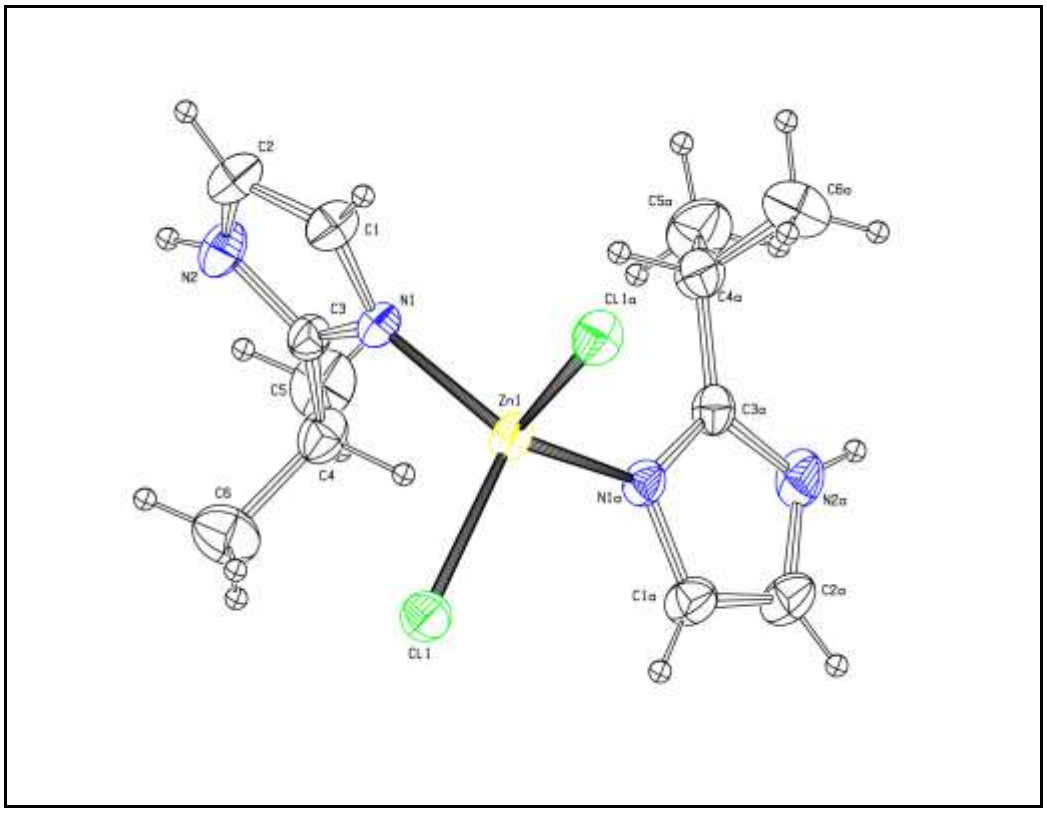


Fig.1.The molecular structure of the title compound, with the atom-numbering scheme. The displacement ellipsoids are drawn at 30% probability level. H atoms are shown as spheres of arbitrary radius.

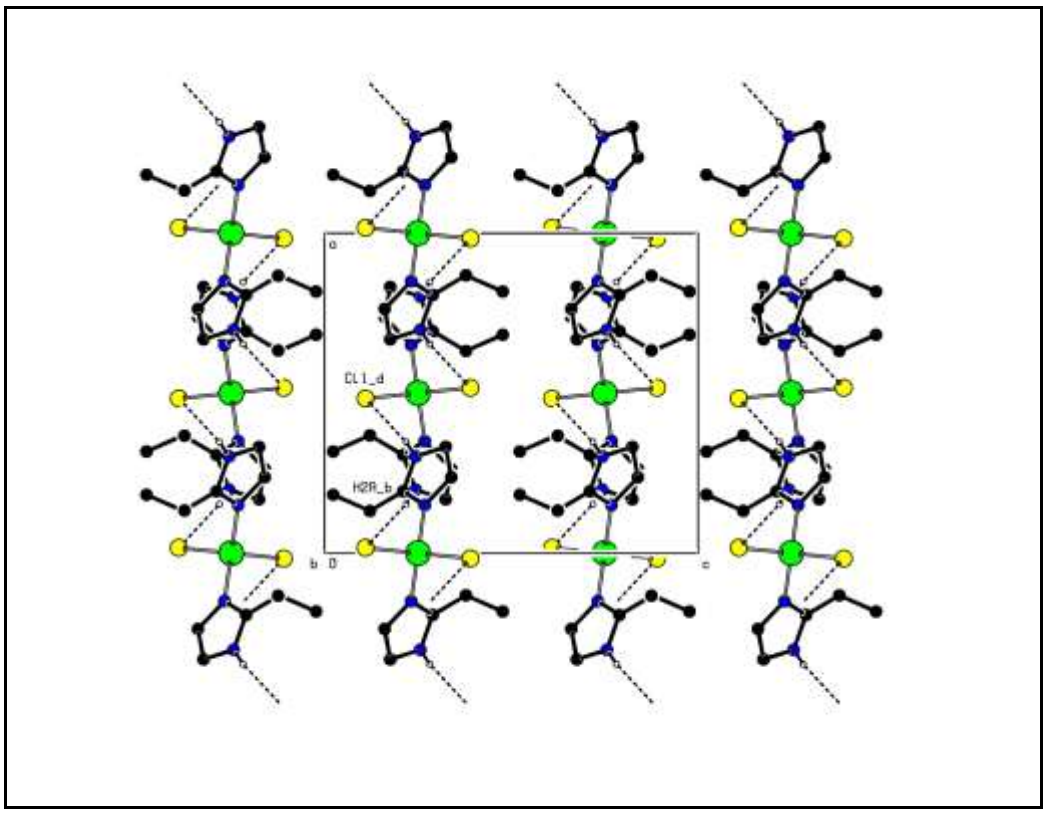


Fig.2. The crystal packing of the title compound, viewed along b axis, showing N2---H2A...Cl1 hydrogen bonds chains parallel to c axis. Hydrogen bond omitted clarity(see Table 2 for details).

Table 3: Selected Bond lengths (Å)Table 4: Selected Bond angles (º)

Bond	Length	Bond	Angle
C(1)-C(2)	1.339(3)	C(2)-C(1)-N(1)	109.3(2)
C(1)-N(1)	1.380(3)	C(2)-C(1)-H(1)	125.4
C(1)-H(1)	0.93	N(1)-C(1)-H(1)	125.4
C(2)-N(2)	1.361(3)	C(1)-C(2)-N(2)	105.5(2)
C(2)-H(2)	0.93	C(1)-C(2)-H(2)	127.2
C(3)-N(1)	1.323(3)	N(2)-C(2)-H(2)	127.2
C(3)-N(2)	1.333(3)	N(1)-C(3)-N(2)	108.8(2)
C(3)-C(4)	1.481(3)	N(1)-C(3)-C(4)	125.5(2)
C(4)-C(6)	1.511(4)	N(2)-C(3)-C(4)	125.7(2)
C(4)-C(5)	1.520(4)	C(3)-C(4)-C(6)	110.2(2)
C(4)-H(4)	0.98	C(3)-C(4)-C(5)	112.6(2)
C(5)-H(5A)	0.96	C(6)-C(4)-C(5)	112.7(2)
C(5)-H(5B)	0.96	C(3)-C(4)-H(4)	107
C(5)-H(5C)	0.96	C(6)-C(4)-H(4)	107
C(6)-H(6A)	0.96	C(5)-C(4)-H(4)	107
C(6)-H(6B)	0.96	C(4)-C(5)-H(5A)	109.5
C(6)-H(6C)	0.96	C(4)-C(5)-H(5B)	109.5
N(1)-Zn(1)	1.9967(18)	H(5A)-C(5)-H(5B)	109.5
N(2)-H(2A)	0.86	C(4)-C(5)-H(5C)	109.5
Zn(1)-N(1)#1	1.9968(18)	H(5A)-C(5)-H(5C)	109.5
Zn(1)-Cl(1)	2.2542(7)	H(5B)-C(5)-H(5C)	109.5
Zn(1)-Cl(1)#1	2.2542(7)	C(4)-C(6)-H(6A)	109.5

Conclusion

The crystal structure analysis of a novel dichloridobis(2-Isopropylimidazole)Zinc(II)compound was studied using x-ray diffraction method. In the crystal, molecule are linked by N---H…Cl hydrogen bonds, forming Zigzag and chains along c axis. There are a number of π—π interactions present linking the ribbons and forming a three dimensional structure.

Acknowledgments

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