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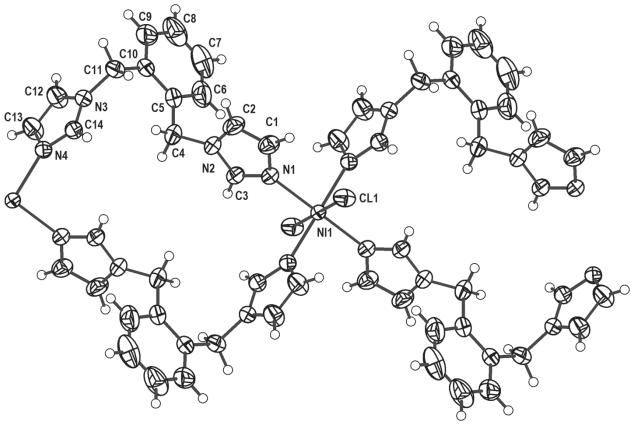
Crystal structure of *catena*-(bis(μ$_2$-1, 2-bis(imidazole-1-ylmethyl)benzene-κ*N:N′*)-dichlororido-nickel(II)), $C_{28}H_{28}C_{l2}N_8Ni$



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Abstract

$C_{28}H_{28}C_{l2}N_8Ni$, monoclinic, $P2_1/c$, $a = 8.521(5)$ Å, $b = 10.255(6))$ Å, $c = 15.414(9)$ Å, $\beta = 91.209(9)°$, $V = 1346.6(13)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0360$, $wR_{ref}(F^2) = 0.0916$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.32 × 0.28 × 0.27 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	9.5 cm^{-1}
Diffractometer, scan mode:	Bruker SMART, φ and ω
$2\theta_{max}$, completeness:	57.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8533, 3401, 0.027
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2786
$N(param)_{refined}$:	178
Programs:	Bruker programs [10, 11], SHELX [12], OLEX2 [13]

Source of material

A mixture of $NiCl_2{\cdot}6H_2O$ (0.024 g, 0.1 mmol), 1,2-bis (imidazole-1-ylmethyl)benzene (1, 2-BIB) (0.046 g, 0.2 mmol), and H_2O (10 mL) was stirred for about 30 min. The resulting solution was sealed in a Teflon-lined stainless autoclave and heated to 393 K for 3 days. The bottle was then rapidly cooled to ambient temperature. Green single crystals (about 76%, based on Ni input) were recovered by vacuum filtration and were dried in air.

Experimental details

The C-bound H atoms were placed at idealized positions (C—H = 0.95Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Discussion

The design and construction of metal-organic coordination polymers is of current interest, owing to their variety of potential applications [1, 2]. 1,2-Bis(imidazole-1-ylmethyl)benzene (1,2-BIB) is a very important nitrogen-containing heterocyclic ligand, and has been widely used in the synthesis of coordination polymers [3, 4]. Its two imidazolyl groups can rotate on the -(CH_2)- group to accommodate the coordination geometries of the central metal atoms in various connection mode. In the compounds reported previously, the ligand exhibits different conformations to coordinate metal centers. The results indicate that this ligand exhibits special ability to form compounds and plays an important role in determining the final molecular conformation. Our research group has reported a few coordination polymers constructed from bis(imidazolyl) ligands. The third order nonlinear optical properties of these compounds in films or in solutions were also discussed [5–7].

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.0000	1.0000	0.5000	0.02810(11)
Cl1	−0.17547(6)	1.06435(5)	0.37806(3)	0.04321(14)
N1	0.06376(19)	0.83528(15)	0.43302(10)	0.0365(4)
N3	0.32413(19)	0.22418(15)	0.35580(10)	0.0366(3)
N4	0.18288(17)	0.09890(15)	0.43864(10)	0.0340(3)
N2	0.1612(2)	0.64656(16)	0.39900(12)	0.0498(5)
C14	0.1810(2)	0.19045(18)	0.38008(12)	0.0355(4)
H14	0.0895	0.2281	0.3577	0.043*
C11	0.3681(3)	0.3210(2)	0.29157(13)	0.0456(5)
H11A	0.2735	0.3579	0.2655	0.055*
H11B	0.4255	0.2781	0.2460	0.055*
C3	0.1260(3)	0.7279(2)	0.46327(14)	0.0468(5)
H3	0.1435	0.7104	0.5219	0.056*
C1	0.0603(3)	0.8203(2)	0.34543(13)	0.0451(5)
H1	0.0212	0.8816	0.3061	0.054*
C10	0.4668(2)	0.42926(19)	0.32850(13)	0.0403(4)
C12	0.4247(3)	0.1475(2)	0.40064(17)	0.0549(6)
H12	0.5335	0.1472	0.3974	0.066*
C5	0.4057(3)	0.5247(2)	0.38130(15)	0.0465(5)
C2	0.1209(3)	0.7050(2)	0.32390(14)	0.0514(5)
H2	0.1327	0.6720	0.2682	0.062*
C13	0.3370(2)	0.0717(2)	0.45089(17)	0.0539(6)
H13	0.3765	0.0089	0.4890	0.065*
C6	0.5012(4)	0.6232(2)	0.41095(18)	0.0673(7)
H6	0.4600	0.6880	0.4460	0.081*
C9	0.6220(3)	0.4353(3)	0.30756(18)	0.0609(7)
H9	0.6641	0.3713	0.2722	0.073*
C4	0.2369(4)	0.5212(2)	0.4072(2)	0.0683(8)
H4A	0.1808	0.4584	0.3712	0.082*
H4B	0.2313	0.4920	0.4670	0.082*
C7	0.6556(4)	0.6278(3)	0.3898(2)	0.0790(9)
H7	0.7193	0.6949	0.4108	0.095*
C8	0.7162(3)	0.5342(3)	0.3380(2)	0.0791(9)
H8	0.8213	0.5372	0.3232	0.095*

As a continuation of our work, we report the synthesis and structure of the title compound.

The asymmetric unit of the title structure is comprised of one Ni(II)ion, one 1,2-BIB molecule, and one chloride ion, as shown in the figure. The Ni(II) atom is located on an inversion centre (symmetry code: 0, 1, 0.5) and is placed in an octahedral coordination environment, defined by four nitrogen atoms from four different 1,2-BIB molecules and two chloride ions. N1, N1(−*x*, 2−*y*, 1−*z*), N4(*x*, 1+*y*, *z*) and N4(−*x*, 1−*y*, 1−*z*) atoms are located on the basal plane. Two chloride ions occupy the apical positions. The bond distances Ni-N are in the range of 2.0586(17) and 2.1008(17) Å, which are all consistent with corresponding bond lengths found in the literature [5–7]. The Ni—Cl bond distance is 2.4669(11)Å, similar to the values observed in the comparable compound [8], but longer than those found in this compound [9]. The 1,2-BIB ligand coordinates to the two metal centers in a trans configuration, similar to that found in comparable structures [5]. In the title compound, each metal center is surrounded by four 1, 2-BIB ligands, resulting in a joint-like chain structure. In another comparable structure, 1,2-BIB is connected to the Ni(II) center to form a two-dimensional layered structure [6].

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References

1. Dhakshinamoorthy, A.; Garcia, H.: Metal-organic frameworks as solid catalysts for the synthesis of nitrogen-containing heterocycles. Chem. Soc. Rev. **43** (2014) 5750–5765.
2. Hu, Z. C.; Deibert, B. J.; Li, J.: Luminescent metal-organic frameworks for chemical sensing and explosive detection. Chem. Soc. Rev. **43** (2014) 5815–5840.
3. Tripuramallu, B. K.; Manna, P.; Das, S. K.: Structural library of coordination polymers based on flexible linkers exploiting the role of linker coordination angle: synthesis, structural characterization and magnetic properties. CrystEngComm **16** (2014) 4816–4833.
4. Song, X. Z.; Song, S. Y.; Zhu, M.; Hao, Z. M.; Meng, X.; Zhao, S. N.; Zhang,H. J.: Employing tripodal carboxylate ligand to construct Co(ii) coordination networks modulated by N-donor ligands: syntheses, structures and magnetic properties. Dalton trans. **42** (2013) 13231–13240.
5. Zhao, N.; Deng, Y. E.; Liu, P.; An, C. X.; Wang, T. X.; Lian, Z. X.: Three coordination polymers constructed from bis(imidazol-l-yl-methyl) benzene: syntheses, structures, and third-order nonlinear optical properties. Transition. Meta. Chem. **40** (2015) 11–19.
6. Zhao, N.; Deng, Y. E.; Liu, P.; An, C. X.; Wang, T. X.; Lian, Z. X.: Syntheses, structures and third-order nonlinear optical properties of three coordination polymers based on bis(imidazol-l-yl-methyl)benzene and aromatic dicarboxylic ligands. Polyhedron **85** (2015) 607–614.
7. Zhao, N.; Liu, P.; An, C. X.; Wang, T. X.; Lian, Z. X.: Structures and third-order nonlinear optical properties of two cobalt(II) coordination polymers constructed from bis(imidazol-l-yl-methyl)benzene and aromatic dicarboxylic ligands. Inorg. Chem. Commun. **50** (2014) 97–100.
8. Zhou, H.; Du, S. W.: Syntheses, crystal structures and magnetism of two new coordination polymers $[Ni(bix)_2Cl_2]n$ and $[Co(bix)Cl_2]_n$. Chinese J. Struct. Chem. **26** (2007) 711–716.
9. Kounavi, K. A.; Moushi, E. E.; Manos, M. J.; Papatriantafyllopoulou, C.; Tasiopoulos A. J.; Nastopoulos, V.: Supramolecular patterns of cationic and neutral Ni(II) complexes from the interplay of hydrogen-bonding, stacking interactions and metal-coordination motifs. CrystEngComm **14** (2012) 6492–6502.
10. Bruker. SADABS. Brucker AXS Inc., Madison, Wisconsin, USA, (2007).
11. Bruker. SMART and SAINT. Brucker AXS Inc., Madison, Wisconsin, USA, (2009).
12. Sheldrick, G. M.: SHELXT-Integrated space-group and crystal-structure determination Acta Cryst. **A71** (2015) 3–8.
13. Dolomanov, O. V.; Bourhis, L.J.; Gildea, R. J; Howard, J. A. K.; Puschmann, H.: OLEX2: a complete structure solution, refinement and analysis program. J. Appl. Cryst. **42** (2009) 339–341.