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Synthesis and Crystal Structure of $[NiL_2(H_2O)_2](ClO_4)_2$ L=MBPT=4-*p*-methylphenyl-3,5-bis-(pyridin-2-yl)-1,2,4-triazole

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Abstract: The Nickel (II) complex, $[Ni(MBPT)_2(H_2O)_2](ClO_4)_2$ (MBPT=4-*p*-methylphenyl-3,5-bis-(pyridin-2-yl)-1,2,4-triazole), was synthesized and its crystal structure determined by X-ray diffraction methods.The complex adopts a distorted octahedral environment made up of two bidentate chelating MBPT ligands in the equatorial plane and two water molecules filling the axial positions.

Keywords: Nickel complex, crystal structure, triaryltriazole.

The substituted 1,2,4-triazoles are very useful ligands in coordination chemistry[1-3]. It is very interesting that some complexes containing substituted 1,2,4-triazoles ligands have the spin-crossover phenomena, which could be used as magnetic materials[4-5]. However, complexes containing triaryltriazole ligands have been little known so far. We have recently synthesized some triaryltriazole compounds[6-7], and we first report here the synthesis and crystal structure of $[Ni(MBPT)_2(H_2O)_2](ClO_4)_2$.

Experimental

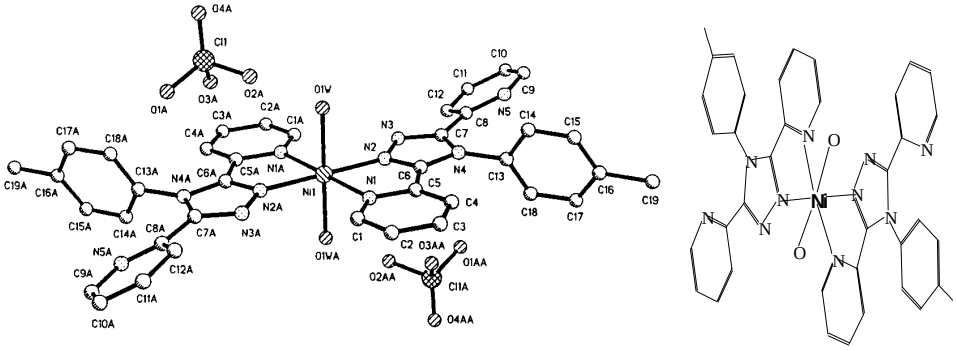
The title complex was obtained by reaction of $Ni(OAc)_2{\cdot}4H_2O$ with MBPT[7] and $NaClO_4{\cdot}H_2O$ in molar ratio of 1:2:2 in ethanol. Anal. For $NiC_{38}H_{34}Cl_2N_{10}O_{10}$. Calcd. C, 49.59; H, 3.72; N, 15.22. Found: C, 49.35; H, 3.89; N, 15.09.
The crystal suitable for X-ray diffraction was obtained by evaporation from a methanol solution.

X-ray crystallography[8]

A colorless slab crystal with dimensions of 0.22x0.16x0.12 mm was selected for X-ray diffraction study. The unit cell parameters and intensity data were collected on a Siemens SMART CCD diffractometer at room temperature using a graphite-monochromated MoKα (λ=0.71073Å) radiation, ω scan mode with $2\theta \geq 50°$. A total of 10886 reflections were collected. 3607 reflections with $I>2\sigma(I)$ were used in the structure determination and refinement. The structure was solved by direct methods and refined on F^2 using full-matrix least-squares procedure. All H-atomic coordinates were fixed at theoretically calculated position and were not refined.

A perspective view of the complex with the atom labelling scheme is shown in **Figure 1** Crystallographic data: $[Ni(C_{19}H_{15}N_5)_2(H_2O)_2](ClO_4)_2$, Mr=920.36, monoclinic, space group $P2_1/c$, a=9.8447(4), b=14.8467(6), c=14.5054(6)Å, β=104.515(1)°, Z=2, V=2052.46(15) $Å^3$, Dc=1.489g/cm^3, F000=948, R=0.070, Rw=0.17. The nickel atom is surrounded by four nitrogen atoms from two MBPT ligands in the equatorial plane and two oxygen atoms from two water molecules in the axial positions to form a distorted octahedral geometry. The MBPT ligand is coordinated to nickel atom *via* N1 atom of a pyridyl ring and N2 atom of the triazole moiety leaving N5 atom of another pyridyl ring and N3 atom of the triazole moiety uncoordinated, which is similar to the coordination mode in the complex $[Ag(MBPT)(PPh_3)_2]$[7]. The Ni-N1 and Ni-N2 bond lengths are 2.117(4) and 2.052(4) Å, respectively, the Ni-O bond length is 2.108(4) Å.

Figure 1



The triazole, pyridine and the methylphenyl rings are all planar and the triazole ring makes dihedral angles of 2.5(3), 25.5(3) and 77.2(3)° respectively with the pyridine and methylphenyl rings. The pyridine rings are oriented at an angle of 26.2(3)° with each other. The perchlorate ion is highly disordered (55:45) and is invloved in intramolecular O-H...O [O1W...O2A=2.87(1)Å; O1W-H1W1...O2A=157°] hydrogen bonding and intermolecular C-H...O [C18...O1A (-x,-y,-z)=3.43(2) Å; C18-H18A...O1A=163°] hydrogen bonding thereby participating in the packing.

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