

# SYNTHESIS AND CHARACTERIZATION OF AZIDO Zn(II) COMPLEX WITH THE CONDENSATION PRODUCT OF 2-ACETILPYRIDINE AND GIRARD'S P REAGENT



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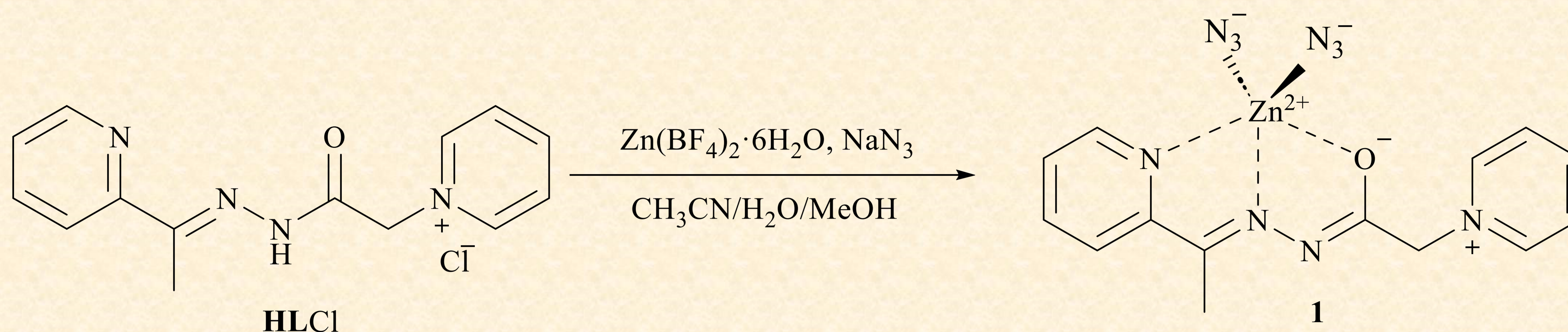
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Hydrazone ligands are one of the most important classes of flexible and versatile polydentate ligands which show very high efficiency in chelating various metal ions. Deprotonation of the –NH group, which is readily achieved in the complexed ligand in particular, results in the formation of tautomeric anionic species (=N–N=C=O or =N–N=C–O), having different coordination properties. Our interest in metal complexes with hydrazone-based ligands is partly due to their potential applications as catalysts and molecular magnets.

In the reaction of HLCI with Zn(BF<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O and NaN<sub>3</sub> in molar ratio 1 : 1 : 4 in acetonitrile/water/methanol mixture of solvents, a mononuclear Zn(II) complex (**1**) was obtained, with composition [ZnL(N<sub>3</sub>)<sub>2</sub>] (Scheme 1).



Scheme 1. Synthesis of [ZnL(N<sub>3</sub>)<sub>2</sub>] complex (**1**).

In complex **1**, the ligand is coordinated in deprotonated, formally neutral, zwitterionic form to Zn(II) ion through the pyridine nitrogen, the imine nitrogen, and the carbonyl oxygen atoms, forming a pentacoordinated complex (Figure 1).

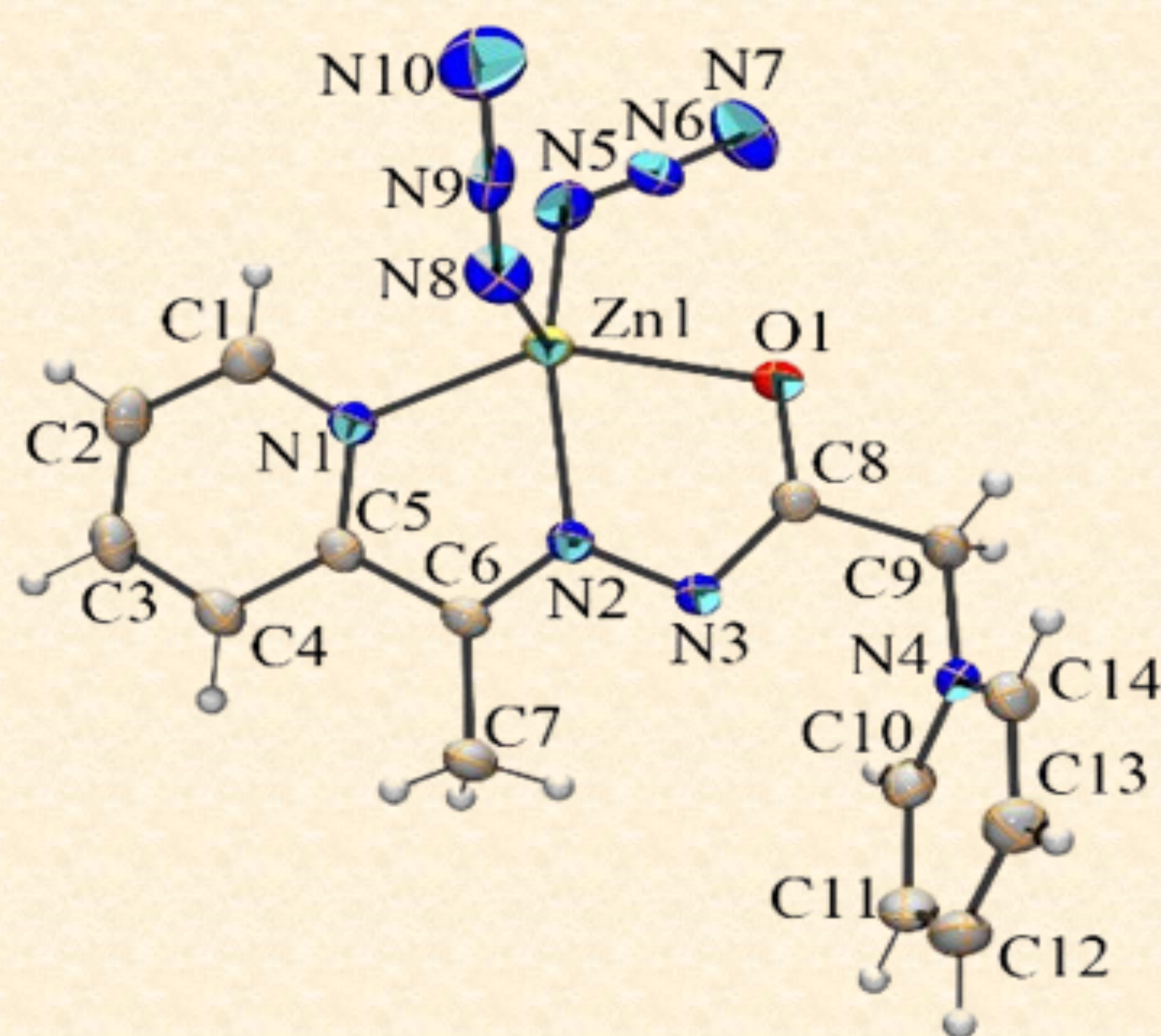


Figure 1. ORTEP representation of the [ZnL(N<sub>3</sub>)<sub>2</sub>] (**1**) complex. Thermal ellipsoids are drawn at the 30% probability level.

Table 4. Crystal data and structure refinement details for **1**.

	<b>1</b>
formula	C <sub>14</sub> H <sub>14</sub> N <sub>10</sub> OZn
Fw (g mol <sup>-1</sup> )	403.72
crystal size (mm)	0.50×0.10×0.10
crystal color	colourless
crystal system	monoclinic
space group	P2 <sub>1</sub> /c
a (Å)	12.3417(5)
b (Å)	8.9990(5)
c (Å)	15.3451(6)
β (°)	101.169(4)
V (Å <sup>3</sup> )	1671.99(13)
Z	4
calcd density (g cm <sup>-3</sup> )	1.604
F(000)	824
no. of collected reflns	15739
no. of independent reflns	3828
R <sub>int</sub>	0.0320
no. of reflns observed	3007
no. parameters	236
R[> 2σ(I)] <sup>a</sup>	0.0331
wR <sub>2</sub> (all data) <sup>b</sup>	0.0823
Goof, S <sup>c</sup>	1.052
maximum/minimum residual electron density	+0.38/−0.30
(e Å <sup>-3</sup> )	

<sup>a</sup>R = Σ||F<sub>o</sub>| − |F<sub>c</sub>||/Σ|F<sub>o</sub>|. <sup>b</sup>wR<sub>2</sub> = {Σ[w(F<sub>o</sub><sup>2</sup> − F<sub>c</sub><sup>2</sup>)<sup>2</sup>]/Σ[w(F<sub>o</sub><sup>2</sup>)<sup>2</sup>]}<sup>1/2</sup>.

<sup>c</sup>S = {Σ[(F<sub>o</sub><sup>2</sup> − F<sub>c</sub><sup>2</sup>)/(n/p)]<sup>1/2</sup> where n is the number of reflections and p is the total number of parameters refined.