Synthesis and characterization of octahedral Ni(II) complex with condensation product of 2-acetylpyridine and Girard's P reagent

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The ligand (HLCl) was synthetized by the reaction of 2-acetylpyridine and Girard's P reagent in molar ratio 1:1 in ethanol. (Scheme 1).

The ligand (HLCl) was synthetized by the reaction of 2-acetylpyridine and Girard's P reagent in molar ratio 1:1 in ethanol. (Scheme 2).

The Ni(II) ion has distorted octahedral coordination geometry. The tridentate ligand (**HL**) is coordinated to the nickel ion with a NNO set of donor atoms forming two five-membered chelate rings and the other three coordination sites are supplemented by azido ligands. The ligand (**HL**) and the $[NiHL(N_3)_3]$ complex were characterized by elemental analysis, IR and UV/Vis spectroscopy and structure of the complex was defined by X-ray analysis.

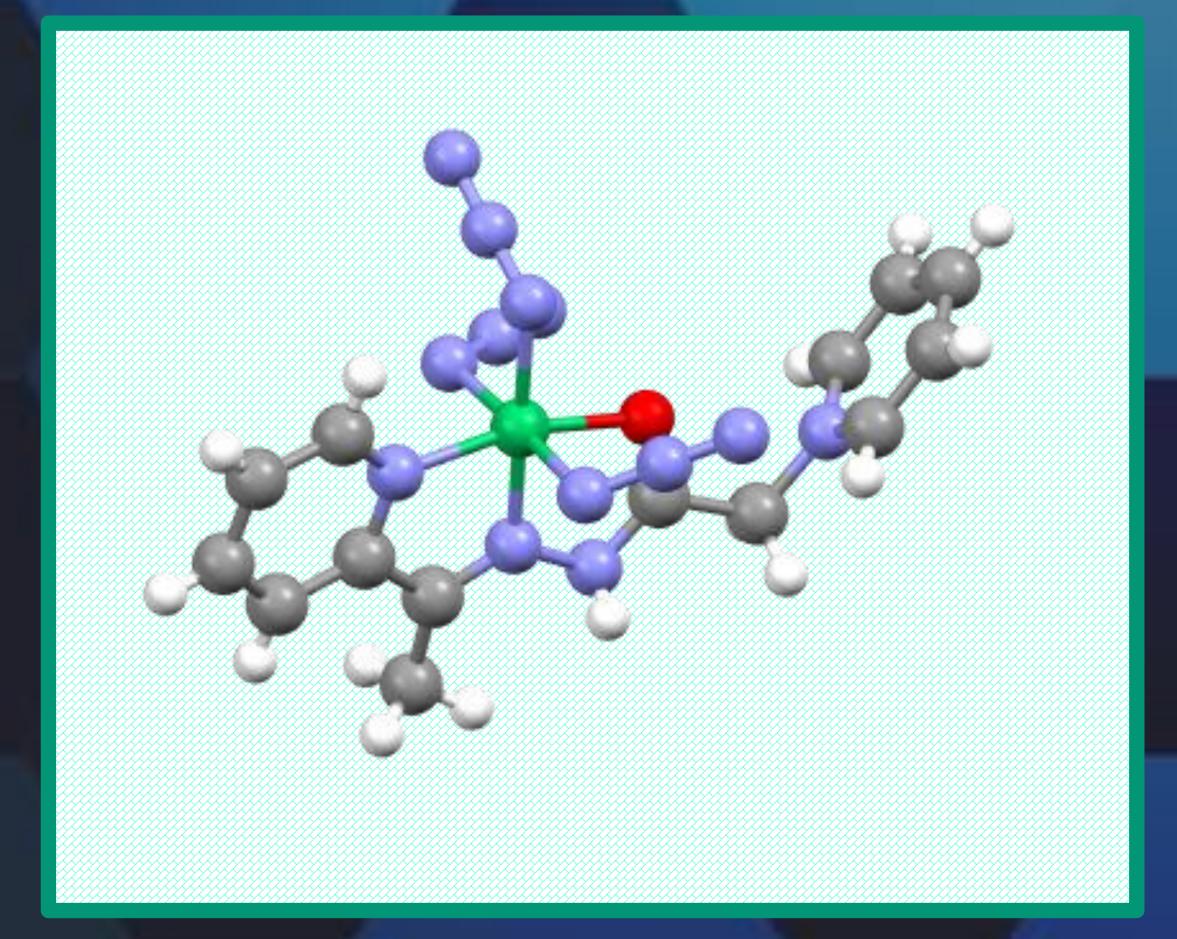


Fig. 1. Structure of complex $[NiHL_2](BF_4)_2$ (complex crystallizes in the triclinic space group P-1).

Crystal Data	
Formula	C ₁₄ H ₁₅ N ₁₃ Ni O
Formula weight	439.07
Crystal system	triclinic
Space group	P-1 (No. 2)
a, b, c [Å]	7.7318(4), 8.6981(6), 14.7200(9)
α, β, γ [°]	78.295(6), 83.810(5), 69.368(6)
V [Å ³]	906.477
Z	2
D _{calc} [g cm ⁻³]	1.609
μ (MoKα) [mm ⁻¹]	1.109
F(000)	450
Data Collection	
Temperature (K)	293
Radiation MoKα [Å]	0.71073
θ range [°]	3.4, 27.485
Dataset	$h = 10, k = 11, l_{max} = 19$
Refinement	
N _{ref} , N _{par}	4159, 263
R, wR, S	0.0419, 0.1058, 1.039
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 0.2160P]$ where $P = (F_o^2 + 2F_c^2)/3$