

Submission to *New Journal of Chemistry*

**Nickel(II) Complexes Chelated by 2,6-Pyridinedicarboxamide:
Syntheses, Characterization, and Ethylene Oligomerization**

Jie Zhang,^a Shaofeng Liu,^{b,*} Antai Li,^a Hongqi Ye,^{a,*} Zhibo Li^b

^a*Department of Chemistry and Engineering, Central South University, Changsha 410083, P. R. China. E-mail: yeslab@csu.edu.cn*

^b*School of Polymer Science and Engineering, Qingdao University of Science and Technology, Qingdao 266042, P. R. China. E-mail: shaofengliu@qust.edu.cn*

Table S1. Crystal data and structure refinement for **Ni5** and **Ni6**.

Complex	Ni5 ·CH ₃ OH·2H ₂ O	Ni6 ·3C ₂ H ₅ OH
Empirical formula	C ₂₇ H ₃₁ Br ₂ N ₃ NiO ₂ ·CH ₃ OH·2H ₂ O	C ₃₁ H ₃₉ Br ₂ N ₃ NiO ₂ ·3CH ₃ OH
Formula weight	714.13	842.38
Temperature / K	173.15	173.15
Crystal system	Monoclinic	Orthorhombic
Space group	P2 ₁ /c	P2 ₁ 2 ₁ 2 ₁
a / Å, b / Å, c / Å	15.331(3), 15.527(3), 14.982(3)	14.859(3), 16.766(4), 16.883(4)
α/°, β/°, γ/°	90, 118.32 (3), 90	90, 90, 90
Volume / Å ³	3139.5(13)	4205.9(16)
Z	4	4
ρ _{calc} / mg mm ⁻³	1.511	1.330
μ / mm ⁻¹	3.203	2.402
F(000)	1456.0	1752.0
Crystal size / mm ³	0.190 × 0.180 × 0.110	0.370 × 0.230 × 0.190
2θ range for data collection	3.018 to 54.978°	5.402 to 55°
Index ranges	-17 ≤ h ≤ 19, -20 ≤ k ≤ 19, -19 ≤ l ≤ 19	-19 ≤ h ≤ 18, -12 ≤ k ≤ 21, -21 ≤ l ≤ 16
Reflections collected	22233	16609
Independent reflections	7137 [R(int) = 0.0515]	9342 [R(int) = 0.0372]
Data/restraints/parameters	7137/28/382	9342/12/470
Goodness-of-fit on F ²	1.235	1.118
Final R indexes [I>2σ (I)]	R ₁ = 0.0806, wR ₂ = 0.1632	R ₁ = 0.0483, wR ₂ = 0.0909
Final R indexes [all data]	R ₁ = 0.0909, wR ₂ = 0.1684	R ₁ = 0.0551, wR ₂ = 0.0945
Largest diff. peak/hole / e Å ⁻³	0.97/-0.67	0.39/-0.49

$$R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|}; wR_2 = \left[\frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)^2]} \right].$$

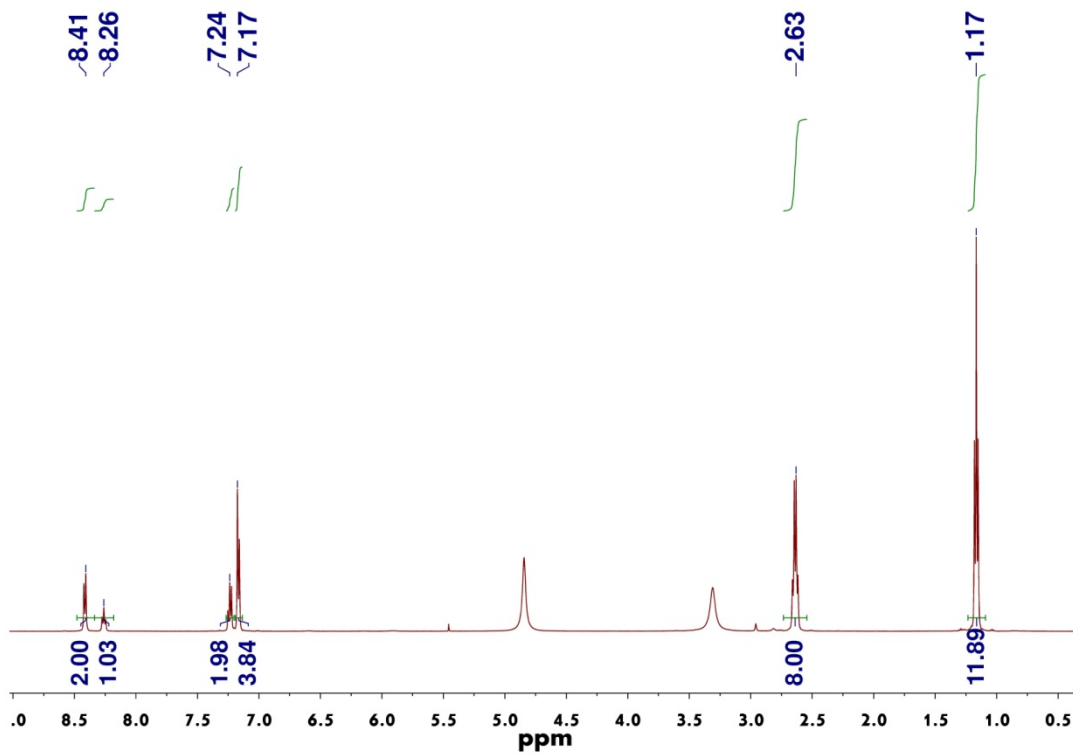


Figure S1. ^1H NMR of Ni5 in CD_3OD .

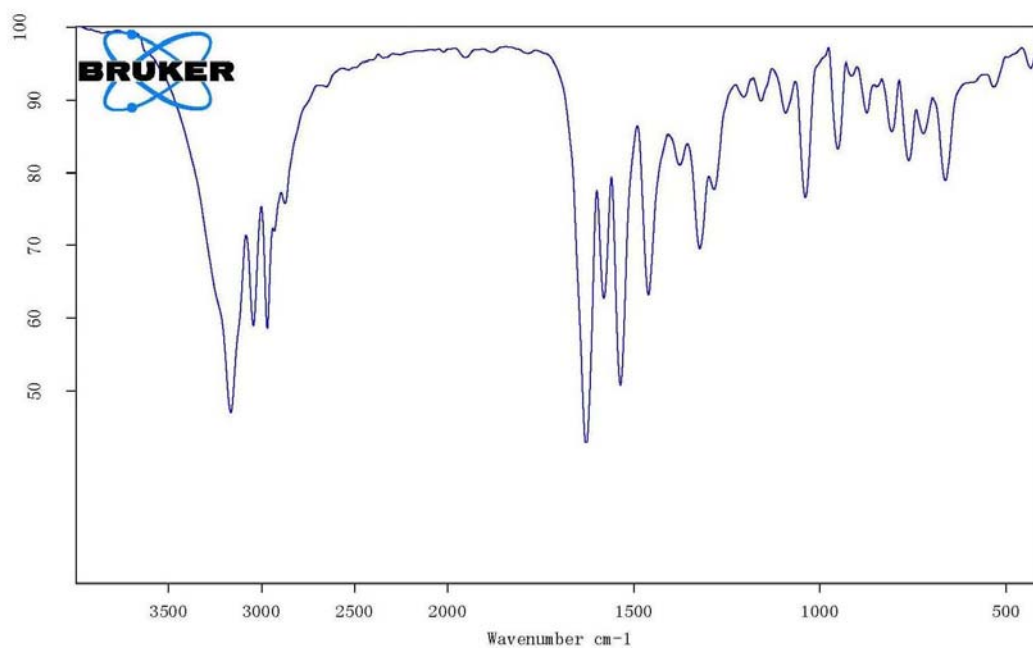


Figure S2. FT-IR of Ni5 yellowish powder.

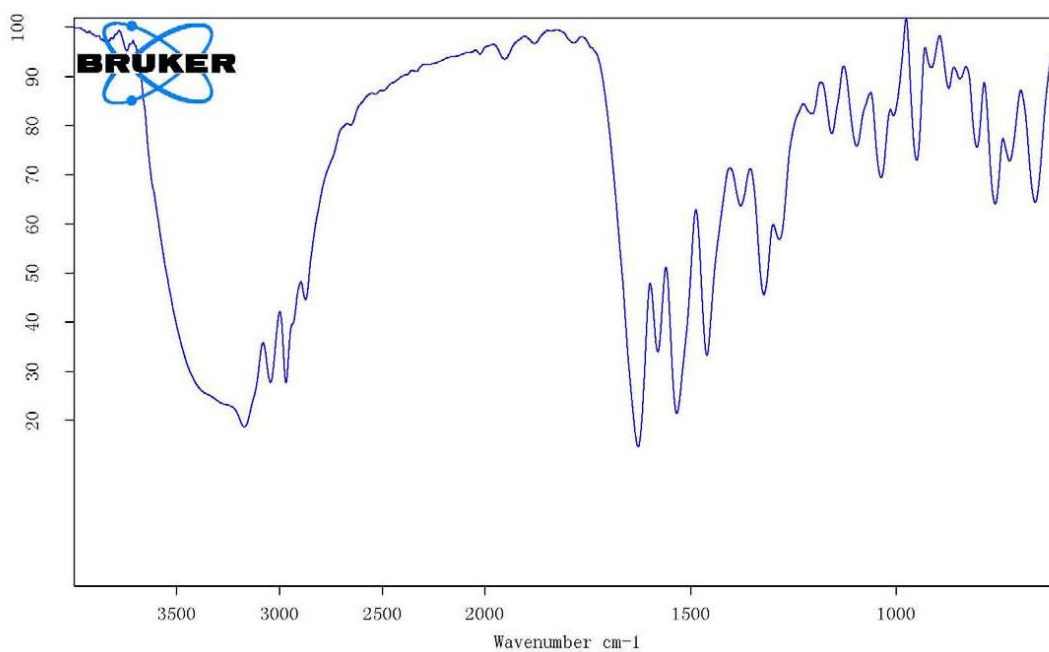


Figure S3. FT-IR of Ni5·CH₃OH·2H₂O green crystal.