

# Support Information

## Urea decomposition mechanism by dinuclear nickel complexes

Christian O. Martin <sup>a, b</sup>, Letícia K. Sebastiany <sup>a</sup>, Alejandro Lopez-Castillo <sup>a</sup>, Rafael S. Freitas <sup>c</sup>, Leandro H. Andrade<sup>d</sup>, Henrique E. Toma <sup>\*d</sup>, Caterina G. C. Marques Netto<sup>\* a</sup>

<sup>a</sup> Department of Chemistry, Universidade Federal de São Carlos, Rod. Washington Luiz, s/n, km 235- São Carlos/SP – Brazil

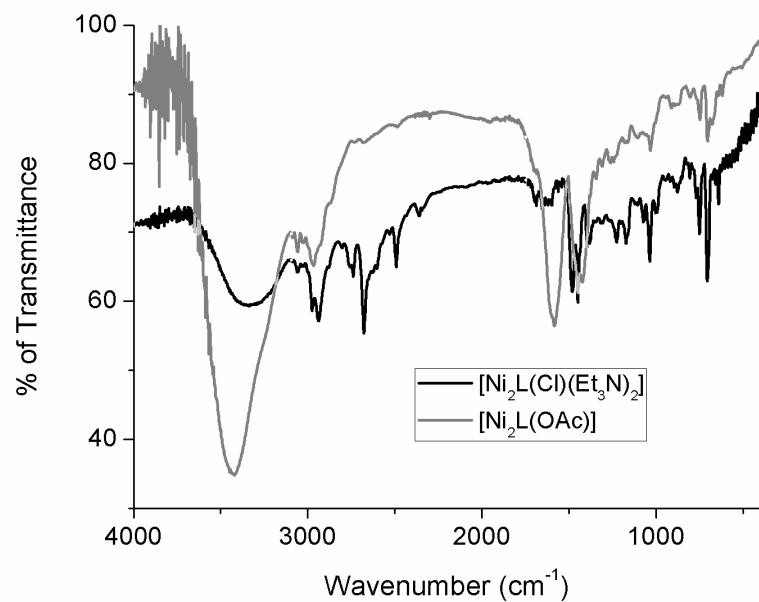
<sup>b</sup> Department of Chemical Engineering, Universidade Federal de São Carlos, Rod. Washington Luiz, s/n, km 235- São Carlos/SP – Brazil

<sup>c</sup> Institute of Physics, Universidade de São Paulo, Rua do Matão, 1371, Cidade Universitária-SP/Brazil

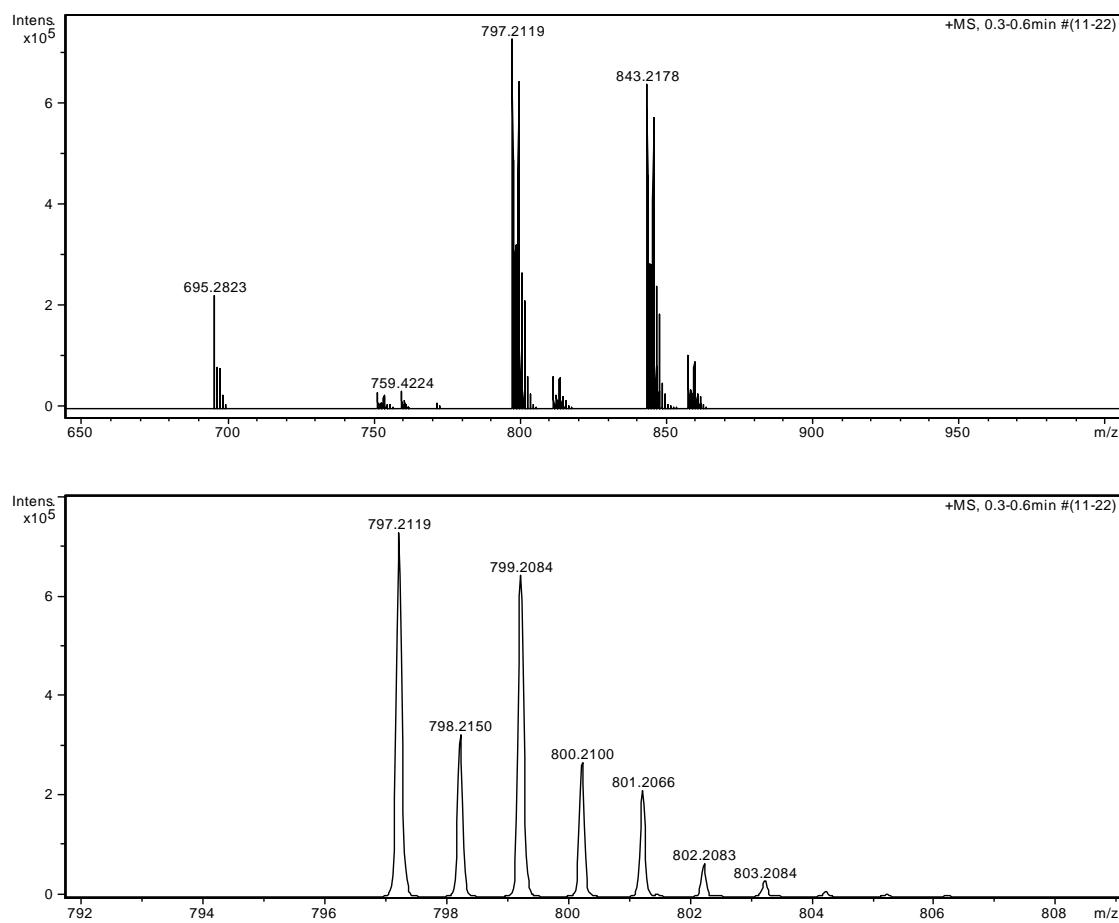
<sup>d</sup> Institute of Chemistry, Universidade de São Paulo, Av. Prof. Lineu Prestes 748, Cidade Universitária-SP/Brazil

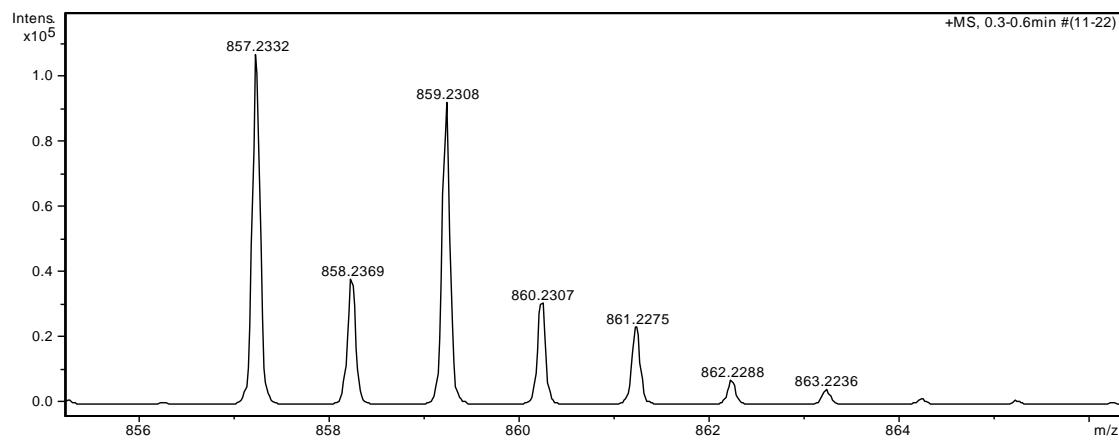
\*Correspondence: HET: [henetoma@iq.usp.br](mailto:henetoma@iq.usp.br); CGCMN: [caterina@ufscar.br](mailto:caterina@ufscar.br)

### Characterization of [Ni<sub>2</sub>L(OAc)] and [Ni<sub>2</sub>L(Cl)(Et<sub>3</sub>N)<sub>2</sub>] complexes

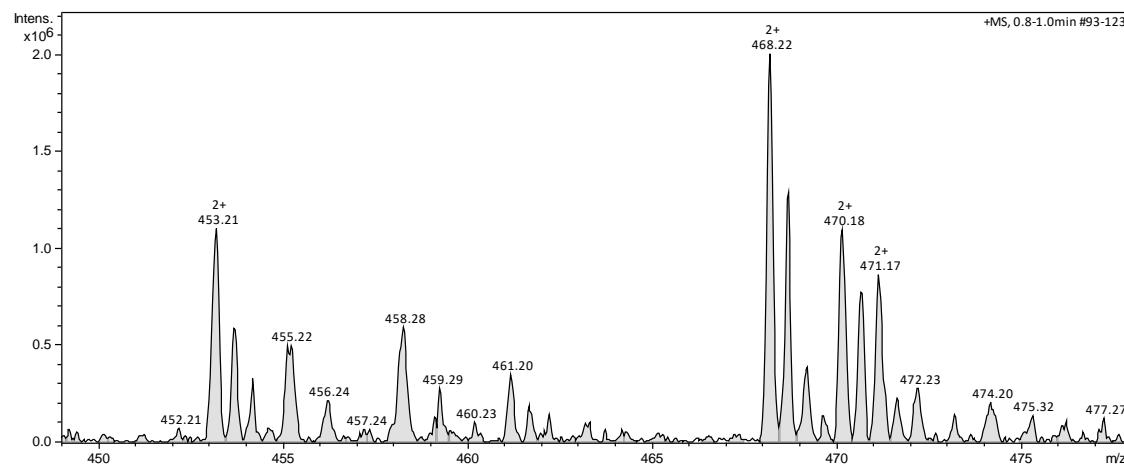
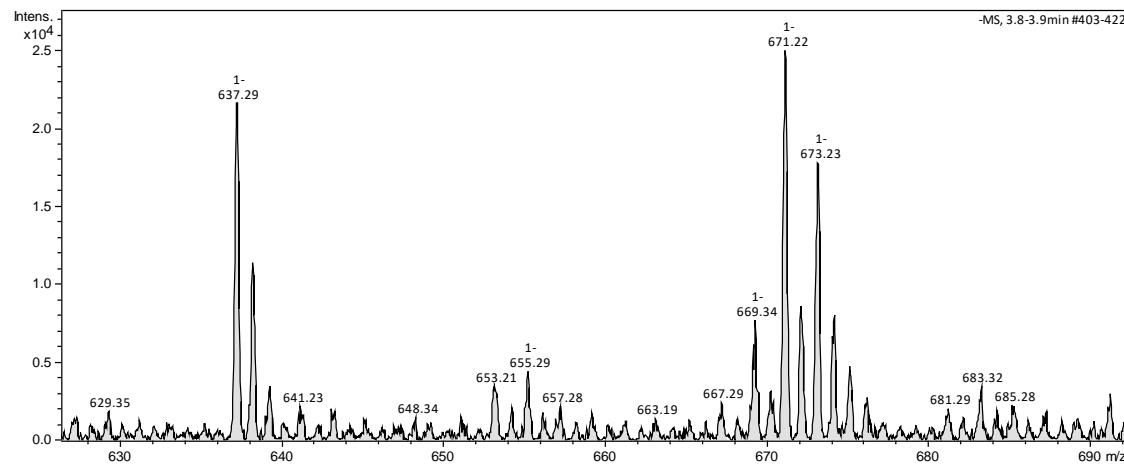


**SI1.** Solid infrared spectra of  $[\text{Ni}_2\text{L}(\text{OAc})]$ (gray line) and  $[\text{Ni}_2\text{L}(\text{Cl})(\text{Et}_3\text{N})_2]$  (black line) complexes.

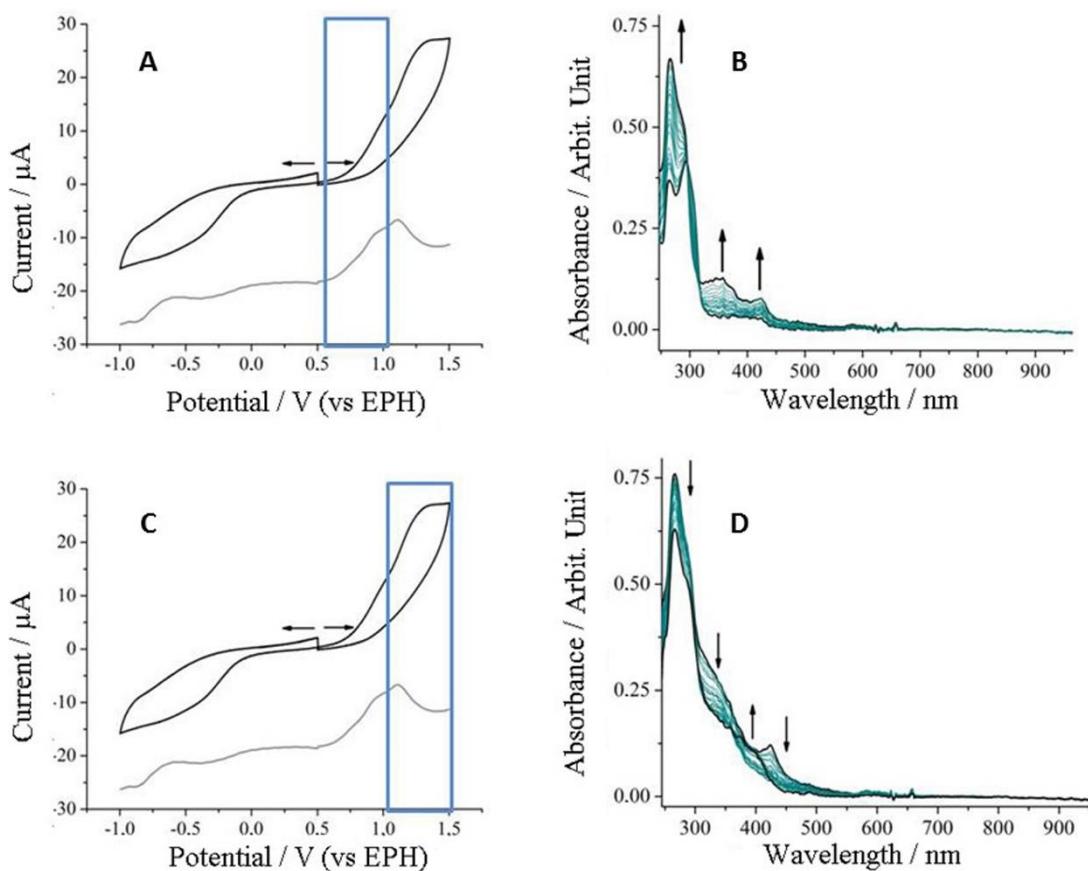




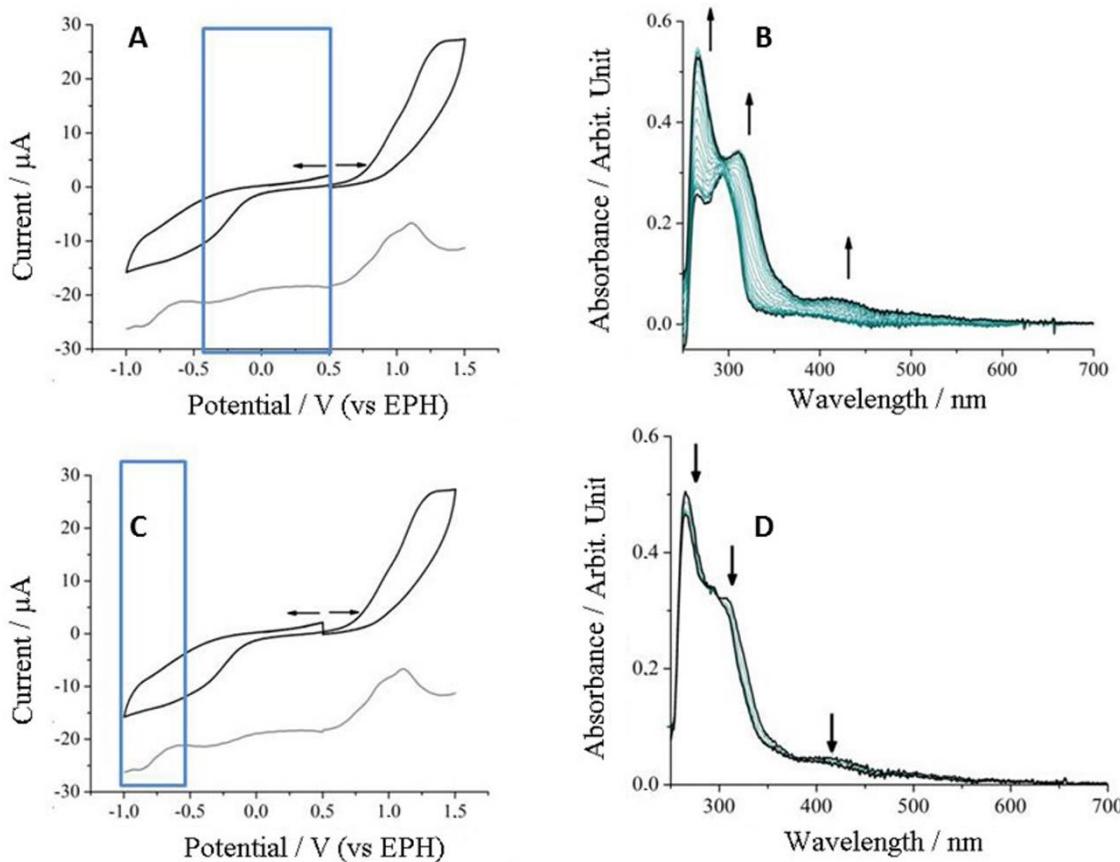
**SI2.** HRMS of  $[\text{Ni}_2\text{L}(\text{OAc})]$ .



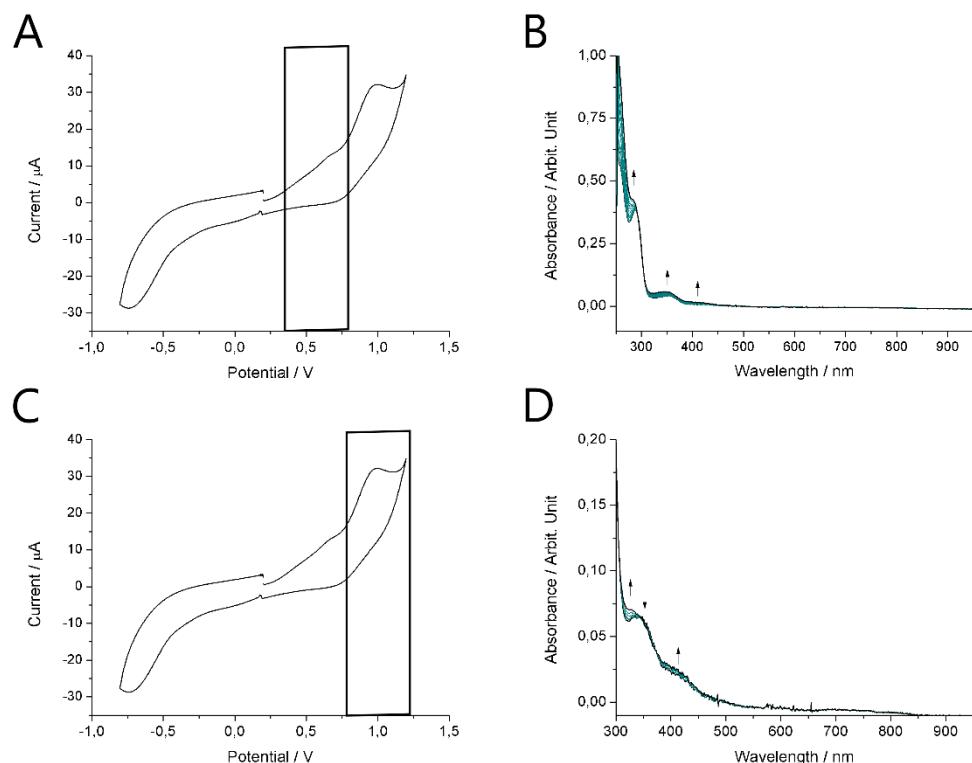
**SI3.** LRMS of  $[\text{Ni}_2\text{L}(\text{Cl})(\text{Et}_3\text{N})_2]$ . Negative mode (top panel) and positive mode (bottom panel).



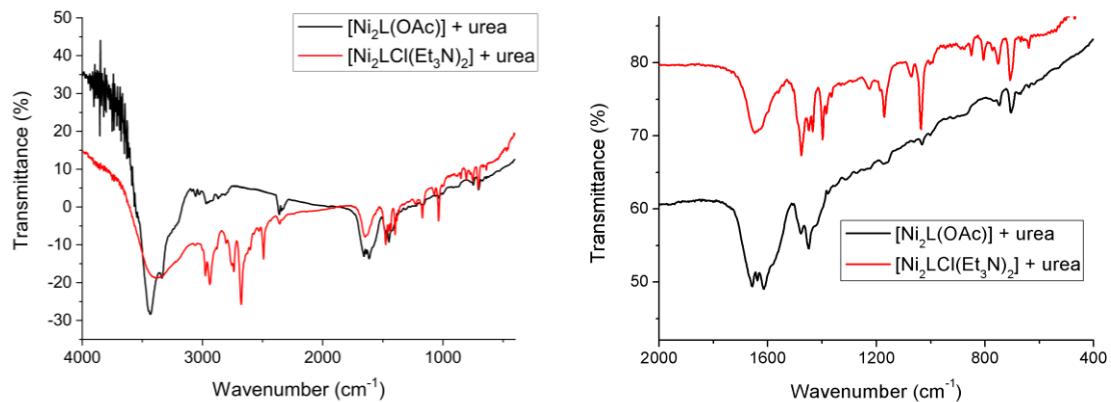
**SI4.** Anodic cyclic voltammetry and corresponding DPV plot for the complex  $[\text{Ni}_2\text{L}(\text{OAc})]$  in DMF and  $0.1 \text{ M}^{-1}$   $\text{TBACIO}_4$  as electrolyte (A and C) and spectroelectrochemistry of the oxidation processes at  $0.63\text{V}$  (B) and  $1.24\text{V}$  (D).



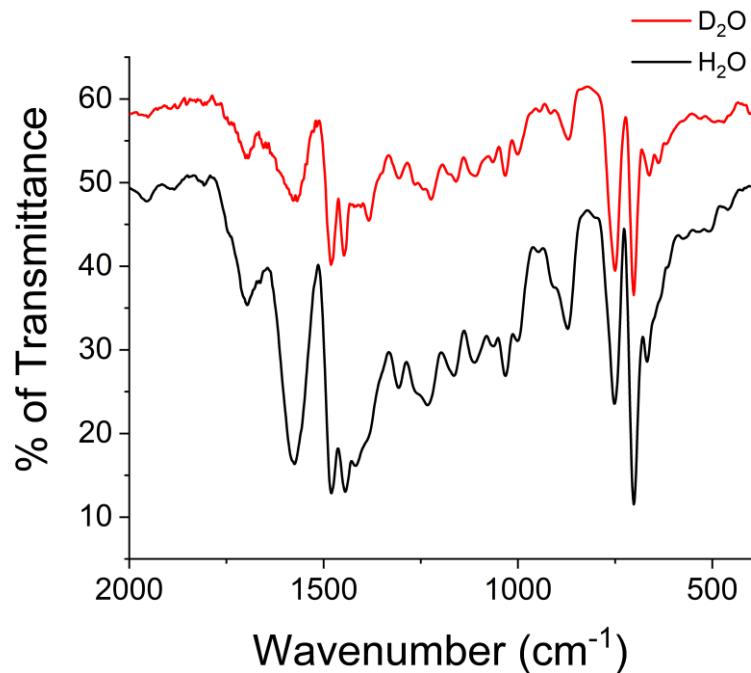
**SI5.** Cathodic cyclic voltammetry and corresponding DPV plot for the complex  $[\text{Ni}_2\text{L}(\text{OAc})]$  in DMF and 0.1 mol  $\text{L}^{-1}$   $\text{TBACIO}_4$  as electrolyte (A and C) and spectroelectrochemistry of the reduction processes at -0,36 (B) and -0,88V (D).



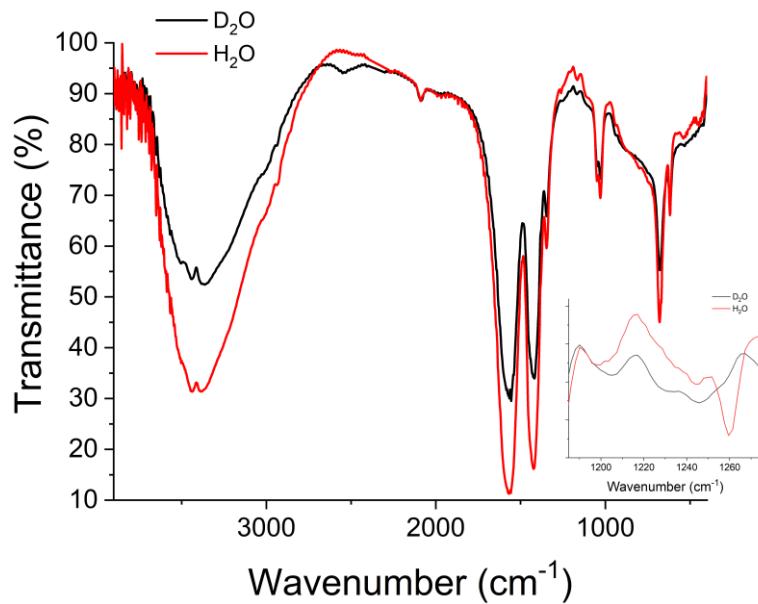
**SI6.** Anodic cyclic voltammetry and corresponding DPV plot for the complex  $[\text{Ni}_2\text{L}(\text{Cl})(\text{Et}_3\text{N})_2]$  in DMF and  $0.1 \text{ M}^{-1}$  TBACIO<sub>4</sub> as electrolyte (A and C) and spectroelectrochemistry of the oxidation processes at 0.5V (B) and 0.8 V(D).



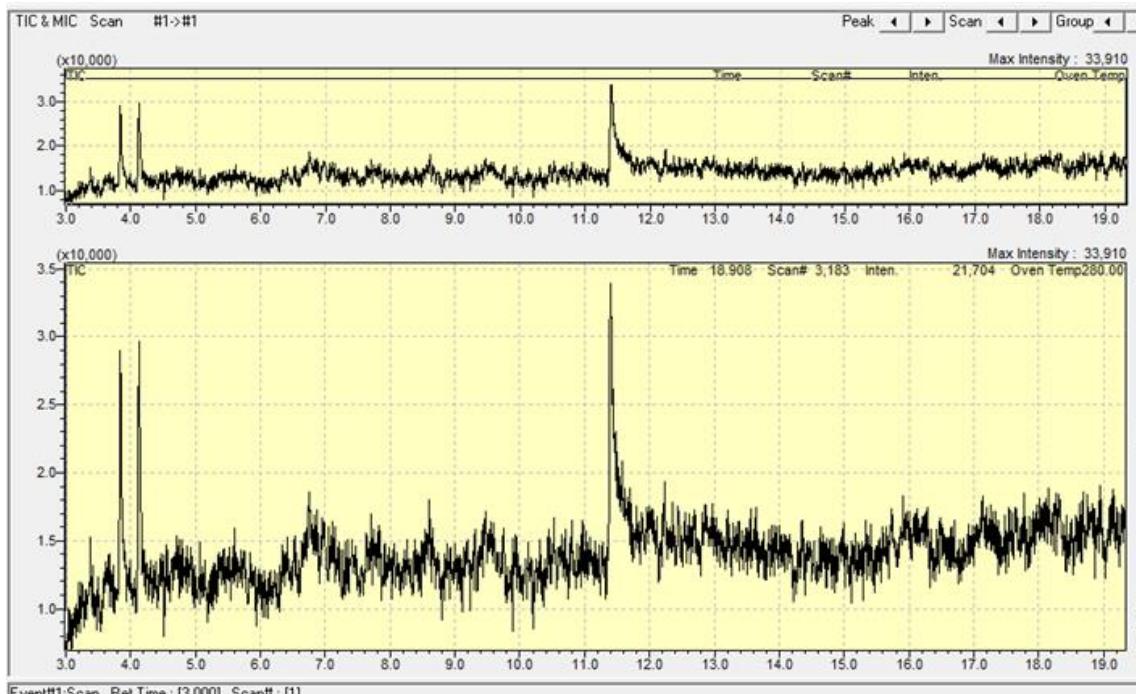
**SI7.** Infrared of coordinated urea to  $[\text{Ni}_2\text{L}(\text{OAc})]$  and  $[\text{Ni}_2\text{L}(\text{Cl})(\text{Et}_3\text{N})_2]$  complexes. Left: spectra from  $4000 \text{ cm}^{-1}$  to  $400 \text{ cm}^{-1}$  and Right: Spectra from  $2000 \text{ cm}^{-1}$  and  $400 \text{ cm}^{-1}$ .



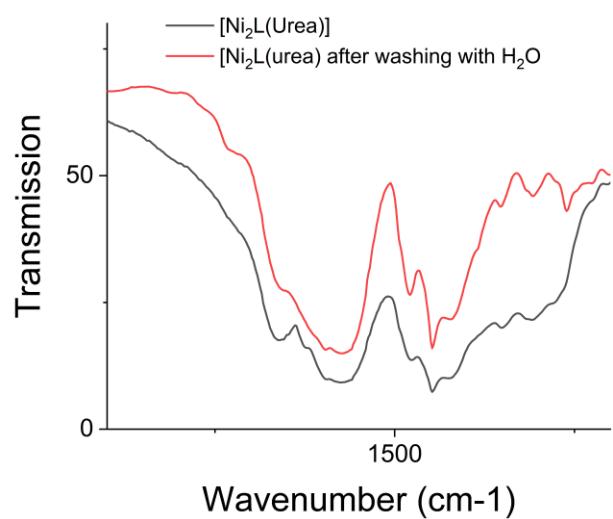
**SI8.** Infrared of the soluble fraction of the reaction between  $[\text{Ni}_2\text{L}(\text{OAc})]$  and water. Black line represents the product obtained after titration with  $\text{H}_2\text{O}$  and red line represents the product obtained after titration with  $\text{D}_2\text{O}$ .



**SI9.** Infrared of the insoluble fraction of the reaction between  $[\text{Ni}_2\text{L}(\text{OAc})]$  and water. Black line represents the product obtained after titration with  $\text{D}_2\text{O}$  and red line represents the product obtained after titration with  $\text{H}_2\text{O}$ . Inset: FTIR spectra between  $1185 \text{ cm}^{-1}$  and  $1275 \text{ cm}^{-1}$ .



**SI10.** GC-MS chromatogram of N-phenylurea decomposition using  $[\text{Ni}_2\text{L}(\text{OAc})]$  as a catalyst. Phenylisocyanate has a retention time of 3.8 min, aniline has a retention time of 4.1 min and N-phenylurea has a retention time of 11.5 min.



**SI11.** Infrared of  $[\text{Ni}_2\text{L}(\text{Urea})]$  before (black line) and after (red line) washing the complex with water.