

## Supplementary Materials

# Relationship between Structure and Zero-Field Splitting of Octahedral Nickel(II) Complexes with a Low-Symmetric Tetradentate Ligand

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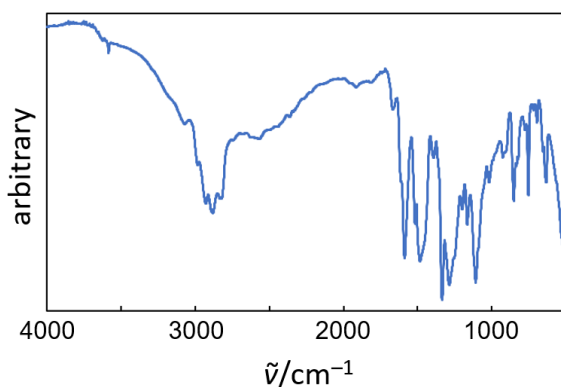
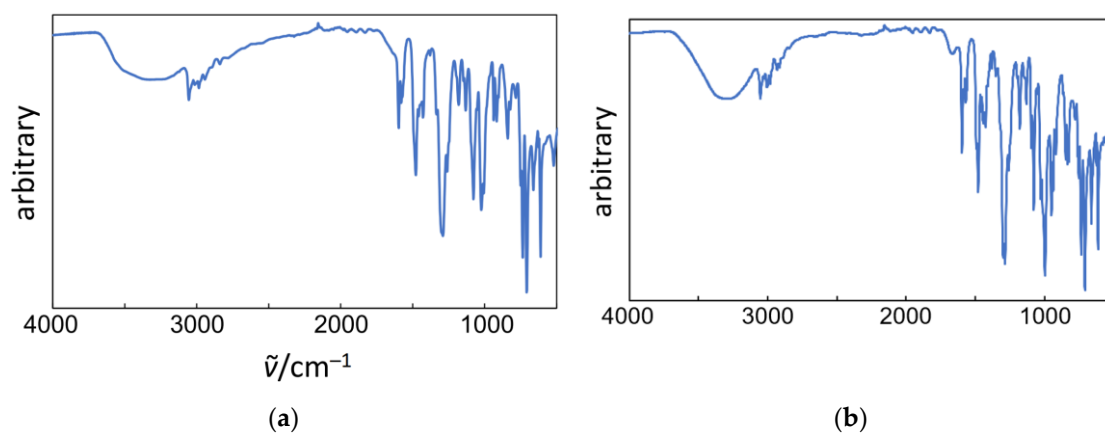
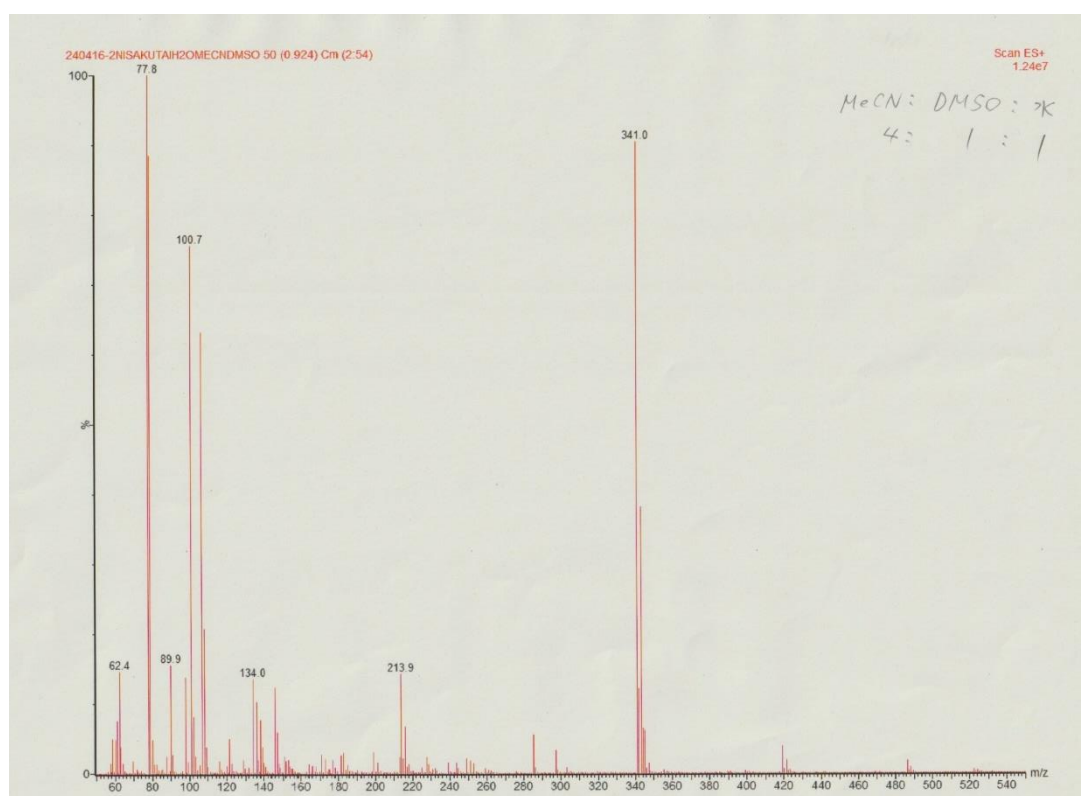


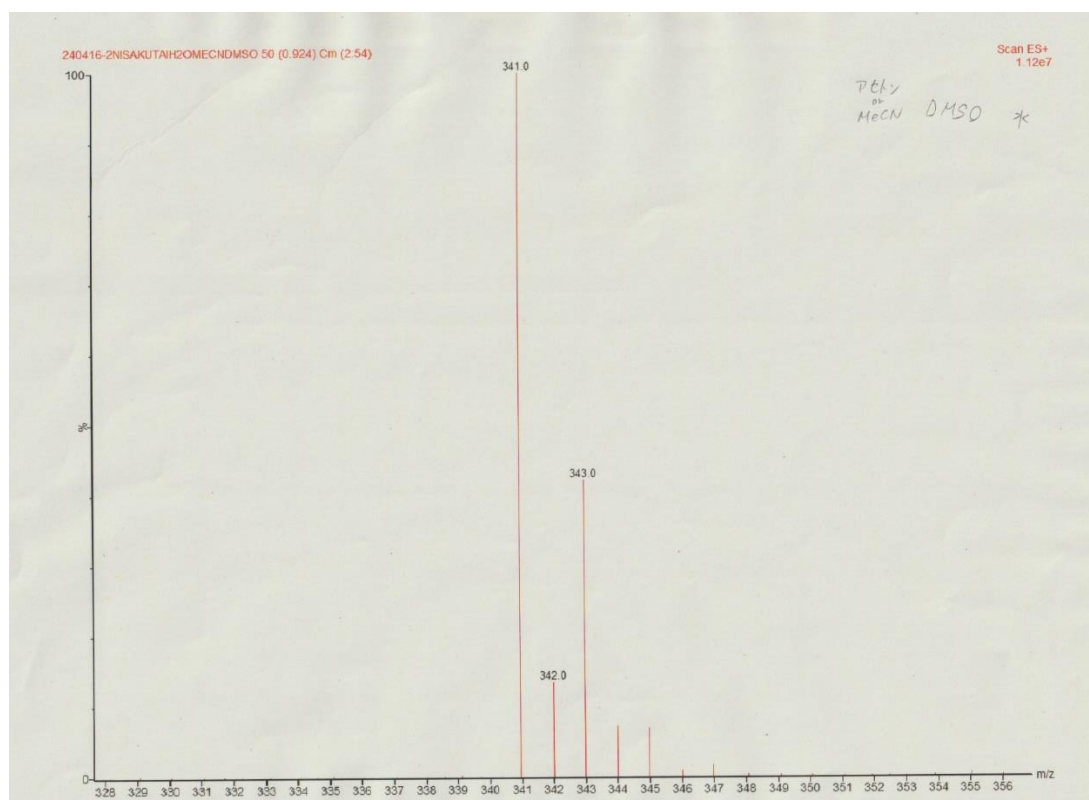
Figure S1. IR spectra of onp<sup>-</sup> ligand.



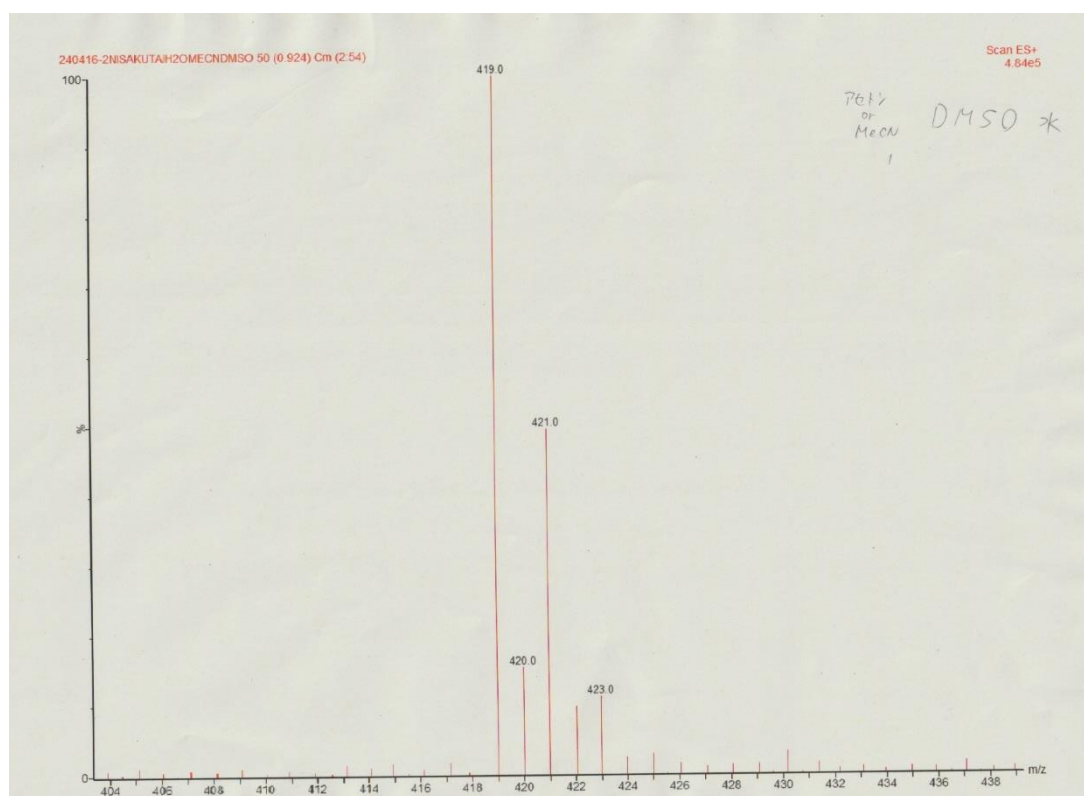
**Figure S2.** IR spectra of the crude product and **1**: (a) the crude product; (b)  $[\text{Ni}(\text{onp})(\text{dmsO})(\text{H}_2\text{O})][\text{BPh}_4] \cdot 2\text{dmsO}$  (**1**).



**Figure S3.** ESI mass spectra of **1** in mixed solvents (acetonitrile: dimethyl sulfoxide:  $\text{H}_2\text{O}$  = 4: 1: 1).



**Figure S4.** ESI mass spectra of **1** in mixed solvents (acetonitrile: dimethyl sulfoxide: H<sub>2</sub>O = 4: 1: 1) at around  $m/z = 341$ .



**Figure S5.** ESI mass spectra of **1** in mixed solvents (acetonitrile: dimethyl sulfoxide: H<sub>2</sub>O = 4: 1: 1) at around  $m/z$  = 419.