

*Supporting Information for:*

**Dual Coordination Modes of Ethylene-Linked NP2 Ligands in  
Cobalt(II) and Nickel(II) Iodides**

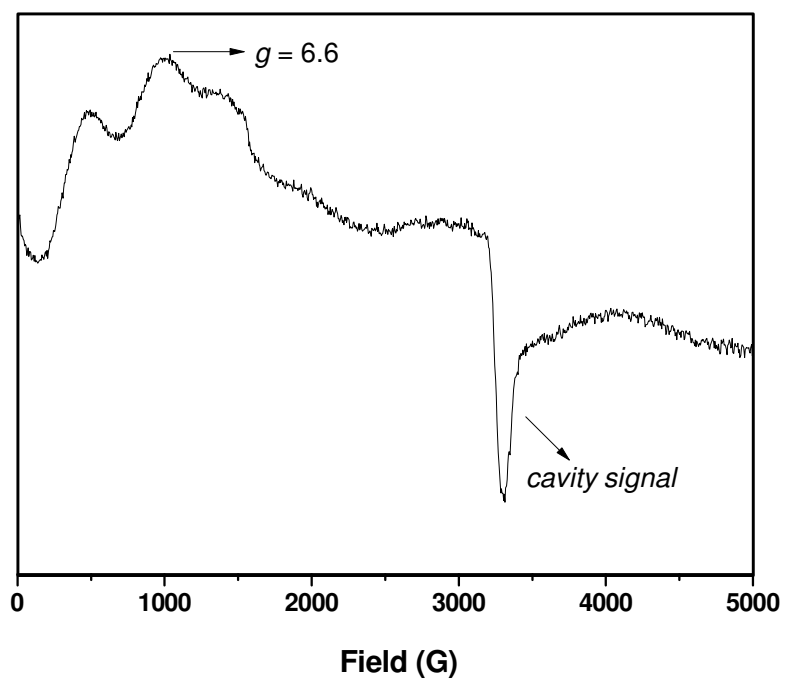
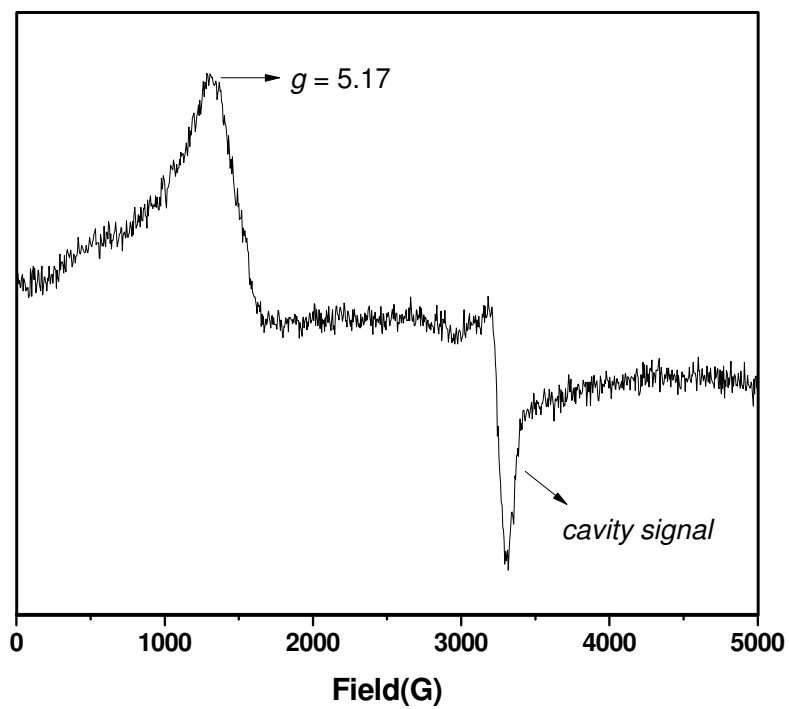
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**Table S1.** Crystal data and refinement parameters for the **Co-2'**, **Co-PNP** and **Ni-PNP** complexes.

|   | <b>Co-2'</b>   | <b>Co-PNP</b>   | <b>Ni-PNP</b>  |
|---|--|---|--|
| empirical formula                             | C <sub>35</sub> H <sub>35</sub> NP <sub>2</sub> CoI <sub>2</sub> | C <sub>32</sub> H <sub>29</sub> NP <sub>2</sub> CoI <sub>2</sub> •C <sub>4</sub> H <sub>8</sub> O | C <sub>32</sub> H <sub>29</sub> NP <sub>2</sub> NiI <sub>2</sub> |
| Fw  | 844.31   | 874.34  | 802.01   |
| color   | dark green   | brown/green   | dark purple  |
| habit   | block  | block   | plate  |
| size (mm)                                     | 0.22 × 0.20 × 0.14   | 0.23 × 0.21 × 0.14  | 0.28 × 0.20 × 0.06   |
| <i>T</i> (K)                                  | 100(2)   | 100(2)  | 100(2)   |
| wavelength (Å)                                | 0.71073  | 0.71073   | 0.71073  |
| lattice system                                | monoclinic   | triclinic   | monoclinic   |
| space group                                   | <i>Cc</i>  | <i>P</i> -1   | <i>P</i> 2 <sub>1</sub> / <i>n</i>                               |
| <i>a</i> (Å)                                  | 14.1550(6)   | 9.9884(4)   | 10.3909(5)   |
| <i>b</i> (Å)                                  | 13.1354(5)   | 11.7808(5)  | 24.7658(11)  |
| <i>c</i> (Å)                                  | 36.1275(14)  | 15.8303(7)  | 12.8704(6)   |
| <i>α</i> (deg)                                | 90   | 101.126(2)  | 90   |
| <i>β</i> (deg)                                | 99.612(2)  | 93.187(2)   | 112.745(2)   |
| <i>γ</i> (deg)                                | 90   | 103.450(2)  | 90   |
| <i>V</i> (Å <sup>3</sup> )                    | 6622.9(5)  | 1767.75(13)   | 3054.5(2)  |
| <i>Z</i>                                      | 8  | 2   | 4  |
| <i>d</i> <sub>calc</sub> (g/cm <sup>3</sup> ) | 1.694  | 1.643   | 1.744  |
| <i>μ</i> (mm <sup>-1</sup> )                  | 2.504  | 2.351   | 2.784  |
| GOF on <i>F</i> <sup>2</sup>                  | 1.372  | 2.236   | 1.749  |
| final <i>R</i> indices                        | <i>R</i> 1 = 0.0325  | <i>R</i> 1 = 0.0358   | <i>R</i> 1 = 0.0243  |
| [ <i>I</i> > 2σ( <i>I</i> )]                  | <i>wR</i> 2 = 0.0580   | <i>wR</i> 2 = 0.0565  | <i>wR</i> 2 = 0.0377   |
| <i>R</i> indices                              | <i>R</i> 1 = 0.0375  | <i>R</i> 1 = 0.0565   | <i>R</i> 1 = 0.0360  |
| all data                                      | <i>wR</i> 2 = 0.0588   | <i>wR</i> 2 = 0.0577  | <i>wR</i> 2 = 0.0385   |



**Figure S1.** Solid EPR spectra of **Co-1** (top) and **Co-3** (bottom) at 4 K.