

## Supporting Information

# New atropisomeric N-N ligands for CO/vinyl arene copolymerization reaction

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**Table S1** U.V.-Visible absorption data for ligands **1-5**.

**Table S2** Selected <sup>1</sup>H NMR data for ligands **1-5** and complexes [Pd(N-N)<sub>2</sub>][PF<sub>6</sub>]<sub>2</sub> **1c-5c**.

**Fig. S1** Variable Temperature NMR of **3** in acetone-*d*<sub>6</sub>.

**Fig. S2** Variable Temperature NMR of **5** in acetone-*d*<sub>6</sub>.

**Table S1** U.V.-Visible absorption data for ligands **1-5**.<sup>a</sup>

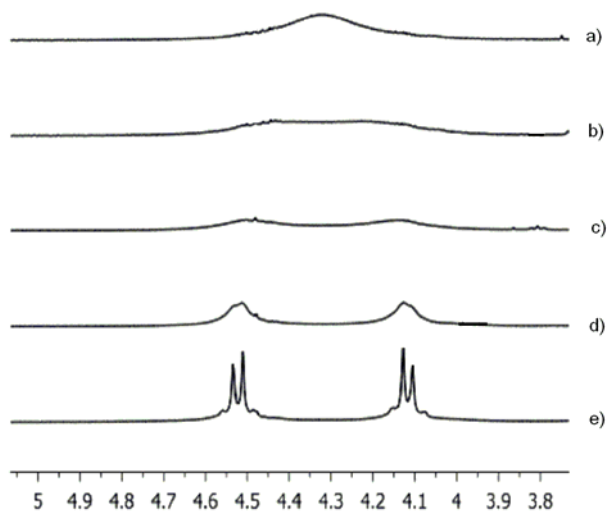
| Ligand          | $\lambda_{\text{max}}$ (95% EtOH)/nm ( $\epsilon/\text{dm}^3 \text{ mol}^{-1} \text{ cm}^{-1}$ ) |
|-----------------|--------------------------------------------------------------------------------------------------|
| 2,2'-bipyridine | 284 (12 800)                                                                                     |
| <b>1</b>        | 288 (8 300)                                                                                      |
| <b>2</b>        | 290 (8 800)                                                                                      |
| <b>3</b>        | 286 (6 000)                                                                                      |
| <b>4</b>        | 292 (2 200)                                                                                      |
| <b>5</b>        | 298 (10 400)                                                                                     |

<sup>a</sup> U.V.-Visible spectra recorded in EtOH ( $5.10^{-5} \text{ mol.L}^{-1}$ ) at 25 °C.

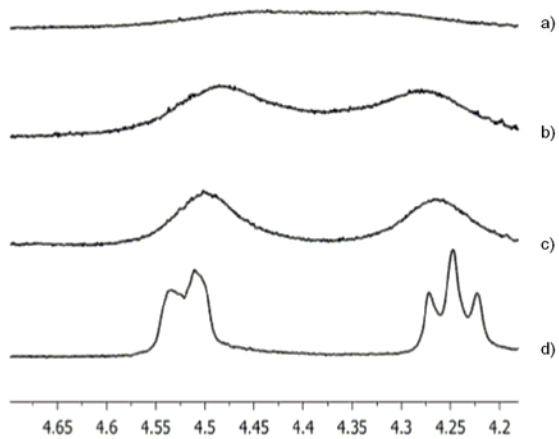
**Table S2** Selected <sup>1</sup>H NMR data for ligands **1-5**<sup>a</sup> and complexes [Pd(N-N)<sub>2</sub>][PF<sub>6</sub>]<sub>2</sub> **1c-5c**.<sup>b</sup>

| Ligand/Complex | H <sup>6,6'</sup> | H <sup>5,5'</sup> | H <sup>4,4'</sup> |
|----------------|-------------------|-------------------|-------------------|
| <b>1</b>       | 8.52              | 7.36              | 7.48              |
| <b>1c</b>      | 8.71              | 8.00              | 8.25              |
| <b>2</b>       | 8.58              | 7.34              | 7.46              |
| <b>2c</b>      | 8.62              | 7.93              | 8.17              |
| <b>3</b>       | 8.63              | 7.39              | 7.50              |
| <b>3c</b>      | 8.70              | 7.96              | 8.21              |
| <b>4</b>       | 8.49              | 7.31              | 7.44              |
| <b>4c</b>      | 8.29              | 7.80              | 7.87              |
| <b>5</b>       | 8.47              | 7.31              | 7.40              |
| <b>5c</b>      | 8.72              | 8.06              | 8.41              |

<sup>a</sup> Spectra recorded in CD<sub>2</sub>Cl<sub>2</sub>, at room temperature. <sup>b</sup> Spectra recorded in acetone-*d*<sub>6</sub>, at room temperature.



**Fig. S1** Variable Temperature NMR of **3** in acetone- $d_6$ : a) 20 °C; b) 11 °C; c) 0 °C; d) -20 °C; e) -40 °C.



**Fig. S2** Variable Temperature NMR of **5** in acetone- $d_6$ : a) 20 °C; b) 0 °C; c) -20 °C; d) -40 °C.