Supporting Information

N-donor functionalized N-heterocyclic carbene nickel(II) complexes in the Kumada coupling

Joris Berding, Thomas F. van Dijkman, Martin Lutz, Anthony L. Spek and Elisabeth Bouwman*

Coordination and Bio-Inorganic Chemistry, Leiden Institute of Chemistry, Leiden University, P.O. Box 9502, 2300 RA, Leiden, The Netherlands, and Bijvoet Center for Biomolecular Research, Crystal and Structural Chemistry, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands

bouwman@chem.leidenuniv.nl

Figure S1. Hydrogen bonding in the crystal structure of 5a
Table S1. Hydrogen bonding geometry in the crystal structure of 5a.
Figure S2. $^1$H NMR spectrum of complex 7 in DMSO.
Figure S3. COSY NMR spectrum of complex 8 in CDCl$_3$.
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References
Figure S1. Discrete hydrogen-bonded aggregate of metal complexes, methanol and water molecules in the asymmetric unit of 5a. C-H hydrogen atoms are omitted for clarity. Geometrical characterizations of the hydrogen bonds are provided in Table S1.

Table S1. Hydrogen bonding geometry in the crystal structure of 5a.

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<tbody>
<tr>
<td>O5-H5O···O19</td>
<td>0.96</td>
<td>1.80</td>
<td>2.740(2)</td>
<td>168</td>
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<td>O6-H6O···O29</td>
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<tr>
<td>O9-H9A···O8</td>
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<td>1.98</td>
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<tr>
<td>O9-H9B···O39</td>
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<td>1.94</td>
<td>2.797(3)</td>
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</table>
Figure S2. $^1$H NMR spectrum of complex 7 in DMSO. The figure was prepared with the program MestReNova.¹

Figure S3. COSY NMR spectrum of complex 8 in CDCl₃. The residual solvent peak is marked with (*). The figure was prepared with the program MestReNova.¹
Figure S4. Quaternion fit of the two independent metal complexes in the crystal structure of 5a, based on the six-membered chelate ring of the first ligand. The calculation was performed with the program PLATON.²
Figure S5. Quaternion fit of the two independent metal complexes in the crystal structure of 8, based on the six-membered chelate ring. Both independent molecules are located on an inversion centre. The calculation was performed with the program PLATON.²
Figure S6. C-H···Ni and C-H···π interactions in the two independent molecules of 8.
H118···Ni1, 2.72 Å; C118···Ni1, 3.579(2) Å; C118-H118···Ni1, 151°; H16A···Cg, 2.54 Å;
C16···Cg, 3.485(2) Å; C16-H16A···Cg, 161°; H27B···Cg, 2.65 Å; C27···Cg, 3.5420(19); C27-
H27B···Cg, 150°.
References