Electronic Supplementary Information for Dalton Transactions

Supporting Information

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

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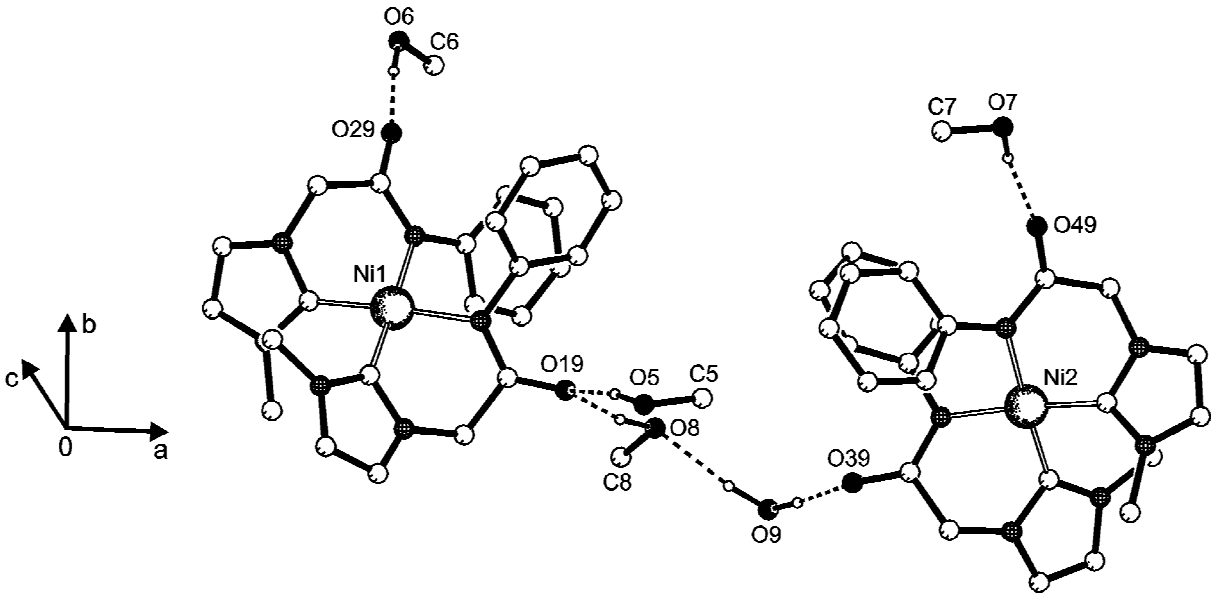

Figure S1. Discrete hydrogen-bonded aggregate of metal complexes, methanol and water molecules in the asymmetric unit of **5a**. C-H hydrogen atoms are omitted for clarity. Geometrical characterizations of the hydrogen bonds are provided in Table S1.

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

	D-H [Å]	H···A [Å]	D····A [Å]	D-H···A [°]
O5-H5O···O19	0.96	1.80	2.740(2)	168
O6-H6O···O29	0.93	1.75	2.675(2)	173
O7-H7O···O49	0.89	1.86	2.731(3)	166
O8-H8O···O19	1.05	1.70	2.737(3)	169
O9-H9A···O8	1.02	1.98	2.934(3)	154
O9-H9B···O39	0.96	1.94	2.797(3)	175

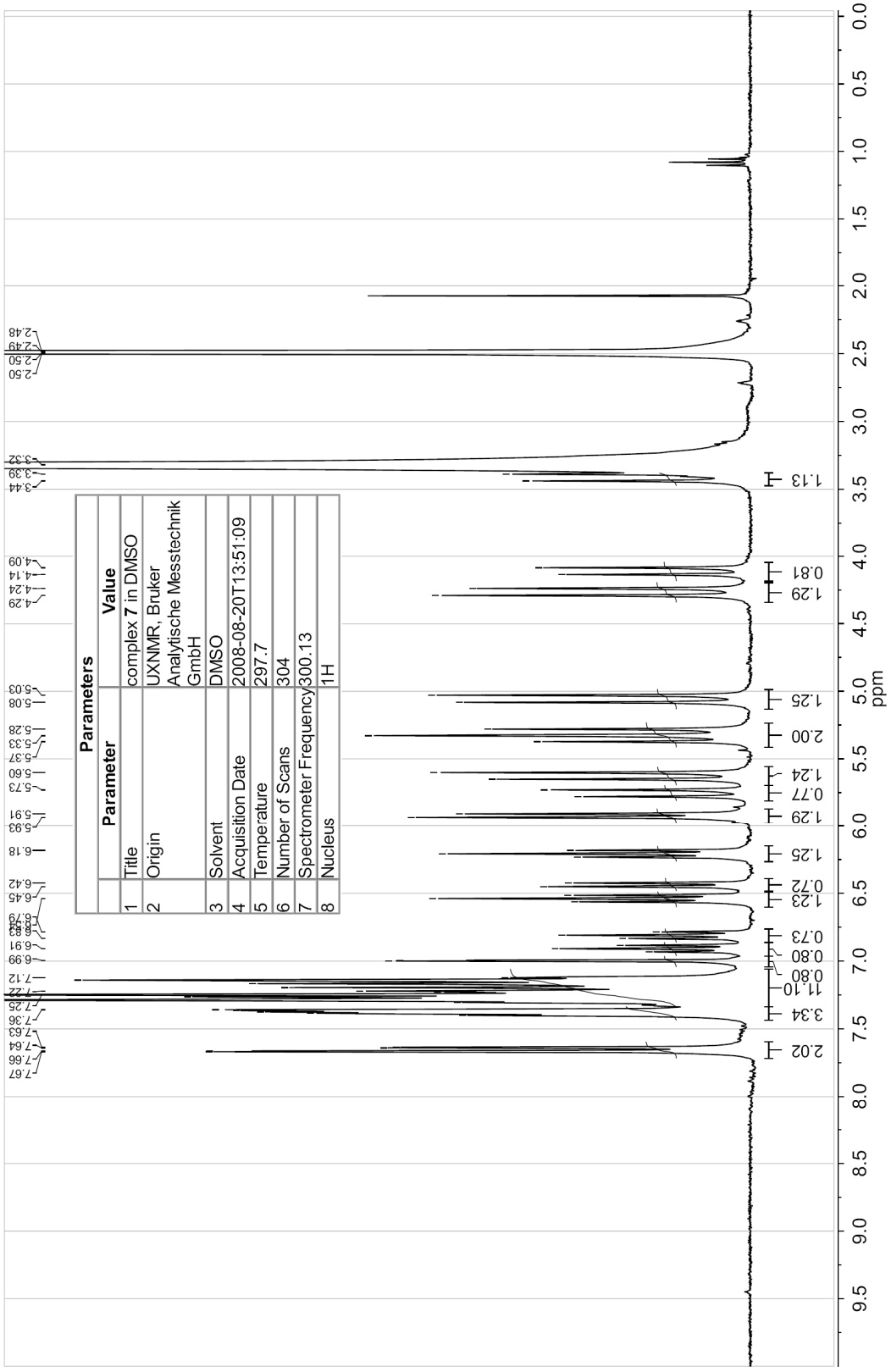

Figure S2. ^{1}H NMR spectrum of complex **7** in DMSO. The figure was prepared with the program MestReNova.[1]

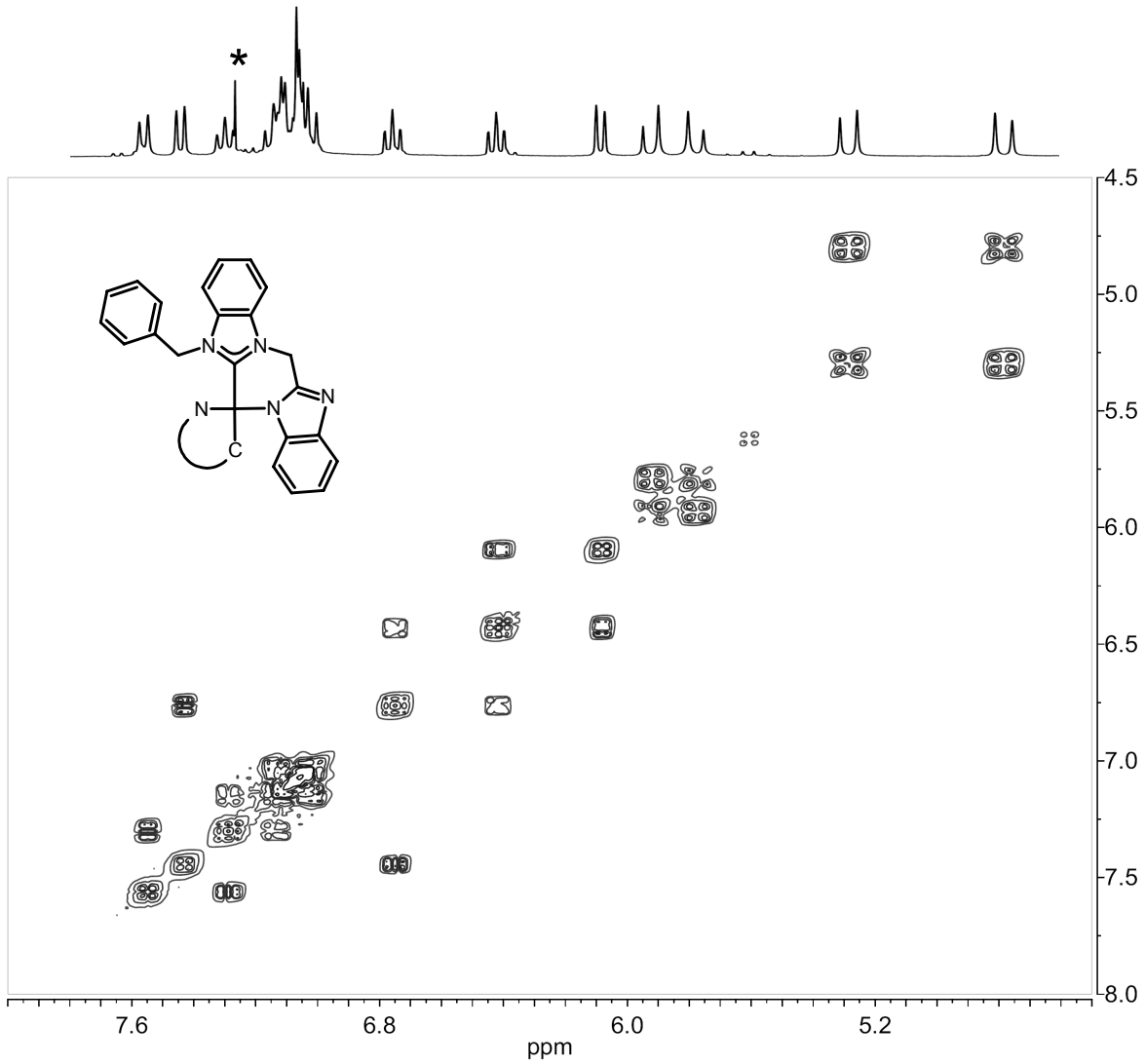

Figure S3. COSY NMR spectrum of complex **8** in $CDCl_3$. The residual solvent peak is marked with (*).The figure was prepared with the program MestReNova.[1]

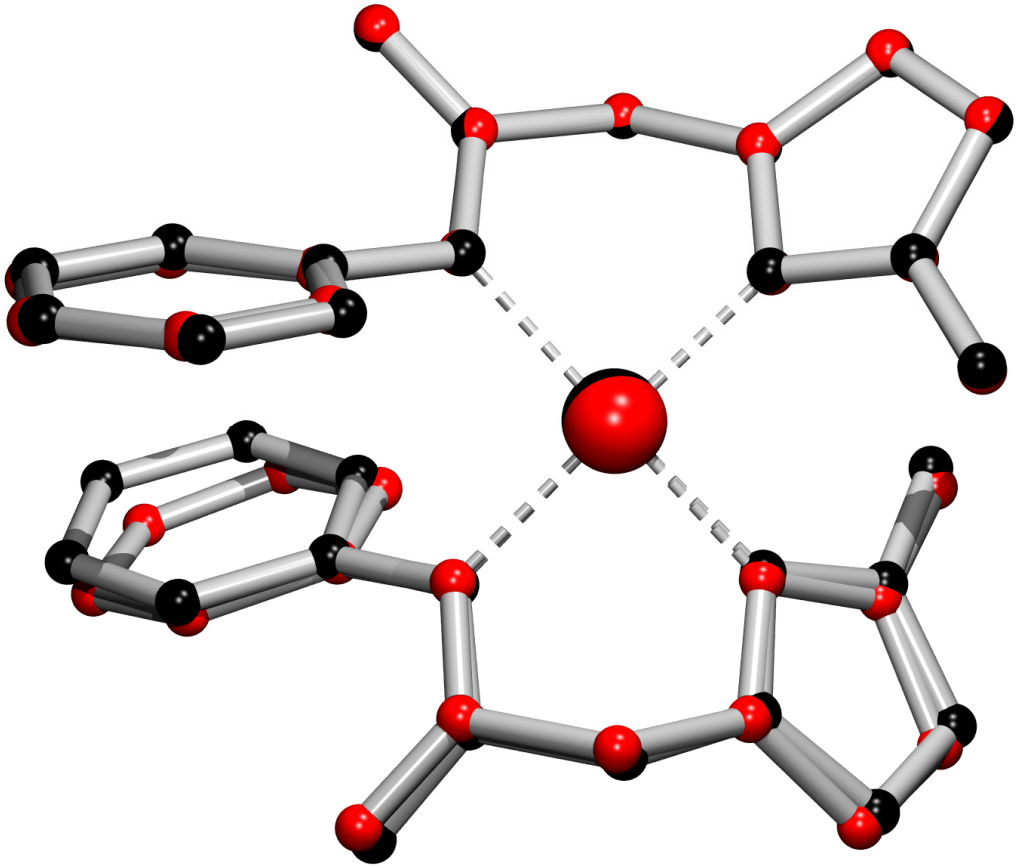

Figure S4. Quaternion fit of the two independent metal complexes in the crystal structure of **5a**, based on the six-membered chelate ring of the first ligand. The calculation was performed with the program PLATON.[2]

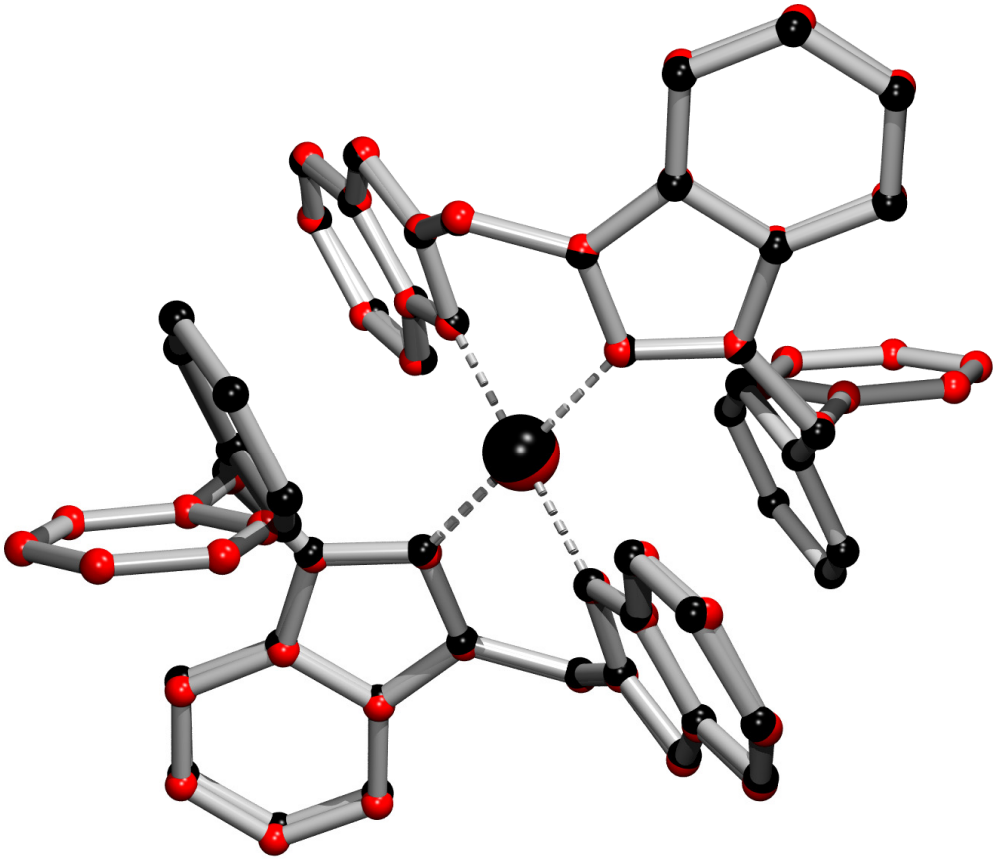

Figure S5. Quaternion fit of the two independent metal complexes in the crystal structure of **8**, based on the six-membered chelate ring. Both independent molecules are located on an inversion centre. The calculation was performed with the program PLATON.[2]

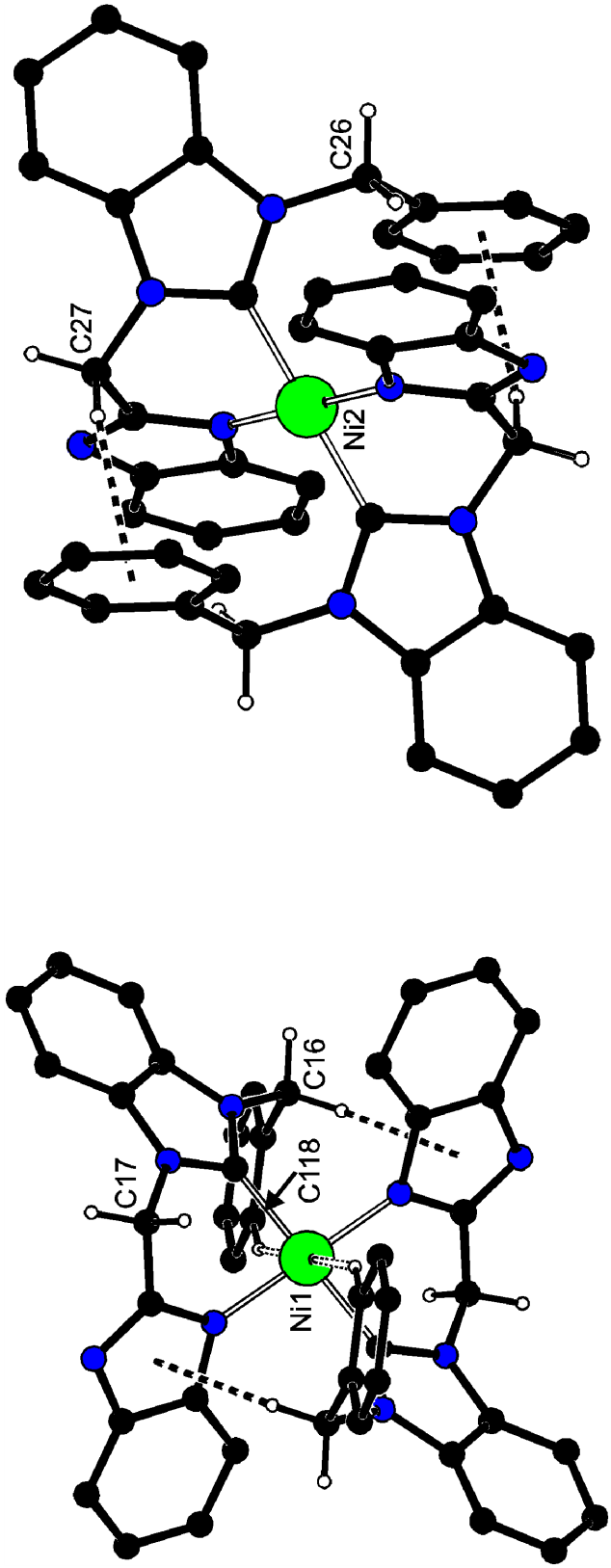

Figure S6. C-H···Ni and C-H···π interactions in the two independent molecules of **8**. H118···Ni1, 2.72 Å; C118···Ni1, 3.579(2) Å; C118-H118···Ni1, 151°; H16A···Cg, 2.54 Å; C16···Cg, 3.485(2) Å; C16-H16A···Cg, 161°; H27B···Cg, 2.65 Å; C27···Cg, 3.5420(19); C27-H27B···Cg, 150°.

References

1 MestReNova, version 5.1.0, Mestrelab Research S.L., Santiago de Compostela, Spain, www.mestrelab.com, 2009.
2 A. L. Spek, *J. Appl. Cryst.*, 2003, **36**, 7.