Article

Benzothiazole Nickelation: an Obstacle to the Catalytic Arylation of Azoles by Cyclopentadienyl Nickel N-Heterocyclic Carbene Complexes

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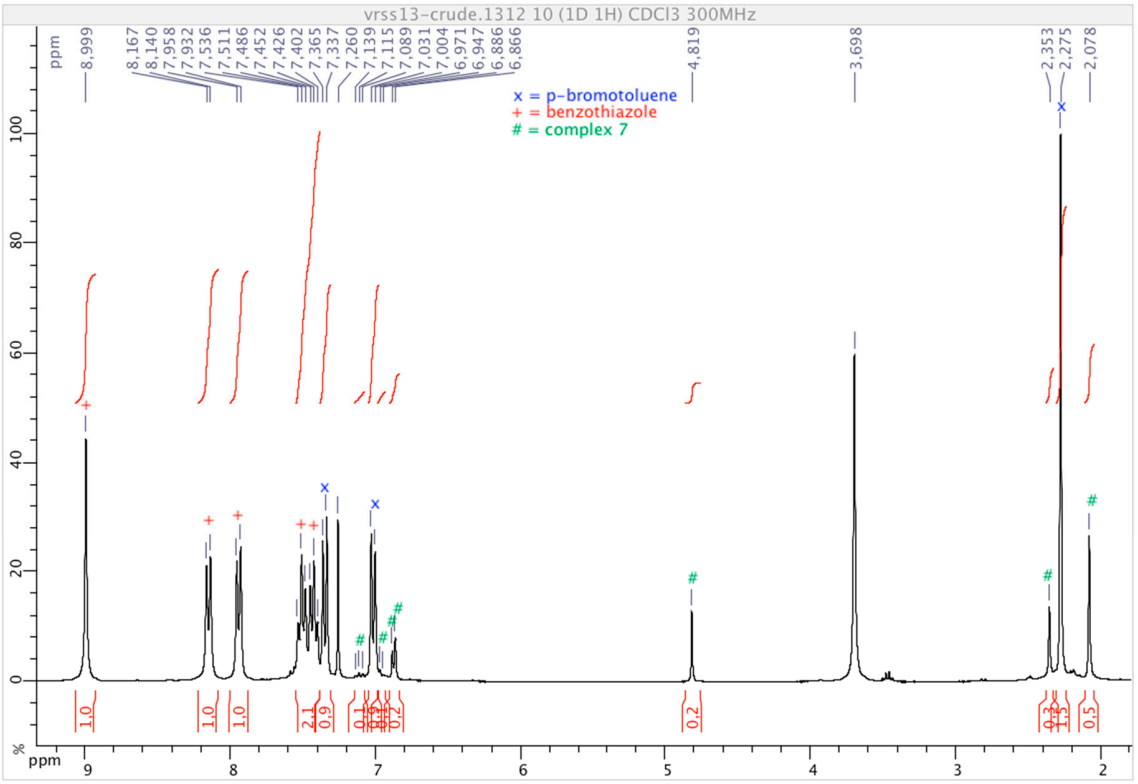

Figure S1. ^{1}H NMR spectrum of a "catalytic" reaction medium after 16 h reaction at 120 °C in 1,4-dioxane between benzothiazole and 4-bromotoluene in the presence of **3** and LiO*t*Bu.

Note: The 'benzothiazole : haloarene : complex **7**' ratio slightly varied from one "catalytic" reaction to another, most probably depending on the evaporation, extraction and filtration steps (see experimental section) but the latter were always the only three compounds observed (see also Fig. S2 and S3).

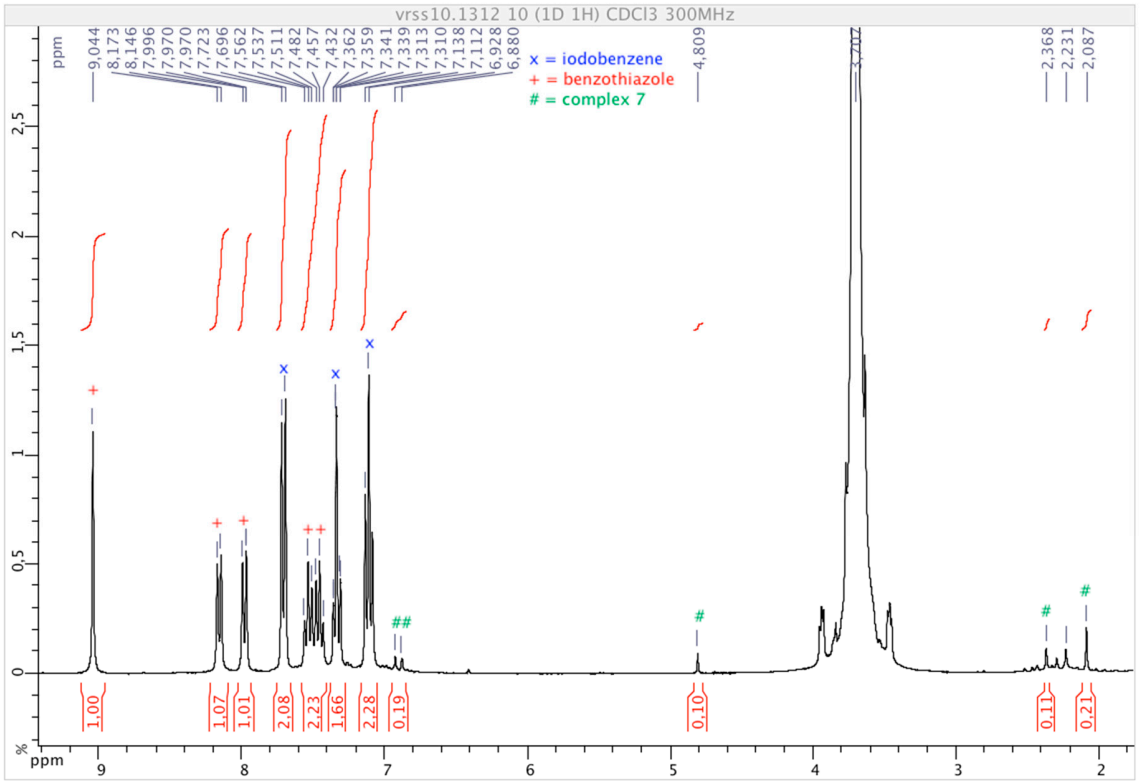

Figure S2. ^{1}H NMR spectrum of a "catalytic" reaction medium after 16 h reaction at 120 °C in 1,4-dioxane between benzothiazole and iodobenzene in the presence of **3** and KO*t*Bu.

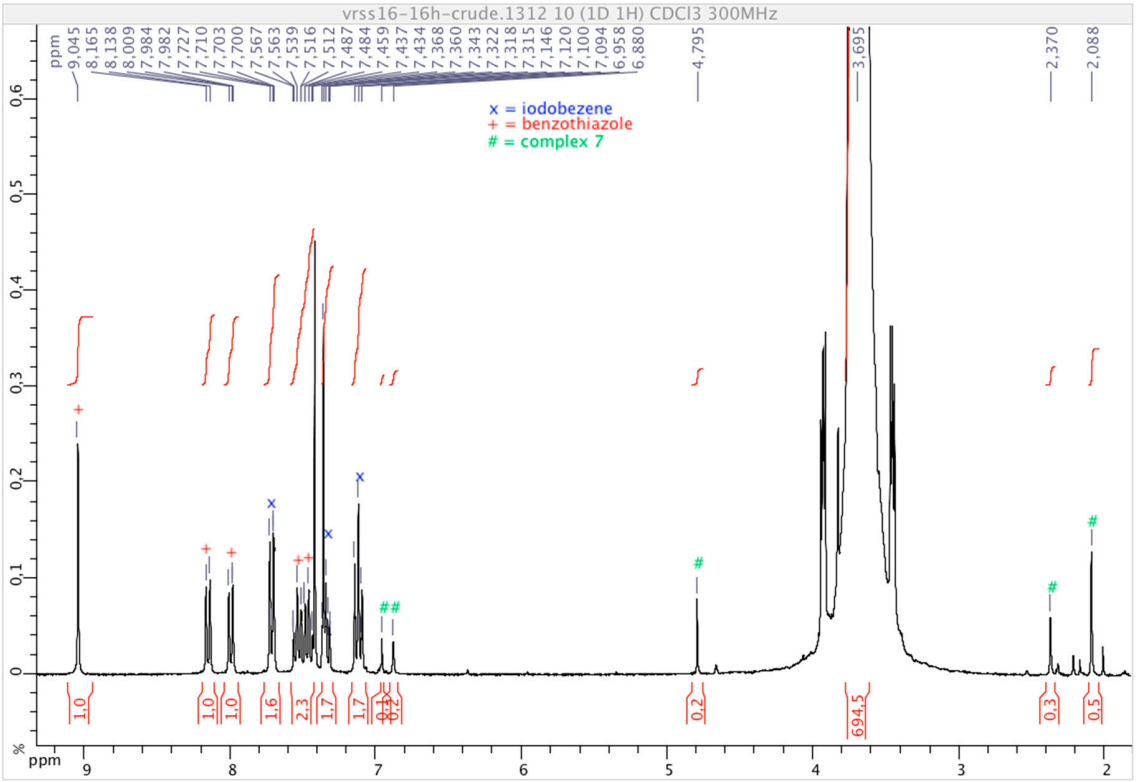

Figure S3. ^{1}H NMR spectrum of a "catalytic" reaction medium after 16 h reaction at 120 °C in 1,4-dioxane between benzothiazole and iodobenzene in the presence of **6** and LiO*t*Bu.

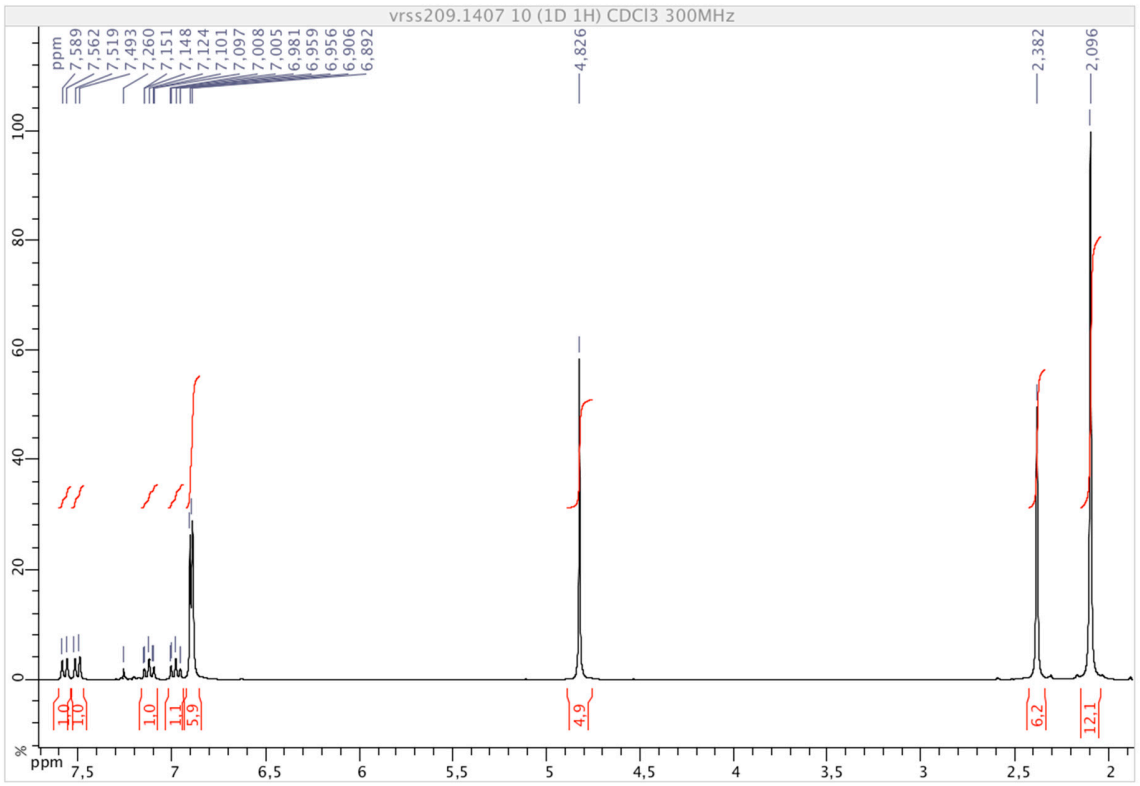

Figure S4. ^{1}H NMR spectrum of [NiCp(C_7H_4NS)(IMes)]

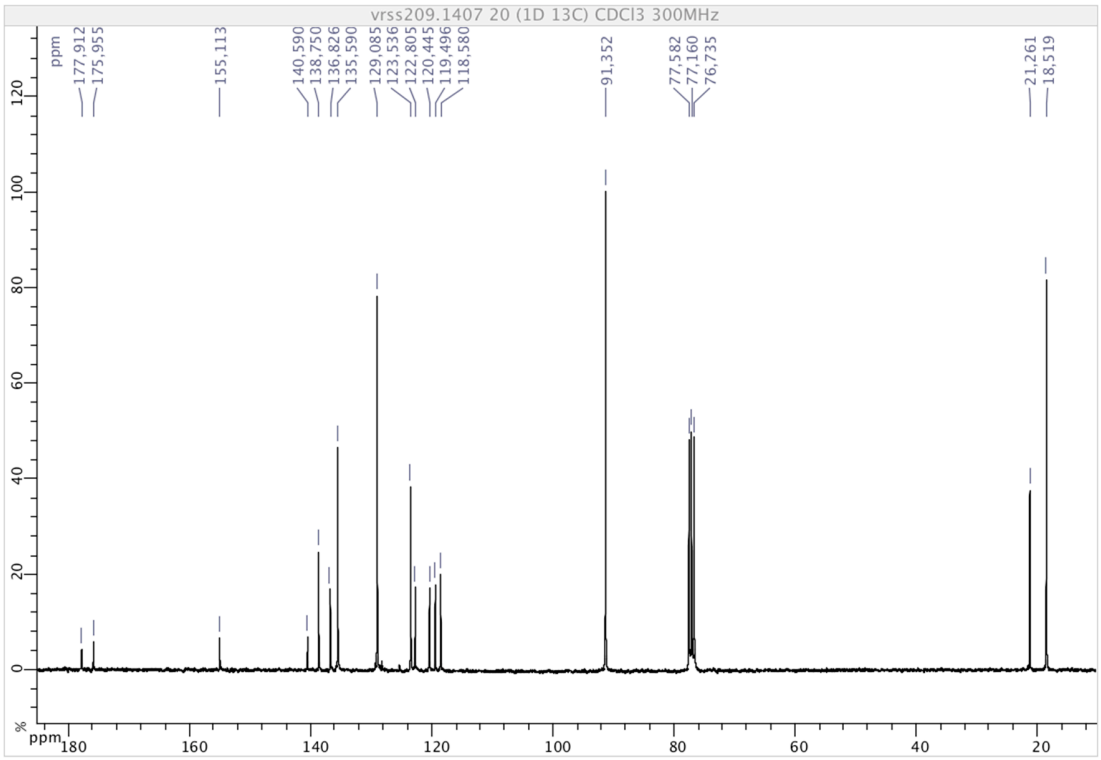

Figure S5. ^{13}C {^{1}H} NMR spectrum of [NiCp(C_7H_4NS)(IMes)]

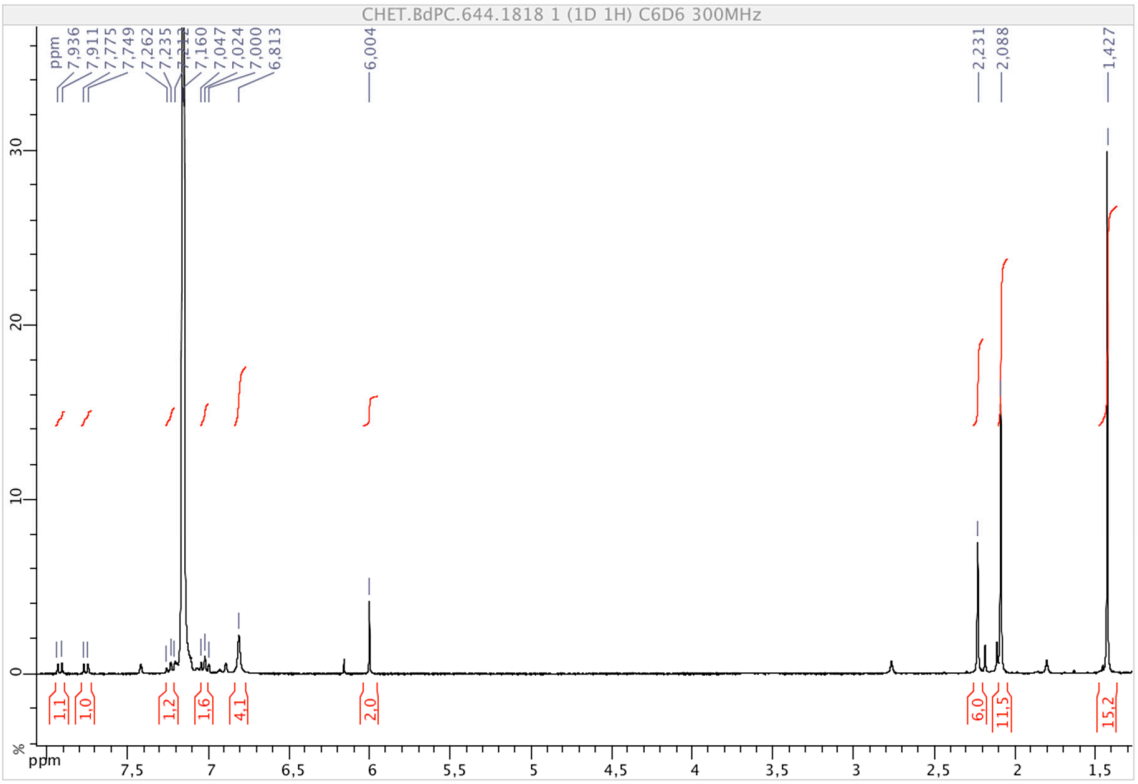

Figure S6. ^{1}H NMR spectrum of [NiCp*(C_7H_4NS)(IMes)]

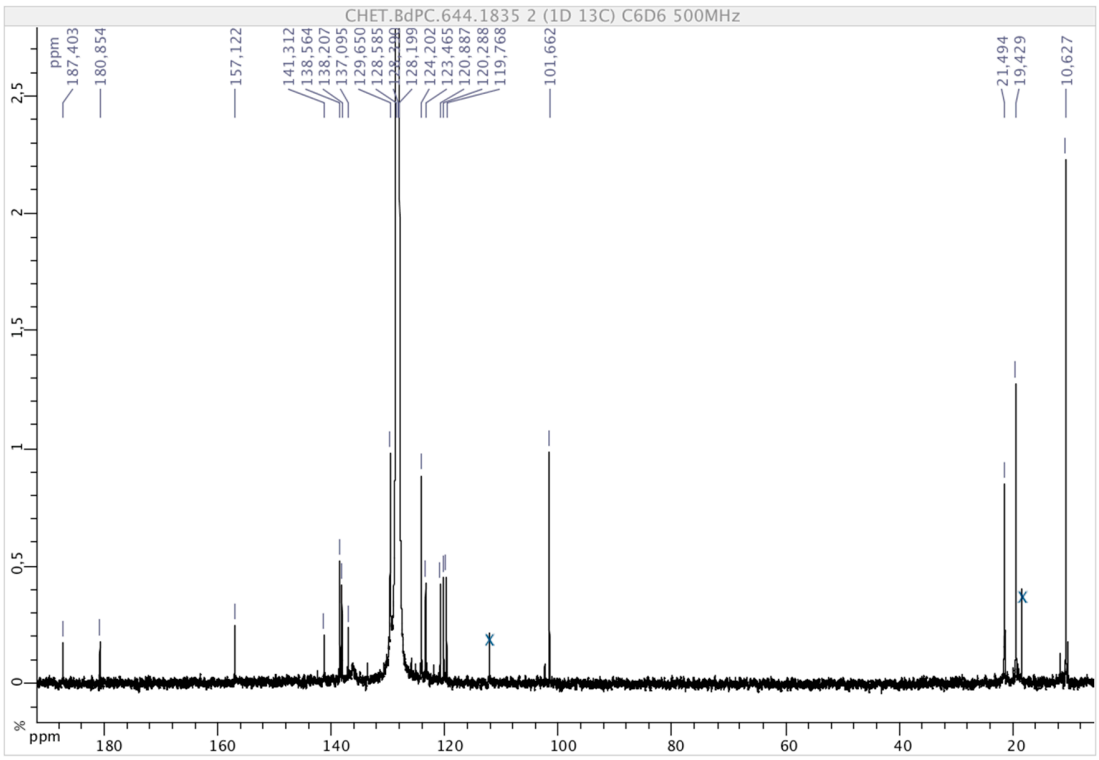

Figure S7. ^{13}C {^{1}H} NMR spectrum of [NiCp*(C_7H_4NS)(IMes)]

Table S1. Crystal data and refinement details of compound **7**.

Compound	**7**
Molecular formula	$C_{33}H_{33}N_3NiS$
Formula weight	562.39
Crystal system	Orthorhombic
Data collection temperature (K)	173(2)
Crystal size (mm)	0.40 × 0.16 × 0.06
Crystal form, colour	Prism, brown
Space group	$P2_12_12_1$
a (Á)	7.6555(4)
b (Á)	9.7436 (5)
c (Á)	37.6422(19)
V (Á^3)	2807.8(2)
Z	4
D_{calcd} (g.cm^{-3})	1.330
Absorption coefficient μ (mm^{-1})	0.792
h, k, l_{max}	4, 12, 49
Measured reflections	11624
Independent reflections, R_{int}	5624, 0.0204
Reflections with I > 2σ(I)	5008
R [$F^2 > 2\sigma(F^2)$]	0.0350
$wR(F^2)$	0.0685
Goodness-of-fit (GOF) on F^2	1.047