

*Supporting Information for:*

**SYNTHESIS OF N-HETEROCYCLIC CARBENE LIGANDS FOR  
SITE-SELECTIVE C-H ALKYLATION BY COOPERATIVE  
NICKEL/ALUMINUM CATALYSIS**

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### X-ray Crystallographic Analysis.

Crystallographic data of (L1)AuCl and (L2)AuCl were summarized in Table S1. Data of (L1)AuCl and (L2)AuCl were collected on a Rigaku/Saturn70 CCD diffractometer using graphite-monochromated Mo K $\alpha$  radiation ( $\lambda = 0.71070 \text{ \AA}$ ) at 143 K, and processed using CrysAlis<sup>Pro</sup> (Agilent).<sup>1</sup> CCDC 1865712 {(L1)AuCl} and CCDC 1865713 {(L2)AuCl} contain the supplementary crystallographic data. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

**Table S1.** Crystallographic data of (L1)AuCl and (L2)AuCl.

compound	(L1)AuCl	(L2)AuCl
empirical formula	C <sub>89</sub> H <sub>96</sub> AuClN <sub>2</sub> O <sub>4</sub>	C <sub>101</sub> H <sub>120</sub> AuClN <sub>2</sub> O <sub>2</sub>
formula weight	1490.17	1626.49
temp / K	143	143
crystal system	monoclinic	triclinic
space group	<i>P</i> 1 2/ <i>c</i> 1 (#13)	<i>P</i> -1 (#2)
<i>a</i> / $\text{\AA}$	14.1726(3)	16.1278(2)
<i>b</i> / $\text{\AA}$	12.8035(2)	24.1654(3)
<i>c</i> / $\text{\AA}$	21.6075(3)	25.8456(4)
$\alpha$ / deg	90.0000	104.9910(12)
$\beta$ / deg	95.1211(16)	106.4080(13)
$\gamma$ / deg	90.0000	104.3830(13)
<i>V</i> / $\text{\AA}^3$	3905.22(12)	8754.2(2)
<i>Z</i>	2	4
observed reflections	11149	46356
unique reflections	11149 (all data)	46356 (all data)
GOF	1.082	0.1070
<i>R</i> 1 (all data), <i>wR</i> 2 (all data) <sup>a</sup>	0.0398, 0.0954	0.1316

[a]  $R1 = \Sigma[|F_o| - |F_c|]/\Sigma|F_o|$ ,  $wR2 = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma w(F_o^2)^2]^{1/2}$ .

<sup>1</sup> CrysAlisPRO: Agilent Technologies Ltd, Yarnton, Oxfordshire, England (2014).













































