

SUPPORTING INFORMATION

REGULAR ARTICLE

**Synthesis and characterization of six-membered pincer nickelacycles and application in alkylation of benzothiazole<sup>†</sup>**

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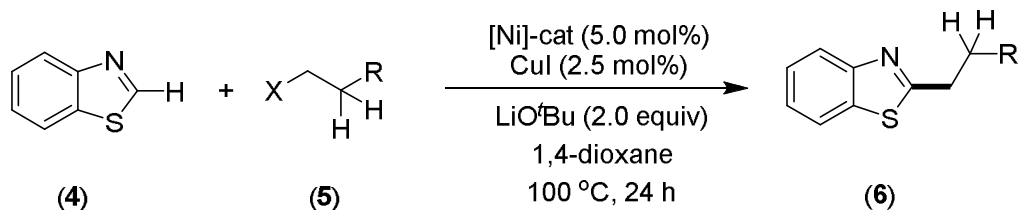
<sup>†</sup> Dedicated to Professor K. C. Kumara Swamy on the occasion of his 60<sup>th</sup> birth anniversary.

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## 1. Alkylation of benzothiazole

**Table S1.** Alkylation of benzothiazole with alkyl halides using various [Ni] catalysts.<sup>a</sup>



Alkyl halides (5)	Products (6)	Yield (%) of products with various [Ni]-catalysts		
		(iPr <sup>4</sup> POCCOP)NiBr (2)	(iPr <sup>4</sup> PCP)NiBr	(iPr <sup>4</sup> POCOP)Ni(OAc)
Me(CH <sub>2</sub> ) <sub>7</sub> -I (5a)	(6a)	91	53	42
Me(CH <sub>2</sub> ) <sub>4</sub> -I (5b)	(6b)	94	72	56
Me(CH <sub>2</sub> ) <sub>11</sub> -I (5c)	(6c)	61	32	7
Ph(CH <sub>2</sub> ) <sub>3</sub> -Br (5d)	(6d)	23	6	2

<sup>a</sup> Reaction conditions: Benzothiazole (0.027 g, 0.2 mmol), alkyl halide (0.4 mmol), [Ni]-catalyst (0.01 mmol, 5.0 mol%), CuI (0.001 g, 0.005 mmol, 2.5 mol%), LiO<sup>t</sup>Bu (0.032 g, 0.4 mmol), 1,4-dioxane (1.0 mL), 100 °C, 24 h. Yields were determined using *n*-dodecane as an internal standard.

## 2. Crystal data and structure refinement for complexes

**Table S2.** Crystal data and structure refinement for complexes **2** and **3**.

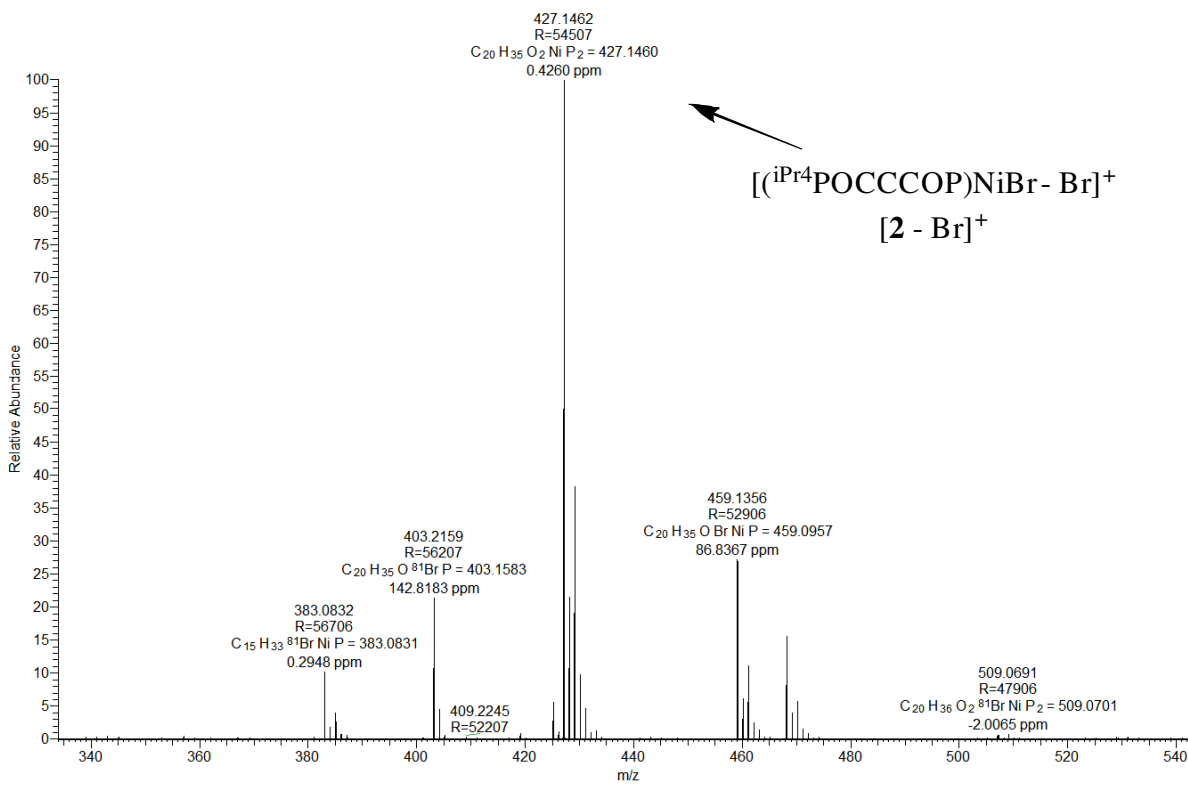
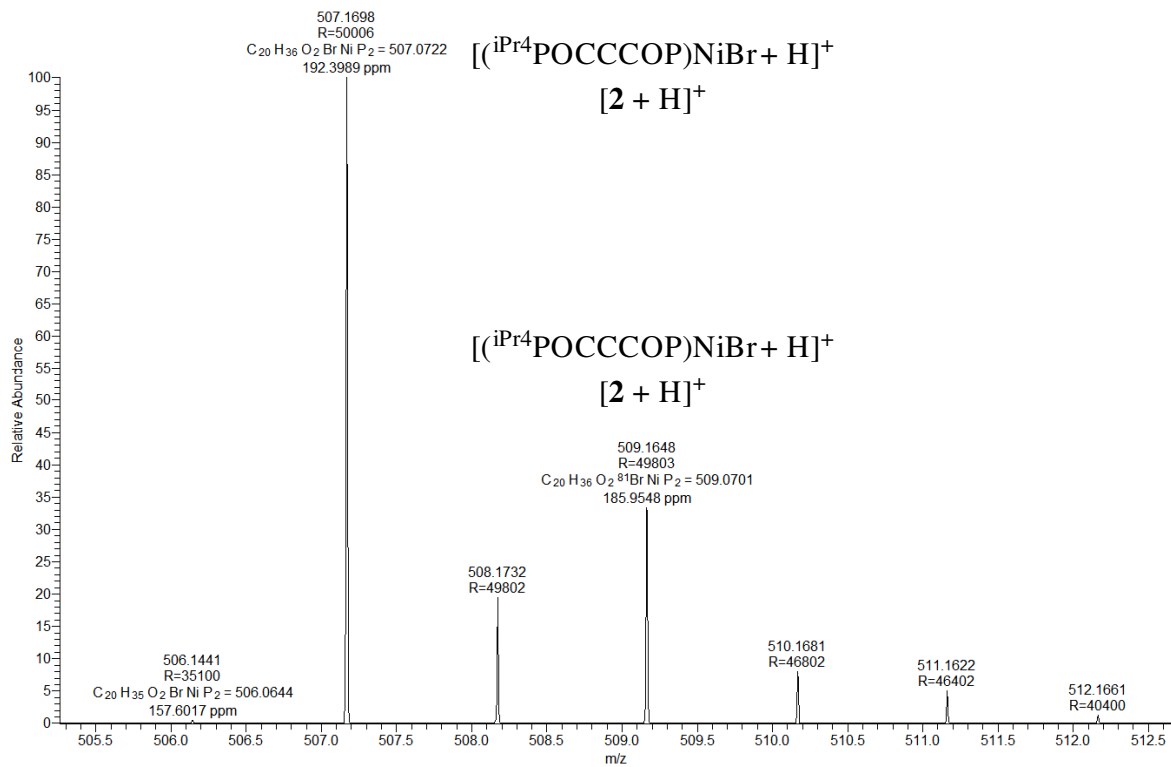
	<b>2</b>	<b>3</b>
Empirical formula	C <sub>20</sub> H <sub>35</sub> BrNiO <sub>2</sub> P <sub>2</sub>	C <sub>22</sub> H <sub>38</sub> NiO <sub>4</sub> P <sub>2</sub>
Formula weight	508.04	487.17
Temperature, K	296(2)	100(2)
Cryst. Syst.	Monoclinic	Triclinic
Space group	C2/c	P-1
<i>a</i> (Å)	7.8480(6)	7.3969(2)
<i>b</i> (Å)	26.140(2)	11.2664(3)
<i>c</i> (Å)	11.5713(9)	14.8162(4)
$\alpha$ (°)	90	93.368(2)
$\beta$ (°)	91.517(4)	96.251(2)
$\gamma$ (°)	90	96.745(2)
<i>V</i> (Å <sup>3</sup> )	2373.0(3)	1215.69(6)
<i>Z</i>	4	2
$\rho$ calcd. Mg/m <sup>3</sup>	1.422	1.331
$\varepsilon$ (mm <sup>-1</sup> )	2.648	0.954
<i>F</i> (000)	1056	520
Crystal size (mm <sup>3</sup> )	0.39 x 0.33 x 0.24	0.32 x 0.21 x 0.15
$\theta$ (min, max) (°)	2.711, 25.000	2.211, 24.998
R(int)	0.0552	0.0281
Independent reflections	2096	4216
Completeness to $\theta$ (%)	99.9	98.5
Max. and min. transmission	0.569, 0.425	0.870, 0.750
Data / restraints / parameters	2096 / 0 / 124	4216 / 0 / 271
GOF on F <sup>2</sup>	1.054	1.071

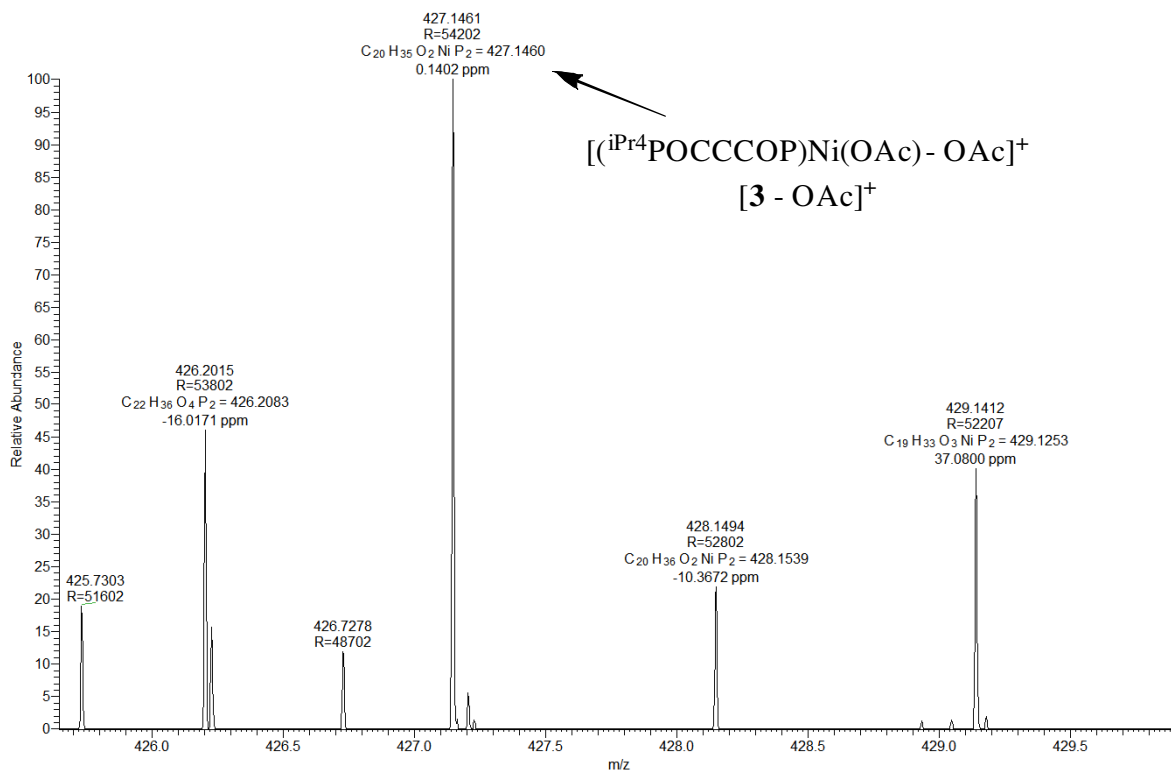
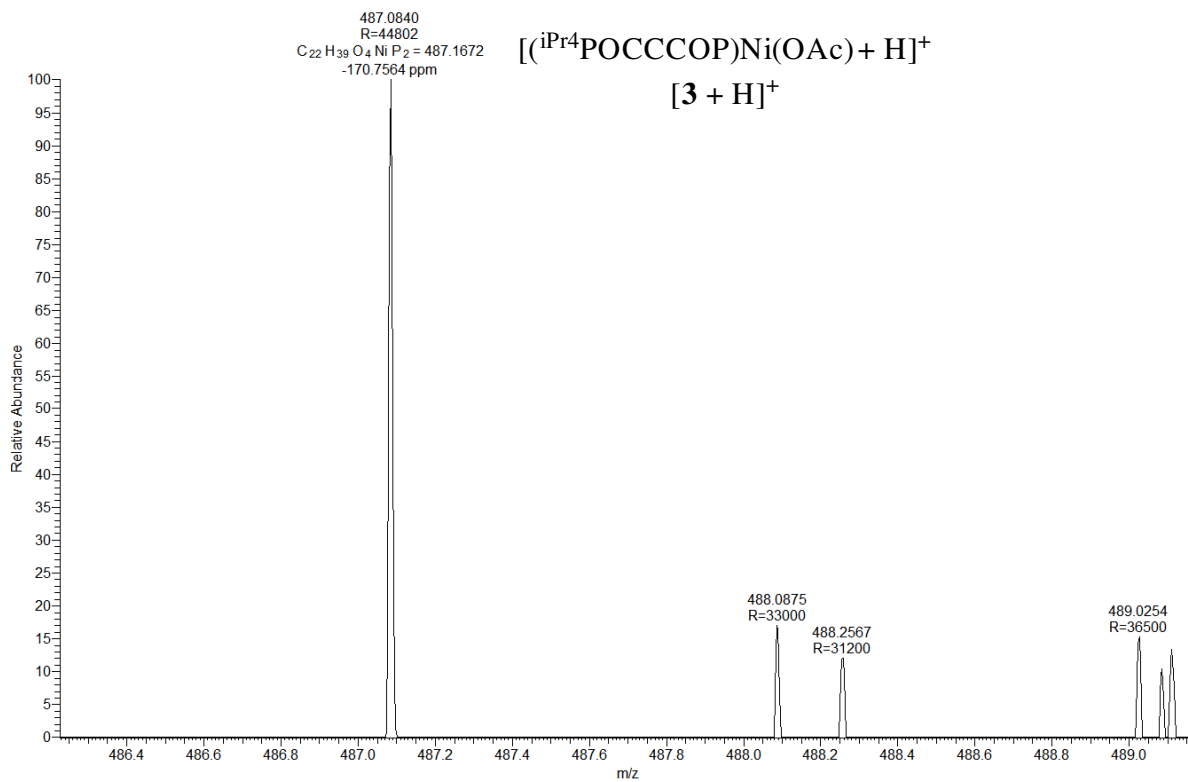
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R1, wR2 ( $I > 2\sigma(I)$ )	0.0306, 0.0785	0.0377, 0.0745
R1, wR2 (all data)	0.0336, 0.080	0.0458, 0.0774

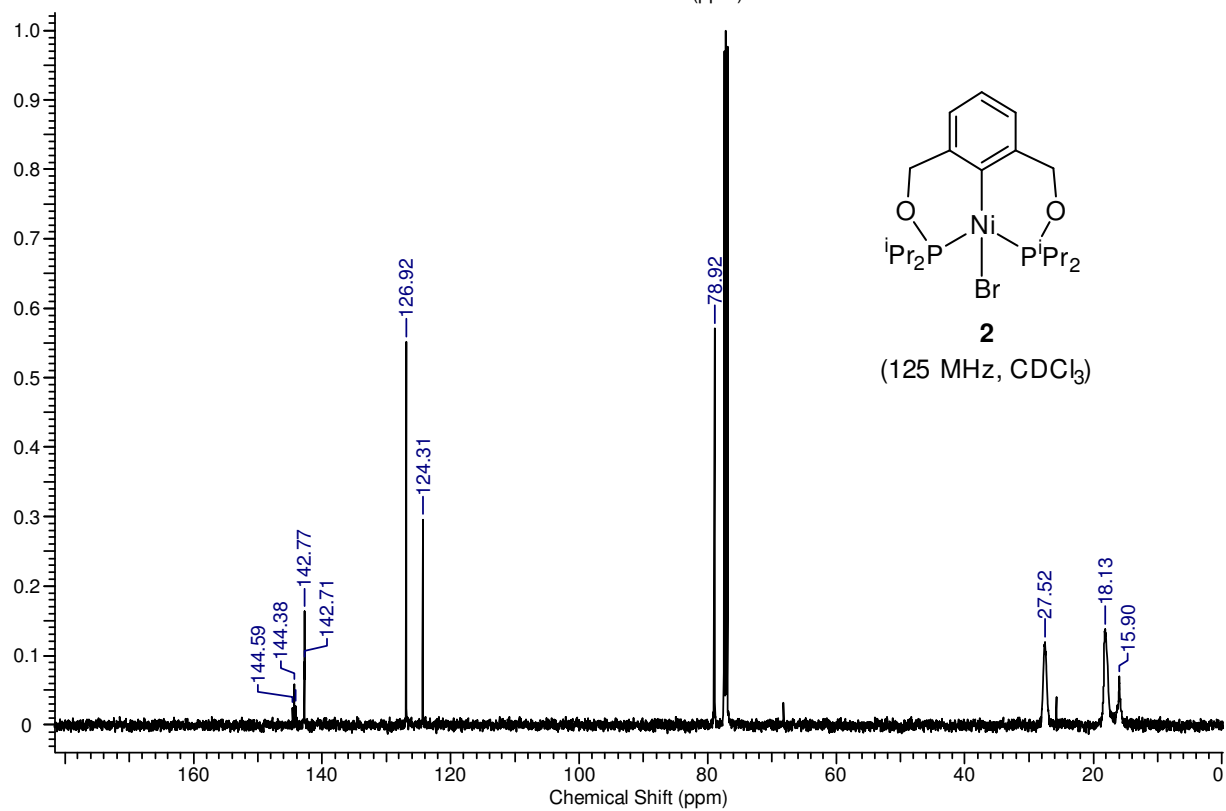
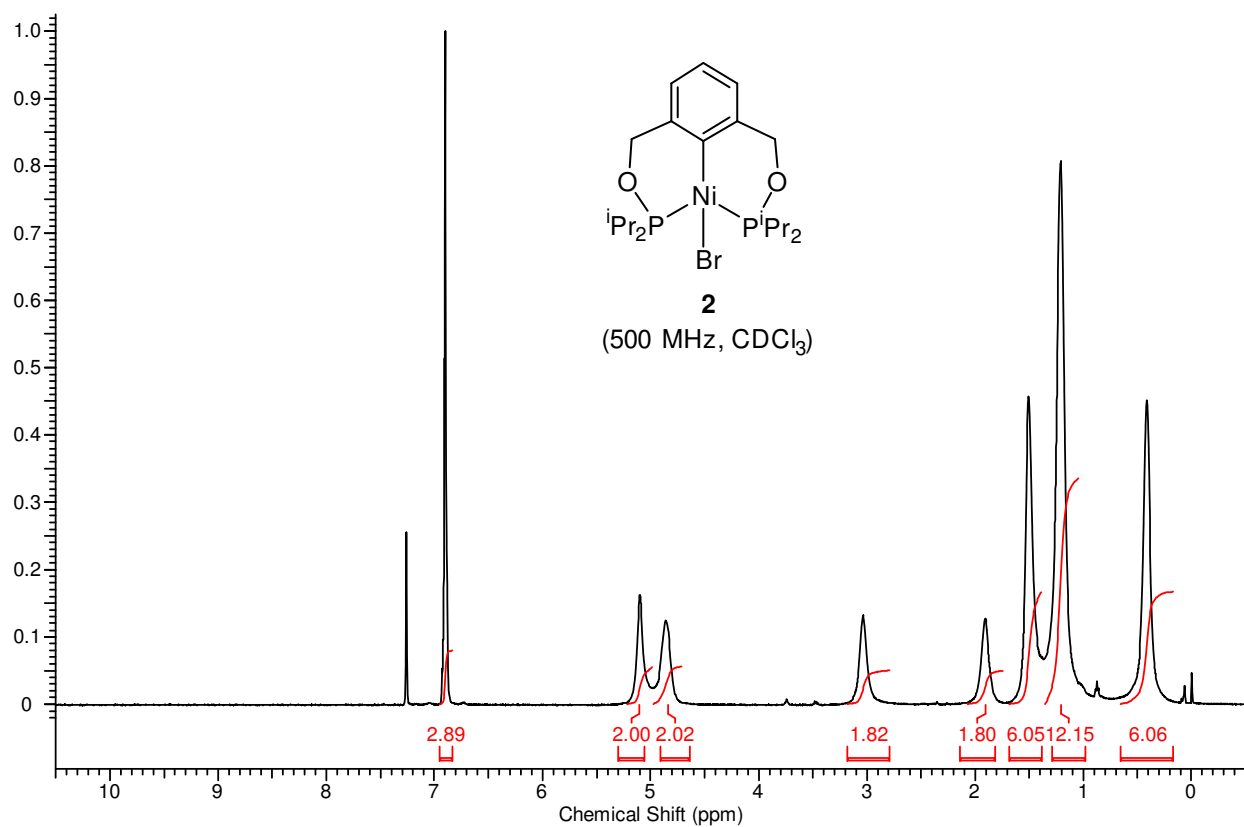
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### 3. HRMS of nickel complexes

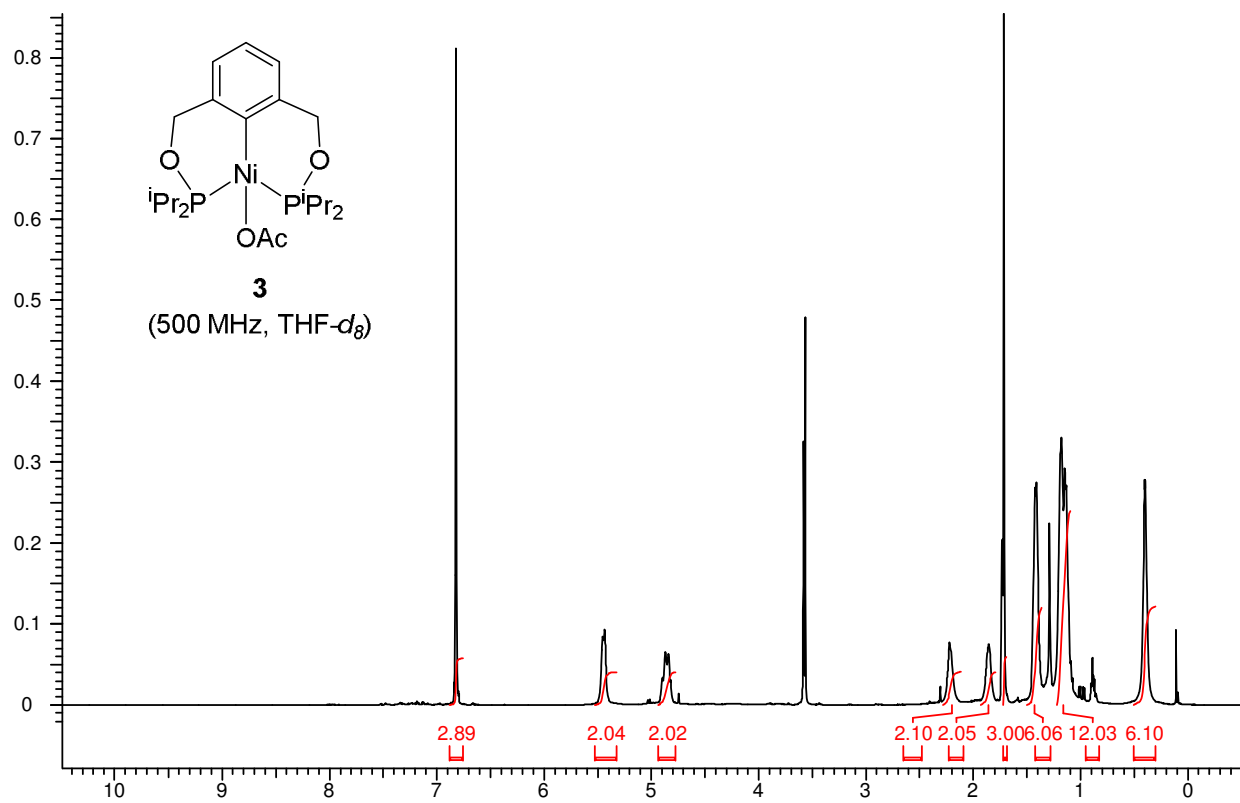
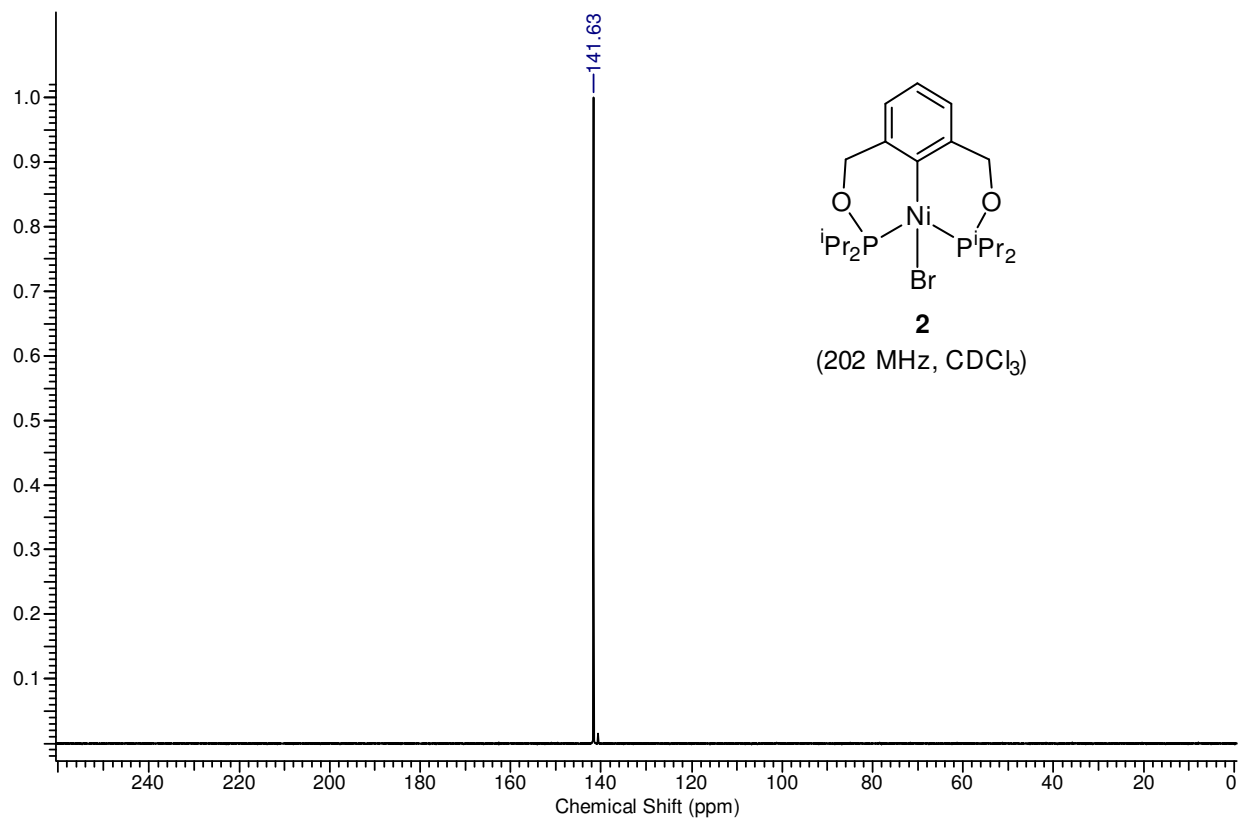


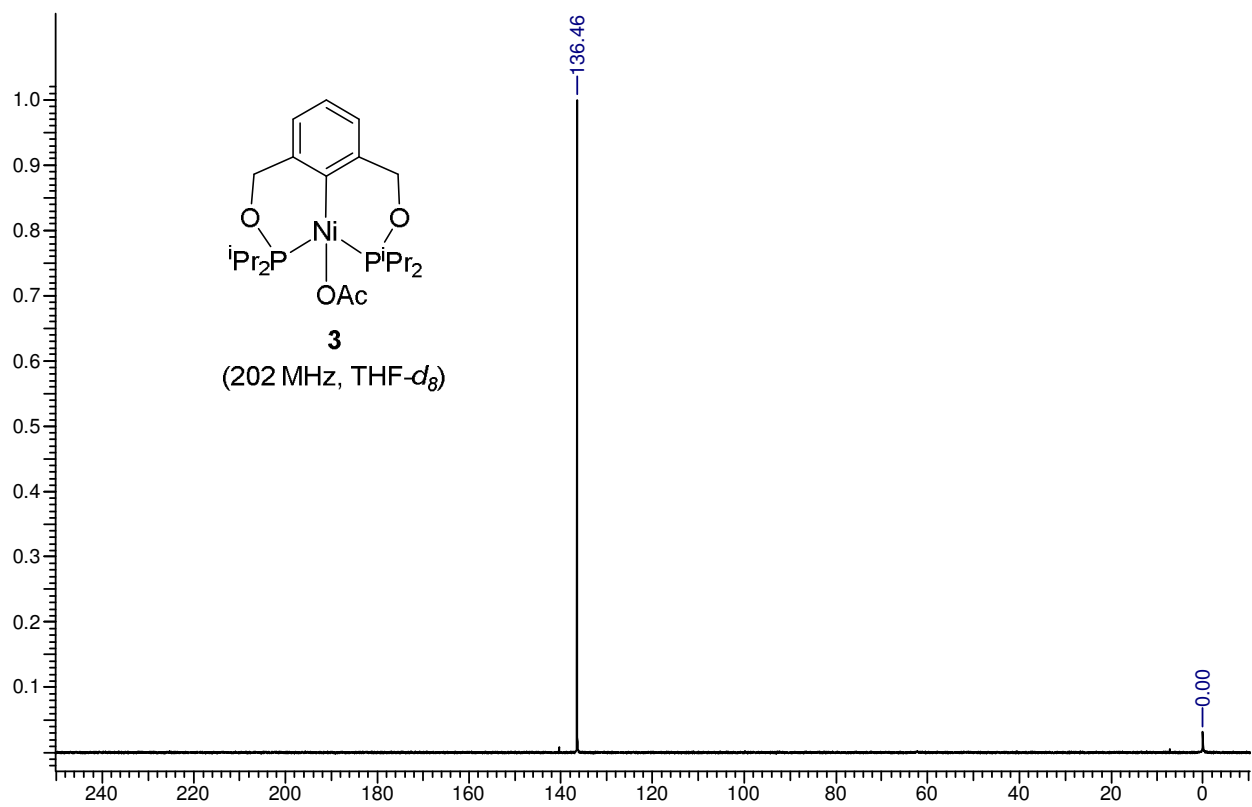
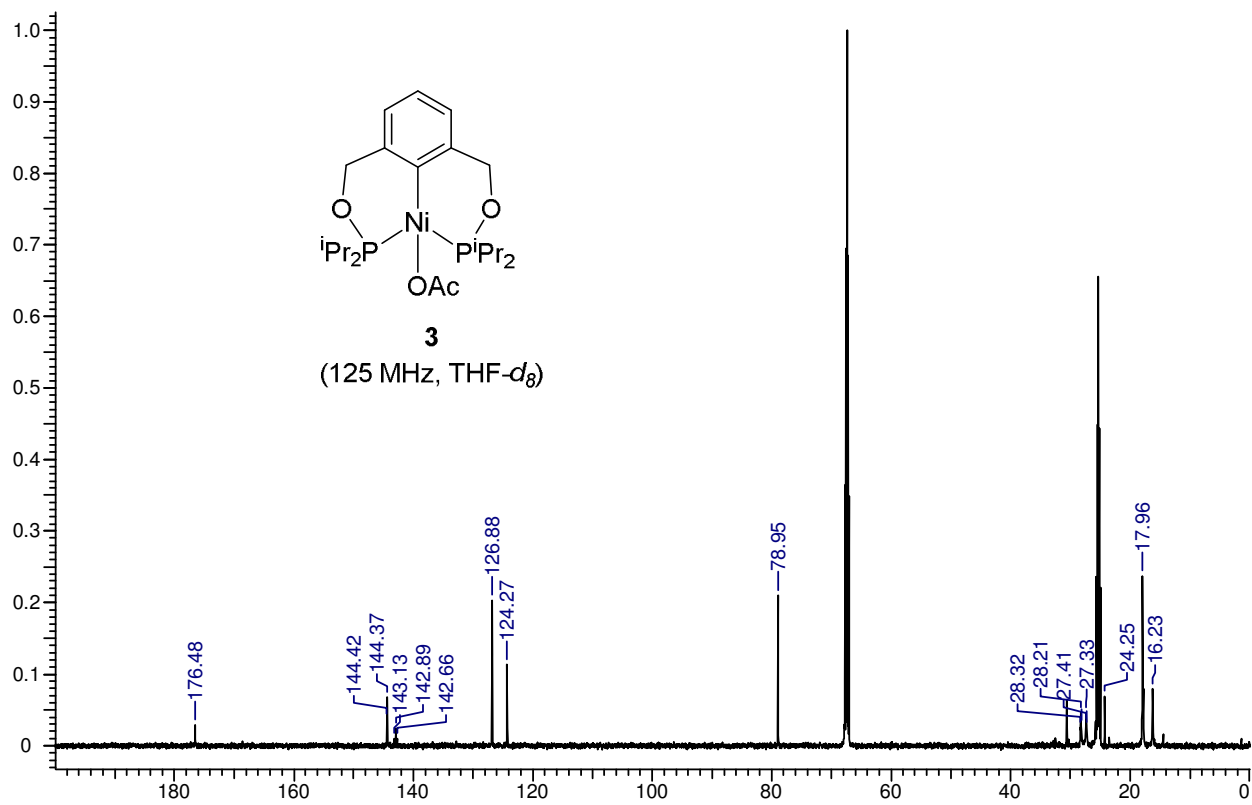


#### 4. NMR spectra of nickel complexes 2 and 3









## 5. GC-MS of 2-Octylated benzothiazole

