**New**

**Easily-preparable N-Heterocyclic Carbene (NHC) Precursors**

**Advantages**
- NHC ligands and catalysts are preparable by heating
- No salt is generated in preparation because of the absence of base

**Applications 1**

**NHC-CO₂ Adducts: Transition metal / NHC complex catalyst preparation**

<table>
<thead>
<tr>
<th>Metal</th>
<th>NHC-CO₂</th>
<th>Metal-NHC complex</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Rh(cod)Cl]₂</td>
<td>[B1045] D5401</td>
<td>Rh(cod)(NHC)Cl</td>
</tr>
<tr>
<td>[Ir(cod)Cl]₂</td>
<td>[C1807] B5603</td>
<td>Ir(cod)(NHC)Cl₂</td>
</tr>
<tr>
<td>Pd(OAc)₂</td>
<td>[P2161] Δ</td>
<td>Pd(NHC)₃(OAc)₂</td>
</tr>
</tbody>
</table>

Procedure:
A mixture of [Rh(cod)Cl]₂ (54 mg) and NHC-CO₂ adduct (2 eq.) is stirred in acetonitrile (3 ml) for 5 min at room temperature in a Schlenk flask, followed by heating at 75 °C for 20 min under an atmosphere of argon. The reaction mixture is dried in vacuo, and washed three times with diethyl ether. The yellow solid obtained is analytically pure (93%).


**NHC Hydrogencarbonate Salts: Transition metal / NHC complex catalyst preparation**

<table>
<thead>
<tr>
<th>Metal</th>
<th>NHC⁺ HCO₃⁻</th>
<th>Metal-NHC complex</th>
</tr>
</thead>
<tbody>
<tr>
<td>(CH₃)₂SAuCl</td>
<td>[C2719] D5513</td>
<td>Au(NHC)Cl</td>
</tr>
</tbody>
</table>

Procedure:
(CH₃)₂SAuCl (11.4 mg), NHC hydrogencarbonate salt (1.2 eq.), and THF (0.7 mL) are put in a capped vial (air atmosphere). After 1 h of stirring at 50 °C, the solution is filtered over silica and dried in vacuo. The Au-NHC complex is obtained as a colorless solid in 95% yield.

Easily-preparable \( N \)-Heterocyclic Carbene (NHC) Precursors

### Applications 2

#### NHC-CO\(_2\) Adducts: NHC-Catalyzed Conjugate Cyanations

\[
\begin{align*}
R^1 & \quad R^1 \\
\text{Me}_3\text{Si-CN} & \quad 10 \text{ mol % D5401} \\
\text{1,4-dioxane, rt} & \quad 25 \text{ examples} \\
\text{>78%} \\
\end{align*}
\]


#### NHC Hydrogencarbonate Salts: NHC-Catalyzed Benzoin Condensations

\[
\begin{align*}
\text{H} & \quad \text{R}^1 \\
\text{10 mol % D5498} & \quad \text{THF, 60 °C, MS3A} \\
\end{align*}
\]


1,3-Dimesitylimidazolium-2-carboxylate 1g [D5401]
1,3-Bis(2,6-diisopropylphenyl)imidazolium-2-carboxylate 1g [B5603]
1,3-Diisopropylimidazolium Hydrogencarbonate (contains varying amounts of 1,3-Diisopropylimidazolium-2-carboxylate) 1g [D5498]
1,3-Di-tert-butylimidazolium Hydrogencarbonate (contains varying amounts of 1,3-Di-tert-butylimidazolium-2-carboxylate) 1g [D5513]

### Related Products

- Chloro(1,5-cyclooctadiene)rhodium(I) Dimer (= \( \text{[Rh(cod)Cl]}_2 \)) 100mg / 1g [B1045]
- Chloro(1,5-cyclooctadiene)iridium(I) Dimer (= \( \text{[Ir(cod)Cl]}_2 \)) 250mg / 1g [C1807]
- Palladium(II) Acetate (Purified) (= \( \text{Pd(OAc)}_2 \)) 1g [P2161]
- Allylpalladium(II) Chloride Dimer (= \( \text{[Pd(allyl)Cl]}_2 \)) 500mg / 1g [A1479]
- Chloro(dimethylsulfide)gold(I) (= \( \text{(CH}_3\text{)}_2\text{SAuCl} \)) 200mg / 1g [C2719]

For further information please refer to our website at www.TCIchemicals.com.