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

**Advantages**
- NHC ligands and catalysts are preparable by heating.
- No salt generated during preparation.
- Applicable under neutral conditions.

### Applications 1

#### NHC-CO\(_2\) Adducts: Transition metal / NHC complex catalyst preparation

<table>
<thead>
<tr>
<th>Metal Complex</th>
<th>NHC-CO(_2) Adduct</th>
<th>Metal-NHC complex</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Rh(cod)Cl](_2)</td>
<td>[D5396]</td>
<td>Rh(cod)(NHC)Cl</td>
</tr>
<tr>
<td>[Ir(cod)Cl](_2)</td>
<td>[D5401]</td>
<td>Ir(cod)(NHC)Cl</td>
</tr>
<tr>
<td>Pd(OAc)(_2)</td>
<td>[B5603]</td>
<td>Pd(NHC)(_3)(OAc)(_2)</td>
</tr>
</tbody>
</table>

**Procedure:**
A mixture of [Rh(cod)Cl]\(_2\) (54 mg) and NHC-CO\(_2\) 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%).

**Cited Reference**

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

<table>
<thead>
<tr>
<th>Metal Complex</th>
<th>NHC*HCO(_3)</th>
<th>Metal-NHC complex</th>
</tr>
</thead>
<tbody>
<tr>
<td>[Pd(allyl)Cl](_2)</td>
<td>D5498</td>
<td>Pd(allyl)(NHC)Cl</td>
</tr>
<tr>
<td>(CH(_3)(_2))(_2)AuCl</td>
<td>D5513</td>
<td>Au(NHC)Cl</td>
</tr>
</tbody>
</table>

**Procedure:**
(CH\(_3\)\(_2\))\(_2\)AuCl (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.

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

Applications 2

NHC-CO₂ Adducts: NHC-Catalyzed Conjugate Cyanations

\[ R^1 \text{Me₃Si-CN} \rightarrow 10 \text{ mol } \% \text{ D5401} \]

\[ \begin{align*}
\text{1,3-Dimethylimidazolium-2-carboxylate} & \quad 1g \quad [D5396] \\
\text{1,3-Dimesitylimidazolium-2-carboxylate} & \quad 1g \quad [D5401] \\
\text{1,3-Bis(2,6-diisopropylphenyl)imidazolium-2-carboxylate} & \quad 1g \quad [B5603] \\
\text{1,3-Diisopropylimidazolium Hydrogencarbonate (contains varying amounts of 1,3-Diisopropylimidazolium-2-carboxylate)} & \quad 1g \quad [D5498] \\
\text{1,3-Di-tert-butylimidazolium Hydrogencarbonate (contains varying amounts of 1,3-Di-tert-butylimidazolium-2-carboxylate)} & \quad 1g \quad [D5513]
\end{align*} \]

NHC Hydrogencarbonate Salts: NHC-Catalyzed Benzoin Condensations

\[ \text{10 mol } \% \text{ D548} \]

\[ \text{THF, 60 °C, MS3A} \]


Related Products

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Chloro(1,5-cyclooctadiene)rhodium(I) Dimer (= [Rh(cod)Cl]₂) 100mg / 1g [B1045]
Chloro(1,5-cyclooctadiene)iridium(I) Dimer (= [Ir(cod)Cl]₂) 250mg / 1g [C1807]
Palladium(II) Acetate (Purified) (= Pd(OAc)₂) 1g [P2161]
Allylpalladium(II) Chloride Dimer (= [Pd(allyl)Cl]₂) 500mg / 1g [A1479]
Chloro(dimethylsulfide)gold(I) (= (CH₃)₂SAuCl) 200mg / 1g [C2719]