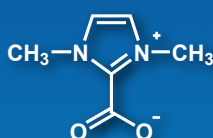
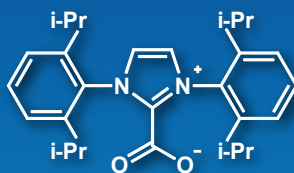


Easily-preparable N-Heterocyclic Carbene (NHC) Precursors

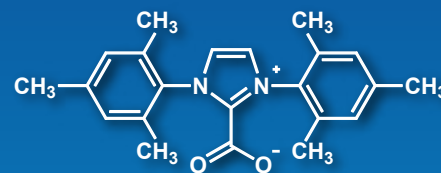
NHC-CO₂ Adducts



1,3-Dimethylimidazolium-
2-carboxylate
1g / 5g
[D5396]

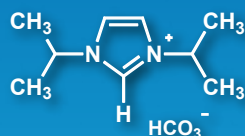


1,3-Bis(2,6-diisopropylphenyl)-
imidazolium-2-carboxylate
1g
[B5603]

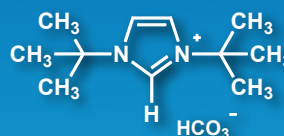


1,3-Dimesitylimidazolium-
2-carboxylate
1g
[D5401]

NHC Hydrogencarbonate Salts



1,3-Diisopropylimidazolium
Hydrogencarbonate
1g
[D5498]



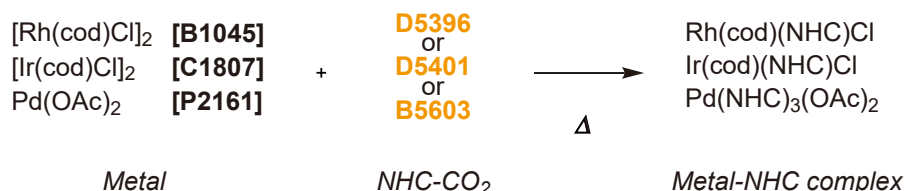
1,3-Di-tert-butylimidazolium
Hydrogencarbonate
1g
[D5513]

Advantages

- NHC ligands and catalysts are preparable by heating.
- No salt generated during preparation.
- Applicable under neutral conditions.
- NHC-CO₂ adducts release CO₂. NHC hydrogencarbonate salts release H₂O and CO₂.

Applications 1

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



Procedure:

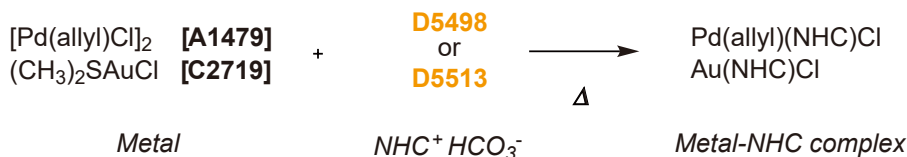
A mixture of [Rh(cod)Cl]₂ (54 mg) and NHC-CO₂ adduct (2 eq.) is stirred in acetonitrile (3 ml) for 5 min at room temperature in a Schlenk flask, followed by heating at 75 °C for 20 min under an atmosphere of argon. The reaction mixture is dried in vacuo, and washed three times with diethyl ether. The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

Reference A. M. Voutchkova, L. N. Appelhans, A. R. Chianese, R. H. Crabtree, *J. Am. Chem. Soc.* **2005**, 127, 17624.
DOI: <http://doi.org/10.1021/ja056625k>

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

Applications 2

NHC Hydrogencarbonate Salts: Transition metal / NHC complex catalyst preparation

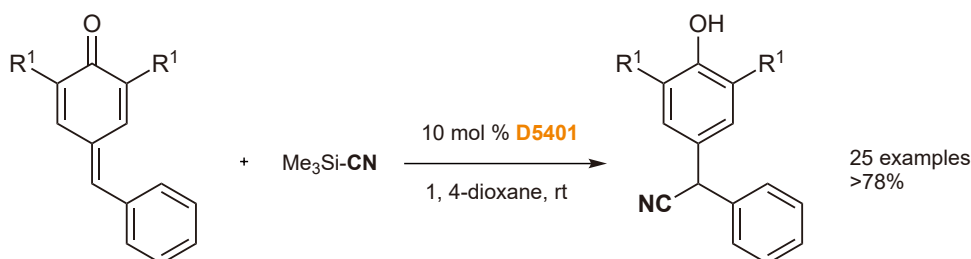


Procedure:

(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.

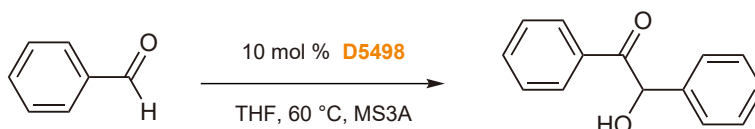
Reference M. Fèvre, J. Pinaud, A. Leteneur, Y. Gnanou, J. Vignolle, D. Taton, *J. Am. Chem. Soc.* **2012**, *134*, 6776. DOI: <http://doi.org/10.1021/ja3005804>

NHC-CO₂ Adducts: NHC-Catalyzed Conjugate Cyanations



Reference P. Goswami, G. Singh, R. V. Anand, *Org. Lett.* **2017**, *19*, 1982. DOI: <http://doi.org/10.1021/acs.orglett.7b00508>

NHC Hydrogencarbonate Salts: NHC-Catalyzed Benzoin Condensations



Reference M. Fèvre, J. Pinaud, A. Leteneur, Y. Gnanou, J. Vignolle, D. Taton, *J. Am. Chem. Soc.* **2012**, *134*, 6776. DOI: <http://doi.org/10.1021/ja3005804>

Related Products

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]

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NHC



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