

New

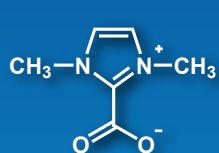
CHEMISTRY

TGI

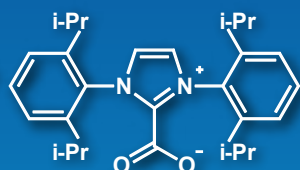
Easily-preparable N-Heterocyclic Carbene (NHC) Precursors

NHC-CO₂ Adducts

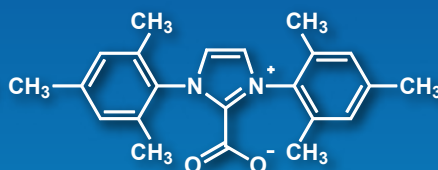
NHC Hydrogencarbonate Salts



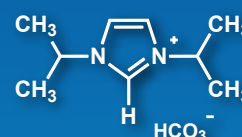
[D5396]



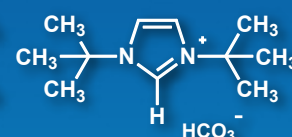
[B5603]



[D5401]



[D5498]



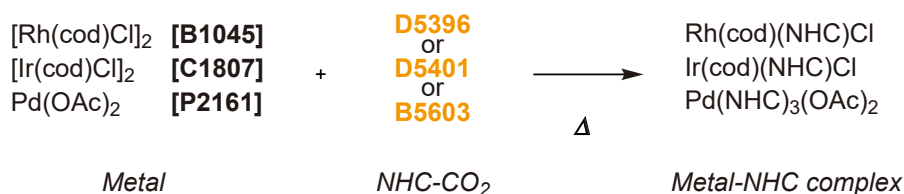
[D5513]

Advantages

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

Applications 1

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

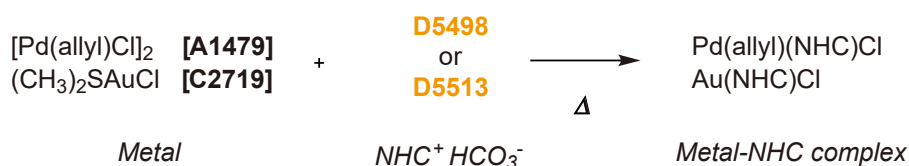


Procedure:

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%).

Cited Reference A. M. Voutchkova, L. N. Appelhans, A. R. Chianese, R. H. Crabtree, *J. Am. Chem. Soc.* **2005**, 127, 17624.

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.

Cited Reference M. Fèvre, J. Pinaud, A. Leteneur, Y. Gnanou, J. Vignolle, D. Taton, *J. Am. Chem. Soc.* **2012**, 134, 6776.

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

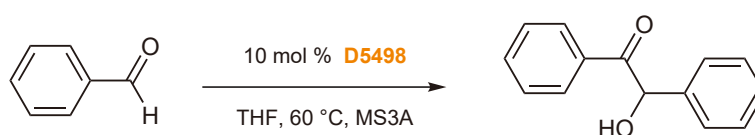
Applications 2

NHC-CO₂ Adducts: NHC-Catalyzed Conjugate Cyanations



Cited Reference P. Goswami, G. Singh, R. V. Anand, *Org. Lett.* **2017**, *19*, 1982.

NHC Hydrogencarbonate Salts: NHC-Catalyzed Benzoin Condensations



Cited Reference M. Fèvre, J. Pinaud, A. Leteneur, Y. Gnanou, J. Vignolle, D. Taton, *J. Am. Chem. Soc.* **2012**, *134*, 6776.

1,3-Dimethylimidazolium-2-carboxylate	1g [D5396]
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-<i>tert</i>-butylimidazolium Hydrogencarbonate (contains varying amounts of 1,3-Di-<i>tert</i>-butylimidazolium-2-carboxylate)	1g [D5513]

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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