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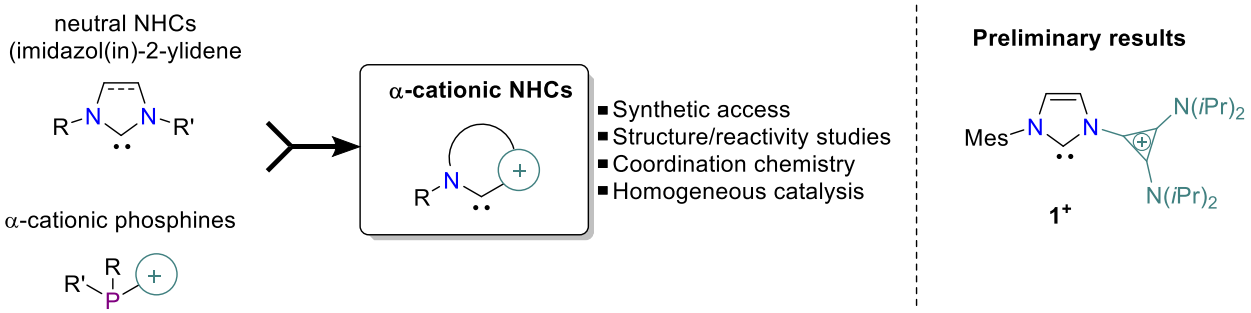
α-CATIONIC N-HETEROCYCLIC CARBENES: SYNTHESIS, COORDINATION CHEMISTRY AND CATALYSIS

Period	6 months beginning not later than: ☐ January ☐ February ☐ March ☐ April ☐ May ☐ June ☐ July ☒ September 2021
Internship supervisor(s)	name: Dr Yves canac, Dr Vincent César e-mail: yves.canac@lcc-toulouse.fr; vincent.cesar@lcc-toulouse.fr group: Molecular design of transition metal pre-catalysts
Location	LCC-CNRS – Toulouse University Paul Sabatier 205 route de Narbonne - BP44099 31077 Toulouse cedex 4 - FRANCE
This research master's degree research project could be followed by a PhD	☒ YES ☐ NO

From mere laboratory oddities, N-Heterocyclic Carbenes (NHCs) have been elevated to compounds of tremendous practical significance in catalysis and synthetic chemistry, with new and exciting applications across the chemical sciences.[1] This ever-growing success is directly related to their unique stereo-electronic properties and the search for new carbenic structures has thus become a priority in order to broaden their application scope.
In line with our research interests,[2] we propose to develop α-cationic NHCs, in which the cationic charge would be directly connected to the carbenic center, in order to maximize the electronic and charge-effects. Interest and impact of these species could be gauged in light of the outstanding results obtained with their phosphine analogues, namely α-cationic phosphines.[3] A proof of concept, we recently reported the cationic NHC **1**$^+$ bearing a N-bounded 2,3-bis(diisopropylamino)cyclopropenium group.[4]



This project is multidisciplinary by nature and will combine synthesis, characterization and reactivity studies, as well as coordination chemistry and catalysis. DFT calculations will complement and support the experimental analysis of their electronic structure, to draw structure/reactivity relationships

References:

[1] M. N. Hopkinson, C. Richter, M. Schedler, F. Glorius, *Nature* **2014**, *510*, 485.
[2] (a) M. Ruamps, N. Lugan, V. César, *Organometallics* **2017**, *36*, 1049; (b) Y. Canac, *Chem. Asian J.* **2018**, *13*, 1872; (c) M. Ruamps, S. Bastin, L. Rechignat, A. Sournia-Saquet, D. A. Valyaev, J.-M. Mouesca, N. Lugan, V. Maurel, V. César, *Chem. Commun.* **2018**, *54*, 7653; (d) R. Taakili, C. Lepetit, C. Duhayon, D. A. Valyaev, N. Lugan, Y. Canac, *Dalton Trans.* **2019**, *48*, 1709.
[3] M. Alcarazo, *Acc. Chem. Res.* **2016**, *49*, 1797.
[4] C. Barthes, C. Duhayon, Y. Canac, V. César, *Chem. Commun.* **2020**, *56*, 3305-3308.

Keywords, areas of expertise	Carbenes, ligand design, coordination chemistry, heterocycles, cations, reactivity, homogeneous catalysis, DFT calculations
Required skills for the internship	Good knowledge in organic chemistry, organometallic chemistry, and advanced characterization techniques (multinuclear NMR, X-Ray diffraction, MS, EPR spectroscopy …). Schlenk line technique, glove box.