

Expanding the chemical space of cobalt synthetic and mechanistic tactics: From Fundamentals to Catalysis



Timeline | 09/2024 to 08/2027



ICIQ People | Pérez-Temprano Group



Budget | 212.500 €



Call | Proyectos I+D
Generación Conocimiento 2023

SUMMARY

COMET The continuous quest for innovative ways of building molecular complexity has converted transition metal-catalyzed CH functionalization and cross-coupling reactions into main thrusts within modern synthetic organic chemistry. Traditionally, these areas have been dominated by precious metal catalysts due to their robustness, efficiency, and the deep understanding on the reaction mechanisms. However, growing global focus on moving towards more sustainable chemical transformations has renewed the interest in incorporating earthabundant first-row transition metals into the organometallic toolkit. Despite this trend, still now, the underutilization of 3d TMs, such as cobalt, remains a long-standing challenge among practitioners of organometallic catalysis. In this context, (pentamethylcyclopentadienyl)cobalt(III) catalysts have emerged as a very powerful tool in site-selective CH functionalization reactions. However, many synthetic and, especially, fundamental questions remain unsolved, including the exploration of their open-shell catalysis. Moreover, the chemistry of their low-valent cobalt(I) analogues has been largely overlooked, despite their potential to significantly impact pivotal fields such as cross-coupling reactions and open up the door to new mechanistic and synthetic possibilities. This project, COMET, seeks to move the organometallic landscape of these cobalt systems to a new dimension of possible reaction manifolds and reactivity patterns. We aim to tackle long-lasting key fundamental and synthetic questions and untap the hidden potential of their open-shell organometallics. To do so, we will uncover and control the principles that govern these transformations by using mechanism as the foundation for reaction design and development.

Task	Year 1			Year 2			Year 3		
	1-4	4-8	8-12	12-16	16-20	20-24	24-28	28-32	32-36
O1	T1.1		MS1						
	T1.2			MS2					
	T1.3		MS3						
	T1.4	MS4							
	T1.5							MS5	
O2	T2.1			MS6					
	T2.2						MS7		
	T2.3					MS8			
					MS9				