



**HAL**  
open science

## Valorization of small molecules: from mechanisms to new reactions

Niklas von Wolff, Joelle Char, Thibault Cantat

► **To cite this version:**

Niklas von Wolff, Joelle Char, Thibault Cantat. Valorization of small molecules: from mechanisms to new reactions. 42<sup>nd</sup> International Conference on Coordination Chemistry (ICCC 2016), Jul 2016, Brest, France. cea-02346073

**HAL Id: cea-02346073**

**<https://hal-cea.archives-ouvertes.fr/cea-02346073>**

Submitted on 4 Nov 2019

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

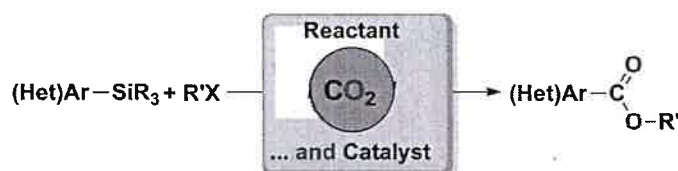
## Valorization of Small Molecules

### From Mechanism to New Reactions

N. von Wolff, J. Char, T. Cantat \*  
CEA Saclay, NIMBE, 91191 Gif-sur-Yvette, France

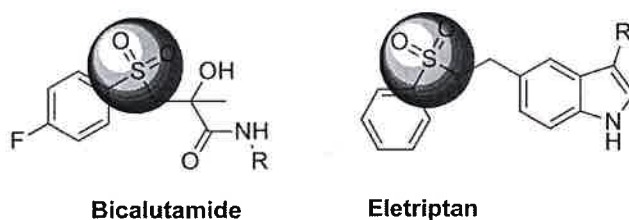
thibault.cantat@cea.fr

Small molecules, such as CO<sub>2</sub>, SO<sub>2</sub>, or nitrous oxides NO<sub>x</sub> are generally regarded as pollutants and wastes. However, recent developments made it possible to think about small molecules as building blocks for organic synthesis, especially using CO<sub>2</sub>. As C–C bonds are universal in organic chemistry, the formation of these bonds from CO<sub>2</sub> is of key interest. We herein report a novel reaction of unactivated organosilanes with CO<sub>2</sub> to form esters and a polyester material for the first time, where CO<sub>2</sub> plays both the role of the reactant and a catalyst.<sup>1</sup>



**Figure 1** CO<sub>2</sub> acts both as reactant and catalyst in the formation of esters from heteroarylsilanes as demonstrated by DFT calculations.

Understanding this reaction and the unique catalytic role of CO<sub>2</sub> using DFT calculations enabled the development of a novel transformation involving SO<sub>2</sub>. For the first time, SO<sub>2</sub> is incorporated in a one-pot one-step process to form aryl alkyl sulfones, a major class of compounds in the organic chemistry with wide applications in synthesis, from pharmaceuticals to natural products.<sup>2</sup>



**Figure 2** Examples of pharmaceuticals bearing the sulfonyl group

1 X. Frogneux, N. von Wolff, P. Thuéry, G. Lefèvre, T. Cantat *Chem. Eur. J.* 10.1002/chem.201505092

2 N. von Wolff, J. Char, T. Cantat, A process for the synthesis of sulfones and sulfonamides, **2015**, EP15306966