



HAL
open science

To Bend or Not to Bend: Is CO2 Bending Required to Promote its Reduction?

Emmanuel Nicolas, Niklas von Wolff, Thibault Cantat

► **To cite this version:**

Emmanuel Nicolas, Niklas von Wolff, Thibault Cantat. To Bend or Not to Bend: Is CO2 Bending Required to Promote its Reduction?. EuCOMC 2017, Jul 2017, Amsterdam, Netherlands. cea-02346348

HAL Id: cea-02346348

<https://cea.hal.science/cea-02346348v1>

Submitted on 5 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.

To Bend or Not to Bend: Is CO₂ Bending Required to Promote its Reduction? [1]

Nicolas, E.; von Wolff, N.; Cantat, T.

LCMCE, NIMBE, CEA, CNRS, Université Paris-Saclay, France

CO₂ reduction is a process actively investigated in order to use CO₂ as a C₁ feedstock for the chemical industry, yet this process is thermodynamically and kinetically challenging.[2] While electrochemical studies, together with the analysis of the Walsh diagram of CO₂, proposed that bending the O–C–O angle is a requirement to promote the reduction of CO₂, this approach is only valid for single electron transfer (SETs) reactions. This paradigm does not apply to hydride-transfer-mediated reductions, for which new rules need to be devised.

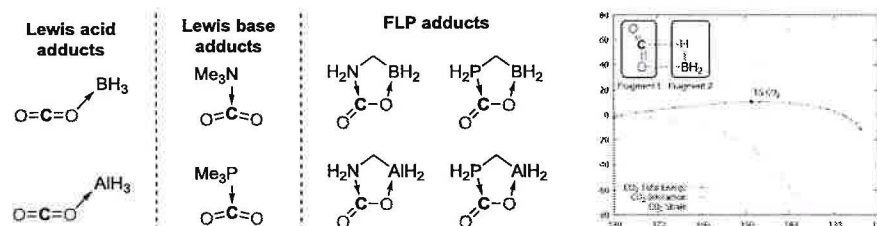


Figure 1 Adducts investigated (left); Example of ASM results (right)

We propose here the use of the Activation Strain Model (ASM) as developed by Bickelhaupt *et al.*[3] to probe the reduction of CO₂ by BH₃, with or without added organocatalysts, which leads to a decorrelation of the respective influences of electronic and steric parameters. We found that slight bending is indeed beneficial to promote CO₂ reduction, but that strong bending is detrimental to the process. Keys for the design of an optimal catalyst are provided.

[1] Nicolas, E.; von Wolff, N., Cantat, T., *Submitted*.

[2] Aresta, M. In *Carbon Dioxide and Organometallics*; Xiao-Bing, L., Ed.; Springer International Publishing, 2016

[3] Wolters, L. P., Bickelhaupt, F. M.; *WIREs Comput. Mol. Sci.* 5, 324 (2015).

E-mail: emmanuel.nicolas@cea.fr

www: <http://iramis.cea.fr/Pisp/thibault.cantat/>