J. Braz. Chem. Soc., Vol. 25, No. 12, S1-S3, 2014.
Printed in Brazil - ©2014 Sociedade Brasileira de Química
0103 - 5053 $6.00+0.00

Supplementary Information

Can Green Dimethyl Carbonate Synthesis be More Effective? A Catalyst Recycling Study Benefiting from Experimental Kinetics and DFT Modeling

Stéphane Chambrey,[a,b] Mahboubeh Poor Kalhor,[c] Henry Chermette[c] and Danielle Ballivet-Tkatchenko*,[a]

[a]*Institut de Chimie Moléculaire de l'Université de Bourgogne, Université de Bourgogne, UMR CNRS 6302 9 Av. Alain Savary, 21000 Dijon, France*

[b]*Unité de Catalyse et Chimie du Solide, Université Lille 1, UMR CNRS 8181 59655 Villeneuve d'Ascq cedex, France*

[c]*Institut des Sciences Analytiques, University of Lyon, Université Lyon 1 (UCBL) and UMR CNRS 5280, 5 rue de la Doua, 69100 Villeurbanne, France*

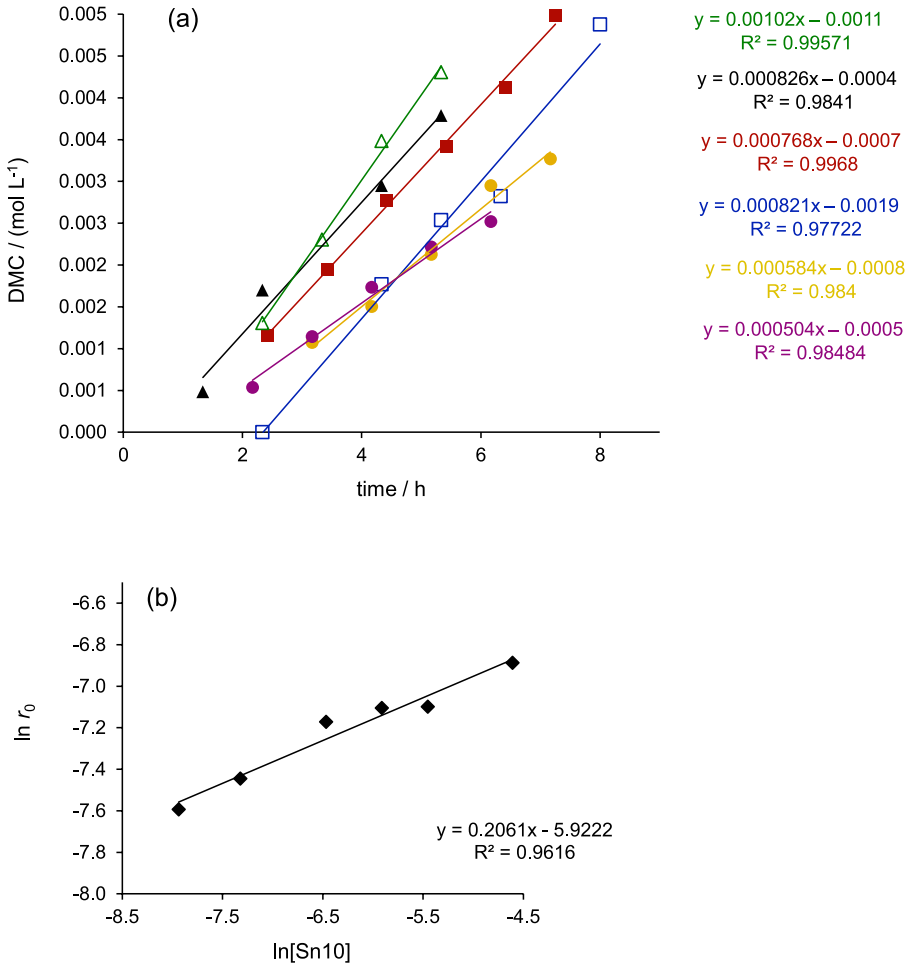


Figure S1. (a) Initial rate of DMC formation with the decatin complex at T = 411 K and P = 22 MPa (concentration range: 0.035 × 10^{-2} to 10^{-2} mol L^{-1}), (b) tin order determination.

*e-mail: ballivet@u-bourgogne.fr

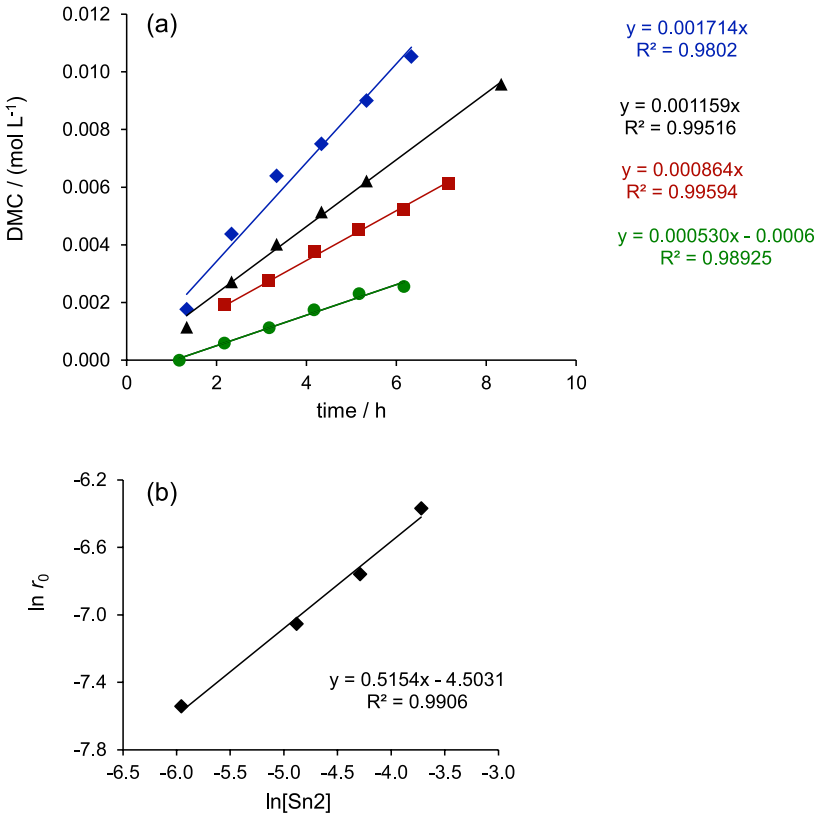


Figure S2. (a) Initial rate of DMC formation with the distannoxane complex at T = 411 K and P = 20 MPa (concentration range: 0.26 × 10^{-2} to 2.4 × 10^{-2} mol L^{-1}), (b) tin order determination.

In Figures S1a and S2a, the zero value of the time scale corresponds to starting heating up to 411 K. Therefore, DMC is analyzed after the reaction mixture has reached 411 K, i.e., after 0.5 h on average. With the decatin complex (Figure S1a), DMC is even analyzed at higher reaction times which suggests the active species is formed after an induction period.

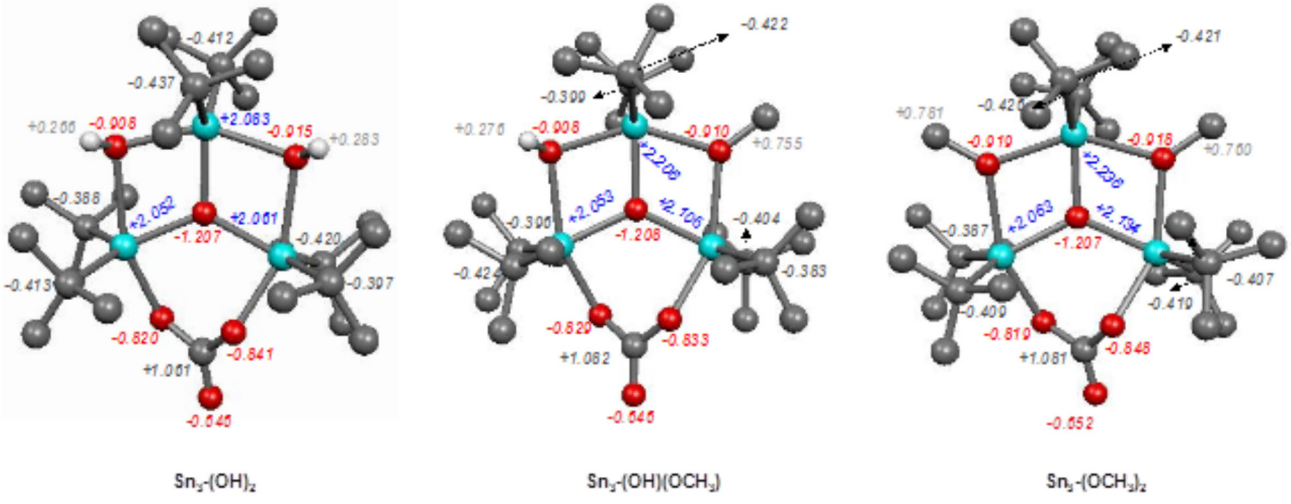


Figure S3. Selected charges in Sn_2-$(OH)_2$, Sn_2-$(OH)(OCH_3)$, and Sn_2-$(OCH_3)_2$.

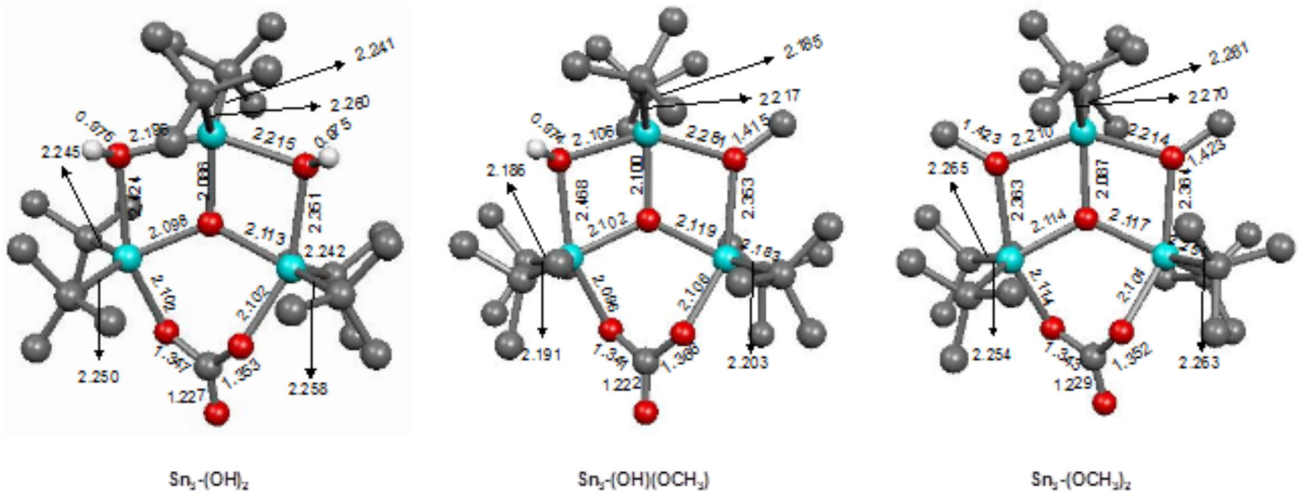
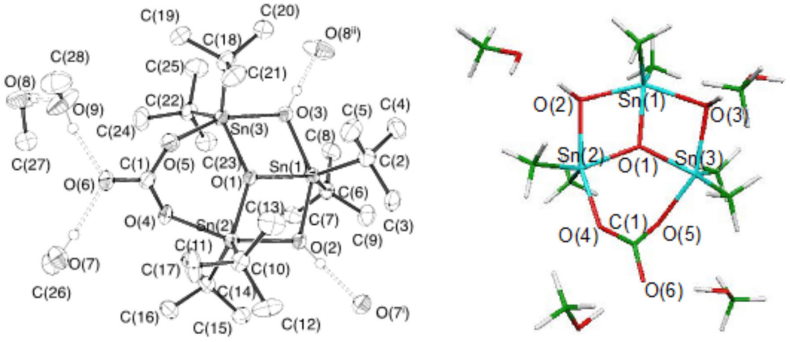


Figure S4. Selected bond lengths in Sn_3-$(OH)_2$, Sn_3-(OH)(OCH_3), and Sn_3-$(OCH_3)_2$.

Table S1. Comparison of selected bond distances (Å) obtained by X-ray analysis[a] for $[^tBu_2Sn(OH)_2][(^tBu_2Sn)_2(O)(CO_3)].3CH_3OH$ and DFT calculations for $[(CH_3)_2Sn(OH)_2]\{[(CH_3)_2Sn]_2(O)(CO_3)\}.3CH_3OH$



Bond distance / Å	X-ray	DFT
C(1)-O(6)	1.266(7)	1.251
C(1)-O(4)	1.280(7)	1.327
C(1)-O(5)	1.310(7)	1.334
Sn(3)-O(1)	2.059(4)	2.092
Sn(2)-O(1)	2.048(4)	2.075
Sn(1)-O(1)	2.080(4)	2.078
Sn(1)-O(3)	2.139(4)	2.203
Sn(1)-O(2)	2.136(4)	2.187

[a]Obtained from the publication of Ballivet-Tkatchenko *et al.*.[1]

Reference

1. Ballivet-Tkatchenko, D.; Burgat, R.; Chambrey, S.; Plasseraud, L.; Richard, P.; *J. Organomet. Chem*. **2006**, *691*, 1498.