OMCOS18

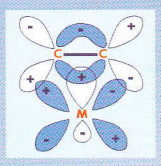
Organometallic Chemistry Directed Towards Organic Synthesis

IUPAC International Symposium

Sitges - Barcelona **2015**

From June 28th to July 2nd

www.omcos2015.com



ICIQ Institut Català d'Investigació Química

RSEQ Real Sociedad Española de Química

IUPAC International Union of Pure and Applied Chemistry

EXCELENCIA SEVERO OCHOA

FINAL PROGRAMME

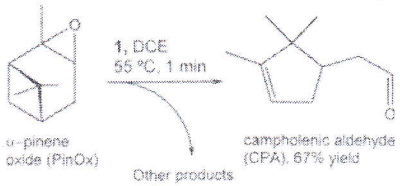
ISOMERISATION OF PINENE OXIDE IN THE PRESENCE OF AN INDENYL MOLYBDENUM CARBONYL COMPLEX

Carla A. Gamelas[a*], Sofia M. Bruno[b], Ana C. Gomes[b], Marta Abrantes[c], M. Conceição Oliveira[c], Anabela A. Valente[b], Filipe A. Almeida Paz[b], Martyn Pillinger[b], Carlos C. Romão[d], Isabel S. Gonçalves[b]

a, Escola Superior de Tecnologia de Setúbal, Instituto Politécnico de Setúbal
b, Department of Chemistry, CICECO - Aveiro Institute of Materials, University of Aveiro, Campus Universitário de Santiago, Aveiro
c, Centro de Química Estrutural, IST, Universidade de Lisboa, Lisboa
d, Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, EAN, Oeiras

* carla.gamelas@estsetubal.ips.pt

The complex $[\{(\eta^5\text{-Ind})Mo(CO)_2(\mu\text{-Cl})\}_2]$ (**1**) has been tested for the catalytic isomerisation of α-pinene oxide (PinOx) to campholenic aldehyde (CPA, see Scheme). Complete conversion of PinOx was achieved within 1 min at 55 °C or 30 min at 35 °C using 1,2-dichloroethane as solvent, giving CPA in 68% yield.[1] Other products included *trans*-carveol, iso-pinocamphone and *trans*-pinocarveol. The stability of **1** under the reaction conditions was investigated by FT-IR spectroscopy and ESI-MS to characterise recovered solids. In the presence of air/moisture **1** undergoes oxidative decarbonylation upon dissolution to give oxomolybdenum species that are proposed to include a tetranuclear oxomolybdenum(V) complex. Conversely, ESI-MS studies of **1** dissolved in dry CH_3CN show mononuclear species of the type $[IndMo(CO)_2(CH_3CN)_n]^+$. The crystal structure of $[(\eta^3\text{-Ind})Mo(CO)_2Cl\text{-}(CH_3CN)_2]$ (**2**) (obtained after dissolution of **1** in CH_3CN) is reported.



References

1. S. M. Bruno, A. C. Gomes, C. A. Gamelas, M. Abrantes, M. C. Oliveira, A. A. Valente, F. A. Almeida Paz, M. Pillinger, C. C. Romão, I. S. Gonçalves, *New J. Chem.* **2014**, *38*, 3172-3180.

Acknowledgment

Funding through CICECO - FCOMP-01-0124-FEDER-037271 (FCT ref. PEst-C/CTM/LA0011/2013) and FCOMP-01-0124-FEDER-029779 (FCT ref. PTDC/QEQ-SUP/1906/2012) is acknowledged.