

## Erratum to: A Curtin-Hammett mechanism for the copolymerization of ethylene and methyl acrylate monomer using a PymNox nickel catalyst as revealed by DFT computational studies

Javier Ramos · Sonia Martínez · Víctor L. Cruz ·  
Javier Martínez-Salazar

Published online: 15 July 2012  
© Springer-Verlag 2012

**Erratum to: J Mol Model (2012) 18:515–523**  
**DOI 10.1007/s00894-011-1093-5**

Concerning the authorship of the works quoted in references 20 and 37, we would like to make clear that the experimental work was done in the group of Brasse et al. [20] while the computational studies were carried out in the group of Ramos et al. [37]. Consequently, the sentence on page 516 should be better clarify by saying that:

“In line with this idea, Brasse et al. [20] modified experimentally Grubbs’ salicylaldiminate catalyst design by replacing the anionic aryloxide ligand with an electrically neutral but isostructural pyridine-*N*-oxide fragment and Ramos et al. [37] studied the corresponding homopolymerisation mechanism.”

Instead of the existing one:

“In line with this idea, we modified Grubbs’ salicylaldiminate catalyst design by replacing the anionic aryloxide ligand with an electrically neutral but isostructural pyridine-*N*-oxide fragment.”

---

The online version of the original article can be found at <http://dx.doi.org/10.1007/s00894-011-1093-5>.

---

J. Ramos (✉) · V. L. Cruz · J. Martínez-Salazar  
BIOPHYM, Departamento de Física Macromolecular,  
Instituto de Estructura de la Materia, CSIC, Serrano 113bis,  
28006 Madrid, Spain  
e-mail: j.ramos@iem.cfmac.csic.es

S. Martínez  
Área de Informática Científica,  
Secretaría General Adjunta de Informática (SGAI),  
CSIC, Pinar 19,  
28006 Madrid, Spain