

Accepted Manuscript

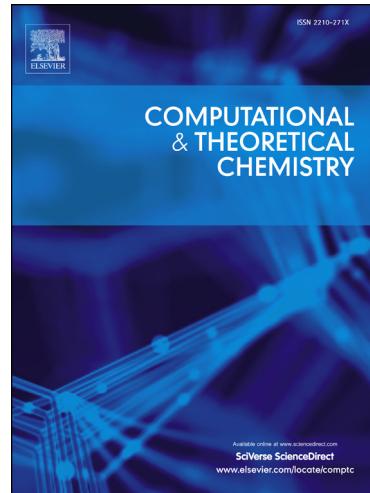
Theoretical Evaluation of Metal-functionalized *rccc* R-Pyrogallol[4]arenes as Media for Molecular Hydrogen Storage

V. Posligua, A. Urbina, L. Rincón, J.-C. Soetens, M.A. Méndez, C.H. Zambrano, F.J. Torres

PII: S2210-271X(15)00351-5

DOI: <http://dx.doi.org/10.1016/j.comptc.2015.08.017>

Reference: COMPTC 1915



To appear in: *Computational & Theoretical Chemistry*

Received Date: 18 July 2015

Revised Date: 27 August 2015

Accepted Date: 28 August 2015

Please cite this article as: V. Posligua, A. Urbina, L. Rincón, J.-C. Soetens, M.A. Méndez, C.H. Zambrano, F.J. Torres, Theoretical Evaluation of Metal-functionalized *rccc* R-Pyrogallol[4]arenes as Media for Molecular Hydrogen Storage, *Computational & Theoretical Chemistry* (2015), doi: <http://dx.doi.org/10.1016/j.comptc.2015.08.017>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Theoretical Evaluation of Metal-functionalized *rccc R-Pyrogallol[4]arenes as Media for Molecular Hydrogen Storage*

V. Posligua^{a,b}, A. Urbina^{a,b}, L. Rincón^c, J.-C. Soetens^d, M. A. Méndez^{a,b,e}, C. H. Zambrano^{a,b},
and F. J. Torres^{a,b,d*}

^a Universidad San Francisco de Quito, Grupo de Química Computacional y Teórica (QCT-USFQ), Departamento de Ingeniería Química, Diego de Robles y Vía Interoceánica, Quito, Ecuador 17-1200-841

^b Universidad San Francisco de Quito, Grupo Ecuatoriano para el Estudio Experimental y Teórico de Nanosistemas –GETNano–, Diego de Robles y Vía Interoceánica, Quito, Ecuador 17-1200-841

^c Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, La Hechicera, Mérida-5101, Venezuela.

^d Université de Bordeaux, ISM, UMR 5255, 351, Cours de la Libération, Talence F-33405, France

^e Universidad San Francisco de Quito, Colegio de Ciencias de la Salud, Edificio de Especialidades Médicas, Hospital de los Valles, Av. Interoceánica Km 12 ½, Quito, Ecuador

* Corresponding author. Email: jtorres@usfq.edu.ec

Download English Version:

<https://daneshyari.com/en/article/5393072>

Download Persian Version:

<https://daneshyari.com/article/5393072>

[Daneshyari.com](https://daneshyari.com)