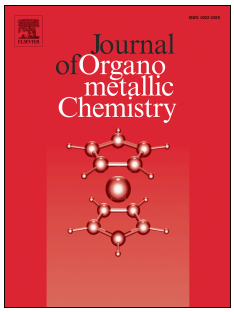
Accepted Manuscript



Light induced nonlinear optical switch in boronated chromophores: a theoretical search towards high contrast switches in the azobenzene series

Norberto Farfan, Cristina C. Jiménez, Margarita Romero-Avila, Rosa Santillan, Isabelle Malfant, Pascal Lacroix

PII: S0022-328X(15)30164-9

DOI: 10.1016/j.jorganchem.2015.09.035

Reference: JOM 19250

To appear in: *Journal of Organometallic Chemistry*

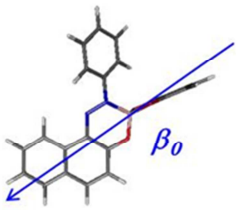
Received Date: 30 June 2015

Revised Date: 15 September 2015

Accepted Date: 28 September 2015

Please cite this article as: N. Farfan, C.C Jiménez, M. Romero-Avila, R. Santillan, I. Malfant, P. Lacroix, Light induced nonlinear optical switch in boronated chromophores: a theoretical search towards high contrast switches in the azobenzene series, *Journal of Organometallic Chemistry* (2015), doi: 10.1016/j.jorganchem.2015.09.035.

DFT computed static hyperpolarizabilities



β_{on}/β_{off} = 8.53

E-**2**

βo = 52.8 x 10^{-30}cm^{5}esu^{-1}
ON

Z-**2**

βo = 6.19 x 10^{-30}cm^{5}esu^{-1}
OFF