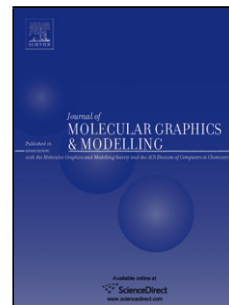


Accepted Manuscript

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PII: S1093-3263(17)30615-0
DOI: <http://dx.doi.org/10.1016/j.jmgm.2017.09.012>
Reference: JMG 7028

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 11-8-2017
Revised date: 12-9-2017
Accepted date: 13-9-2017

Please cite this article as: Li-Xue Jing, Li Wang, Jin-Ting Ye, Zhen-Zhen Chen, He Chen, Yong-Qing Qiu, Theoretical investigation on second-order nonlinear optical properties of ruthenium alkynyl–dihydroazulene/vinylheptafulvene complexes, Journal of Molecular Graphics and Modelling <http://dx.doi.org/10.1016/j.jmgm.2017.09.012>

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Theoretical investigation on second-order nonlinear optical properties of Ruthenium Alkynyl–Dihydroazulene/Vinylheptafulvene complexes

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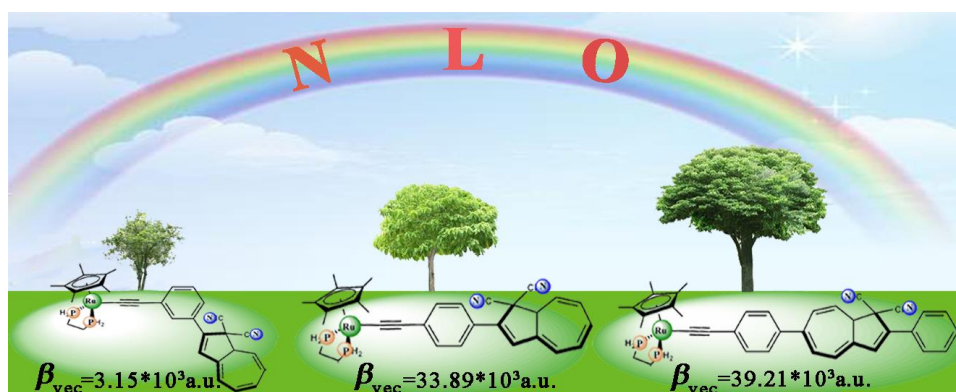
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Graphical abstract

The para-position of the Ru acetylide and additional a p-phenylene spacer greatly increase the second-order NLO responses.



Highlights

- The β_{vec} value can be efficiently tuned by the position of the Ru acetylide.
- The differences on NLO properties are attributed to the more

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