

Accepted Manuscript

Role of dispersion corrected hybrid GGA class in accurately calculating the bond dissociation energy of carbon halogen bond: A benchmark study

Naveen Kosar, Tariq Mahmood, Khurshid Ayub



PII: S0022-2860(17)31159-6

DOI: [10.1016/j.molstruc.2017.08.104](https://doi.org/10.1016/j.molstruc.2017.08.104)

Reference: MOLSTR 24242

To appear in: *Journal of Molecular Structure*

Received Date: 23 July 2017

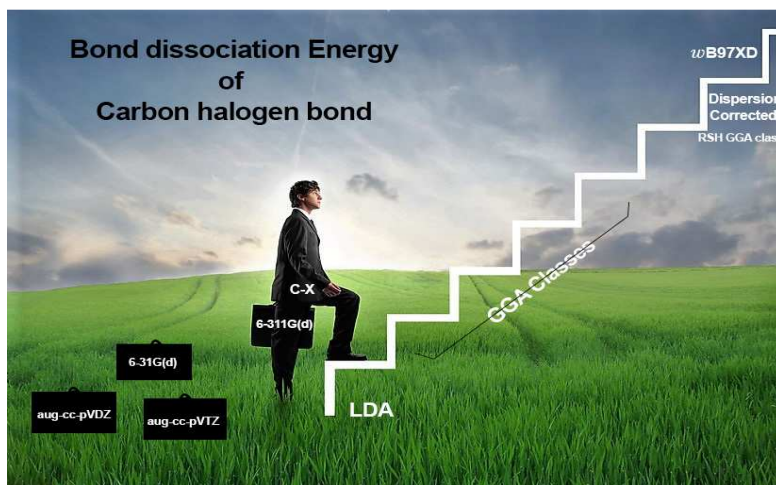
Revised Date: 20 August 2017

Accepted Date: 24 August 2017

Please cite this article as: N. Kosar, T. Mahmood, K. Ayub, Role of dispersion corrected hybrid GGA class in accurately calculating the bond dissociation energy of carbon halogen bond: A benchmark study, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2017.08.104.

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.

Graphical abstract



Download English Version:

<https://daneshyari.com/en/article/5159914>

Download Persian Version:

<https://daneshyari.com/article/5159914>

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