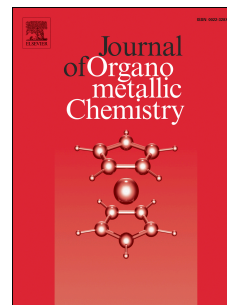


Accepted Manuscript

Direct energetic evaluation of aromaticity by cleaving the rings of cyclic compounds

Ke An, Jun Zhu



PII: S0022-328X(18)30047-0

DOI: [10.1016/j.jorganchem.2018.01.038](https://doi.org/10.1016/j.jorganchem.2018.01.038)

Reference: JOM 20276

To appear in: *Journal of Organometallic Chemistry*

Received Date: 30 October 2017

Revised Date: 17 January 2018

Accepted Date: 22 January 2018

Please cite this article as: K. An, J. Zhu, Direct energetic evaluation of aromaticity by cleaving the rings of cyclic compounds, *Journal of Organometallic Chemistry* (2018), doi: 10.1016/j.jorganchem.2018.01.038.

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.

Direct Energetic Evaluation of Aromaticity by Cleaving the Rings of Cyclic Compounds

Ke An, and Jun Zhu *

State Key Laboratory of Physical Chemistry of Solid Surfaces and Collaborative Innovation Center of Chemistry for Energy Materials (iChEM), Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005

Email: jun.zhu@xmu.edu.cn

Highlights:

1. An energetic criterion based on the original definition of aromaticity by cleaving the (anti)aromatic rings was proposed.
2. A strong correlation between ASE and ISE in the S_0 state ($R^2 = 0.947$) was achieved.
3. The T_1 state (anti)aromaticity can also be estimated via this method.
4. Moderate correlation was found between the ASE and NICS(1)_{zz} values.
5. This method could be also applied to bicyclic species and organometallics.

Download English Version:

<https://daneshyari.com/en/article/7756050>

Download Persian Version:

<https://daneshyari.com/article/7756050>

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