

Accepted Manuscript

Computational study on the mechanisms and reaction pathways of the Brominated Alkyl Radical ($\text{CHBr}_2/\text{CBr}_3$) with NO_2 reactions

Yunju Zhang, Ruojing Song, Yuxi Sun, Jingyu Sun, Yong-guo Liu, Rongshun Wang

PII: S2210-271X(17)30326-2

DOI: <http://dx.doi.org/10.1016/j.comptc.2017.07.006>

Reference: COMPTC 2568

To appear in: *Computational & Theoretical Chemistry*

Received Date: 19 April 2017

Revised Date: 9 July 2017

Accepted Date: 10 July 2017



Please cite this article as: Y. Zhang, R. Song, Y. Sun, J. Sun, Y-g. Liu, R. Wang, Computational study on the mechanisms and reaction pathways of the Brominated Alkyl Radical ($\text{CHBr}_2/\text{CBr}_3$) with NO_2 reactions, *Computational & Theoretical Chemistry* (2017), doi: <http://dx.doi.org/10.1016/j.comptc.2017.07.006>

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.

Computational study on the mechanisms and reaction pathways of the Brominated Alkyl Radical ($\text{CHBr}_2/\text{CBr}_3$) with NO_2 reactions

Yunju Zhang,^{1,5*} Ruojing Song,¹ Yuxi Sun,^{1,2,5} Jingyu Sun,⁴ Yong-guo, Liu,⁵

Rongshun, Wang,³

¹*Key Laboratory of Photoinduced Functional Materials, Mianyang Normal University,*

Mianyang 621000, PR China

²*Key Laboratory of Life-Organic Analysis, Qufu Normal University, Qufu 273165, PR*

China

³*Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal*

University, Renmin Road 5268. Changchun, Jilin 130024, P. R. China

⁴*Hubei Collaborative Innovation Center for Rare Metal Chemistry, Hubei Key*

Laboratory of Pollutant Analysis & Reuse Technology, College of Chemistry and

Chemical engineering, Hubei Normal University, Cihu Road 11, Huangshi, Hubei

435002, P. R. China

⁵*Beijing Technology and Business University, Beijing 100048, PR China*

Abstract:

Mechanisms and reaction channels of the CHBr_2 and CBr_3 with NO_2 reactions have been studied by quantum chemistry methods. The calculated results indicating that the title reactions can take place on either the singlet or triplet potential energy surfaces (PES) and the pathways on the triplet PES should be much less competitive than that on the singlet PES. On the singlet surface, CHBr_2 radical can associate with NO_2 to barrierlessly generate adduct IM1 (CHBr_2NO_2), followed by isomerization to IM2a (*trans-cis-CHBr}_2\text{ONO}*) and IM2b (*trans-trans-CHBr}_2\text{ONO}*), which can easily

Download English Version:

<https://daneshyari.com/en/article/5392342>

Download Persian Version:

<https://daneshyari.com/article/5392342>

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