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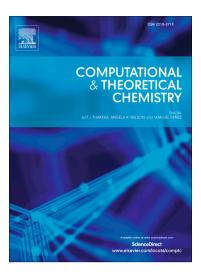
PII: S2210-271X(17)30326-2

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 (CHBr₂/CBr₃) with NO₂ reactions, *Computational & Theoretical Chemistry* (2017), doi: http://dx.doi.org/10.1016/j.comptc.2017.07.006

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Computational study on the mechanisms and reaction pathways of the Brominated Alkyl Radical (CHBr₂/CBr₃) with NO₂ reactions

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Mechanisms and reaction channels of the CHBr₂ and CBr₃ with NO₂ 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, CHBr₂ radical can associate with NO₂ to barrierlessly generate adduct IM1 (CHBr₂NO₂), followed by isomerization to IM2a (*trans-cis-*CHBr₂ONO) and IM2b (*trans-trans-*CHBr₂ONO), which can easily

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