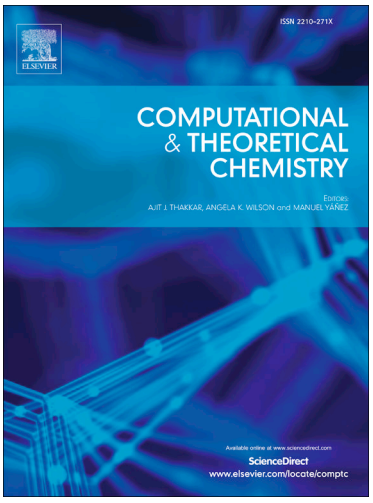

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Computational study on the mechanisms and reaction pathways of the Brominated Alkyl Radical ($CHBr_2$/CBr_3) with NO_2 reactions

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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*-$CHBr_2ONO$) and IM2b (*trans-trans*-$CHBr_2ONO$), which can easily