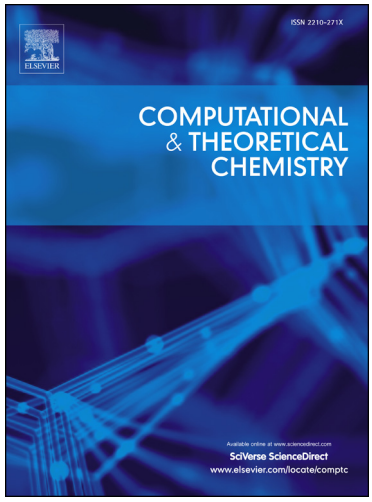

Further Studies into the Photodissociation Pathways of Phenylperoxyl Radicals

Xin He, Zeng-Xia Zhao, Hong-Xing Zhang

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Further Studies into the Photodissociation Pathways of Phenylperoxyl Radicals

Xin He, Zeng-Xia Zhao*, Hong-Xing Zhang*

International Joint Research Laboratory of Nano-Micro Architecture Chemistry, Institute of Theoretical Chemistry, Jilin University, 130023 Changchun, China.

*Corresponding author. Tel.: +86 18943121798

e-mail: zxzhaojlu@gmail.com

Abstract: In this work, we report performed a high level ab initio study on the low-lying electronic states of C_6H_5OO, utilizing complete active space self-consistent field (CASSCF) and multiconfiguration second-order perturbation theory (CASPT2) method, and the contracted ANO-L basis set have been taken into account. The potential energy curves for the four lowest states associated with the lowest dissociation limit of C_6H_5OO radical. The calculated results clearly assigned the experimentally observed photodissociation channels leading to C_6H_5O (X^2A, 2^2A) + $O(^3P_g)$ and C_6H_5 (X^2A) + $O_2(X^3\Sigma_g^-, 1^1\Delta_g , 1^1\Sigma_g^+)$.

Keywords: CASSCF, CASPT2, photodissociation, phenylperoxyl radical